

# Package ‘LaMa’

October 28, 2026

**Type** Package

**Title** Fast Numerical Maximum Likelihood Estimation for Latent Markov Models

**Version** 3.0.0

**Description** A variety of latent Markov models, including hidden Markov models, hidden semi-Markov models, state-space models and continuous-time variants can be formulated and estimated within the same framework via directly maximising the likelihood function using the so-called forward algorithm. Applied researchers often need custom models that standard software does not easily support. Writing tailored 'R' code offers flexibility but suffers from slow estimation speeds. We address these issues by providing easy-to-use functions (written in 'C++' for speed) for common tasks like the forward algorithm. These functions can be combined into custom models in a Lego-type approach, offering up to 10-20 times faster estimation via standard numerical optimisers. To aid in building fully custom likelihood functions, several vignettes are included that show how to simulate data from and estimate all the above model classes.

**URL** <https://janolefi.github.io/LaMa/>

**License** MIT + file LICENSE

**Encoding** UTF-8

**Imports** Rcpp, stats, utils, methods, Matrix, splines2, mgcv, MASS, numDeriv, RTMBdist (>= 1.1.0)

**LinkingTo** Rcpp, RcppArmadillo

**Depends** R (>= 3.5.0), RTMB (>= 2.0)

**RoxygenNote** 7.3.3

**Suggests** knitr, rmarkdown, testthat (>= 3.0.0), PHSM, MSwM, scales

**VignetteBuilder** knitr

**Config/testthat/edition** 3

**LazyData** true

**NeedsCompilation** yes

**Author** Jan-Ole Fischer [aut, cre] (ORCID:

<<https://orcid.org/0009-0004-1556-9053>>)

**Maintainer** Jan-Ole Fischer <jan-ole.fischer@mailbox.org>

**Repository** CRAN

**Date/Publication** 2026-10-28 14:30:08 UTC

## Contents

|                                 |    |
|---------------------------------|----|
| calc_trackInd . . . . .         | 4  |
| cosinor . . . . .               | 4  |
| ddwell . . . . .                | 5  |
| dgmrf2 . . . . .                | 6  |
| forward . . . . .               | 8  |
| forward_g . . . . .             | 10 |
| forward_hsmm . . . . .          | 13 |
| forward_ihsmm . . . . .         | 14 |
| forward_p . . . . .             | 17 |
| forward_phsmm . . . . .         | 19 |
| forward_s . . . . .             | 21 |
| forward_sp . . . . .            | 22 |
| gamma2 . . . . .                | 24 |
| gdeterminant . . . . .          | 25 |
| generator . . . . .             | 25 |
| generator_g . . . . .           | 27 |
| lama . . . . .                  | 28 |
| LaMaColors . . . . .            | 29 |
| logLik.LaMaModel . . . . .      | 30 |
| make_matrices_dens . . . . .    | 31 |
| MCreport . . . . .              | 32 |
| minmax . . . . .                | 34 |
| minmax0_smooth . . . . .        | 35 |
| modmat . . . . .                | 35 |
| multistart . . . . .            | 37 |
| nessi . . . . .                 | 40 |
| penalty . . . . .               | 40 |
| penalty2 . . . . .              | 42 |
| penalty_uni . . . . .           | 45 |
| plot.LaMaModel . . . . .        | 46 |
| plot.LaMaResiduals . . . . .    | 47 |
| predict.LaMa_matrices . . . . . | 49 |
| predict.smoothdens . . . . .    | 50 |
| pred_matrix . . . . .           | 51 |
| print.LaMaModel . . . . .       | 52 |
| print.LaMa_matrices . . . . .   | 52 |
| process_hid_formulas . . . . .  | 53 |
| pseudo_res . . . . .            | 54 |
| qreml . . . . .                 | 57 |

|                               |     |
|-------------------------------|-----|
| qreml_old . . . . .           | 62  |
| rep_sp . . . . .              | 66  |
| scores . . . . .              | 67  |
| sdreportMC . . . . .          | 68  |
| sdreport_outer . . . . .      | 70  |
| simulate.LaMaModel . . . . .  | 71  |
| skewnorm . . . . .            | 73  |
| smoothdens . . . . .          | 74  |
| statedens . . . . .           | 76  |
| stateprobs . . . . .          | 78  |
| stateprobs_g . . . . .        | 79  |
| stateprobs_p . . . . .        | 81  |
| stationary . . . . .          | 82  |
| stationary_ct . . . . .       | 83  |
| stationary_p . . . . .        | 84  |
| stationary_p_sparse . . . . . | 85  |
| stationary_sparse . . . . .   | 86  |
| summary.LaMaModel . . . . .   | 87  |
| summary.qremlModel . . . . .  | 88  |
| tpm . . . . .                 | 88  |
| tpm_ct . . . . .              | 90  |
| tpm_emb . . . . .             | 91  |
| tpm_emb_g . . . . .           | 92  |
| tpm_g . . . . .               | 93  |
| tpm_g2 . . . . .              | 95  |
| tpm_hsmm . . . . .            | 96  |
| tpm_hsmm2 . . . . .           | 97  |
| tpm_ihsmm . . . . .           | 98  |
| tpm_p . . . . .               | 99  |
| tpm_phsmm . . . . .           | 101 |
| tpm_phsmm2 . . . . .          | 102 |
| tpm_thinned . . . . .         | 104 |
| trex . . . . .                | 105 |
| trigBasisExp . . . . .        | 105 |
| viterbi . . . . .             | 106 |
| viterbi_g . . . . .           | 107 |
| viterbi_p . . . . .           | 108 |
| vm . . . . .                  | 109 |
| wrpcauchy . . . . .           | 110 |
| zero_inflate . . . . .        | 111 |
| %sp% . . . . .                | 112 |

---

|               |                                                                                           |
|---------------|-------------------------------------------------------------------------------------------|
| calc_trackInd | <i>Calculate the index of the first observation of each track based on an ID variable</i> |
|---------------|-------------------------------------------------------------------------------------------|

---

### Description

Function to conveniently calculate the trackInd variable that is needed internally when fitting a model to longitudinal data with multiple tracks.

### Usage

```
calc_trackInd(ID)
```

### Arguments

|    |                                                                                |
|----|--------------------------------------------------------------------------------|
| ID | ID variable of track IDs that is of the same length as the data to be analysed |
|----|--------------------------------------------------------------------------------|

### Value

A vector of indices of the first observation of each track which can be passed to the forward and forward\_g to sum likelihood contributions of each track

### Examples

```
uniqueID = c("Animal1", "Animal2", "Animal3")
ID = rep(uniqueID, c(100, 200, 300))
trackInd = calc_trackInd(ID)
```

---

|         |                                      |
|---------|--------------------------------------|
| cosinor | <i>Trigonometric basis expansion</i> |
|---------|--------------------------------------|

---

### Description

Builds a design matrix of sin/cos pairs for use in models with periodic predictors. Can be used directly or inside formulas passed to modmat (where expansion is handled automatically).

### Usage

```
cosinor(x, period = 24)
```

### Arguments

|        |                                                                                                                           |
|--------|---------------------------------------------------------------------------------------------------------------------------|
| x      | Numeric vector of the periodic variable.                                                                                  |
| period | Numeric vector of period lengths, e.g. 24 for a daily cycle with hourly data or c(24, 12) for a daily + semi-daily cycle. |

## Details

The resulting columns form the basis for linear predictors of the form

$$\eta_t = \beta_0 + \sum_k \left( \beta_{1k} \sin\left(\frac{2\pi x_t}{\text{period}_k}\right) + \beta_{2k} \cos\left(\frac{2\pi x_t}{\text{period}_k}\right) \right).$$

## Value

A numeric matrix with  $2 * \text{length}(\text{period})$  columns named  $\sin(2\pi x / \text{period}) / \cos(2\pi x / \text{period})$ .

## Examples

```
cosinor(1:24, period = 24)
cosinor(1:24, period = c(24, 12, 6))

## In model formulas (expand_cosinor handles the expansion):
form <- ~ x + temp * cosinor(hour, c(24, 12))
data <- data.frame(x = runif(24), temp = rnorm(24, 20), hour = 1:24)
modmat <- modmat(form, data = data)
```

---

|        |                                                                                   |
|--------|-----------------------------------------------------------------------------------|
| ddwell | <i>State dwell-time distributions of periodically inhomogeneous Markov chains</i> |
|--------|-----------------------------------------------------------------------------------|

---

## Description

Computes the dwell-time distribution of a periodically inhomogeneous Markov chain for a given transition probability matrix.

## Usage

```
ddwell(x, Gamma, time = NULL, state = NULL)
```

## Arguments

|       |                                                                                                                                                                                          |
|-------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x     | vector of (non-negative) dwell times to compute the dwell-time distribution for                                                                                                          |
| Gamma | array of L unique transition probability matrices of a periodically inhomogeneous Markov chain, with dimensions $c(N, N, L)$ , where N is the number of states and L is the cycle length |
| time  | integer vector of time points in 1:L at which to compute the dwell-time distribution. If NULL, the overall dwell-time distribution is computed.                                          |
| state | integer vector of state indices for which to compute the dwell-time distribution. If NULL, dwell-time distributions for all states are returned in a named list.                         |

## Details

For Markov chains whose transition probabilities vary only periodically, which is achieved for example by expressing the transition probability matrix as a periodic function of the time of day using `tpm_p` or `cosinor`, the probability distribution of time spent in a state can be computed analytically. This function computes said distribution, either for a specific time point (conditioning on transitioning into the state at that time point) or for the overall distribution (conditioning on transitioning into the state at any time point).

## Value

either time-varying dwell-time distribution(s) if time is specified, or overall dwell-time distribution if time is NULL. If more than one state is specified, a named list over states is returned.

## References

When using this function, please cite:

Koslik, J. O., Feldmann, C. C., Mews, S., Michels, R., & Langrock, R. (2025). Inference on the state process of periodically inhomogeneous hidden Markov models for animal behavior. *The Annals of Applied Statistics*, 19(4), 2724–2737.

## Examples

```
# setting parameters for trigonometric link
beta = matrix(c(-1, 2, -1, -2, 1, -1), nrow = 2, byrow = TRUE)
Gamma = tpm_p(beta = beta, degree = 1)

# at specific times and for specific state
ddwell(1:20, Gamma, time = 1:4, state = 1)
# results in 4x20 matrix

# or overall distribution for all states
ddwell(1:20, Gamma)
# results in list of length 2, each element is a vector of length 20
```

---

dgmrf2

---

*Reparametrised multivariate Gaussian distribution*


---

## Description

Density function of the multivariate Gaussian distribution reparametrised in terms of its precision matrix (inverse variance). This implementation is particularly useful for defining the **joint log-likelihood** with penalised splines or i.i.d. random effects that have a multivariate Gaussian distribution with fixed precision/ penalty matrix  $\lambda S$ . As  $S$  is fixed and only scaled by  $\lambda$ , it is more efficient to precompute the determinant of  $S$  (for the normalisation constant) and only scale the quadratic form by  $\lambda$  when multiple spline parameters/ random effects with different  $\lambda$ 's but the same penalty matrix  $S$  are evaluated.

**Usage**

```
dgmrf2(x, mu = 0, S, lambda, logdetS = NULL, log = FALSE)
```

**Arguments**

|         |                                                                                                                                                                                                                                       |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x       | density evaluation point, either a vector or a matrix                                                                                                                                                                                 |
| mu      | mean parameter. Either scalar or vector                                                                                                                                                                                               |
| S       | unscaled precision matrix                                                                                                                                                                                                             |
| lambda  | precision scaling parameter<br>Can be a vector if x is a matrix. Then each row of x is evaluated with the corresponding lambda. This is beneficial from an efficiency perspective because the determinant of S is only computed once. |
| logdetS | Optional precomputed log determinant of the precision matrix S. If the precision matrix does not depend on parameters, it can be precomputed and passed to the function.                                                              |
| log     | logical; if TRUE, densities are returned on the log scale.                                                                                                                                                                            |

**Details**

This implementation allows for automatic differentiation with RTMB.

**Value**

vector of density values

**Examples**

```
x = matrix(runif(30), nrow = 3)

# iid random effects
S = diag(10)
sigma = c(1, 2, 3) # random effect standard deviations
lambda = 1 / sigma^2
d = dgmrf2(x, 0, S, lambda)

# P-splines
L = diff(diag(10), diff = 2) # second-order difference matrix
S = t(L) %*% L
lambda = c(1,2,3)
d = dgmrf2(x, 0, S, lambda, log = TRUE)
```

---

forward

---

*Forward algorithm to calculate the HMM log-likelihood*


---

### Description

Calculates the log-likelihood of a sequence of observations under a hidden Markov model using the **forward algorithm** (Zucchini, MacDonald & Langrock, 2016).

### Usage

```
forward(
  delta,
  Gamma,
  allprobs,
  trackID = NULL,
  logspace = FALSE,
  bw = NULL,
  report = TRUE,
  ad = NULL,
  tod = NULL
)
```

### Arguments

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial distribution; either <ul style="list-style-type: none"> <li>• a vector of length nStates, or</li> <li>• a matrix of dimension c(nTracks, nStates), if trackID is provided, or</li> <li>• "stationary", for the (periodically) stationary distribution of Gamma at the start of each track (see 'Details').</li> </ul>                                                                                                                          |
| Gamma    | transition probability matrix; either <ul style="list-style-type: none"> <li>• a matrix of dimension c(nStates, nStates),</li> <li>• an array of dimension c(nStates, nStates, nTracks) if trackID is provided,</li> <li>• an array of dimension c(nStates, nStates, nObs) for time-varying transition probabilities, or</li> <li>• an array of dimension c(nStates, nStates, L) for periodic transition probabilities, if tod is provided.</li> </ul> |
| allprobs | matrix of state-dependent probabilities or density values of dimension c(nObs, nStates)                                                                                                                                                                                                                                                                                                                                                                |
| trackID  | optional vector of length nObs containing nTracks unique IDs that separate tracks (see 'Details'). The observations of each track need to be consecutive.                                                                                                                                                                                                                                                                                              |
| logspace | logical; if TRUE, allprobs is assumed to be on the log-scale, improving numerical stability for small probabilities.                                                                                                                                                                                                                                                                                                                                   |

|        |                                                                                                                                                                                                                                                                                                                                                  |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| bw     | optional positive integer specifying the bandwidth for a banded approximation of the forward algorithm, inducing a banded Hessian w.r.t. the observations. Defaults to NULL (exact algorithm). Approximation error decays geometrically in bw. Only used with automatic differentiation; otherwise the exact likelihood is computed.             |
| report | logical; if TRUE (default), delta, Gamma, allprobs, and trackID are reported from the fitted model. Requires ad = TRUE.                                                                                                                                                                                                                          |
| ad     | logical; whether to use automatic differentiation. Determined automatically — for debugging only.                                                                                                                                                                                                                                                |
| tod    | optional integer vector of length nObs with values in 1, ..., L, indexing the slices of Gamma for periodic models (e.g. time of day with L = 24 for hourly data). $\text{Gamma}[, , \text{tod}[t]]$ is the transition into time t, hence the periodically stationary initial distribution is <code>stationary_p(Gamma, tod[1] %% L + 1)</code> . |

## Details

If trackID is provided, the total log-likelihood is the sum of each track's likelihood contribution. In this case, Gamma can be

- a matrix (same transition probabilities for each track),
- an array of dimension  $c(\text{nStates}, \text{nStates}, \text{nTracks})$  (track-specific transition probability matrix), or
- an array of dimension  $c(\text{nStates}, \text{nStates}, \text{nObs})$  for time-varying transition probabilities, or
- an array of dimension  $c(\text{nStates}, \text{nStates}, L)$  for periodic transition probabilities, if tod is provided.

Additionally, delta can be a vector (same initial distribution for each track) or a matrix of dimension  $c(\text{nTracks}, \text{nStates})$  (track-specific initial distributions).

With `delta = "stationary"`, the initial distribution of each track is computed from Gamma:

- the stationary distribution of Gamma (or of its slice for each track, if track-specific),
- the periodically stationary distribution at the first time point of each track, if tod is provided (see [stationary\\_p](#)),
- the stationary distribution of the first slice of each track, for time-varying transition probabilities, i.e. at the covariate values of the first observation.

This requires Gamma to contain transition probability matrices (not, e.g., sub-stochastic matrices), which is checked without automatic differentiation. The computed delta is reported as a matrix of dimension  $c(\text{nTracks}, \text{nStates})$ .

**Note:** forward should only be called **once** in the likelihood function, with a trackID argument for multiple tracks. Downstream functions like [lama](#), [viterbi](#), [stateprobs](#) or [pseudo\\_res](#) rely on the quantities it reports, and only those of the last call are kept.

## Value

HMM log-likelihood for given data and parameters

## References

Zucchini, W., MacDonald, I.L., & Langrock, R. (2016). *Hidden Markov Models for Time Series: An Introduction Using R* (2nd ed.). Chapman & Hall/CRC.

Mews, Koslik, & Langrock (2025). How to build your latent Markov model: The role of time and space. *Statistical Modelling*, 25(6), 481–507.

## See Also

Other forward algorithms: [forward\\_g\(\)](#), [forward\\_hsmm\(\)](#), [forward\\_ihsmm\(\)](#), [forward\\_p\(\)](#), [forward\\_phsmm\(\)](#)

## Examples

```
## negative log likelihood function
nll = function(par, step) {
  # parameter transformations for unconstrained optimisation
  Gamma = tpm(par[1:2]) # multinomial logit link
  delta = stationary(Gamma) # stationary HMM
  mu = exp(par[3:4])
  sigma = exp(par[5:6])
  # calculate all state-dependent probabilities
  allprobs = matrix(1, length(step), 2)
  ind = which(!is.na(step))
  for(j in 1:2) allprobs[ind,j] = dgamma2(step[ind], mu[j], sigma[j])
  # simple forward algorithm to calculate log-likelihood
  -forward(delta, Gamma, allprobs)
}

## fitting an HMM to the trex data
par = c(-2,-2,          # initial tpm params (logit-scale)
        log(c(0.3, 2.5)), # initial means for step length (log-transformed)
        log(c(0.2, 1.5))) # initial sds for step length (log-transformed)
mod = nlm(nll, par, step = trex$step[1:1000])
```

---

forward\_g

*Forward algorithm with time-varying transition probability matrix*

---

## Description

Calculates the log-likelihood of a sequence of observations under a hidden Markov model with time-varying transition probabilities using the **forward algorithm** (Zucchini, MacDonald & Langrock, 2016).

## Usage

```
forward_g(
  delta,
  Gamma,
  allprobs,
```

```

    trackID = NULL,
    logspace = FALSE,
    bw = NULL,
    report = TRUE,
    ad = NULL
)

```

## Arguments

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial distribution; either <ul style="list-style-type: none"> <li>• a vector of length nStates, or</li> <li>• a matrix of dimension c(nTracks, nStates), if trackID is provided.</li> </ul>                                                                                                                                                                                                                                        |
| Gamma    | array of transition probability matrices of dimension c(nStates, nStates, nObs), where the first slice of each track is ignored as there is no transition into the start of a track.<br>For a single track, an array of dimension c(nStates, nStates, nObs-1) is also accepted.<br>This function also supports continuous-time HMMs, where each slice is a Markov semigroup $\Gamma(\Delta t) = \exp(Q\Delta t)$ for generator $Q$ . |
| allprobs | matrix of state-dependent probabilities or density values of dimension c(nObs, nStates)                                                                                                                                                                                                                                                                                                                                              |
| trackID  | optional vector of length nObs containing nTracks unique IDs that separate tracks (see ‘Details’). The observations of each track need to be consecutive.                                                                                                                                                                                                                                                                            |
| logspace | logical; if TRUE, allprobs is assumed to be on the log-scale, improving numerical stability for small probabilities.                                                                                                                                                                                                                                                                                                                 |
| bw       | optional positive integer specifying the bandwidth for a banded approximation of the forward algorithm, inducing a banded Hessian w.r.t. the observations. Defaults to NULL (exact algorithm). Approximation error decays geometrically in bw. Only used with automatic differentiation; otherwise the exact likelihood is computed.                                                                                                 |
| report   | logical; if TRUE (default), delta, Gamma, allprobs, and trackID are reported from the fitted model. Requires ad = TRUE.                                                                                                                                                                                                                                                                                                              |
| ad       | logical; whether to use automatic differentiation. Determined automatically — for debugging only.                                                                                                                                                                                                                                                                                                                                    |

## Details

**Deprecated:** please use [forward](#) for all model types instead.

If trackID is provided, the total log-likelihood will be the sum of each track’s likelihood contribution. In this case, Gamma must be an array of dimension c(nStates, nStates, nObs), matching the number of rows of allprobs. For each track, the transition matrix at the beginning of the track will be ignored (as there is no transition between tracks). Additionally, delta can be a vector (same initial distribution for each track) or a matrix of dimension c(nTracks, nStates) (different initial distribution for each track).

**Note:** When there are multiple tracks, for compatibility with downstream functions like [viterbi\\_g](#), [stateprobs\\_g](#) or [pseudo\\_res](#), forward\_g should only be called **once** with a trackID argument.

**Value**

HMM log-likelihood for given data and parameters

**References**

Zucchini, W., MacDonald, I.L., & Langrock, R. (2016). *Hidden Markov Models for Time Series: An Introduction Using R* (2nd ed.). Chapman & Hall/CRC.

Mews, Koslik, & Langrock (2025). How to build your latent Markov model: The role of time and space. *Statistical Modelling*, 25(6), 481–507.

**See Also**

Other forward algorithms: [forward\(\)](#), [forward\\_hsmm\(\)](#), [forward\\_ihsmm\(\)](#), [forward\\_p\(\)](#), [forward\\_phsmm\(\)](#)

**Examples**

```
## Simple usage
Gamma = array(c(0.9, 0.2, 0.1, 0.8), dim = c(2,2,10))
delta = c(0.5, 0.5)
allprobs = matrix(0.5, 10, 2)
forward_g(delta, Gamma, allprobs)

## Full model fitting example
## negative log likelihood function
nll = function(par, step, Z) {
  # parameter transformations for unconstrained optimisation
  beta = matrix(par[1:6], nrow = 2)
  Gamma = tpm_g(Z, beta) # multinomial logit link for each time point
  delta = stationary(Gamma[,1]) # stationary HMM
  mu = exp(par[7:8])
  sigma = exp(par[9:10])
  # calculate all state-dependent probabilities
  allprobs = matrix(1, length(step), 2)
  ind = which(!is.na(step))
  for(j in 1:2) allprobs[ind,j] = dgamma2(step[ind], mu[j], sigma[j])
  # simple forward algorithm to calculate log-likelihood
  -forward_g(delta, Gamma, allprobs)
}

## fitting an HMM to the trex data
par = c(-1.5, -1.5,          # initial tpm intercepts (logit-scale)
        rep(0, 4),         # initial tpm slopes
        log(c(0.3, 2.5)),  # initial means for step length (log-transformed)
        log(c(0.2, 1.5)))  # initial sds for step length (log-transformed)
mod = nlm(nll, par, step = trex$step[1:500], Z = cosinor(trex$tod[1:500]))
```

---

|              |                                                                                                                                                                                                                                                                                                                                                                      |
|--------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| forward_hsmm | <i>Rhref<a href="https://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock">https://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock</a>Forward algorithm for homogeneous hidden semi-Markov models</i> |
|--------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

## Description

Calculates the (approximate) log-likelihood of a sequence of observations under a homogeneous hidden semi-Markov model using a modified **forward algorithm**.

## Usage

```
forward_hsmm(
  dm,
  omega,
  allprobs,
  trackID = NULL,
  delta = NULL,
  eps = 1e-10,
  report = TRUE
)
```

## Arguments

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dm       | list of length nStates containing vectors of dwell-time probability mass functions (PMFs) for each state. The vector lengths correspond to the approximating state aggregate sizes, hence there should be little probability mass not covered by these.                                                                                                                                                                                                                                                                                                                                                                                                  |
| omega    | matrix of dimension c(nStates, nStates) of conditional transition probabilities, also called embedded transition probability matrix.<br><br>Contains the transition probabilities given that the current state is left. Hence, the diagonal elements need to be zero and the rows need to sum to one. Can be constructed using <a href="#">tpm_emb</a> .                                                                                                                                                                                                                                                                                                 |
| allprobs | matrix of state-dependent probabilities/ density values of dimension c(nObs, nStates) which will automatically be converted to the appropriate dimension.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| trackID  | optional vector of length nObs containing IDs<br><br>If provided, the total log-likelihood will be the sum of each track's likelihood contribution. In this case, dm can be a nested list, where the top layer contains k dm lists as described above. omega can then also be an array of dimension c(nStates, nStates, nTracks) with one conditional transition probability matrix for each track. Furthermore, instead of a single vector delta corresponding to the initial distribution, a delta matrix of initial distributions, of dimension c(nTracks, nStates), can be provided, such that each track starts with it's own initial distribution. |

|        |                                                                                                                                                                               |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta  | optional vector of initial state probabilities of length nStates<br>By default, the stationary distribution is computed (which is typically recommended).                     |
| eps    | small value to avoid numerical issues in the approximating transition matrix construction. Usually, this should not be changed.                                               |
| report | logical, indicating whether initial distribution, approximating transition probability matrix and allprobs matrix should be reported from the fitted model. Defaults to TRUE. |

Details

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs, where the state duration distribution is explicitly modelled by a distribution on the positive integers. For direct numerical maximum likelihood estimation, HSMMs can be represented as HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities.

This function is designed to be used with automatic differentiation based on the R package RTMB. It will be very slow without it!

Value

HSMM log-likelihood for given data and parameters

References

Langrock, R., & Zucchini, W. (2011). Hidden Markov models with arbitrary state dwell-time distributions. *Computational Statistics & Data Analysis*, 55(1), 715-724.

Koslik, J. O. (2025). Hidden semi-Markov models with inhomogeneous state dwell-time distributions. *Computational Statistics & Data Analysis*, 209, 108171.

See Also

Other forward algorithms: `forward()`, `forward_g()`, `forward_ihsmm()`, `forward_p()`, `forward_phsmm()`

Examples

# currently no examples

---

|               |                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|---------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| forward_ihsmm | <i>Rhref<a href="https://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock">https://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock</a>Forward algorithm for hidden semi-Markov models with inhomogeneous state durations and/ or conditional transition probabilities</i> |
|---------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

Description

Calculates the (approximate) log-likelihood of a sequence of observations under an inhomogeneous hidden semi-Markov model using a modified **forward algorithm**.

**Usage**

```
forward_ihsmm(
  dm,
  omega,
  allprobs,
  trackID = NULL,
  delta = NULL,
  startInd = NULL,
  eps = 1e-10,
  report = TRUE
)
```

**Arguments**

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dm       | <p>list of length nStates containing matrices (or vectors) of dwell-time probability mass functions (PMFs) for each state.</p> <p>If the dwell-time PMFs are constant, the vectors are the PMF of the dwell-time distribution fixed in time. The vector lengths correspond to the approximating state aggregate sizes, hence there should be little probability mass not covered by these.</p> <p>If the dwell-time PMFs are inhomogeneous, the matrices need to have n rows, where n is the number of observations. The number of columns again corresponds to the size of the approximating state aggregates.</p> <p>In the latter case, the first <math>\max(\text{sapply}(\text{dm}, \text{ncol})) - 1</math> observations will not be used because the first approximating transition probability matrix needs to be computed based on the first <math>\max(\text{sapply}(\text{dm}, \text{ncol}))</math> covariate values (represented by dm).</p> |
| omega    | <p>matrix of dimension <math>c(\text{nStates}, \text{nStates})</math> or array of dimension <math>c(\text{nStates}, \text{nStates}, \text{nObs})</math> of conditional transition probabilities, also called embedded transition probability matrix.</p> <p>It contains the transition probabilities given the current state is left. Hence, the diagonal elements need to be zero and the rows need to sum to one. Such a matrix can be constructed using <a href="#">tpm_emb</a> and an array using <a href="#">tpm_emb_g</a>.</p>                                                                                                                                                                                                                                                                                                                                                                                                                     |
| allprobs | matrix of state-dependent probabilities/ density values of dimension $c(\text{nObs}, \text{nStates})$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| trackID  | <p>trackID optional vector of length nObs containing IDs</p> <p>If provided, the total log-likelihood will be the sum of each track's likelihood contribution. Instead of a single vector delta corresponding to the initial distribution, a delta matrix of initial distributions, of dimension <math>c(\text{nTracks}, \text{nStates})</math>, can be provided, such that each track starts with its own initial distribution.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| delta    | <p>optional vector of initial state probabilities of length N</p> <p>By default, instead of this, the stationary distribution is computed corresponding to the first approximating transition probability matrix of each track is computed. Contrary to the homogeneous case, this is not theoretically motivated but just for convenience.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| startInd | <p>optional integer index at which the forward algorithm starts.</p> <p>When approximating inhomogeneous HSMMs by inhomogeneous HMMs, the first transition probability matrix that can be constructed is at time <code>max(sapply(dm, ncol))</code> (as it depends on the previous covariate values). Hence, when not provided, <code>startInd</code> is chosen to be <code>max(sapply(dm, ncol))</code>. Fixing <code>startInd</code> at a value <b>larger</b> than <code>max(aggregate sizes)</code> is useful when models with different aggregate sizes are fitted to the same data and are supposed to be compared. In that case it is important that all models use the same number of observations.</p> |
| eps      | <p>small value to avoid numerical issues in the approximating transition matrix construction. Usually, this should not be changed.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| report   | <p>logical, indicating whether initial distribution, approximating transition probability matrix and <code>allprobs</code> matrix should be reported from the fitted model. Defaults to TRUE.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |

## Details

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs, where the state duration distribution is explicitly modelled by a distribution on the positive integers. This function can be used to fit HSMMs where the state-duration distribution and/ or the conditional transition probabilities vary with covariates. For direct numerical maximum likelihood estimation, HSMMs can be represented as HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities.

This function is designed to be used with automatic differentiation based on the R package RTMB. It will be very slow without it!

## Value

HSMM log-likelihood for given data and parameters

## References

Koslik, J. O. (2025). Hidden semi-Markov models with inhomogeneous state dwell-time distributions. *Computational Statistics & Data Analysis*, 209, 108171.

## See Also

Other forward algorithms: [forward\(\)](#), [forward\\_g\(\)](#), [forward\\_hsmm\(\)](#), [forward\\_p\(\)](#), [forward\\_phsmm\(\)](#)

## Examples

# currently no examples

---

|           |                                                                                                                                                                                                                                                                                                                                                                                    |
|-----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| forward_p | <a href="https://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock">Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock</a> Forward algorithm with for periodically varying transition probability matrices |
|-----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

## Description

Calculates the log-likelihood of a sequence of observations under a hidden Markov model with periodically varying transition probabilities using the **forward algorithm**.

## Usage

```
forward_p(
  delta,
  Gamma,
  allprobs,
  tod,
  trackID = NULL,
  ad = NULL,
  report = TRUE,
  logspace = FALSE
)
```

## Arguments

|          |                                                                                                                                                                                                                                                                                                                                                                                     |
|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial or stationary distribution of length nStates, or matrix of dimension c(nTracks, nStates) for nTracks independent tracks, if trackID is provided                                                                                                                                                                                                                             |
| Gamma    | array of transition probability matrices of dimension c(nStates, nStates, L). Here we use the definition $\Pr(S_t = j \mid S_{t-1} = i) = \gamma_{ij}^{(t)}$ such that the transition probabilities between time point $t - 1$ and $t$ are an element of $\Gamma^{(t)}$ .                                                                                                           |
| allprobs | matrix of state-dependent probabilities/ density values of dimension c(nObs, nStates)                                                                                                                                                                                                                                                                                               |
| tod      | (Integer valued) variable for cycle indexing in 1, ..., L, mapping the data index to a generalised time of day (length nObs)<br>For half-hourly data L = 48. It could, however, also be day of year for daily data and L = 365.                                                                                                                                                     |
| trackID  | optional vector of length nObs containing IDs<br>If provided, the total log-likelihood will be the sum of each track's likelihood contribution. Instead of a single vector delta corresponding to the initial distribution, a delta matrix of initial distributions of dimension c(nTracks, nObs), can be provided, such that each track starts with it's own initial distribution. |
| ad       | optional logical, indicating whether automatic differentiation with RTMB should be used. By default, the function determines this itself.                                                                                                                                                                                                                                           |

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| report   | logical, indicating whether delta, Gamma, allprobs, and potentially trackID should be reported from the fitted model. Defaults to TRUE, but only works if ad = TRUE, as it uses the RTMB package.<br><b>Caution:</b> When there are multiple tracks, for compatibility with downstream functions like <a href="#">viterbi_p</a> , <a href="#">stateprobs_p</a> or <a href="#">pseudo_res</a> , forward_p should only be called <b>once</b> with a trackID argument. |
| logspace | logical, indicating whether the probabilities/ densities in the allprobs matrix are on log-scale. If so, internal computations are also done on log-scale which is numerically more robust when the entries are very small.                                                                                                                                                                                                                                         |

## Details

**Deprecated:** please use [forward](#) with argument tod instead.

When the transition probability matrix only varies periodically (e.g. as a function of time of day), there are only  $L$  unique matrices if  $L$  is the period length (e.g.  $L = 24$  for hourly data and time-of-day variation). Thus, it is much more efficient to only calculate these  $L$  matrices and index them by a time variable (e.g. time of day or day of year) instead of calculating such a matrix for each index in the data set (which would be redundant). This function allows for that by only expecting a transition probability matrix for each time point in a period and an integer valued  $(1, \dots, L)$  time variable that maps the data index to the according time.

## Value

HMM log-likelihood for given data and parameters

## See Also

Other forward algorithms: [forward\(\)](#), [forward\\_g\(\)](#), [forward\\_hsmm\(\)](#), [forward\\_ihsmm\(\)](#), [forward\\_phsmm\(\)](#)

## Examples

```
## negative log likelihood function
nll = function(par, step, tod) {
  # parameter transformations for unconstrained optimisation
  beta = matrix(par[1:6], nrow = 2)
  Gamma = tpm_p(1:24, beta = beta) # multinomial logit link for each time point
  delta = stationary_p(Gamma, tod[1] %% 24 + 1) # stationary HMM
  mu = exp(par[7:8])
  sigma = exp(par[9:10])
  # calculate all state-dependent probabilities
  allprobs = matrix(1, length(step), 2)
  ind = which(!is.na(step))
  for(j in 1:2) allprobs[ind,j] = dgamma2(step[ind], mu[j], sigma[j])
  # simple forward algorithm to calculate log-likelihood
  -forward_p(delta, Gamma, allprobs, tod)
}

## fitting an HMM to the nessi data
par = c(-2,-2,          # initial tpm intercepts (logit-scale)
        rep(0, 4),      # initial tpm slopes
```

```

      log(c(0.3, 2.5)), # initial means for step length (log-transformed)
      log(c(0.2, 1.5))) # initial sds for step length (log-transformed)
mod = nlm(nll, par, step = trex$step[1:500], tod = trex$tod[1:500])

```

forward\_phsmm

*Rhref<https://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock>Forward algorithm for hidden semi-Markov models with periodically inhomogeneous state durations and/ or conditional transition probabilities*

## Description

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs, where the state duration distribution is explicitly modelled by a distribution on the positive integers. This function can be used to fit HSMMs where the state-duration distribution and/ or the conditional transition probabilities vary with covariates. For direct numerical maximum likelihood estimation, HSMMs can be represented as HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities.

This function can be used to fit HSMMs where the state-duration distribution and/ or the conditional transition probabilities vary periodically. In the special case of periodic variation (as compared to arbitrary covariate influence), this version is to be preferred over `forward_ihsmm` because it computes the **correct periodically stationary distribution** and no observations are lost for the approximation.

This function is designed to be used with automatic differentiation based on the R package RTMB. It will be very slow without it!

## Usage

```

forward_phsmm(
  dm,
  omega,
  allprobs,
  tod,
  trackID = NULL,
  delta = NULL,
  eps = 1e-10,
  report = TRUE
)

```

## Arguments

**dm** list of length `nStates` containing matrices (or vectors) of dwell-time probability mass functions (PMFs) for each state.

If the dwell-time PMFs are constant, the vectors are the PMF of the dwell-time distribution fixed in time. The vector lengths correspond to the approximating

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
|----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|          | state aggregate sizes, hence there should be little probability mass not covered by these.<br>If the dwell-time PMFs are inhomogeneous, the matrices need to have $L$ rows, where $L$ is the cycle length. The number of columns again correspond to the size of the approximating state aggregates.                                                                                                                                                    |
| omega    | matrix of dimension $c(nStates, nStates)$ or array of dimension $c(nStates, nStates, L)$ of conditional transition probabilities, also called embedded transition probability matrix<br>It contains the transition probabilities given the current state is left. Hence, the diagonal elements need to be zero and the rows need to sum to one. Such a matrix can be constructed using <code>tpm_emb</code> and an array using <code>tpm_emb_g</code> . |
| allprobs | matrix of state-dependent probabilities/ density values of dimension $c(nObs, nStates)$                                                                                                                                                                                                                                                                                                                                                                 |
| tod      | (Integer valued) variable for cycle indexing in $1, \dots, L$ , mapping the data index to a generalised time of day (length $nObs$ ). For half-hourly data $L = 48$ . It could, however, also be day of year for daily data and $L = 365$ .                                                                                                                                                                                                             |
| trackID  | optional vector of length $nObs$ containing IDs<br>If provided, the total log-likelihood will be the sum of each track's likelihood contribution. Instead of a single vector <code>delta</code> corresponding to the initial distribution, a <code>delta</code> matrix of initial distributions, of dimension $c(nTracks, nStates)$ , can be provided, such that each track starts with its own initial distribution.                                   |
| delta    | Optional vector of initial state probabilities of length $nStates$ . By default, instead of this, the stationary distribution is computed corresponding to the first approximating t.p.m. of each track is computed. Contrary to the homogeneous case, this is not theoretically motivated but just for convenience.                                                                                                                                    |
| eps      | small value to avoid numerical issues in the approximating transition matrix construction. Usually, this should not be changed.                                                                                                                                                                                                                                                                                                                         |
| report   | logical, indicating whether initial distribution, approximating transition probability matrix and <code>allprobs</code> matrix should be reported from the fitted model. Defaults to TRUE.                                                                                                                                                                                                                                                              |

## Details

Calculates the (approximate) log-likelihood of a sequence of observations under a periodically inhomogeneous hidden semi-Markov model using a modified **forward algorithm**.

## Value

HsMM log-likelihood for given data and parameters

## References

Koslik, J. O. (2025). Hidden semi-Markov models with inhomogeneous state dwell-time distributions. *Computational Statistics & Data Analysis*, 209, 108171.

## See Also

Other forward algorithms: `forward()`, `forward_g()`, `forward_hsmm()`, `forward_ihsmm()`, `forward_p()`

**Examples**

```
# currently no examples
```

---

|           |                                                                                                                                                                                                                                                                                                                                                                                                         |
|-----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| forward_s | <i><a href="https://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock">Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock</a>Forward algorithm for hidden semi-Markov models with homogeneous transition probability matrix</i> |
|-----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

**Description**

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs that can be approximated by HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities.

**Usage**

```
forward_s(delta, Gamma, allprobs, sizes)
```

**Arguments**

|          |                                                                                                                                                    |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial or stationary distribution of length $N$ , or matrix of dimension $c(k, N)$ for $k$ independent tracks, if trackID is provided             |
| Gamma    | transition probability matrix of dimension $c(M, M)$                                                                                               |
| allprobs | matrix of state-dependent probabilities/ density values of dimension $c(n, N)$ which will automatically be converted to the appropriate dimension. |
| sizes    | state aggregate sizes that are used for the approximation of the semi-Markov chain.                                                                |

**Value**

log-likelihood for given data and parameters

**Examples**

```
## generating data from homogeneous 2-state HSMM
mu = c(0, 6)
lambda = c(6, 12)
omega = matrix(c(0,1,1,0), nrow = 2, byrow = TRUE)
# simulation
# for a 2-state HSMM the embedded chain always alternates between 1 and 2
s = rep(1:2, 100)
C = x = numeric(0)
for(t in 1:100){
  dt = rpois(1, lambda[s[t]])+1 # shifted Poisson
  C = c(C, rep(s[t], dt))
  x = c(x, rnorm(dt, mu[s[t]], 1.5)) # fixed sd 2 for both states
}
```

```
## negative log likelihood function
mllk = function(theta.star, x, sizes){
  # parameter transformations for unconstraint optimization
  omega = matrix(c(0,1,1,0), nrow = 2, byrow = TRUE) # omega fixed (2-states)
  lambda = exp(theta.star[1:2]) # dwell time means
  dm = list(dpois(1:sizes[1]-1, lambda[1]), dpois(1:sizes[2]-1, lambda[2]))
  Gamma = tpm_hsmm2(omega, dm)
  delta = stationary(Gamma) # stationary
  mu = theta.star[3:4]
  sigma = exp(theta.star[5:6])
  # calculate all state-dependent probabilities
  allprobs = matrix(1, length(x), 2)
  for(j in 1:2){ allprobs[,j] = dnorm(x, mu[j], sigma[j]) }
  # return negative for minimization
  -forward_s(delta, Gamma, allprobs, sizes)
}

## fitting an HSMM to the data
theta.star = c(log(5), log(10), 1, 4, log(2), log(2))
mod = nlm(mllk, theta.star, x = x, sizes = c(20, 30), stepmax = 5)
```

forward\_sp

Rhref<https://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrock>Forward algorithm for hidden semi-Markov models with periodically varying transition probability matrices

## Description

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs that can be approximated by HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities. Recently, this inference procedure has been generalised to allow either the dwell-time distributions or the conditional transition probabilities to depend on external covariates such as the time of day. This special case is implemented here. This function allows for that, by expecting a transition probability matrix for each time point in a period, and an integer valued  $(1, \dots, L)$  time variable that maps the data index to the according time.

## Usage

```
forward_sp(delta, Gamma, allprobs, sizes, tod)
```

## Arguments

|       |                                                                                                                                                                                                                                                                     |
|-------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta | initial or stationary distribution of length $N$ , or matrix of dimension $c(k, N)$ for $k$ independent tracks, if trackID is provided                                                                                                                              |
| Gamma | array of transition probability matrices of dimension $c(M, M, L)$ .<br>Here we use the definition $\Pr(S_t = j \mid S_{t-1} = i) = \gamma_{ij}^{(t)}$ such that the transition probabilities between time point $t - 1$ and $t$ are an element of $\Gamma^{(t)}$ . |

|          |                                                                                                                                                                                                                                          |
|----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| allprobs | matrix of state-dependent probabilities/ density values of dimension $c(n, N)$ which will automatically be converted to the appropriate dimension.                                                                                       |
| sizes    | state aggregate sizes that are used for the approximation of the semi-Markov chain.                                                                                                                                                      |
| tod      | (Integer valued) variable for cycle indexing in $1, \dots, L$ , mapping the data index to a generalised time of day (length $n$ ). For half-hourly data $L = 48$ . It could, however, also be day of year for daily data and $L = 365$ . |

## Value

log-likelihood for given data and parameters

## Examples

```
## generating data from homogeneous 2-state HSMM
mu = c(0, 6)
beta = matrix(c(log(4), log(6), -0.2, 0.2, -0.1, 0.4), nrow=2)
# time varying mean dwell time
Lambda = exp(cbind(1, cosinor(1:24))%*%t(beta))
omega = matrix(c(0, 1, 1, 0), nrow = 2, byrow = TRUE)
# simulation
# for a 2-state HSMM the embedded chain always alternates between 1 and 2
s = rep(1:2, 100)
C = x = numeric(0)
tod = rep(1:24, 50) # time of day variable
time = 1
for(t in 1:100){
  dt = rpois(1, Lambda[tod[time], s[t]])+1 # dwell time depending on time of day
  time = time + dt
  C = c(C, rep(s[t], dt))
  x = c(x, rnorm(dt, mu[s[t]], 1.5)) # fixed sd 2 for both states
}
tod = tod[1:length(x)]

## negative log likelihood function
mllk = function(theta.star, x, sizes, tod){
  # parameter transformations for unconstraint optimization
  omega = matrix(c(0, 1, 1, 0), nrow = 2, byrow = TRUE) # omega fixed (2-states)
  mu = theta.star[1:2]
  sigma = exp(theta.star[3:4])
  beta = matrix(theta.star[5:10], nrow=2)
  # time varying mean dwell time
  Lambda = exp(cbind(1, cosinor(1:24))%*%t(beta))
  dm = list()
  for(j in 1:2){
    dm[[j]] = sapply(1:sizes[j]-1, dpois, lambda = Lambda[,j])
  }
  Gamma = tpm_phsmm2(omega, dm)
  delta = stationary_p(Gamma, tod[1])
  # calculate all state-dependent probabilities
  allprobs = matrix(1, length(x), 2)
  for(j in 1:2){ allprobs[,j] = dnorm(x, mu[j], sigma[j]) }
```

```

    # return negative for minimization
    -forward_sp(delta, Gamma, allprobs, sizes, tod)
  }

  ## fitting an HSMM to the data
  theta.star = c(1, 4, log(2), log(2), # state-dependent parameters
                log(4), log(6), rep(0,4)) # state process parameters dm
  # mod = nlm(mllk, theta.star, x = x, sizes = c(10, 15), tod = tod, stepmax = 5)

```

gamma2

*Reparametrised gamma distribution***Description**

Density, distribution function, quantile function and random generation for the gamma distribution reparametrised in terms of mean and standard deviation.

**Usage**

```

dgamma2(x, mean = 1, sd = 1, log = FALSE)

pgamma2(q, mean = 1, sd = 1, lower.tail = TRUE, log.p = FALSE)

qgamma2(p, mean = 1, sd = 1, lower.tail = TRUE, log.p = FALSE)

rgamma2(n, mean = 1, sd = 1)

```

**Arguments**

|            |                                                                                                    |
|------------|----------------------------------------------------------------------------------------------------|
| x, q       | vector of quantiles                                                                                |
| mean       | mean parameter, must be positive scalar.                                                           |
| sd         | standard deviation parameter, must be positive scalar.                                             |
| log, log.p | logical; if TRUE, probabilities/ densities $p$ are returned as $\log(p)$ .                         |
| lower.tail | logical; if TRUE, probabilities are $P[X \leq x]$ , otherwise, $P[X > x]$ .                        |
| p          | vector of probabilities                                                                            |
| n          | number of observations. If $\text{length}(n) > 1$ , the length is taken to be the number required. |

**Details**

This implementation allows for automatic differentiation with RTMB.

**Value**

dgamma2 gives the density, pgamma2 gives the distribution function, qgamma2 gives the quantile function, and rgamma2 generates random deviates.

**Examples**

```
x = rgamma2(1)
d = dgamma2(x)
p = pgamma2(x)
q = qgamma2(p)
```

---

gdeterminant

*Computes generalised determinant*


---

**Description**

Computes generalised determinant

**Usage**

```
gdeterminant(x, eps = NULL, log = TRUE)
```

**Arguments**

|     |                                                                                           |
|-----|-------------------------------------------------------------------------------------------|
| x   | symmetric matrix                                                                          |
| eps | eigenvalues smaller than this will be treated as zero                                     |
| log | logical. If TRUE, the log-determinant is returned. If FALSE, the determinant is returned. |

**Value**

generalised log-determinant of x

---

generator

*Build the generator matrix of a continuous-time Markov chain*


---

**Description**

This function builds the **infinitesimal generator matrix** for a **continuous-time Markov chain** from an unconstrained parameter vector.

**Usage**

```
generator(
  beta,
  Z = NULL,
  Eta = NULL,
  byrow = FALSE,
  report = TRUE,
  param = NULL
)
```

## Arguments

|        |                                                                                                                                                                                                                                                   |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| beta   | parameters; either <ul style="list-style-type: none"> <li>• a vector of length <math>nStates * (nStates-1)</math>, or</li> <li>• a matrix of dimension <math>c(nStates * (nStates-1), p+1)</math> if design matrix Z is also provided.</li> </ul> |
| Z      | optional covariate design matrix with or without intercept column, i.e. of dimension $c(nObs, p)$ or $c(nObs, p+1)$ . If provided, beta needs to be a matrix of dimension $c(nStates * (nStates-1), p+1)$ .                                       |
| Eta    | optional pre-calculated matrix of linear predictors of dimension $c(nObs, nStates * (nStates-1))$ . If provided, Z and beta will be ignored.                                                                                                      |
| byrow  | logical indicating if the generator matrix should be filled by row                                                                                                                                                                                |
| report | logical, indicating whether the generator matrix Q should be reported from the fitted model. Defaults to TRUE, but only works if when automatic differentiation with RTMB is used.                                                                |
| param  | deprecated, please use argument beta instead.                                                                                                                                                                                                     |

## Details

Off-diagonal entries are calculated as  $\exp(\beta_i)$  to ensure positivity. The diagonal entries are then set to the negative row sums, which is required for generator matrices.

If a design matrix Z or a matrix of linear predictors Eta is provided, the function will automatically call [generator\\_g](#) to build the generator matrix based on the design matrix and coefficient matrix. In that case, the argument beta needs to be a matrix of coefficients of dimension  $c(nStates * (nStates-1), p+1)$ , where the first column contains the intercepts.

## Value

infinitesimal generator matrix of dimension  $c(nStates, nStates)$  or array of such matrices of dimension  $c(nStates, nStates, nObs)$  if Z or Eta is provided.

## See Also

Other transition probability matrix functions: [generator\\_g\(\)](#), [tpm\(\)](#), [tpm\\_ct\(\)](#), [tpm\\_emb\(\)](#), [tpm\\_emb\\_g\(\)](#), [tpm\\_g\(\)](#), [tpm\\_g2\(\)](#), [tpm\\_p\(\)](#)

## Examples

```
# 2 states: 2 free off-diagonal elements
generator(rep(-1, 2))
# 3 states: 6 free off-diagonal elements
generator(rep(-2, 6))
```

generator\_g

*Build generator matrices of a continuous-time Markov chain***Description**

This function builds **infinitesimal generator matrices** for a **continuous-time Markov chain** based on a design matrix and coefficient matrix.

**Usage**

```
generator_g(Z, beta, Eta = NULL, byrow = FALSE, report = TRUE)
```

**Arguments**

|        |                                                                                                                                                                                                 |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Z      | Covariate design matrix with or without intercept column, i.e. of dimension $c(n_{\text{obs}}, p)$ or $c(n_{\text{obs}}, p+1)$ . If not provided, intercept column is added automatically.      |
| beta   | Matrix of coefficients for the off-diagonal elements of the generator matrix of dimension $c(n_{\text{states}} * (n_{\text{states}}-1), p+1)$ . First columns contains the intercepts.          |
| Eta    | optional pre-calculated matrix of linear predictors of dimension $c(n_{\text{obs}}, n_{\text{states}} * (n_{\text{states}}-1))$ . If provided, no Z and beta are necessary and will be ignored. |
| byrow  | logical indicating if the generator matrices should be filled by row                                                                                                                            |
| report | logical, indicating whether the generator matrices Q should be reported from the fitted model. Defaults to TRUE, but only works if when automatic differentiation with RTMB is used.            |

**Details**

**Deprecated:** please use [generator](#)(beta, Z) for all model types instead.

Off-diagonal entries are calculated as  $\exp(Z\beta_i)$  to ensure positivity. The diagonal entries are then set to the negative row sums, which is required for generator matrices.

**Value**

array of infinitesimal generator matrices of dimension  $c(n_{\text{states}}, n_{\text{states}}, n_{\text{obs}})$

**See Also**

Other transition probability matrix functions: [generator\(\)](#), [tpm\(\)](#), [tpm\\_ct\(\)](#), [tpm\\_emb\(\)](#), [tpm\\_emb\\_g\(\)](#), [tpm\\_g\(\)](#), [tpm\\_g2\(\)](#), [tpm\\_p\(\)](#)

**Examples**

```
# 2 states: 2 free off-diagonal elements
generator(rep(-1, 2))
# 3 states: 6 free off-diagonal elements
generator(rep(-2, 6))
```

lama

*Build a LaMaModel from an optimised RTMB object***Description**

Having fitted a latent Markov model using automatic differentiation via RTMB, this function calls RTMB's `obj$report()` and does some additional processing. This then yields estimated parameters on their natural scale, allows for convenient calculation of AIC and BIC, state-decoding, and residual calculation. `print()` gives a short overview of the model, `summary()` the estimates. `report()` is the deprecated old name of `lama()`.

**Usage**

```
lama(obj)

report(obj)
```

**Arguments**

`obj`                      Optimised RTMB object

**Details**

The number of observations (used by BIC) is the number of rows of the reported `allprobs` that are not all 1, i.e. missing observations are not counted. This assumes that `forward` is called only once in the likelihood function.

**Value**

A model object of class "LaMaModel" containing a list with the reported quantities from the RTMB object, along estimated parameters (`par`), the log-likelihood (`llk`), number of parameters (`df`) and observations (`nobs`), and the maximum gradient component (`mgc`) at the estimate. It also contains `obj` itself (not a copy), so that functions like `MCreport` or `scores` can be called on the model object.

**Examples**

```
data <- trex[1:200,]

# initial parameters and observations
par <- list(
  log_mu = log(c(0.3, 1)),      # initial means for step length (log-transformed)
  log_sigma = log(c(0.2, 0.7)), # initial sds for step length (log-transformed)
  eta = rep(-2, 2)              # initial t.p.m. parameters (on logit scale)
)
dat <- list(
  step = data$step,             # hourly step lengths
  nStates = 2                   # number of hidden states
)
```

```

# likelihood function
nll <- function(par) {
  getAll(par, dat)
  Gamma <- tpm(eta)
  delta <- stationary(Gamma)
  mu <- exp(log_mu); REPORT(mu)
  sigma <- exp(log_sigma); REPORT(sigma)
  allprobs <- matrix(1, length(step), nStates)
  ind <- which(!is.na(step))
  for(j in 1:nStates) {
    allprobs[ind,j] <- dgamma2(step[ind], mu[j], sigma[j])
  }
  -forward(delta, Gamma, allprobs)
}

# automatic differentiation and optimisation
obj <- MakeADFun(nll, par, silent = TRUE)
opt <- nlminb(obj$par, obj$fn, obj$gr)

### reporting ###
mod <- lama(obj)
mod          # short overview
summary(mod) # estimated state process and reported quantities

# estimated parameters
mod$par

# estimated quantities on natural scale
mod$mu
mod$sigma
mod$Gamma

# information criteria
AIC(mod)
BIC(mod)

# state decoding
states <- viterbi(mod = mod) # global decoding
probs <- stateprobs(mod = mod) # local decoding

# residual calculation
pres <- pseudo_res(data$step, # observation sequence
                    "gamma2", # distribution family
                    list(mean = mod$mu, sd = mod$sigma), # parameters for that family
                    mod = mod) # model object

# or from the model object alone, and plotted
plot(mod)

```

**Description**

Generate a colour-blind-friendly palette

**Usage**

```
LaMaColors(ncolors)
```

**Arguments**

`ncolors`                Number of colours to return; at most 10

**Value**

A colour palette of length `ncolors`

**Examples**

```
cb <- LaMaColors(3)
```

---

|                               |                                                     |
|-------------------------------|-----------------------------------------------------|
| <code>logLik.LaMaModel</code> | <i>Extract log-likelihood from LaMaModel object</i> |
|-------------------------------|-----------------------------------------------------|

---

**Description**

Extract log-likelihood from LaMaModel object

**Usage**

```
## S3 method for class 'LaMaModel'
logLik(object, ...)
```

**Arguments**

`object`                A model fitted using RTMB and obtained via `lama(obj)` of class "LaMaModel"

`...`                    Additional arguments (not used)

**Value**

An object of class "logLik"

---

|                    |                                                                                               |
|--------------------|-----------------------------------------------------------------------------------------------|
| make_matrices_dens | <i>Build a standardised P-Spline design matrix and the associated P-Spline penalty matrix</i> |
|--------------------|-----------------------------------------------------------------------------------------------|

---

## Description

This function builds the B-spline design matrix for a given data vector. Importantly, the B-spline basis functions are normalised such that the integral of each basis function is 1, hence this basis can be used for spline-based density estimation, when the basis functions are weighted by non-negative weights summing to one.

## Usage

```
make_matrices_dens(
  x,
  k,
  type = "real",
  degree = 3,
  knots = NULL,
  diff_order = 2,
  pow = 0.5,
  npoints = 10000
)
```

## Arguments

|            |                                                                                                                                                                                                                                                                                                                                       |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x          | data vector                                                                                                                                                                                                                                                                                                                           |
| k          | number of basis functions                                                                                                                                                                                                                                                                                                             |
| type       | type of the data, either "real" for data on the reals, "positive" for data on the positive reals or "circular" for circular data like angles.                                                                                                                                                                                         |
| degree     | degree of the B-spline basis functions, defaults to cubic B-splines                                                                                                                                                                                                                                                                   |
| knots      | optional vector of knots (including the boundary knots) to be used for basis construction. If not provided, the knots are placed equidistantly for "real" and "circular" and using polynomial spacing for "positive".<br>For "real" and "positive" $k - \text{degree} + 1$ knots are needed, for "circular" $k + 1$ knots are needed. |
| diff_order | order of differencing used for the P-Spline penalty matrix. Defaults to second-order differences.                                                                                                                                                                                                                                     |
| pow        | power for polynomial knot spacing, only used for type = "positive"                                                                                                                                                                                                                                                                    |
| npoints    | number of points used in the numerical integration for normalizing the B-spline basis functions                                                                                                                                                                                                                                       |

**Value**

list containing the design matrix  $Z$ , the penalty matrix  $S$ , the prediction design matrix  $Z_{\text{predict}}$ , the prediction grid  $x_{\text{seq}}$ , and details for the basis expansion.

The penalty matrix leaves out the last coefficient, which is fixed at zero for identifiability.

**Examples**

```
set.seed(1)
# real-valued
x <- rnorm(100)
modmat <- make_matrices_dens(x, k = 20)
# positive-continuous
x <- rgamma2(100, mean = 5, sd = 2)
modmat <- make_matrices_dens(x, k = 20, type = "positive")
# circular
x <- rvm(100, mu = 0, kappa = 2)
modmat <- make_matrices_dens(x, k = 20, type = "circular")
# bounded in an interval
x <- rbeta(100, 1, 2)
modmat <- make_matrices_dens(x, k = 20)
```

---

MCreport

---

*Sample parameters from approximate Gaussian posterior distribution*


---

**Description**

Efficient Monte Carlo sampling of parameters (and REPORTed quantities) from the approximate posterior of an (R)TMB model. See [sdreport](#) for details on posterior variance-covariance in random effects models.

**Usage**

```
MCreport(
  obj,
  nSamples = 1000,
  include_random_pars = TRUE,
  report = FALSE,
  Q = NULL,
  ...
)
```

**Arguments**

|                       |                                                                                                                                     |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| <code>obj</code>      | Optimised RTMB object generated by <a href="#">MakeADFun</a> , or a model object from <a href="#">lama</a> or <a href="#">qrem1</a> |
| <code>nSamples</code> | Number of samples to draw                                                                                                           |

|                     |                                                                                                                                                                                                                                                |
|---------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| include_random_pars | Logical; Should random parameters be included in the output?                                                                                                                                                                                   |
| report              | Logical; Should REPORTed quantities be sampled as well? Defaults to FALSE because this may be slow depending on your model.                                                                                                                    |
| Q                   | Optional precalculated sparse precision matrix returned by <code>sdreport(..., getJointPrecision = TRUE)\$jointPrecision</code> . If not provided, computed internally using <code>sdreport</code> . Only used for models with random effects. |
| ...                 | For internal use only                                                                                                                                                                                                                          |

## Details

**Caution:** This has nothing to do with Bayesian posterior sampling. It is simple Monte Carlo sampling from a Gaussian distribution with mean at the MLE and covariance given by the inverse of the Hessian (for fixed effects models) or the joint precision matrix (for random effects models). This is a common approach to get an approximate idea of parameter uncertainty around the MLE, but it relies on large-sample asymptotics.

Sampling random effects from their posterior as compared to calculating marginal standard deviations like [sdreport](#) is particularly useful for multidimensional random effects (e.g. for locations  $x$  and  $y$ ) where pointwise confidence intervals (e.g. along a path) based on standard deviations are not possible.

## Value

A list structured like the original parameter list used in the [MakeADFun](#) call (potentially including additional REPORTed quantities). Each entry is a list with `nSamples` entries.

## Examples

```
step <- trex$step[1:2000] # subsetting trex data
N <- 2                    # 2 states

# custom likelihood
nll <- function(par) {
  getAll(par)
  Gamma <- tpm(eta)
  delta <- stationary(Gamma)
  mu <- exp(log_mu); REPORT(mu)
  sigma <- exp(log_sigma); REPORT(sigma)
  allprobs <- matrix(1, length(step), N)
  for(j in 1:N) allprobs[,j] <- dgamma2(step, mu[j], sigma[j])
  -forward(delta, Gamma, allprobs)
}

# initial parameters in named list
par0 <- list(eta = rep(-1.5,2),
             log_mu = log(c(0.3, 2.5)),
             log_sigma = log(c(0.3, 1.5)))

# constructing AD object
obj <- MakeADFun(nll, par0, silent = TRUE)
```

```
# optimising
opt <- nlminb(obj$par, obj$fn, obj$gr)

# sampling from distribution of the MLE
samples <- MCreport(obj, nSamples = 10, report = TRUE)
```

---

minmax

*AD-compatible minimum and maximum functions*


---

## Description

These functions compute the parallel minimum/ maximum of two vector-valued inputs and are compatible with automatic differentiation using RTMB.

## Usage

```
min2(x, y)
```

```
max2(x, y)
```

## Arguments

|   |               |
|---|---------------|
| x | first vector  |
| y | second vector |

## Value

min2 returns the parallel minimum and max2 the parallel maximum of x and y

## Examples

```
x <- c(1, 4, 8, 2)
y <- c(2, 5, 3, 7)
min2(x, y)
max2(x, y)
```

---

|                |                                                                                     |
|----------------|-------------------------------------------------------------------------------------|
| minmax0_smooth | <i>Smooth approximations to <math>\max(x, 0)</math> and <math>\min(x, 0)</math></i> |
|----------------|-------------------------------------------------------------------------------------|

---

**Description**

Smooth approximations to  $\max(x, 0)$  and  $\min(x, 0)$

**Usage**

```
max0_smooth(x, rho = 20)
```

```
min0_smooth(x, rho = 20)
```

**Arguments**

|     |                                                                 |
|-----|-----------------------------------------------------------------|
| x   | a vector of values                                              |
| rho | smoothing parameter, larger values lead to closer approximation |

**Value**

the approximate maximum or minimum of x and 0

**Examples**

```
x <- seq(-1, 1, by = 0.1)
min0_smooth(x)
max0_smooth(x)
```

---

|        |                                                                                                                         |
|--------|-------------------------------------------------------------------------------------------------------------------------|
| modmat | <i>Build the design and the penalty matrix for models involving penalised splines based on a formula and a data set</i> |
|--------|-------------------------------------------------------------------------------------------------------------------------|

---

**Description**

Build the design and the penalty matrix for models involving penalised splines based on a formula and a data set

**Usage**

```
modmat(formula, data, knots = NULL)
```

```
make_matrices(formula, data, knots = NULL)
```

## Arguments

|         |                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| formula | <p>formula as used in mgcv. Formulas can be right-side only, or contain a response variable, which is just extracted for naming.</p> <p>Can also be a list of formulas, which are then processed separately. In that case, both a named list of right-side only formulas or a list of formulas with response variables can be provided.</p>                                                                                               |
| data    | data frame containing all the variables on the right side of the formula(s)                                                                                                                                                                                                                                                                                                                                                               |
| knots   | <p>optional list containing user specified knot values for each covariate to be used for basis construction. For most bases the user simply supplies the knots to be used, which must match up with the k value supplied (note that the number of knots is not always just k). See mgcv documentation for more details.</p> <p>If formula is a list, this needs to be a named (based on the response variables) list over such lists.</p> |

## Details

make\_matrices() is the former name of modmat() and still works.

## Value

a list of class LaMa\_matrices containing:

|         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Z       | design matrix (or list of such matrices if formula is a list))                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| S       | list of penalty matrices (with names based on the response terms of the formulas as well as the smooth terms and covariates). For tensorproduct smooths, corresponding entries are themselves lists, containing the $d$ marginal penalty matrices if $d$ is the dimension of the tensor product)                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| pardim  | list of parameter dimensions (fixed and penalised separately) for each formula, for ease of setting up initial parameters                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| coef    | list of coefficient vectors filled with zeros of the correct length for each formula, for ease of setting up initial parameters                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| sp0     | <p>named vector of <b>initial penalty strengths</b>, with one entry per penalty matrix and names matching S (a smooth with several penalties, e.g. a tensor product, contributes one entry each, named &lt;smooth&gt;.&lt;margin&gt;).</p> <p>These are <code>initial.sp</code>'s guesses times 100, capped at 1e6; the inner optimisation is better behaved when it starts constrained, and the outer iteration relaxes the penalty from there.</p> <p>It can be passed straight to <code>penalty</code> or <code>penalty2</code> when each smooth appears once. When a smooth is replicated, e.g. one spline per state, use <code>rep_sp</code>, as a single <code>rep()</code> over <code>sp0</code> is only correct for some models.</p> |
| formula | the formula(s) as supplied, in the same nesting as Z                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| data    | the data frame used for the model(s)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| gam     | unfitted mgcv: : gam object used for construction of Z and S (or list of such objects if formula is a list). Its X element is not kept, as it is returned as Z                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |

|       |                                                                                                                               |
|-------|-------------------------------------------------------------------------------------------------------------------------------|
| gam0  | fitted mgcv::gam which is used internally to create prediction design matrices (or list of such objects if formula is a list) |
| knots | knot list used in the basis construction (or named list over such lists if formula is a list)                                 |

### See Also

[predict.LaMa\\_matrices](#) for prediction design matrix construction based on the model matrices object created by this function.

### Examples

```
data = data.frame(x = runif(100),
                  y = runif(100),
                  g = factor(rep(1:10, each = 10)))

# univariate thin plate regression spline
modmat = modmat(~ s(x), data)
# univariate P-spline
modmat = modmat(~ s(x, bs = "ps"), data)
# adding random intercept
modmat = modmat(~ s(g, bs = "re") + s(x, bs = "ps"), data)
# tensorproduct of x and y
modmat = modmat(~ s(x) + s(y) + ti(x,y), data)
# multiple formulas at once
modmat = modmat(list(mu ~ s(x) + y, sigma ~ s(g, bs = "re")), data = data)
```

---

multistart

---

*Optimise an RTMB object from several starting values*


---

### Description

Latent Markov models often have several local optima of the likelihood. `multistart()` optimises `obj` from several starting values: the first is `obj$par` (the initial parameters), the others are random perturbations of it on the working scale. Afterwards, [lama\(obj\)](#) builds the model from the best fit, as RTMB keeps the parameters with the lowest negative log-likelihood it evaluated.

### Usage

```
multistart(
  obj,
  nstarts = 20,
  sd = 1,
  starts = NULL,
  scale = c("fixed", "unit_info"),
  stop = c("bayes", "hits", "none"),
  hits = 3,
  sd_max = 2,
```

```

    tol = 1e-06,
    seed = NULL,
    optimizer = stats::nlminb,
    silent = FALSE,
    ...
)

```

## Arguments

|                        |                                                                                                                                                                                                         |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>obj</code>       | RTMB object from <code>MakeADFun()</code>                                                                                                                                                               |
| <code>nstarts</code>   | maximum number of starts, including <code>obj\$par</code>                                                                                                                                               |
| <code>sd</code>        | standard deviation of the perturbations on the working scale: a number, a vector of the length of <code>obj\$par</code> , or a named list with one value per parameter (names as in the parameter list) |
| <code>starts</code>    | optional matrix of starting values, one per row, with columns as <code>obj\$par</code> ; then <code>nstarts</code> and <code>sd</code> are ignored                                                      |
| <code>scale</code>     | "fixed" for perturbations of <code>obj\$par</code> with <code>sd</code> , or "unit_info" for perturbations of the first fit scaled by the unit information, see 'Details'                               |
| <code>stop</code>      | stopping rule: "bayes" (not used for given starts), "hits" or "none", see 'Details'                                                                                                                     |
| <code>hits</code>      | number of times the best optimum needs to be reached for <code>stop = "hits"</code>                                                                                                                     |
| <code>sd_max</code>    | largest standard deviation for <code>scale = "unit_info"</code>                                                                                                                                         |
| <code>tol</code>       | relative tolerance for two runs to reach the same optimum                                                                                                                                               |
| <code>seed</code>      | optional seed for the random number generator                                                                                                                                                           |
| <code>optimizer</code> | optimisation function called as <code>optimizer(par, fn, gr, ...)</code> , returning <code>par</code> and objective (like <code>nlminb</code> ) or value (like <code>optim</code> )                     |
| <code>silent</code>    | logical; if TRUE, nothing is printed                                                                                                                                                                    |
| <code>...</code>       | further arguments passed to <code>optimizer</code>                                                                                                                                                      |

## Details

**Stopping.** Two runs reach the same optimum if their negative log-likelihoods differ by less than `tol` (relative), so permuted states (label switching) count as the same optimum. Only converged runs (convergence code 0 and maximum gradient component below 0.01) count for stopping. In any case, at most `nstarts` starts are run.

- `stop = "bayes"` uses the Bayesian stopping rule of Boender and Rinnooy Kan (1987): after  $k$  runs with  $w$  distinct optima, the expected number of optima is  $w(k-1)/(k-w-2)$ , and `multistart()` stops when this is below  $w + 0.5$ , i.e. probably no optimum is missed. The rule assumes that the starts are independent draws from one distribution, so only the random starts count, not the first run from `obj$par`, and it is not used for given starts. It needs at least 8 converged random starts.
- `stop = "hits"` stops once the best optimum was reached `hits` times.

**Caution.** Stopping does not mean that the global optimum was found. "No optimum missed" only refers to the distribution of the starts: optima far away from it, or with a small basin of attraction, can be missed. For example, with a very small sd, all starts converge to the same optimum and the rule stops quickly, although other starts might find a better one. So choose sd wide enough and still check the fit.

### Scatter.

- With `scale = "fixed"`, the starts are `obj$par` plus normal noise with standard deviation `sd`. As most working parameters are on log or logit scale, `sd = 1` is a relative change, so one value usually fits all parameters. Parameters on identity scale (e.g. means of normal distributions) may need their own sd, given as a named list like `list(eta = 1, mu = 5)`.
- With `scale = "unit_info"`, the starts are drawn around the first fit from a normal distribution with covariance  $nH^{-1}$ , where  $H$  is the Hessian of the negative log-likelihood and  $n$  the number of observations. This is the information of a single observation (unit information), which does not shrink with  $n$  and takes correlations of the parameters into account. Standard deviations are capped at `sd_max`, for weakly identified parameters. If the Hessian is not positive definite (or `allprobs` is not reported, so  $n$  is unknown), the fixed sd is used instead.

### Value

output of optimizer for the best run, with two more elements: `runs`, a data frame with the negative log-likelihood `nll`, convergence code and maximum gradient component `mgc` of each run, and `starts`, the matrix of starting values used.

### References

Boender, C. G. E., & Rinnooy Kan, A. H. G. (1987). Bayesian stopping rules for multistart global optimization methods. *Mathematical Programming*, 37(1), 59-80.

### Examples

```
nll <- function(par) {
  getAll(par, dat)
  Gamma <- tpm(eta)
  mu <- exp(log_mu); REPORT(mu)
  allprobs <- cbind(dgamma2(step, mu[1], exp(log_sigma[1])),
                    dgamma2(step, mu[2], exp(log_sigma[2])))
  -forward(stationary(Gamma), Gamma, allprobs)
}
dat <- list(step = trex$step[1:500])
par <- list(eta = c(-2, -2), log_mu = log(c(0.3, 2.5)), log_sigma = log(c(0.2, 1.5)))
obj <- MakeADFun(nll, par, silent = TRUE)

opt <- multistart(obj, seed = 1)
opt$runs
mod <- lama(obj) # best fit

# starts scaled by the first fit
opt <- multistart(obj, scale = "unit_info", seed = 1)
```

---

|       |                                            |
|-------|--------------------------------------------|
| nessi | <i>Loch Ness Monster Acceleration Data</i> |
|-------|--------------------------------------------|

---

**Description**

A small group of researchers managed to put an accelerometer on the Loch Ness Monster and collected data for a few days. Now we have a data set of the overall dynamic body acceleration (ODBA) of the creature.

**Usage**

nessi

**Format**

A data frame with 5.000 rows and 3 variables:

- ODBA** overall dynamci body acceleration
- logODBA** logarithm of overall dynamic body acceleration
- state** hidden state variable

**Source**

Generated for example purposes.

---

|         |                                                 |
|---------|-------------------------------------------------|
| penalty | <i>Computes penalty based on quadratic form</i> |
|---------|-------------------------------------------------|

---

**Description**

This function computes quadratic penalties of the form

$$0.5 \sum_i \lambda_i b_i^T S_i b_i,$$

with smoothing parameters  $\lambda_i$ , coefficient vectors  $b_i$ , and fixed penalty matrices  $S_i$ .

It is intended to be used inside the **penalised negative log-likelihood function** when fitting models with penalised splines or simple random effects via **quasi restricted maximum likelihood** (qREML) with the [qrem1](#) function. For [qrem1](#) to work, the likelihood function needs to be compatible with the RTMB R package to enable automatic differentiation.

**Usage**

penalty(re\_coef, S, sp, lambda)

**Arguments**

|         |                                                                                                                                                                                                                                                                                                                                                                                                                |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| re_coef | coefficient vector/ matrix or list of coefficient vectors/ matrices<br>Each list entry corresponds to a different smooth/ random effect with its own associated penalty matrix in S. When several smooths/ random effects of the same kind are present, it is convenient to pass them as a matrix, where each row corresponds to one smooth/ random effect. This way all rows can use the same penalty matrix. |
| S       | fixed penalty matrix or list of penalty matrices matching the structure of re_coef and also the dimension of the individuals smooths/ random effects                                                                                                                                                                                                                                                           |
| sp      | penalty strength parameter vector that has a length corresponding to the <b>total number</b> of random effects/ spline coefficients in re_coef<br>E.g. if re_coef contains one vector and one matrix with 4 rows, then sp needs to be of length 5.                                                                                                                                                             |
| lambda  | former name of sp, still works                                                                                                                                                                                                                                                                                                                                                                                 |

**Details**

**Caution:** The formatting of re\_coef needs to match the structure of the parameter list in your penalised negative log-likelihood function, i.e. you cannot have two random effect vectors of different names (different list elements in the parameter list), combine them into a matrix inside your likelihood and pass the matrix to penalty. If these are separate random effects, each with its own name, they need to be passed as a list to penalty. Moreover, the ordering of re\_coef needs to match the character vector random specified in [qrem1](#).

**Value**

returns the penalty value and reports to [qrem1](#).

**References**

Koslik, J. O. (2024). Efficient smoothness selection for nonparametric Markov-switching models via quasi restricted maximum likelihood. arXiv preprint arXiv:2411.11498.

**See Also**

[qrem1](#) for the **qREML** algorithm

**Examples**

```
# Example with a single random effect
re = rep(0, 5)
S = diag(5)
sp = 1
penalty(re, S, sp)

# Example with two random effects,
# where one element contains two random effects of similar structure
re = list(matrix(0, 2, 5), rep(0, 4))
S = list(diag(5), diag(4))
```

```

sp = c(1,1,2) # length = total number of random effects
penalty(re, S, sp)

# Full model-fitting example

data = trex[1:1000,] # subset

# initial parameter list
par = list(logmu = log(c(0.3, 2.5)), # step mean
           logsigma = log(c(0.3, 1.5)), # step sd
           beta0 = c(-2,-2), # state process intercept
           betaspline = matrix(rep(0, 18), nrow = 2)) # state process spline coefs

# data object with initial penalty strength sp
dat = list(step = data$step, # step length
           tod = data$tod, # time of day covariate
           N = 2, # number of states
           sp = rep(10,2)) # initial penalty strength

# building model matrices
modmat = modmat(~ s(tod, bs = "cp"),
               data = data.frame(tod = 1:24),
               knots = list(tod = c(0,24))) # wrapping points
dat$Z = modmat$Z # spline design matrix
dat$S = modmat$S # penalty matrix

# penalised negative log-likelihood function
pnll = function(par) {
  getAll(par, dat) # makes everything contained available without $
  Gamma = tpm_g(Z, cbind(beta0, betaspline)) # transition probabilities
  delta = stationary_p(Gamma, t = tod[1] %% 24 + 1) # initial distribution
  mu = exp(logmu) # step mean
  sigma = exp(logsigma) # step sd
  # calculating all state-dependent densities
  allprobs = matrix(1, nrow = length(step), ncol = N)
  ind = which(!is.na(step)) # only for non-NA obs.
  for(j in 1:N) allprobs[ind,j] = dgamma2(step[ind],mu[j],sigma[j])
  -forward_g(delta, Gamma[,tod], allprobs) +
    penalty(betaspline, S, sp) # this does all the penalization work
}

# model fitting
mod = qreml(pnll, par, dat, random = "betaspline")

```

## Description

This function computes a quadratic penalty of the form

$$0.5 \sum_i \lambda_i b^T S_i b,$$

with smoothing parameters  $\lambda_i$ , coefficient vector  $b$ , and fixed penalty matrices  $S_i$ . This generalises the `penalty` by allowing subsets of the coefficient vector  $b$  to be penalised multiple times with different smoothing parameters, which is necessary for **tensor products**, **functional random effects** or **adaptive smoothing**.

It is intended to be used inside the **penalised negative log-likelihood function** when fitting models with penalised splines or simple random effects via **quasi restricted maximum likelihood** (qREML) with the `qrem1` function. For `qrem1` to work, the likelihood function needs to be compatible with the RTMB R package to enable automatic differentiation.

## Usage

```
penalty2(re_coef, S, sp, lambda)
```

## Arguments

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>re_coef</code> | list of coefficient vectors/ matrices<br>Each list entry corresponds to a different smooth/ random effect with its own associated penalty matrix or penalty-matrix list in <code>S</code> . When several smooths/ random effects of the same kind are present, it is convenient to pass them as a matrix, where each row corresponds to one smooth/ random effect. This way all rows can use the same penalty matrix.                                                                                                                                                                                             |
| <code>S</code>       | list of fixed penalty matrices matching the structure of <code>re_coef</code> .<br>This means if <code>re_coef</code> is of length 3, then <code>S</code> needs to be a list of length 3. Each entry needs to be either a penalty matrix, matching the dimension of the corresponding entry in <code>re_coef</code> , or a list with multiple penalty matrices for tensor products.                                                                                                                                                                                                                               |
| <code>sp</code>      | penalty strength parameter vector that has a length corresponding to the provided <code>re_coef</code> and <code>S</code> .<br>Specifically, for entries with one penalty matrix, <code>nrow(re_coef[[i]])</code> parameters are needed. For entries with <code>k</code> penalty matrices, <code>k * nrow(re_coef[[i]])</code> parameters are needed.<br>E.g. if <code>re_coef[[1]]</code> is a vector and <code>re_coef[[2]]</code> a matrix with 4 rows, <code>S[[1]]</code> is a list of length 2 and <code>S[[2]]</code> is a matrix, then <code>sp</code> needs to be of length <code>1 * 2 + 4 = 6</code> . |
| <code>lambda</code>  | former name of <code>sp</code> , still works                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |

## Details

**Caution:** The formatting of `re_coef` needs to match the structure of the parameter list in your penalised negative log-likelihood function, i.e. you cannot have two random effect vectors of different names (different list elements in the parameter list), combine them into a matrix inside your

likelihood and pass the matrix to `penalty`. If these are separate random effects, each with its own name, they need to be passed as a list to `penalty`. Moreover, the ordering of `re_coef` needs to match the character vector `random` specified in `qrem1`.

### Value

returns the penalty value and reports to `qrem1`.

### See Also

`qrem1` for the **qREML** algorithm

### Examples

```
# Example with a single random effect
re = rep(0, 5)
S = diag(5)
sp = 1
penalty(re, S, sp)

# Example with two random effects,
# where one element contains two random effects of similar structure
re = list(matrix(0, 2, 5), rep(0, 4))
S = list(diag(5), diag(4))
sp = c(1,1,2) # length = total number of random effects
penalty(re, S, sp)

# Full model-fitting example

data = trex[1:1000,] # subset

# initial parameter list
par = list(logmu = log(c(0.3, 2.5)), # step mean
           logsigma = log(c(0.3, 1.5)), # step sd
           beta0 = c(-2,-2), # state process intercept
           betaspline = matrix(rep(0, 18), nrow = 2)) # state process spline coeffs

# data object with initial penalty strength sp
dat = list(step = data$step, # step length
           tod = data$tod, # time of day covariate
           N = 2, # number of states
           sp = rep(10,2)) # initial penalty strength

# building model matrices
modmat = modmat(~ s(tod, bs = "cp"),
               data = data.frame(tod = 1:24),
               knots = list(tod = c(0,24))) # wrapping points
dat$Z = modmat$Z # spline design matrix
dat$S = modmat$S # penalty matrix

# penalised negative log-likelihood function
pnll = function(par) {
```

```

getAll(par, dat) # makes everything contained available without $
Gamma = tpm_g(Z, cbind(beta0, betaspline)) # transition probabilities
delta = stationary_p(Gamma, t = tod[1] %% 24 + 1) # initial distribution
mu = exp(logmu) # step mean
sigma = exp(logsigma) # step sd
# calculating all state-dependent densities
allprobs = matrix(1, nrow = length(step), ncol = N)
ind = which(!is.na(step)) # only for non-NA obs.
for(j in 1:N) allprobs[ind,j] = dgamma2(step[ind],mu[j],sigma[j])
-forward_g(delta, Gamma[,tod], allprobs) +
  penalty(betaspline, S, sp) # this does all the penalisation work
}

# model fitting
mod = qreml(pnll, par, dat, random = "betaspline")

```

---

|             |                                                                                 |
|-------------|---------------------------------------------------------------------------------|
| penalty_uni | <i>Penalty approximation of unimodality constraints for univariates smooths</i> |
|-------------|---------------------------------------------------------------------------------|

---

## Description

Penalty approximation of unimodality constraints for univariates smooths

## Usage

```
penalty_uni(coef, m, kappa = 1000, concave = TRUE, rho = 20)
```

## Arguments

|         |                                                                                                                                                                                     |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| coef    | coefficient vector of matrix on which to apply the unimodality penalty                                                                                                              |
| m       | vector of indices for the position of the coefficient mode. If coef is a vector, must be of length 1. Otherwise, must be of length equal to nrow(coef)                              |
| kappa   | global scaling factor for the penalty                                                                                                                                               |
| concave | logical; if TRUE (default), the penalty enforces increasing until the mode then decreasing. If the coefficients should decrease until the mode, then increase, set concave = FALSE. |
| rho     | control parameter for smooth approximation to $\min(x, 0)$ used internally. For large values, gets closer to true minimum function but less stable.                                 |

## Value

a numeric value of the penalty for the given coefficients

## Examples

```
## coefficient vector
coef <- c(1, 2, 3, 2, 1)
# mode at position 3
penalty_uni(coef, m = 3) # basically zero
#' # mode at position 2
penalty_uni(coef, m = 2) # large positive penalty

## coefficient matrix
coef <- rbind(coef, coef)
m <- c(1, 4)
penalty_uni(coef, m)
```

---

|                |                                |
|----------------|--------------------------------|
| plot.LaMaModel | <i>Plot a LaMaModel object</i> |
|----------------|--------------------------------|

---

## Description

Plots the pseudo-residuals of a model from [lama](#) or [qrem1](#), computed by [pseudo\\_res](#) from the model object alone, with one row of plots per data stream, or the estimated state-dependent densities of each data stream built with [statedens](#).

## Usage

```
## S3 method for class 'LaMaModel'
plot(x, type = c("residuals", "statedens"), stream = NULL, ...)
```

## Arguments

|        |                                                                                                          |
|--------|----------------------------------------------------------------------------------------------------------|
| x      | model object of class "LaMaModel"                                                                        |
| type   | "residuals" (default) for the pseudo-residuals, "statedens" for the state-dependent densities            |
| stream | optional names of the data streams to plot, by default all                                               |
| ...    | further arguments passed to <a href="#">plot.LaMaResiduals</a> , or for type = "statedens" see 'Details' |

## Details

For type = "statedens", each data stream is shown as a histogram with the state-dependent densities (probabilities for discrete distributions) weighted by the state probabilities, and their sum, the marginal density, as a dashed line. The weighted density of state  $j$  is the mean over the observations of  $p_{tj}f_j(x; \theta_{tj})$ , which allows for parameters that depend on covariates, several tracks and inhomogeneous state processes. This needs allprobs to be the product of matrices from [statedens](#), which is checked.

Further arguments for type = "statedens":

weights state probabilities  $p_{tj}$ : "stateprobs" (default) for the local state probabilities from [stateprobs](#), "viterbi" for the states decoded by [viterbi](#), "stationary" for the stationary distribution (averaged over tracks, or over the cycle for periodic models), or a vector of length nStates

col colours of the states, defaults to [LaMaColors](#)

lwd line width

n number of grid points for continuous distributions

legend position of the legend, e.g. "topright" (default), or FALSE for none

... arguments passed to plot() of the histogram, e.g. breaks, main, xlab, xlim, ylim or border

Several streams are shown side by side, unless par(mfrow) has been set.

### Value

for type = "residuals" the pseudo-residuals, for type = "statedens" a list with the grid x, the weighted state-dependent densities density (one column per state), the state weights and the observations data (or a list of these for several streams), invisibly

### Examples

```
dat <- list(step = trex$step[1:500], angle = trex$angle[1:500])
nll <- function(par) {
  getAll(par, dat)
  Gamma <- tpm(eta)
  allprobs <- statedens(step, dgamma2, exp(log_mu), exp(log_sigma)) *
    statedens(angle, dvm, 0, exp(log_kappa))
  -forward(stationary(Gamma), Gamma, allprobs)
}
par <- list(eta = c(-2, -2), log_mu = log(c(0.3, 2.5)), log_sigma = log(c(0.2, 1.5)),
  log_kappa = log(c(0.2, 1.5)))
obj <- MakeADFun(nll, par, silent = TRUE)
opt <- nlmnb(obj$par, obj$fn, obj$gr)
mod <- lama(obj)

plot(mod) # pseudo-residuals
plot(mod, type = "statedens") # state-dependent densities of both streams
plot(mod, type = "statedens", stream = "step", weights = "viterbi",
  breaks = 40, xlab = "step length")
```

---

plot.LaMaResiduals      *Plot pseudo-residuals*

---

### Description

Plot pseudo-residuals computed by [pseudo\\_res](#). The QQ plot shows a pointwise 95% band (in gray) for the sample quantiles under a correct model.

**Usage**

```
## S3 method for class 'LaMaResiduals'
plot(
  x,
  col = "darkblue",
  lwd = 1.5,
  main = NULL,
  breaks = "Sturges",
  axis.lab = list(qq = c("Theoretical quantiles", "Sample quantiles"), hist =
    c("Pseudo-residuals", "Density"), acf = c("Lag", "ACF")),
  ...
)
```

**Arguments**

|          |                                                                                                                                                                                  |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x        | pseudo-residuals as returned by <code>pseudo_res</code> . For several data streams (from <code>pseudo_res(mod)</code> ), one row of plots per stream, titled by the stream name. |
| col      | character, color for the QQ-line (and density curve if <code>histogram = TRUE</code> )                                                                                           |
| lwd      | numeric, line width for the QQ-line (and density curve if <code>histogram = TRUE</code> )                                                                                        |
| main     | optional character vector of main titles for the plots of length 2 (or 3 if <code>histogram = TRUE</code> )                                                                      |
| breaks   | breaks argument passed to <code>hist</code>                                                                                                                                      |
| axis.lab | labels used for the x and y axis of each plot (named list)                                                                                                                       |
| ...      | currently ignored. For method consistency                                                                                                                                        |

**Value**

NULL, plots the pseudo-residuals in a 3-panel layout

**Examples**

```
## pseudo-residuals for the trex data
step = trex$step[1:1000]
angle = trex$angle[1:1000]

nll = function(par){
  getAll(par)
  Gamma = tpm(logitGamma)
  delta = stationary(Gamma)
  mu = exp(logMu); REPORT(mu)
  sigma = exp(logSigma); REPORT(sigma)
  kappa = exp(logKappa); REPORT(kappa)
  allprobs = matrix(1, length(step), 2)
  ind = which(!is.na(step) & !is.na(angle))
  for(j in 1:2) {
    allprobs[ind,j] = dgamma2(step[ind], mu[j], sigma[j]) *
      dvm(angle[ind], 0, kappa[j])
  }
}
```

```

    -forward(delta, Gamma, allprobs)
  }

par = list(logitGamma = c(-2,-2),
          logMu = log(c(0.3, 2.5)),
          logSigma = log(c(0.3, 1.5)),
          logKappa = log(c(0.1, 1.7)))

obj = MakeADFun(nll, par, silent = TRUE)
opt = nlminb(obj$par, obj$fn, obj$gr)

mod = lama(obj)

pres_step = pseudo_res(step,      # observations
                      "gamma2",  # family that is used
                      list(mean = mod$mu, sd = mod$sigma), # the family's parameters
                      mod = mod) # model object
pres_angle = pseudo_res(angle,
                      "vm",
                      list(mu = 0, kappa = mod$kappa),
                      mod = mod)

# separate plots
plot(pres_step)
plot(pres_angle)

# together
par(mfrow = c(2,3))
plot(pres_step, main = c("", "Step Length", ""),
     axis.lab = list(hist = c("Step residuals", "Density")))
plot(pres_angle, main = c("", "Turning Angle", ""),
     axis.lab = list(hist = c("Angle residuals", "Density")))

# or from the model object alone, one row per stream
plot(pseudo_res(mod))

```

---

`predict.LaMa_matrices` *Build the prediction design matrix based on new data and model\_matrices object created by [modmat](#)*

---

## Description

Build the prediction design matrix based on new data and `model_matrices` object created by [modmat](#)

## Usage

```

## S3 method for class 'LaMa_matrices'
predict(object, newdata, what = NULL, exclude = NULL, ...)

```

**Arguments**

|         |                                                                                                                                                                                                                                  |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| object  | model matrices object as returned from <a href="#">modmat</a>                                                                                                                                                                    |
| newdata | data frame containing the variables in the formula and new data for which to evaluate the basis                                                                                                                                  |
| what    | optional character string specifying which formula to use for prediction if object contains multiple formulas.                                                                                                                   |
| exclude | optional vector of terms to set to zero in the predicted design matrix. Useful for predicting main effects only when e.g. <code>s(..., bs = "re")</code> terms are present. See <code>mgcv::predict.gam</code> for more details. |
| ...     | for method consistency only                                                                                                                                                                                                      |

**Value**

prediction design matrix for newdata with the same basis as used for object

**See Also**

[modmat](#) for creating objects of class `LaMa_matrices` which can be used for prediction by this function.

**Examples**

```
# single formula
modmat = modmat(~ s(x), data.frame(x = 1:10))
Z_p = predict(modmat, data.frame(x = 1:10 - 0.5))
# with multiple formulas
modmat = modmat(list(mu ~ s(x), sigma ~ s(x, bs = "ps")), data = data.frame(x = 1:10))
Z_p = predict(modmat, data.frame(x = 1:10 - 0.5), what = "mu")
# nested formula list
form = list(stream1 = list(mu ~ s(x), sigma ~ s(x, bs = "ps")))
modmat = modmat(form, data = data.frame(x = 1:10))
Z_p = predict(modmat, data.frame(x = 1:10 - 0.5), what = c("stream1", "mu"))
```

---

predict.smoothdens      *Estimated smooth densities*

---

**Description**

Evaluates the smooth densities built with [smoothdens](#) for given spline coefficients, e.g. to plot the estimated state-dependent densities.

**Usage**

```
## S3 method for class 'smoothdens'
predict(object, coef, x = NULL, ...)
```

**Arguments**

|        |                                                                                            |
|--------|--------------------------------------------------------------------------------------------|
| object | object of class "smoothdens" for one data stream                                           |
| coef   | coefficient matrix, one row per state, without the last column fixed at zero               |
| x      | optional points to evaluate the densities at, defaults to the prediction grid object\$xseq |
| ...    | unused                                                                                     |

**Value**

list with the points x and the matrix density of densities, one row per point and one column per state

**Examples**

```
x = c(rnorm(100, 0, 1), rnorm(100, 5, 1))
dens = smoothdens(x, par = list(mean = c(0, 5), sd = c(1, 1)))
# densities at the initial coefficients
pred = predict(dens, coef = dens$coef)
matplot(pred$x, pred$density, type = "l", lty = 1)
```

---

|             |                                                                                                                         |
|-------------|-------------------------------------------------------------------------------------------------------------------------|
| pred_matrix | <i>Build the prediction design matrix based on new data and model_matrices object created by <a href="#">modmat</a></i> |
|-------------|-------------------------------------------------------------------------------------------------------------------------|

---

**Description**

**Deprecated.** Use [predict](#) on the object returned by [modmat](#) instead, which does the same thing: `predict(modmat, newdata)` in place of `pred_matrix(modmat, newdata)`.

**Usage**

```
pred_matrix(model_matrices, newdata, what = NULL, exclude = NULL)
```

**Arguments**

|                |                                                                                                                                                                                                                                   |
|----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| model_matrices | model_matrices object as returned from <a href="#">modmat</a>                                                                                                                                                                     |
| newdata        | data frame containing the variables in the formula and new data for which to evaluate the basis                                                                                                                                   |
| what           | optional character string specifying which formula to use for prediction if model_matrices contains multiple formulas.                                                                                                            |
| exclude        | optional vector of terms to set to zero in the predicted design matrix. Useful for predicting main effects only when e.g. <code>sd(..., bs = "re")</code> terms are present. See <code>mgcv::predict.gam</code> for more details. |

**Value**

prediction design matrix for newdata with the same basis as used for model\_matrices

**See Also**

[predict](#), which replaces this function

**Examples**

```
modmat = modmat(~ s(x), data.frame(x = 1:10))
# deprecated:
# Z_p = pred_matrix(modmat, data.frame(x = 1:10 - 0.5))
# use instead:
Z_p = predict(modmat, data.frame(x = 1:10 - 0.5))
```

---

|                 |                                 |
|-----------------|---------------------------------|
| print.LaMaModel | <i>Print a LaMaModel object</i> |
|-----------------|---------------------------------|

---

**Description**

Prints a short overview of a model from [lama](#) or [qrem1](#): the state process, observations, parameters, log-likelihood, AIC and BIC, and the names of the reported quantities. Use `summary()` for the estimates.

**Usage**

```
## S3 method for class 'LaMaModel'
print(x, ...)
```

**Arguments**

|     |                                   |
|-----|-----------------------------------|
| x   | model object of class "LaMaModel" |
| ... | additional arguments (not used)   |

**Value**

x, invisibly

---

|                     |                                     |
|---------------------|-------------------------------------|
| print.LaMa_matrices | <i>Print a LaMa_matrices object</i> |
|---------------------|-------------------------------------|

---

**Description**

Print a LaMa\_matrices object

**Usage**

```
## S3 method for class 'LaMa_matrices'
print(x, ...)
```

**Arguments**

`x`                      object of class `LaMa_matrices` as returned by `modmat`  
`...`                    ignored

**Value**

`x`, invisibly. Called for its side effect of printing.

**See Also**

[modmat](#)

---

|                      |                                                                                       |
|----------------------|---------------------------------------------------------------------------------------|
| process_hid_formulas | <i>Process and standardise formulas for the state process of hidden Markov models</i> |
|----------------------|---------------------------------------------------------------------------------------|

---

**Description**

Process and standardise formulas for the state process of hidden Markov models

**Usage**

```
process_hid_formulas(formulas, nStates, ref = NULL)
```

**Arguments**

`formulas`            formulas for the transition process of a hidden Markov model, either as a single formula, a list of formulas, or a matrix.  
`nStates`            number of states of the Markov chain  
`ref`                optional vector of reference categories for each state, defaults to `1:nStates`. If provided, must be of length `nStates` and contain valid state indices. If a formula matrix is provided, this cannot be specified because reference categories are specified by one "." entry in each row.

**Value**

named list of formulas of length `nStates * (nStates - 1)`, where each formula corresponds to a transition from state  $i$  to state  $j$ , excluding transitions from  $i$  to `ref[i]`.

## Examples

```
# single formula for all non-reference category elements
formulas = process_hid_formulas(~ s(x), nStates = 3)
# now a list of length 6 with names tr.ij, not including reference categories

# different reference categories
formulas = process_hid_formulas(~ s(x), nStates = 3, ref = c(1,1,1))

# different formulas for different entries (and only for 2 of 6)
formulas = list(tr.12 ~ s(x), tr.23 ~ s(y))
formulas = process_hid_formulas(formulas, nStates = 3, ref = c(1,1,1))
# also a list of length 6, remaining entries filled with tr.ij ~ 1

# matrix input with reference categories
formulas = matrix(c(".", "~ s(x)", "~ s(y)",
                    "~ g", ". ", "~ I(x^2)",
                    "~ y", "~ 1", ". "),
                  nrow = 3, byrow = TRUE)
# dots define reference categories
formulas = process_hid_formulas(formulas, nStates = 3)
```

---

pseudo\_res

*Calculate pseudo-residuals*

---

## Description

For HMMs, pseudo-residuals are used to assess the overall goodness-of-fit of the model. These are based on the cumulative distribution function (CDF)

$$F_{X_t}(x_t) = F(x_t \mid x_1, \dots, x_{t-1})$$

and can be used to quantify whether an observation is extreme relative to its model-implied distribution.

This function calculates such residuals via the probability integral transform, based on the local state probabilities obtained by [stateprobs](#) and the respective parametric family.

## Usage

```
pseudo_res(
  obs,
  dist,
  par,
  stateprobs = NULL,
  mod = NULL,
  normal = TRUE,
  discrete = NULL,
  randomise = TRUE
)
```

**Arguments**

|            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| obs        | vector of observations (of length nObs), or a model object from <a href="#">lama</a> (or the RTMB object), in which case nothing else is needed (see ‘Details’)                                                                                                                                                                                                                                                                                                                                                                                                                             |
| dist       | character string specifying which parametric CDF to use (e.g., "norm" for normal or "pois" for Poisson) or CDF function to evaluate directly. If a discrete CDF function is passed, the discrete argument needs to be set to TRUE because this cannot be determined automatically.                                                                                                                                                                                                                                                                                                          |
| par        | named parameter list for the parametric CDF<br>Names need to correspond to the parameter names in the specified distribution (e.g. list(mean = c(1, 2), sd = c(1, 1)) for a normal distribution and 2 states). This argument is as flexible as the parametric distribution allows. For example you can have a matrix of parameters with one row for each observation and one column for each state.                                                                                                                                                                                         |
| stateprobs | matrix of local state probabilities for each observation (of dimension c(nObs, nStates)) as computed by <a href="#">stateprobs</a>                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| mod        | optional model object containing required quantities<br>When using automatic differentiation either with RTMB::MakeADFun or <a href="#">qrem1</a> and include <a href="#">forward</a> in your likelihood function, the objects needed for state decoding are automatically reported after model fitting. Hence, you can pass the model object obtained from obj\$report(), <a href="#">lama</a> or <a href="#">qrem1</a> directly to this function and avoid calculating local state probabilities manually. In this case, a call should look like pseudo_res(obs, "norm", par, mod = mod). |
| normal     | logical, if TRUE, returns Gaussian pseudo residuals<br>These will be approximately standard normally distributed if the model is correct.                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| discrete   | logical, if TRUE, computes discrete pseudo residuals (which slightly differ in their definition)<br>By default, will be determined using dist argument, but only works for standard discrete distributions. When used with a special discrete distribution, set to TRUE manually.                                                                                                                                                                                                                                                                                                           |
| randomise  | for discrete pseudo residuals only. Logical, if TRUE, return randomised pseudo residuals. Recommended for discrete observations.                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

**Details**

Pseudo-residuals are based on the probability integral transform. If the cumulative distribution function (CDF)  $F$  of a random variable  $X$  is known, then  $F(X)$  is uniformly distributed on  $[0, 1]$ . Applying the standard normal quantile function  $\Phi^{-1}$  then gives a residual that is approximately standard normal under the model.

For discrete-valued observations, the CDF is a step function, so the residual is not uniquely defined. One can compute a "lower" and "upper" pseudo-residual corresponding to  $F(X - 1)$  and  $F(X)$ , respectively. If randomise = TRUE, a value is drawn uniformly between the lower and upper bounds. In this case, the resulting pseudo-residuals are again approximately standard normal after applying the standard normal quantile function.

**Model object only:** `pseudo_res(mod)` needs no observations, family or parameters. It evaluates the likelihood function stored in the model again, with each density (e.g. `dgamma2()`) replaced by its CDF (`pgamma2()`) with the same arguments, so that the likelihood function itself builds the CDFs in place of `allprobs`. This works for loops over states or time, `cbind()`, covariate-dependent parameters, densities on the log scale, mixtures within a state and several data streams (multiplied, or summed on the log scale), giving one set of residuals per stream, named after the data variable. Before, it checks that the densities enter `allprobs` as a product or mixture, so that swapping in CDFs is valid. If not, e.g. for densities transformed by hand (truncation, Jacobians, zero inflation via indicators) or a latent variable integrated out inside `allprobs`, it stops, and `pseudo_res(obs, dist, par, mod = mod)` needs to be used instead. Densities in your own helper functions called by the likelihood function are found as well, and [qrem1](#) models work like models from [lama](#). The likelihood function needs to call [forward](#) once (use `trackID` for several tracks), and it is evaluated with the data as they are when `pseudo_res()` is called.

## Value

vector of pseudo residuals of class `LaMaResiduals` or list containing lower, upper, and mean if discrete residuals are not randomised. For `pseudo_res(mod)` with several data streams, a named list of these, one per stream, also of class `LaMaResiduals`.

## See Also

[plot.LaMaResiduals](#) for plotting pseudo-residuals.

## Examples

```
## continuous-valued observations
obs = rnorm(100)
stateprobs = matrix(0.5, nrow = 100, ncol = 2)
par = list(mean = c(1,2), sd = c(1,1))
pres = pseudo_res(obs, "norm", par, stateprobs)

## discrete-valued observations
obs = rpois(100, lambda = 1)
par = list(lambda = c(1,2))
pres = pseudo_res(obs, "pois", par, stateprobs)

## custom CDF function
obs = rnbinom(100, size = 1, prob = 0.5)
par = list(size = c(0.5, 2), prob = c(0.4, 0.6))
pres = pseudo_res(obs, pnbinom, par, stateprobs,
                  discrete = TRUE)
# if discrete CDF function is passed, 'discrete' needs to be set to TRUE

## no CDF function available, only density (artificial example)
obs = rnorm(100)
par = list(mean = c(1,2), sd = c(1,1))
# construct CDF using numerical integration
cdf = function(x, mean, sd) integrate(dnorm, -Inf, x, mean = mean, sd = sd)$value
pres = pseudo_res(obs, cdf, par, stateprobs)
```

```

### Full model fit example ###
step = trex$step[1:500]

nll = function(par){
  getAll(par)
  Gamma = tpm(logitGamma)
  delta = stationary(Gamma)
  mu = exp(logMu); REPORT(mu)
  sigma = exp(logSigma); REPORT(sigma)
  allprobs = matrix(1, length(step), 2)
  ind = which(!is.na(step))
  for(j in 1:2) allprobs[ind,j] = dgamma2(step[ind], mu[j], sigma[j])
  -forward(delta, Gamma, allprobs)
}

par = list(logitGamma = c(-2,-2),
          logMu = log(c(0.3, 2.5)),
          logSigma = log(c(0.3, 1.5)))

obj = MakeADFun(nll, par, silent = TRUE)
opt = nlminb(obj$par, obj$fn, obj$gr)

mod = lama(obj)

pres = pseudo_res(step,      # observation sequence
                  "gamma2",  # parametric family that was used
                  list(mean = mod$mu, sd = mod$sigma), # parameters for that family
                  mod = mod) # model object

# or, from the model object alone
pres = pseudo_res(mod)

plot(pres)

```

---

|       |                                                                                                                                         |
|-------|-----------------------------------------------------------------------------------------------------------------------------------------|
| qrem1 | <i>Automatic smoothness selection for arbitrary statistical models with penalised splines, simple random effects, or tensorproducts</i> |
|-------|-----------------------------------------------------------------------------------------------------------------------------------------|

---

## Description

Efficiently fits models involving quadratic penalties of the form

$$\sum_i \lambda_i b^T S_i b,$$

by combining automatic differentiation via RTMB with a custom implementation of the extended Fellner-Schall update.

Users only need to supply a custom penalised log-likelihood function that calls `penalty()` or `penalty2()`.

**Usage**

```
qrem1(
  pnll,
  par,
  dat,
  random,
  map = NULL,
  silent = 1,
  spname = NULL,
  tol_edf = 0.01,
  maxiter = 100,
  alpha = 0.1,
  tol = 0.01,
  smoothing = 1,
  method = "BFGS",
  lsp_max = 15,
  step_small = 0.05,
  max_halve = 6,
  control = list(),
  spHess = FALSE,
  joint_unc = FALSE,
  saveall = FALSE
)
```

**Arguments**

|        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| pnll   | penalised negative log-likelihood function that is structured as dictated by RTMB and uses the <a href="#">penalty</a> or <a href="#">penalty2</a> function to compute the penalty                                                                                                                                                                                                                                                                                                                    |
| par    | named list of initial parameters                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| dat    | initial data list that contains the data used in the likelihood function, hyper-parameters, and the <b>initial penalty strength</b> vector, called sp or lambda (see spname)                                                                                                                                                                                                                                                                                                                          |
| random | vector of names of the random effects/ penalised parameters in par<br><b>Caution:</b> The ordering of random needs to match the order of the random effects passed to penalty.                                                                                                                                                                                                                                                                                                                        |
| map    | optional map argument, containing factor vectors to indicate parameter sharing or fixing                                                                                                                                                                                                                                                                                                                                                                                                              |
| silent | integer silencing level: 0 corresponds to full printing of inner and outer iterations, 1 to printing of outer iterations only, and 2 to no printing                                                                                                                                                                                                                                                                                                                                                   |
| spname | optional name of the penalty strength vector in dat.<br>By default, dat\$sp is used if present, otherwise dat\$lambda. Hence, if dat contains sp, lambda is free to be used for something else, e.g. the mean of a Poisson distribution. In the likelihood function, the penalty strengths are accessed by the same name, e.g. penalty(beta, S, sp), as qrem1() replaces them with the current values in each iteration. The returned model object stores them under this name as well, e.g. mod\$sp. |

|            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| tol_edf    | <p>convergence tolerance on the <b>effective degrees of freedom</b>.</p> <p>This is the primary convergence criterion. The iteration stops once no smooth's effective degrees of freedom has changed by more than tol_edf across the last four outer iterations, provided the step in <math>\log(\lambda)</math> is also small. The effective degrees of freedom are what say whether the <b>fitted smooth</b> is still changing, and unlike a tolerance on the restricted likelihood they mean the same thing on every model, being measured in effective parameters rather than in nats. The penalty strengths themselves are a poor proxy: <math>\lambda</math> can slide along a flat ridge for many iterations, moving substantially in relative terms, while neither the criterion nor the fit changes appreciably.</p> |
| maxiter    | maximum number of outer iterations                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| alpha      | <p>smallest factor by which a penalty strength may <b>decrease</b> in one outer iteration, a number in <math>[0, 1)</math>. Defaults to 0.1.</p> <p>Penalty strengths are free to increase as fast as the update proposes, but cannot collapse faster than this per iteration. Reducing a penalty strength too quickly can push the inner optimisation into a local optimum or a numerically awkward region, which matters more here than in a GAM because the likelihood is user-written. Set to zero to remove the floor entirely. Step length is handled separately, by max_half and the adaptive multiplier.</p>                                                                                                                                                                                                          |
| tol        | <p><b>fallback</b> convergence tolerance, on the restricted log-likelihood. Defaults to 0.01.</p> <p>Used only when the effective degrees of freedom are not trustworthy, i.e. when they fall outside <math>[0, K_i]</math>, which happens when the data Hessian is indefinite (see tol_edf and the returned edf_valid). The iteration then stops once the restricted log-likelihood has changed by less than tol over the last four outer iterations. A tolerance in nats is not comparable across models, which is why it is the fallback rather than the primary criterion.</p>                                                                                                                                                                                                                                            |
| smoothing  | optional scaling factor for the final penalty strength parameters. Increasing this beyond one leads to a smoother final model                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| method     | inner optimisation method to be used by <code>optim</code> . Defaults to "BFGS"                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| lsp_max    | largest value allowed for $\log(\lambda)$ . Defaults to 15, as in mgcv, i.e. penalty strengths saturate at roughly $3.3e6$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| step_small | size of a step in $\log(\lambda)$ below which the step multiplier is allowed to double. Defaults to 0.05, as in mgcv                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| max_half   | <p>maximum number of times a step that decreases the restricted likelihood is halved before it is accepted anyway. Defaults to 6.</p> <p>mgcv never shortens below the full Fellner-Schall step and accepts a worse one instead, which for a user-written likelihood can drift downhill for tens of iterations.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| control    | list of control parameters for <code>optim</code> to use in the inner optimisation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| spHess     | logical, if TRUE, the sparse automatic differentiation Hessian is used for evaluation. The factorisation is dense either way                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| joint_unc  | logical, if TRUE, joint RTMB object is returned allowing for joint uncertainty quantification                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| saveall    | logical, if TRUE, then all model objects from each iteration are saved in the final model object                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |

## Details

Step size control follows the extended Fellner-Schall implementation in `mgcv` while convergence is judged on the effective degrees of freedom (differing from `mgcv`).

**The criterion.** The penalty strengths are chosen to maximise the Laplace-approximate restricted log-likelihood

$$V(\lambda) = \ell_p(\hat{b}; \lambda) + \frac{1}{2} \log |S_\lambda|_+ - \frac{1}{2} \log |J|,$$

where  $\ell_p$  is the penalised log-likelihood at its mode  $\hat{b}$ ,  $S_\lambda = \sum_i \lambda_i S_i$ ,  $|\cdot|_+$  denotes the product of the positive eigenvalues, and  $J$  is the Hessian of the penalised negative log-likelihood at  $\hat{b}$ . Every outer iteration refits the inner problem to obtain  $\hat{b}$  and  $J$ , so one call is a sequence of complete model fits, each warm started at the previous one.

**The update.** The penalty strengths are updated multiplicatively,  $\lambda_i \leftarrow \lambda_i r_i$ , by the extended Fellner-Schall ratio

$$r_i = \frac{\text{tr}(S_\lambda^- S_i) - \text{tr}(J^{-1} S_i)}{\hat{b}^T S_i \hat{b}},$$

which equals one exactly where  $\partial V / \partial \lambda_i = 0$  and otherwise moves  $\lambda_i$  in the direction of the gradient, without ever making it negative. For a smooth carrying a single penalty the first trace is  $\text{rank}(S_i) / \lambda_i$ , obtained once from an eigendecomposition instead of at every iteration. Only the diagonal blocks of  $J^{-1}$  enter, and these come from the Cholesky factor by triangular solves rather than from a full inverse.

**Step control.** The step is taken in  $\log \lambda$  and scaled by a multiplier that persists across iterations: it doubles while the criterion keeps improving and is halved, up to `max_half` times, while it does not. A step that still worsens the criterion after that many halvings is accepted, which is the only way the iteration can move downhill. In addition no penalty strength may fall by more than a factor `alpha` in one iteration, and  $\log \lambda$  is capped at `lsp_max`. The fit returned is the best iterate seen, not necessarily the last one.

**Convergence.** The iteration stops once no smooth's effective degrees of freedom

$$\text{edf}_i = K_i - \text{tr}(J^{-1} \lambda_i S_i)$$

has moved by more than `tol_edf` over the last four iterations, provided the step in  $\log \lambda$  is also small; see `tol_edf`. Being eigenvalue sums, the effective degrees of freedom must lie in  $[0, K_i]$ , and they leave that range only if the data Hessian is indefinite, in which case the traces driving the update are not the quantities the method assumes. That is reported rather than repaired, through the returned `edf_valid` and a warning, and the criterion then falls back to `tol` on the restricted log-likelihood.

**Numerics.**  $J$  is the exact automatic differentiation Hessian, which matters because the finite differencing error of `optimHess` is of the same order as the criterion differences the convergence test has to resolve. It is factorised by a pivoted Cholesky decomposition after scaling to a unit diagonal; should it not be positive definite, a ridge is added and reported through the returned `hessian_repaired`.

**Uncertainty.** The returned `outer_hessian()` gives the Hessian of the negative restricted log-likelihood in the penalty strengths, which `sdreport_outer` turns into standard errors. Note that these describe the curvature of  $V$  only, and treat the approximation to it as exact.

**Value**

model object of class "qrem1Model", inheriting from "LaMaModel" (see [lama](#)), carrying the fitted quantities, the smoothness selection diagnostics shown by [summary.qrem1Model](#), and `outer_hessian()`, the outer Hessian that [sdreport\\_outer](#) turns into standard errors

**References**

Wood, S. N., & Fasiolo, M. (2017). A generalized Fellner-Schall method for smoothing parameter optimization with application to Tweedie location, scale and shape models. *Biometrics*, 73(4), 1071-1081.

Koslik, J. O. (2024). Efficient smoothness selection for nonparametric Markov-switching models via quasi restricted maximum likelihood. arXiv preprint arXiv:2411.11498.

**See Also**

[penalty](#) and [penalty2](#) to compute the penalty inside the likelihood function, and [qrem1\\_old](#) for the original algorithm

**Examples**

```
data = trex[1:2000,] # subset of the data

# initial parameter list
par = list(logmu = log(c(0.3, 2.5)), # step mean
           logsigma = log(c(0.3, 1.5)), # step sd
           beta0 = c(-2,-2), # state process intercept
           beta_spline = matrix(rep(0, 18), nrow = 2)) # state process spline coeffs

# data object with initial penalty strength sp
dat = list(step = data$step, # step length
           tod = data$tod, # time of day covariate
           N = 2, # number of states
           sp = rep(20,2)) # initial penalty strength

# building model matrices
modmat = modmat(~ s(tod, bs = "cp"),
                data = data.frame(tod = 1:24),
                knots = list(tod = c(0,24))) # wrapping points
dat$Z = modmat$Z # spline design matrix
dat$S = modmat$S # penalty matrix

# penalised negative log-likelihood function
pnll = function(par) {
  getAll(par, dat) # makes everything contained available without $
  Gamma = tpm(cbind(beta0, beta_spline), Z) # transition probabilities
  delta = stationary_p(Gamma, t = tod[1] %% 24 + 1) # initial distribution
  mu = exp(logmu) # step mean
  sigma = exp(logsigma) # step sd
  # calculating all state-dependent densities
  allprobs = matrix(1, nrow = length(step), ncol = N)
  ind = which(!is.na(step)) # only for non-NA obs.
```

```

    for(j in 1:N) allprobs[ind,j] = dgamma2(step[ind],mu[j],sigma[j])
  -forward(delta, Gamma[, ,tod], allprobs) +
    penalty(beta_spline, S, sp) # this does all the penalization work
}

# model fitting
mod = qreml(pnll, par, dat, random = "beta_spline", silent = 2)

```

---

|           |                                                                                |
|-----------|--------------------------------------------------------------------------------|
| qreml_old | <i>Quasi restricted maximum likelihood (qREML) algorithm, previous version</i> |
|-----------|--------------------------------------------------------------------------------|

---

## Description

This algorithm can be used very flexibly to fit statistical models that involve **penalised splines** or simple **i.i.d. random effects**, i.e. that have penalties of the form

$$0.5 \sum_i \lambda_i b_i^T S_i b_i,$$

with smoothing parameters  $\lambda_i$ , coefficient vectors  $b_i$ , and fixed penalty matrices  $S_i$ .

The **qREML** algorithm is typically much faster than REML or marginal ML using the full Laplace approximation method, but may be slightly less accurate regarding the estimation of the penalty strength parameters.

qreml\_old is the previous implementation, kept for reference. Use [qreml](#), which estimates the same quantities with a better behaved outer iteration.

Under the hood, qreml\_old uses the R package RTMB for automatic differentiation in the inner optimisation. The user has to specify the **penalised negative log-likelihood function** pnll structured as dictated by RTMB and use the [penalty](#) function to compute the quadratic-form penalty inside the likelihood.

## Usage

```

qreml_old(
  pnll,
  par,
  dat,
  random,
  map = NULL,
  silent = 1,
  psname = "lambda",
  alpha = 0.3,
  smoothing = 1,
  maxiter = 100,
  tol = 1e-04,
  max_half = 5,
  method = "BFGS",

```

```

control = list(),
conv_crit = "relchange",
spHess = FALSE,
joint_unc = FALSE,
saveall = FALSE
)

```

## Arguments

|           |                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| pnll      | <p>penalised negative log-likelihood function that is structured as dictated by RTMB and uses the <a href="#">penalty</a> function from LaMa to compute the penalty</p> <p>Needs to be a function of the named list of initial parameters par only.</p>                                                                                                                                                                                       |
| par       | <p>named list of initial parameters</p> <p>The random effects/ spline coefficients can be vectors or matrices, the latter summarising several random effects of the same structure, each one being a row in the matrix.</p>                                                                                                                                                                                                                   |
| dat       | <p>initial data list that contains the data used in the likelihood function, hyperparameters, and the <b>initial penalty strength</b> vector</p> <p>If the initial penalty strength vector is <b>not</b> called lambda, the name it has in dat needs to be specified using the pname argument below. Its length needs to match the to the total number of random effects.</p>                                                                 |
| random    | <p>vector of names of the random effects/ penalised parameters in par</p> <p><b>Caution:</b> The ordering of random needs to match the order of the random effects passed to <a href="#">penalty</a> inside the likelihood function.</p>                                                                                                                                                                                                      |
| map       | <p>optional map argument, containing factor vectors to indicate parameter sharing or fixing.</p> <p>Needs to be a named list for a subset of fixed effect parameters or penalty strength parameters. For example, if the model has four penalty strength parameters, map[[pname]] could be factor(c(NA, 1, 1, 2)) to fix the first penalty strength parameter, estimate the second and third jointly, and estimate the fourth separately.</p> |
| silent    | <p>integer silencing level: 0 corresponds to full printing of inner and outer iterations, 1 to printing of outer iterations only, and 2 to no printing.</p>                                                                                                                                                                                                                                                                                   |
| pname     | <p>optional name given to the penalty strength parameter in dat. Defaults to "lambda".</p>                                                                                                                                                                                                                                                                                                                                                    |
| alpha     | <p>optional hyperparameter for exponential smoothing of the penalty strengths.</p> <p>For larger values smoother convergence is to be expected but the algorithm may need more iterations.</p>                                                                                                                                                                                                                                                |
| smoothing | <p>optional scaling factor for the final penalty strength parameters</p> <p>Increasing this beyond one will lead to a smoother final model. Can be an integer or a vector of length equal to the length of the penalty strength parameter.</p>                                                                                                                                                                                                |
| maxiter   | <p>maximum number of iterations in the outer optimisation over the penalty strength parameters.</p>                                                                                                                                                                                                                                                                                                                                           |
| tol       | <p>Convergence tolerance for the penalty strength parameters.</p>                                                                                                                                                                                                                                                                                                                                                                             |

|           |                                                                                                                                                                                                                                                                                                                                                                                                                                         |
|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| max_halve | maximum number of step halvings per outer iteration.<br>After each update of the penalty strength parameters, the restricted log-likelihood is compared to its value in the previous iteration. If it decreased, the step (on the log scale) is repeatedly halved until it does not, or until max_halve halvings have been made. This makes the outer iteration monotone and hence more robust. Set to zero to switch step halving off. |
| method    | optimisation method to be used by <code>optim</code> . Defaults to "BFGS", but might be changed to "L-BFGS-B" for high-dimensional settings.                                                                                                                                                                                                                                                                                            |
| control   | list of control parameters for <code>optim</code> to use in the inner optimisation. Here, <code>optim</code> uses the BFGS method which cannot be changed.<br>We advise against changing the default values of <code>reltol</code> and <code>maxit</code> as this can decrease the accuracy of the Laplace approximation.                                                                                                               |
| conv_crit | character, convergence criterion for the penalty strength parameters. Can be "relchange" (default) or "gradient".                                                                                                                                                                                                                                                                                                                       |
| spHess    | logical, if TRUE, sparse AD Hessian is used in each outer iteration. If your Hessian is large and sparse (many cross derivatives are 0), this will speed up the computations a lot. If your Hessian is dense, this will slow down the computations slightly and might require significantly more memory.                                                                                                                                |
| joint_unc | logical, if TRUE, joint RTMB object is returned allowing for joint uncertainty quantification                                                                                                                                                                                                                                                                                                                                           |
| saveall   | logical, if TRUE, then all model objects from each iteration are saved in the final model object.                                                                                                                                                                                                                                                                                                                                       |

### Value

model object of class 'qremlModel'. This is a list containing:

|                    |                                                                                                                                                                                                         |
|--------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ...                | everything that is reported inside <code>pnl1</code> using <code>RTMB::REPORT()</code> . When using forward, <code>tpm_g</code> , etc., this may involve automatically reported objects.                |
| obj                | RTMB AD object containing the final conditional model fit                                                                                                                                               |
| psname             | final penalty strength parameter vector                                                                                                                                                                 |
| all_psname         | list of all penalty strength parameter vectors over the iterations                                                                                                                                      |
| par                | named estimated parameter list in the same structure as the initial <code>par</code> . Note that the name <code>par</code> is not fixed but depends on the original name of your <code>par</code> list. |
| relist_par         | function to convert the estimated parameter vector to the estimated parameter list. This is useful for uncertainty quantification based on sampling from a multivariate normal distribution.            |
| par_vec            | estimated parameter vector                                                                                                                                                                              |
| llk                | unpenalised log-likelihood at the optimum                                                                                                                                                               |
| n_fixpar           | number of fixed, i.e. unpenalised, parameters                                                                                                                                                           |
| edf                | overall effective number of parameters                                                                                                                                                                  |
| all_edf            | list of effective number of parameters for each smooth                                                                                                                                                  |
| Hessian_condtional | final Hessian of the conditional penalised fit                                                                                                                                                          |
| obj_joint          | if <code>joint_unc = TRUE</code> , joint RTMB object for joint uncertainty quantification in model and penalty parameters.                                                                              |

## References

Koslik, J. O. (2024). Efficient smoothness selection for nonparametric Markov-switching models via quasi restricted maximum likelihood. arXiv preprint arXiv:2411.11498.

## See Also

[penalty](#) and [penalty2](#) to compute the penalty inside the likelihood function

## Examples

```
data = trex[1:1000,] # subset

# initial parameter list
par = list(logmu = log(c(0.3, 2.5)), # step mean
          logsigma = log(c(0.3, 1.5)), # step sd
          beta0 = c(-2,-2), # state process intercept
          betaspline = matrix(rep(0, 18), nrow = 2)) # state process spline coeffs

# data object with initial penalty strength lambda
dat = list(step = data$step, # step length
          tod = data$tod, # time of day covariate
          N = 2, # number of states
          lambda = rep(10,2)) # initial penalty strength

# building model matrices
modmat = modmat(~ s(tod, bs = "cp"),
               data = data.frame(tod = 1:24),
               knots = list(tod = c(0,24))) # wrapping points
dat$Z = modmat$Z # spline design matrix
dat$S = modmat$S # penalty matrix

# penalised negative log-likelihood function
pnll = function(par) {
  getAll(par, dat) # makes everything contained available without $
  Gamma = tpm_g(Z, cbind(beta0, betaspline), ad = TRUE) # transition probabilities
  delta = stationary_p(Gamma, t = tod[1] %% 24 + 1, ad = TRUE) # initial distribution
  mu = exp(logmu) # step mean
  sigma = exp(logsigma) # step sd
  # calculating all state-dependent densities
  allprobs = matrix(1, nrow = length(step), ncol = N)
  ind = which(!is.na(step)) # only for non-NA obs.
  for(j in 1:N) allprobs[ind,j] = dgamma2(step[ind],mu[j],sigma[j])
  -forward_g(delta, Gamma[,tod], allprobs) +
    penalty(betaspline, S, lambda) # this does all the penalization work
}

# model fitting
mod = qremL_old(pnll, par, dat, random = "betaspline", silent = 2)
```

---

|        |                                                                |
|--------|----------------------------------------------------------------|
| rep_sp | <i>Repeat initial penalty strengths for replicated smooths</i> |
|--------|----------------------------------------------------------------|

---

## Description

Expands the `sp0` element of a `modmat` object into a `sp` vector for `penalty` or `penalty2`, when each smooth is used more than once, for example one spline per state or per off-diagonal element of the transition probability matrix.

## Usage

```
rep_sp(model_matrices, N)
```

## Arguments

`model_matrices` object of class `LaMa_matrices` as returned by `modmat`

`N` number of replicates. Either a single number used for every smooth, or one number per smooth, i.e. per element of `model_matrices$S`

## Details

`sp` runs over replicates **within** each smooth, so for a tensor product the margins vary fastest. A single `rep()` over `sp0` therefore only gives the right answer for some models, silently producing the right length but the wrong values for others. This function repeats each smooth's penalty strengths separately, which is always correct.

## Value

named numeric vector of initial penalty strengths, of the length and in the order expected for `sp`

## See Also

`modmat`, which computes `sp0`

## Examples

```
modmat = modmat(~ s(x) + ti(x, y), data.frame(x = runif(100), y = runif(100)))
modmat$sp0      # one value per penalty
rep_sp(modmat, 2) # ready to use as 'sp' for two replicates of each smooth
```

---

|        |                                            |
|--------|--------------------------------------------|
| scores | <i>Per-observation score contributions</i> |
|--------|--------------------------------------------|

---

## Description

Computes the score contribution of each observation,

$$u_t = \frac{\partial}{\partial \theta} \log p(x_t \mid x_1, \dots, x_{t-1}),$$

for a model whose negative log-likelihood function calls [forward](#). Their column sums are the gradient of the log-likelihood. They are the building block for robust (sandwich) standard errors, e.g. cluster-robust ones via `rowsum(U, ID)`.

## Usage

```
scores(obj, par = NULL)
```

## Arguments

|                  |                                                                                                                                                                 |
|------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>obj</code> | optimised RTMB object from <a href="#">MakeADFun</a> , or a model object from <a href="#">lama</a> or <a href="#">qrem1</a>                                     |
| <code>par</code> | optional parameter vector like <code>obj\$par</code> , e.g. <code>opt\$par</code> . Defaults to the estimates (for <a href="#">qrem1</a> models the final fit). |

## Details

Each log-likelihood contribution in [forward](#) gets a weight  $w_t$ . The gradient of the weighted log-likelihood is linear in the weights, so its derivative w.r.t.  $w_t$  is  $u_t$ . This needs one tape of the gradient and one reverse sweep per parameter. The weights are handed to [forward](#) internally, so the likelihood function does not need to change.

The likelihood function is taken from `obj` and evaluated again, with the data as they are when `scores()` is called. Parameters fixed via `map` are respected, and the columns correspond to `obj$par`, like `obj$gr()` and `obj$he()`.

If the likelihood function calls [forward](#) several times, e.g. once per track, the rows of the result follow the order of these calls. Only [forward](#) (and its deprecated `_g` and `_p` versions) is supported, and models with random effects are not.

## Value

matrix of score contributions of dimension `c(nObs, length(obj$par))`

## Examples

```
nll <- function(par) {
  getAll(par)
  Gamma <- tpm(eta)
  delta <- stationary(Gamma)
  allprobs <- cbind(dgamma2(step, mu[1], sigma[1]),
```

```

      dgamma2(step, mu[2], sigma[2]))
    -forward(delta, Gamma, allprobs)
  }
  step <- trex$step[1:200]
  par <- list(eta = c(-2, -2), mu = c(0.3, 2.5), sigma = c(0.2, 1.5))
  obj <- MakeADFun(nll, par, silent = TRUE)
  opt <- nlmnb(obj$par, obj$fn, obj$gr)
  mod <- lama(obj)
  U <- scores(mod)
  colSums(U) # ~ 0 at the MLE

```

---

sdreportMC

*Monte Carlo version of sdreport*


---

## Description

After optimisation of an AD model, `sdreportMC` can be used to calculate samples of confidence intervals of all model parameters and `REPORT()`ed quantities including nonlinear functions of random effects and parameters.

## Usage

```

sdreportMC(
  obj,
  what,
  nSamples = 1000,
  Hessian = NULL,
  CI = FALSE,
  probs = c(0.025, 0.975)
)

```

## Arguments

|                       |                                                                                                                                                 |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>obj</code>      | object returned by <code>MakeADFun()</code> after optimisation or model of class <code>qrem1Model</code> as returned by <a href="#">qrem1</a> . |
| <code>what</code>     | vector of strings with names of parameters and/or <code>REPORT()</code> ed quantities to be reported                                            |
| <code>nSamples</code> | number of samples to draw from the multivariate normal distribution of the MLE                                                                  |
| <code>Hessian</code>  | optional Hessian matrix. If not provided, it will be computed from the object                                                                   |
| <code>CI</code>       | logical. If <code>TRUE</code> , only confidence intervals instead of samples will be returned                                                   |
| <code>probs</code>    | vector of probabilities for the confidence intervals (ignored if no CIs are computed)                                                           |

## Details

This function simply samples from the approximate multivariate normal distribution of the maximum likelihood estimate (MLE) of the parameters

$$\hat{\theta} \sim N(\theta, H^{-1}),$$

where  $H$  is the Hessian matrix of the negative log-likelihood function at the MLE. It then returns either the sampled parameters or `REPORT()`ed transformations of them. If `CI = TRUE`, it does not return the samples but directly computes confidence intervals.

If you are interested in several quantities, calling `sdreportMC` once with a vector `what` will generally be faster than calling it several times with single elements of `what`.

## Value

named list corresponding to the elements of `what`. Each element has the structure of the corresponding quantity with an additional dimension added for the samples. For example, if a quantity is a vector, the list contains a matrix. If a quantity is a matrix, the list contains an array. If quantity is an array, the list contains an array with one extra dimension.

## Examples

```
# fitting an HMM to the trex data and running sdreportMC
## negative log-likelihood function
nll = function(par) {
  getAll(par, dat) # makes everything contained available without $
  Gamma = tpm(eta) # computes transition probability matrix from unconstrained eta
  delta = stationary(Gamma) # computes stationary distribution
  # exponentiating because all parameters strictly positive
  mu = exp(logmu)
  sigma = exp(logsigma)
  kappa = exp(logkappa)
  # reporting statements for sdreportMC
  REPORT(mu)
  REPORT(sigma)
  REPORT(kappa)
  # calculating all state-dependent densities
  allprobs = matrix(1, nrow = length(step), ncol = N)
  ind = which(!is.na(step) & !is.na(angle)) # only for non-NA obs.
  for(j in 1:N){
    allprobs[ind,j] = dgamma2(step[ind],mu[j],sigma[j])*dvm(angle[ind],0,kappa[j])
  }
  -forward(delta, Gamma, allprobs) # simple forward algorithm
}

## initial parameter list
par = list(
  logmu = log(c(0.3, 1)),          # initial means for step length (log-transformed)
  logsigma = log(c(0.2, 0.7)),    # initial sds for step length (log-transformed)
  logkappa = log(c(0.2, 0.7)),    # initial concentration for turning angle (log-transformed)
  eta = rep(-2, 2)                # initial t.p.m. parameters (on logit scale)
)
```

```

## data and hyperparameters
dat = list(
  step = trex$step[1:500], # hourly step lengths
  angle = trex$angle[1:500], # hourly turning angles
  N = 2
)

## creating AD function
obj = MakeADFun(nll, par, silent = TRUE) # creating the objective function

## optimising
opt = nlminb(obj$par, obj$fn, obj$gr) # optimization

## running sdreportMC
# `mu` has report statement, `delta` is automatically reported by `forward()`
sdrMC = sdreportMC(obj,
  what = c("mu", "delta"),
  nSamples = 50)
dim(sdrMC$delta)
# now a matrix with 50 samples (rows)

```

---

|                |                                                                              |
|----------------|------------------------------------------------------------------------------|
| sdreport_outer | <i>Report uncertainty of the estimated smoothing parameters or variances</i> |
|----------------|------------------------------------------------------------------------------|

---

## Description

Computes standard deviations for the smoothing parameters of a model object returned by `qrem1` using the delta method.

## Usage

```
sdreport_outer(mod, invert = FALSE)
```

## Arguments

|                     |                                                                                                                                                                    |
|---------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>mod</code>    | model objects as returned by <a href="#">qrem1</a>                                                                                                                 |
| <code>invert</code> | optional logical; if TRUE, the inverse smoothing parameters (variances) are returned along with the transformed standard deviations obtained via the delta method. |

## Details

The computations are based on the approximate gradient of the restricted log likelihood. The outer Hessian is computed by finite differencing of this gradient. If the inverse smoothing parameters are requested, the standard deviations are transformed to the variances using the delta method.

**Value**

list containing report matrix summarising parameters and standard deviations as well as the outer Hessian matrix.

**Examples**

```
## no examples
```

---

|                    |                                     |
|--------------------|-------------------------------------|
| simulate.LaMaModel | <i>Simulate from a fitted model</i> |
|--------------------|-------------------------------------|

---

**Description**

Simulates states and observations from a model fitted with [forward](#) and [statedens](#). By default, this is done on the observed design: the tracks and their lengths, the initial distribution `delta`, the transition probabilities `Gamma` and the parameters of the state-dependent densities are those reported by the model, i.e. conditional on the observed covariates. Simulating for new covariates is not possible; instead, rebuild the likelihood function for the new data and call [lama](#) on the resulting object.

**Usage**

```
## S3 method for class 'LaMaModel'
simulate(
  object,
  nsim = 1,
  seed = NULL,
  rdens = NULL,
  random = FALSE,
  fill_na = FALSE,
  ...
)
```

**Arguments**

|                     |                                                                                                                                                                                                                                                                                        |
|---------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>object</code> | model object from <a href="#">lama</a> or <a href="#">qrem1</a> that was built with <a href="#">statedens</a>                                                                                                                                                                          |
| <code>nsim</code>   | number of simulations                                                                                                                                                                                                                                                                  |
| <code>seed</code>   | optional seed for the random number generator                                                                                                                                                                                                                                          |
| <code>rdens</code>  | optional named list of random number generators of the data streams, for densities without one named by replacing the leading d with r (e.g. from <a href="#">zero_inflate</a> ). The first argument is the number of draws, the others are the parameters as in the density.          |
| <code>random</code> | logical; if TRUE, <code>obj\$simulate()</code> of RTMB is used, so that random effects are drawn from their distribution first, see ‘Details’. The data streams are those passed to <a href="#">statedens</a> . Default is FALSE, which keeps the reported (estimated) random effects. |

|         |                                                                                                                                                                                                                                                                        |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| fill_na | logical; if TRUE, missing observations of the data are filled in by simulated values (their parameters need to be defined, e.g. covariates must not be missing). Default is FALSE, which keeps them missing. Streams that are missing completely are always simulated. |
| ...     | currently not used                                                                                                                                                                                                                                                     |

## Details

The states are drawn as in the decoding functions, so that all types of Gamma that `forward` accepts (homogeneous, track-specific, time-varying, periodic) work, as does a continuous-time model with one transition matrix per time interval (the simulation is then conditional on the observed time points). Each data stream is drawn from the random number generator belonging to its density, e.g. `rgamma2` for `dgamma2`.

Missing observations of the data stay missing (unless `fill_na = TRUE`), except for a stream that is missing completely: such a placeholder (e.g. `step = rep(NA, n)`) lets you simulate from a likelihood function without data, see the examples.

Models with random effects are by default simulated conditional on the estimated random effects. With `random = TRUE`, RTMB draws the random effects first, which requires that the density of each random effect is evaluated in the likelihood function *before* the random effect is used, either by `u %~% dnorm(...)` or by `nll <- nll - sum(dnorm(u, ..., log = TRUE))` (or another density). The states and data are then simulated given these draws, so that every simulation has new random effects. This also requires that `allprobs` is the product of the data streams built by `statedens`, with each data stream passed once.

## Value

data frame with the columns `trackID` (index of the track, if used), `state` and one column per data stream, for `nsim = 1`, else a list of `nsim` such data frames.

## Examples

```
nll <- function(par) {
  getAll(par, dat)
  Gamma <- tpm(eta)
  allprobs <- statedens(step, dgamma2, exp(log_mu), exp(log_sigma)) *
    statedens(angle, dvm, 0, exp(log_kappa))
  -forward(stationary(Gamma), Gamma, allprobs)
}
dat <- list(step = trex$step[1:500], angle = trex$angle[1:500])
par <- list(eta = c(-2, -2), log_mu = log(c(0.3, 2.5)), log_sigma = log(c(0.2, 1.5)),
  log_kappa = log(c(0.2, 1.5)))
obj <- MakeADFun(nll, par, silent = TRUE)
opt <- nlminb(obj$par, obj$fn, obj$gr)
mod <- lama(obj)

sim <- simulate(mod, seed = 1)
head(sim)

# simulate without data: all-NA streams as placeholders, parameters of your choice, then refit
dat$step <- dat$angle <- rep(NA, 500)
```

```

obj0 <- MakeADFun(nll, par, silent = TRUE)
sim <- simulate(lama(obj0), seed = 1)
dat$step <- sim$step; dat$angle <- sim$angle
obj1 <- MakeADFun(nll, par, silent = TRUE)
opt1 <- nlminb(obj1$par, obj1$fn, obj1$gr)

# random effects: RTMB draws them first, then the states and data are simulated given them
nll_re <- function(par) {
  getAll(par, dat)
  u ~% dnorm(0, exp(log_su)) # track-level random effect on the mean step length in state 1
  mu <- exp(cbind(log_mu[1] + u[id], log_mu[2]))
  Gamma <- tpm(eta)
  .nll <- .nll - forward(stationary(Gamma), Gamma, statedens(step, dgamma2, mu, exp(log_sigma)), id)
  .nll
}
dat <- list(step = trex$step[1:500], id = rep(1:5, each = 100))
par_re <- list(eta = c(-2, -2), log_mu = log(c(0.3, 2.5)), log_sigma = log(c(0.2, 1.5)),
              log_su = log(0.3), u = rep(0, 5))
obj_re <- MakeADFun(nll_re, par_re, random = "u", silent = TRUE)
sim_re <- simulate(lama(obj_re), random = TRUE, seed = 1)

```

---

skewnorm

*Skew normal distribution*


---

## Description

Density, distribution function, quantile function and random generation for the skew normal distribution.

## Usage

```

dskewnorm(x, xi = 0, omega = 1, alpha = 0, log = FALSE)

pskewnorm(q, xi = 0, omega = 1, alpha = 0, lower.tail = TRUE, log.p = FALSE)

qskewnorm(p, xi = 0, omega = 1, alpha = 0, lower.tail = TRUE, log.p = FALSE)

rskewnorm(n, xi = 0, omega = 1, alpha = 0)

```

## Arguments

|                         |                                                                                      |
|-------------------------|--------------------------------------------------------------------------------------|
| <code>x, q</code>       | vector of quantiles                                                                  |
| <code>xi</code>         | location parameter                                                                   |
| <code>omega</code>      | scale parameter, must be positive.                                                   |
| <code>alpha</code>      | skewness parameter, +/- Inf is allowed.                                              |
| <code>log, log.p</code> | logical; if TRUE, probabilities/ densities $p$ are returned as $\log(p)$ .           |
| <code>lower.tail</code> | logical; if TRUE (default), probabilities are $P[X \leq x]$ , otherwise $P[X > x]$ . |

|   |                                                                                                           |
|---|-----------------------------------------------------------------------------------------------------------|
| p | vector of probabilities                                                                                   |
| n | number of observations. If <code>length(n) &gt; 1</code> , the length is taken to be the number required. |

### Details

This implementation of `dskewnorm` allows for automatic differentiation with RTMB while the other functions are imported from the `sn` package.

### Value

`dskewnorm` gives the density, `pskewnorm` gives the distribution function, `qskewnorm` gives the quantile function, and `rskewnorm` generates random deviates.

### Examples

```
x = rskewnorm(1)
d = dskewnorm(x)
p = pskewnorm(x)
q = qskewnorm(p)
```

---

smoothdens

---

*Build the design and penalty matrices for smooth density estimation*


---

### Description

This high-level function can be used to prepare objects needed to estimate mixture models of smooth densities using P-Splines.

### Usage

```
smoothdens(
  x,
  par,
  type = "real",
  k = 25,
  knots = NULL,
  degree = 3,
  diff_order = 2,
  pow = 0.5,
  npoints = 10000
)
```

## Arguments

|            |                                                                                                                                                                                                                                                                                                                                                                                              |
|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x          | data vector for one data stream, or named data frame or list of several data streams                                                                                                                                                                                                                                                                                                         |
| par        | list of initial means and sds ("real", "positive") or means and concentrations ("circular", called kappa or concentration), one value per state. For several data streams, a named list of such lists.                                                                                                                                                                                       |
| type       | type of each data stream, either "real" for data on the reals, "positive" for data on the positive reals or "circular" for angular data.                                                                                                                                                                                                                                                     |
| k          | number of basis functions for each data stream                                                                                                                                                                                                                                                                                                                                               |
| knots      | optional vector of knots (including the boundary knots) to be used for basis construction, for several data streams a named list of such vectors. If not provided, the knots are placed equidistantly for "real" and "circular" and using polynomial spacing for "positive".<br>For "real" and "positive" $k - \text{degree} + 1$ knots are needed, for "circular" $k + 1$ knots are needed. |
| degree     | degree of the B-spline basis functions for each data stream, defaults to cubic B-splines                                                                                                                                                                                                                                                                                                     |
| diff_order | order of differencing used for the P-Spline penalty matrix for each data stream. Defaults to second-order differences.                                                                                                                                                                                                                                                                       |
| pow        | power for polynomial knot spacing, only used for type = "positive"                                                                                                                                                                                                                                                                                                                           |
| npoints    | number of points used in the numerical integration for normalizing the B-spline basis functions<br>type, k, degree, diff_order, pow and npoints can be of length 1 or one per data stream (named or in the order of x).                                                                                                                                                                      |

## Details

Under the hood, [make\\_matrices\\_dens](#) is used for the actual construction of the design and penalty matrices.

You can provide one or multiple data streams of different types (real, positive, circular) and specify initial means and standard deviations/ concentrations for each data stream. This information is then converted into suitable spline coefficients. smoothdens then constructs the design and penalty matrices for standardised B-splines basis functions (integrating to one) for each data stream. For types "real" and "circular" the knots are placed equidistant in the range of the data, for type "positive" the knots are placed using polynomial spacing.

The last spline coefficient of each state is fixed at zero for identifiability, hence coef has  $k - 1$  columns. density(beta) takes care of this: it maps the coefficient matrix to the allprobs matrix, with rows of missing observations equal to one.

## Value

For one data stream, an object of class "smoothdens": a list containing the design matrix Z, the penalty matrix S, the initial coefficients coef, the prediction design matrix Z\_predict, the prediction grid xseq, details for the basis expansion basis, and the function density(beta). For several data streams, a named list of such objects.

**See Also**

[predict](#) for the estimated densities

**Examples**

```
## one data stream, mixture of two normals
x = c(rnorm(100, 0, 1), rnorm(100, 5, 1))
dens = smoothdens(x, par = list(mean = c(0, 5), sd = c(1, 1)))

Z = dens$Z # design matrix
S = dens$S # penalty matrix
beta = dens$coef # initial coefficients
allprobs = dens$density(beta) # use this in the likelihood function

## 3 data streams
data = data.frame(x1 = rnorm(100, mean = 0, sd = 1),
                  x2 = rgamma2(100, mean = 5, sd = 3),
                  x3 = rvm(100, mu = 0, kappa = 2))

par = list(x1 = list(mean = 0, sd = 1),
           x2 = list(mean = 5, sd = 3),
           x3 = list(mean = 0, kappa = 2))

dens = smoothdens(data, par, type = c("real", "positive", "circular"))

# objects for x1
Z1 = dens$x1$Z
allprobs = dens$x1$density(dens$x1$coef) *
  dens$x2$density(dens$x2$coef) *
  dens$x3$density(dens$x3$coef)
```

---

statedens

*State-dependent densities of one data stream*


---

**Description**

Builds the matrix of state-dependent densities (or probabilities) of one data stream, as used in the allprobs matrix of [forward](#). Several data streams that are conditionally independent given the state are combined by multiplying their matrices.

**Usage**

```
statedens(x, dens, ..., nStates = NULL, log = FALSE)
```

**Arguments**

|      |                                                                                                                                         |
|------|-----------------------------------------------------------------------------------------------------------------------------------------|
| x    | vector of observations of length nObs, possibly containing NAs                                                                          |
| dens | density function, e.g. <a href="#">dnorm</a> , <a href="#">dgamma2</a> or <a href="#">dvm</a> , with the observations as first argument |

|         |                                                                    |
|---------|--------------------------------------------------------------------|
| ...     | parameters of dens, see ‘Details’                                  |
| nStates | number of states. Only needed if all parameters are single values. |
| log     | logical; if TRUE, log-densities are returned                       |

## Details

Each parameter in ... can be

- a single value, used for all states,
- a vector of length nStates, one value per state, or
- a matrix of dimension c(nObs, nStates), one value per observation and state, e.g. from a regression on covariates.

Missing observations contribute nothing to the likelihood, so their rows are 1 (0 with log = TRUE). As each data stream gets its own matrix, a missing value in one stream does not remove the observations of the others.

With log = TRUE, the log-densities are returned, to be added over data streams and used with forward(..., logspace = TRUE). They are computed by dens(..., log = TRUE) if dens has an argument log, otherwise as log(dens(...)) (e.g. for densities from [zero\\_inflate](#)).

In obj\$simulate() of RTMB, x is registered as data and simulated by [forward](#), see [simulate.LaMaModel](#).

Writing the loop over states by hand is equally valid and gives the same result. statedens() is just a shortcut.

## Value

matrix of dimension c(nObs, nStates)

## Examples

```
step <- trex$step[1:200]
angle <- trex$angle[1:200]
mu <- c(0.3, 2.5); sigma <- c(0.2, 1.5); kappa <- c(0.2, 1.5)

# one data stream
allprobs <- statedens(step, dgamma2, mu, sigma)

# the same by hand
allprobs2 <- matrix(1, length(step), 2)
ind <- which(!is.na(step))
for(j in 1:2) allprobs2[ind, j] <- dgamma2(step[ind], mu[j], sigma[j])
all.equal(allprobs, allprobs2)

# two data streams, mean of the turning angle the same in both states
allprobs <- statedens(step, dgamma2, mu, sigma) * statedens(angle, dvm, 0, kappa)

# on the log scale, for forward(..., logspace = TRUE)
logprobs <- statedens(step, dgamma2, mu, sigma, log = TRUE) +
  statedens(angle, dvm, 0, kappa, log = TRUE)
```

stateprobs

*Calculate conditional local state probabilities in HMMs***Description**

Computes

$$\Pr(\text{State}_t = j \mid X_1, \dots, X_T)$$

for a given HMM.

**Usage**

```
stateprobs(
  delta,
  Gamma,
  allprobs,
  trackID = NULL,
  mod = NULL,
  forecast = FALSE,
  tod = NULL
)
```

**Arguments**

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial distribution; either <ul style="list-style-type: none"> <li>• a vector of length nStates,</li> <li>• a matrix of dimension c(nTracks, nStates) if trackID is provided, or</li> <li>• a model object as for mod, so that mod can be passed as the first argument</li> </ul>                                                                                                                                                                    |
| Gamma    | transition probability matrix; either <ul style="list-style-type: none"> <li>• a matrix of dimension c(nStates, nStates),</li> <li>• an array of dimension c(nStates, nStates, nTracks) if trackID is provided,</li> <li>• an array of dimension c(nStates, nStates, nObs) for time-varying transition probabilities, or</li> <li>• an array of dimension c(nStates, nStates, L) for periodic transition probabilities, if tod is provided</li> </ul> |
| allprobs | matrix of state-dependent probabilities or density values of dimension c(nObs, nStates)                                                                                                                                                                                                                                                                                                                                                               |
| trackID  | optional vector of length nObs containing nTracks unique IDs that separate tracks. The observations of each track need to be consecutive.                                                                                                                                                                                                                                                                                                             |
| mod      | optional model object containing delta, Gamma, allprobs, and optionally trackID. When using RTMB: :MakeADFun or qrem1 with forward in the likelihood, these are reported automatically after model fitting and the object returned by obj\$report(), lama or qrem1 can be passed directly.                                                                                                                                                            |

|          |                                                                                                                                |
|----------|--------------------------------------------------------------------------------------------------------------------------------|
| forecast | logical, indicating if forecast probabilities $\Pr(\text{State}_t = j \mid X_1, \dots, X_{t-1})$ should be calculated instead. |
| tod      | optional integer vector of length nObs with values in 1, ..., L, indexing the slices of Gamma for periodic models              |

**Value**

matrix of conditional state probabilities of dimension  $c(\text{nObs}, \text{nStates})$

**See Also**

Other decoding functions: [stateprobs\\_g\(\)](#), [stateprobs\\_p\(\)](#), [viterbi\(\)](#), [viterbi\\_g\(\)](#), [viterbi\\_p\(\)](#)

**Examples**

```
Gamma = tpm(c(-1,-2))
delta = stationary(Gamma)
allprobs = matrix(runif(10), nrow = 10, ncol = 2)

probs = stateprobs(delta, Gamma, allprobs)
```

---

|              |                                                                               |
|--------------|-------------------------------------------------------------------------------|
| stateprobs_g | <i>Calculate conditional local state probabilities for inhomogeneous HMMs</i> |
|--------------|-------------------------------------------------------------------------------|

---

**Description**

Computes

$$\Pr(\text{State}_t = j \mid X_1, \dots, X_T)$$

for inhomogeneous HMMs

**Usage**

```
stateprobs_g(
  delta,
  Gamma,
  allprobs,
  trackID = NULL,
  mod = NULL,
  forecast = FALSE
)
```

**Arguments**

|          |                                                                                                                                                                                                                                                                                                                                                             |
|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial distribution; either <ul style="list-style-type: none"> <li>• a vector of length nStates, or</li> <li>• a matrix of dimension c(nTracks, nStates) if trackID is provided</li> </ul>                                                                                                                                                                 |
| Gamma    | array of transition probability matrices of dimension c(nStates, nStates, nObs), where the first slice of each track is ignored as there is no transition into the start of a track. For a single track, an array of dimension c(nStates, nStates, nObs-1) is also accepted.                                                                                |
| allprobs | matrix of state-dependent probabilities or density values of dimension c(nObs, nStates)                                                                                                                                                                                                                                                                     |
| trackID  | optional vector of length nObs containing nTracks unique IDs that separate tracks. The observations of each track need to be consecutive.                                                                                                                                                                                                                   |
| mod      | optional model object containing delta, Gamma, allprobs, and optionally trackID. When using RTMB::MakeADFun or <a href="#">qrem1</a> with <a href="#">forward_g</a> in the likelihood, these are reported automatically after model fitting and the object returned by obj\$report(), <a href="#">lama</a> or <a href="#">qrem1</a> can be passed directly. |
| forecast | logical, indicating if forecast probabilities $\Pr(\text{State}_t = j \mid X_1, \dots, X_{t-1})$ should be calculated instead.                                                                                                                                                                                                                              |

**Details**

**Deprecated:** please use [stateprobs](#) for all model types instead.

**Value**

matrix of conditional state probabilities of dimension c(nObs, nStates)

**See Also**

Other decoding functions: [stateprobs\(\)](#), [stateprobs\\_p\(\)](#), [viterbi\(\)](#), [viterbi\\_g\(\)](#), [viterbi\\_p\(\)](#)

**Examples**

```
Gamma = tpm_g(runif(10), matrix(c(-1,-1,1,-2), nrow = 2, byrow = TRUE))
delta = c(0.5, 0.5)
allprobs = matrix(runif(20), nrow = 10, ncol = 2)

probs = stateprobs_g(delta, Gamma[,,-1], allprobs)
```

---

|              |                                                                                            |
|--------------|--------------------------------------------------------------------------------------------|
| stateprobs_p | <i>Calculate conditional local state probabilities for periodically inhomogeneous HMMs</i> |
|--------------|--------------------------------------------------------------------------------------------|

---

### Description

Computes

$$\Pr(S_t = j \mid X_1, \dots, X_T)$$

for periodically inhomogeneous HMMs

### Usage

```
stateprobs_p(
  delta,
  Gamma,
  allprobs,
  tod,
  trackID = NULL,
  mod = NULL,
  forecast = FALSE
)
```

### Arguments

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial or stationary distribution of length N, or matrix of dimension c(k,N) for k independent tracks, if trackID is provided<br>This could e.g. be the periodically stationary distribution (for each track) as computed by <a href="#">stationary_p</a> .                                                                                                                                                                                                                                                                                                                                                   |
| Gamma    | array of transition probability matrices for each time point in the cycle of dimension c(N,N,L), where L is the length of the cycle.                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| allprobs | matrix of state-dependent probabilities/ density values of dimension c(n, N)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| tod      | (Integer valued) variable for cycle indexing in 1, ..., L, mapping the data index to a generalised time of day (length n). For half-hourly data L = 48. It could, however, also be day of year for daily data and L = 365.                                                                                                                                                                                                                                                                                                                                                                                     |
| trackID  | optional vector of k track IDs, if multiple tracks need to be decoded separately. The observations of each track need to be consecutive.                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| mod      | optional model object containing initial distribution delta, transition probability matrix Gamma, matrix of state-dependent probabilities allprobs, and potentially a trackID variable<br>If you are using automatic differentiation either with RTMB: <a href="#">:MakeADFun</a> or <a href="#">qrem1</a> and include <a href="#">forward_p</a> in your likelihood function, the objects needed for state decoding are automatically reported after model fitting. Hence, you can pass the model object obtained from obj\$report(), <a href="#">lama</a> or <a href="#">qrem1</a> directly to this function. |
| forecast | logical, indicating if forecast probabilities $\Pr(S_t = j \mid X_1, \dots, X_{t-1})$ should be calculated instead.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

**Details**

**Deprecated:** please use [stateprobs](#) with argument `tod` instead.

**Value**

matrix of conditional state probabilities of dimension  $c(n,N)$

**See Also**

Other decoding functions: [stateprobs\(\)](#), [stateprobs\\_g\(\)](#), [viterbi\(\)](#), [viterbi\\_g\(\)](#), [viterbi\\_p\(\)](#)

**Examples**

```
L = 24
beta = matrix(c(-1, 2, -1, -2, 1, -1), nrow = 2, byrow = TRUE)
Gamma = tpm_p(1:L, L, beta, degree = 1)
delta = stationary_p(Gamma, 2) # for tod[1] = 1
allprobs = matrix(runif(200), nrow = 100, ncol = 2)
tod = rep(1:24, 5)[1:100]

probs = stateprobs_p(delta, Gamma, allprobs, tod)
```

---

stationary

---

*Compute the stationary distribution of a homogeneous Markov chain*


---

**Description**

A homogeneous, finite state Markov chain that is irreducible and aperiodic converges to a unique stationary distribution, here called  $\delta$ . As it is stationary, this distribution satisfies

$$\delta\Gamma = \delta,$$

subject to  $\sum_{j=1}^N \delta_j = 1$ , where  $\Gamma$  is the transition probability matrix. This function solves the linear system of equations above.

**Usage**

```
stationary(Gamma)
```

**Arguments**

|       |                                                                                                                                                                                            |
|-------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Gamma | transition probability matrix of dimension $c(N,N)$ or array of such matrices of dimension $c(N,N,nTracks)$ if the stationary distribution should be computed for several matrices at once |
|-------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

**Value**

either a single stationary distribution of the Markov chain (vector of length  $N$ ) or a matrix of stationary distributions of dimension  $c(nTracks,N)$  with one stationary distribution in each row

**See Also**

[tpm](#) to create a transition probability matrix using the multinomial logistic link (softmax)

Other stationary distribution functions: [stationary\\_ct\(\)](#), [stationary\\_p\(\)](#)

**Examples**

```
# single matrix
Gamma = tpm(c(rep(-2,3), rep(-3,3)))
delta = stationary(Gamma)
# multiple matrices
Gamma = array(Gamma, dim = c(3,3,10))
Delta = stationary(Gamma)
```

---

|               |                                                                              |
|---------------|------------------------------------------------------------------------------|
| stationary_ct | <i>Compute the stationary distribution of a continuous-time Markov chain</i> |
|---------------|------------------------------------------------------------------------------|

---

**Description**

A well-behaved continuous-time Markov chain converges to a unique stationary distribution, here called  $\pi$ . This distribution satisfies

$$\pi Q = 0,$$

subject to  $\sum_{j=1}^N \pi_j = 1$ , where  $Q$  is the infinitesimal generator of the Markov chain. This function solves the linear system of equations above for a given generator matrix.

**Usage**

```
stationary_ct(Q)
```

```
stationary_cont(Q)
```

**Arguments**

$Q$  infinitesimal generator matrix of dimension  $c(N, N)$  (dense or sparse, e.g. from `Matrix`) or array of such matrices of dimension  $c(N, N, nTracks)$  if the stationary distribution should be computed for several matrices at once

**Value**

either a single stationary distribution of the continuous-time Markov chain (vector of length  $N$ ) or a matrix of stationary distributions of dimension  $c(nTracks, N)$  with one stationary distribution in each row

**See Also**

[generator](#) to create a generator matrix

Other stationary distribution functions: [stationary\(\)](#), [stationary\\_p\(\)](#)

**Examples**

```
# single matrix
Q = generator(c(-2,-2))
Pi = stationary_ct(Q)
# multiple matrices
Q = array(Q, dim = c(2,2,10))
Pi = stationary_ct(Q)
```

---

|              |                                                                                          |
|--------------|------------------------------------------------------------------------------------------|
| stationary_p | <i>Periodically stationary distribution of a periodically inhomogeneous Markov chain</i> |
|--------------|------------------------------------------------------------------------------------------|

---

**Description**

Computes the periodically stationary distribution of a periodically inhomogeneous Markov chain.

**Usage**

```
stationary_p(Gamma, t = NULL, ad = NULL)
```

**Arguments**

|       |                                                                                                                                                                                                                      |
|-------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Gamma | array of transition probability matrices of dimension c(N,N,L)                                                                                                                                                       |
| t     | integer index of the time point in the cycle, for which to calculate the stationary distribution<br><br>If t is not provided, the function calculates all stationary distributions for each time point in the cycle. |
| ad    | optional logical, indicating whether automatic differentiation with RTMB should be used. By default, the function determines this itself.                                                                            |

**Details**

If the transition probability matrix of an inhomogeneous Markov chain varies only periodically (with period length  $L$ ), it converges to a so-called periodically stationary distribution. This happens, because the thinned Markov chain, which has a full cycle as each time step, has homogeneous transition probability matrix

$$\Gamma_t = \Gamma^{(t)} \Gamma^{(t+1)} \dots \Gamma^{(t+L-1)}$$

for all  $t = 1, \dots, L$ . The stationary distribution for time  $t$  satisfies  $\delta^{(t)} \Gamma_t = \delta^{(t)}$ . Here,  $\text{Gamma}[ , , t]$  is the transition from  $t$  to  $t+1$ . [forward](#) with `tod` uses  $\text{Gamma}[ , , \text{tod}[t]]$  for the transition into  $t$ , so there, the initial distribution is `stationary_p(Gamma, tod[1] %% L + 1)`, and `stationary_p(Gamma)[c(2:L, 1), ]` has the distribution at `tod = k` in row  $k$ .

This function calculates said periodically stationary distribution.

**Value**

either the periodically stationary distribution at time  $t$  or all periodically stationary distributions.

## References

When using this function, please cite:

Koslik, J. O., Feldmann, C. C., Mews, S., Michels, R., & Langrock, R. (2025). Inference on the state process of periodically inhomogeneous hidden Markov models for animal behavior. *The Annals of Applied Statistics*, 19(4), 2724–2737.

## See Also

[tpm\\_p](#) and [tpm\\_g](#) to create multiple transition matrices based on a cyclic variable or design matrix

Other stationary distribution functions: [stationary\(\)](#), [stationary\\_ct\(\)](#)

## Examples

```
# setting parameters for trigonometric link
beta = matrix(c(-1, 2, -1, -2, 1, -1), nrow = 2, byrow = TRUE)
Gamma = tpm_p(beta = beta, degree = 1)
# periodically stationary distribution for specific time point
delta = stationary_p(Gamma, 4)

# all periodically stationary distributions
Delta = stationary_p(Gamma)
```

---

|                     |                                                       |
|---------------------|-------------------------------------------------------|
| stationary_p_sparse | <i>Sparse version of</i> <a href="#">stationary_p</a> |
|---------------------|-------------------------------------------------------|

---

## Description

This function computes the periodically stationary distribution of a Markov chain given a list of **L sparse** transition probability matrices. Compatible with automatic differentiation by RTMB

## Usage

```
stationary_p_sparse(Gamma, t = NULL)
```

## Arguments

|       |                                                                                                                                                                                                               |
|-------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Gamma | sist of length L containing sparse transition probability matrices for one cycle.                                                                                                                             |
| t     | integer index of the time point in the cycle, for which to calculate the stationary distribution If t is not provided, the function calculates all stationary distributions for each time point in the cycle. |

## Value

either the periodically stationary distribution at time t or all periodically stationary distributions.

## Examples

```
## periodic HSMM example (here the approximating tpm is sparse)
N = 2 # number of states
L = 24 # cycle length
# time-varying mean dwell times
Z = cosinor(1:L, period = L) # trigonometric basis functions design matrix
beta = matrix(c(2, 2, 0.1, -0.1, -0.2, 0.2), nrow = 2)
Lambda = exp(cbind(1, Z) %*% t(beta))
sizes = c(20, 20) # approximating chain with 40 states
# state dwell-time distributions
dm = lapply(1:N, function(i) sapply(1:sizes[i]-1, dpois, lambda = Lambda[,i]))
omega = matrix(c(0,1,1,0), nrow = N, byrow = TRUE) # embedded t.p.m.

# calculating extended-state-space t.p.m.s
Gamma = tpm_phsmm(omega, dm)
# Periodically stationary distribution for specific time point
delta = stationary_p_sparse(Gamma, 4)

# All periodically stationary distributions
Delta = stationary_p_sparse(Gamma)
```

---

|                   |                                                     |
|-------------------|-----------------------------------------------------|
| stationary_sparse | <i>Sparse version of <a href="#">stationary</a></i> |
|-------------------|-----------------------------------------------------|

---

## Description

This is function computes the stationary distribution of a Markov chain with a given **sparse** transition probability matrix. Compatible with automatic differentiation by RTMB

## Usage

```
stationary_sparse(Gamma)
```

## Arguments

|       |                                                          |
|-------|----------------------------------------------------------|
| Gamma | sparse transition probability matrix of dimension c(N,N) |
|-------|----------------------------------------------------------|

## Value

stationary distribution of the Markov chain with the given transition probability matrix

## Examples

```
## HSMM example (here the approximating tpm is sparse)
# building the t.p.m. of the embedded Markov chain
omega = matrix(c(0,1,1,0), nrow = 2, byrow = TRUE)
# defining state aggregate sizes
sizes = c(20, 30)
# defining state dwell-time distributions
```

```

lambda = c(5, 11)
dm = list(dpois(1:sizes[1]-1, lambda[1]), dpois(1:sizes[2]-1, lambda[2]))
# calculating extended-state-space t.p.m.
Gamma = tpm_hsmm(omega, dm)
delta = stationary_sparse(Gamma)

```

---

|                   |                                      |
|-------------------|--------------------------------------|
| summary.LaMaModel | <i>Summary of a LaMaModel object</i> |
|-------------------|--------------------------------------|

---

## Description

Summarises a model from [lama](#) or [qrem1](#). Besides the overview of `print()`, this contains

- for a homogeneous state process (or one per track) with at most 10 states: the transition probability matrix (or generator matrix  $Q$  in continuous time, if reported, e.g. by `tpm_ct`), its stationary distribution and mean dwell times, averaged over tracks if there is one per track,
- for a periodic state process: the stationary distribution averaged over the cycle, i.e. the long-run proportion of time spent in each state,
- the quantities reported by the likelihood function via `REPORT()`: numeric vectors of length equal to the number of states are shown as one table with a column per state, other small objects separately, and large ones only by name,
- log-likelihood, AIC, BIC and the maximum gradient component at the estimate.

## Usage

```

## S3 method for class 'LaMaModel'
summary(object, ...)

## S3 method for class 'summary.LaMaModel'
print(x, digits = max(3, getOption("digits") - 3), ...)

```

## Arguments

|                     |                                       |
|---------------------|---------------------------------------|
| <code>object</code> | model object of class "LaMaModel"     |
| <code>...</code>    | additional arguments (not used)       |
| <code>x</code>      | object of class "summary.LaMaModel"   |
| <code>digits</code> | number of significant digits to print |

## Value

`summary()` returns an object of class "summary.LaMaModel", a list containing the quantities shown, e.g. `Gamma`, `stationary`, `dwell` and `bystate`. `print()` returns `x` invisibly.

---

|                    |                                       |
|--------------------|---------------------------------------|
| summary.qrem1Model | <i>Summary of a qrem1Model object</i> |
|--------------------|---------------------------------------|

---

## Description

Summarises a model from [qrem1](#): the summary of [summary.LaMaModel](#), plus the effective degrees of freedom and smoothing parameters of the smooth terms and diagnostics of the smoothness selection.

## Usage

```
## S3 method for class 'qrem1Model'
summary(object, ...)

## S3 method for class 'summary.qrem1Model'
print(x, digits = max(3, getOption("digits") - 3), ...)
```

## Arguments

|        |                                       |
|--------|---------------------------------------|
| object | model object of class "qrem1Model"    |
| ...    | additional arguments (not used)       |
| x      | object of class "summary.qrem1Model"  |
| digits | number of significant digits to print |

## Value

summary() returns an object of class "summary.qrem1Model", extending "summary.LaMaModel" by edf, lambda and selection. print() returns x invisibly.

---

|     |                                                                                    |
|-----|------------------------------------------------------------------------------------|
| tpm | <i>Build the transition probability matrix from unconstrained parameter vector</i> |
|-----|------------------------------------------------------------------------------------|

---

## Description

Markov chains are parametrised in terms of a transition probability matrix  $\Gamma$ , for which each row contains a conditional probability distribution of the next state given the current state. Hence, each row has entries between 0 and 1 that need to sum to one.

For numerical optimisation, we parameterise in terms of unconstrained parameters, thus this function computes said matrix from an unconstrained parameter vector via the inverse multinomial logistic link (also known as softmax) applied to each row.

**Usage**

```
tpm(
  beta,
  Z = NULL,
  Eta = NULL,
  byrow = FALSE,
  ref = NULL,
  ad = NULL,
  report = TRUE,
  param = NULL
)
```

**Arguments**

|        |                                                                                                                                                                                                                                                            |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| beta   | parameters; either <ul style="list-style-type: none"> <li>• a vector of length <math>nStates * (nStates - 1)</math>, or</li> <li>• a matrix of dimension <math>c(nStates * (nStates - 1), p + 1)</math> if design matrix Z is also provided.</li> </ul>    |
| Z      | optional covariate design matrix with or without intercept column, i.e. of dimension $c(nObs, p)$ or $c(nObs, p + 1)$ . If provided, beta needs to be a matrix of dimension $c(nStates * (nStates - 1), p + 1)$ .                                          |
| Eta    | optional pre-calculated matrix of linear predictors of dimension $c(nObs, nStates * (nStates - 1))$ . If provided, Z and beta will be ignored.                                                                                                             |
| byrow  | logical indicating if each transition probability matrix should be filled by row. Defaults to FALSE, but should be set to TRUE if one wants to work with a matrix of beta parameters returned by popular HMM packages like moveHMM, momentuHMM, or hmmTMB. |
| ref    | optional integer vector of length nStates giving, for each row, the column index of the reference state (its predictor is fixed to 0). Defaults to the diagonal ( $ref = 1:nStates$ ).                                                                     |
| ad     | logical; whether to use automatic differentiation. Determined automatically — for debugging only.                                                                                                                                                          |
| report | logical; if TRUE (default), delta, Gamma, allprobs, and trackID are reported from the fitted model. Requires $ad = TRUE$ .                                                                                                                                 |
| param  | deprecated, please use argument beta instead.                                                                                                                                                                                                              |

**Value**

Transition probability matrix of dimension  $c(nStates, nStates)$  or array of such matrices of dimension  $c(nStates, nStates, nObs)$  if Z or Eta is provided.

**See Also**

Other transition probability matrix functions: [generator\(\)](#), [generator\\_g\(\)](#), [tpm\\_ct\(\)](#), [tpm\\_emb\(\)](#), [tpm\\_emb\\_g\(\)](#), [tpm\\_g\(\)](#), [tpm\\_g2\(\)](#), [tpm\\_p\(\)](#)

## Examples

```
## homogeneous Markov chain
# 2 states: 2 = 2*(2-1) free off-diagonal elements
par <- rep(-2, 2)
Gamma <- tpm(par)
# 3 states: 6 = 3*(3-1) free off-diagonal elements
par <- rep(-3, 6)
Gamma <- tpm(par)
# 4 states: 12 = 4*(4-1) free off-diagonal elements
par <- rep(-4, 12)
Gamma <- tpm(par)

## inhomogeneous Markov chain
# t.p.m. depends on covariates
z1 <- runif(100); z2 <- runif(100) # 2 covariates
Z <- cbind(1, z1, z2) # design matrix
beta0 <- c(-2, -2); beta1 = c(1, -2); beta2 = c(2, -1) # coefficients for intercept and covariates
beta <- cbind(beta0, beta1, beta2) # coefficient matrix; with intercepts!
Gamma <- tpm(beta, Z) # array with 100 slices
```

---

tpm\_ct

---

*Calculate continuous time transition probabilities*


---

## Description

A continuous-time Markov chain is described by an infinitesimal generator matrix  $Q$ . When observing data at time points  $t_1, \dots, t_n$  the transition probabilities between  $t_i$  and  $t_{i+1}$  are calculated as

$$\Gamma(\Delta t_i) = \exp(Q\Delta t_i),$$

where  $\exp()$  is the matrix exponential. The mapping  $\Gamma(\Delta t)$  is also called the **Markov semigroup**. This function calculates all transition matrices based on a given generator and time differences.

## Usage

```
tpm_ct(Q, timediff, rates = NULL, ad = NULL, report = TRUE)
```

```
tpm_cont(Q, timediff, rates = NULL, ad = NULL, report = TRUE)
```

## Arguments

|                       |                                                                                                                                                                                                                                                                 |
|-----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $Q$                   | infinitesimal generator matrix of the continuous-time Markov chain of dimension $c(nStates, nStates)$                                                                                                                                                           |
| <code>timediff</code> | time differences between observations of length <code>nObs-1</code> when based on <code>nObs</code> observations                                                                                                                                                |
| <code>rates</code>    | optional vector of state-dependent rates for MM(M)PP fitting. For the MM(M)PP likelihood, the matrices needed in the forward algorithm are $\exp((Q - \Lambda)\Delta t)$ , where $\Lambda$ is a diagonal matrix with the state-dependent rates on the diagonal. |

|        |                                                                                                                                           |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------|
| ad     | optional logical, indicating whether automatic differentiation with RTMB should be used. By default, the function determines this itself. |
| report | logical, indicating whether Q should be reported from the fitted model. Defaults to TRUE, but only works if ad = TRUE.                    |

### Value

array of continuous-time transition matrices of dimension  $c(nStates, nStates, nObs-1)$

### See Also

Other transition probability matrix functions: [generator\(\)](#), [generator\\_g\(\)](#), [tpm\(\)](#), [tpm\\_emb\(\)](#), [tpm\\_emb\\_g\(\)](#), [tpm\\_g\(\)](#), [tpm\\_g2\(\)](#), [tpm\\_p\(\)](#)

### Examples

```
# building a Q matrix for a 3-state cont.-time Markov chain
Q = generator(rep(-2, 6))

# draw random time differences
timediff = rexp(100, 10)

# compute all transition matrices
Gamma = tpm_cont(Q, timediff)
```

---

|         |                                                                                                        |
|---------|--------------------------------------------------------------------------------------------------------|
| tpm_emb | <i>Build the embedded transition probability matrix of an HSMM from unconstrained parameter vector</i> |
|---------|--------------------------------------------------------------------------------------------------------|

---

### Description

Hidden semi-Markov models are defined in terms of state durations and an **embedded** transition probability matrix that contains the conditional transition probabilities given that the **current state is left**. This matrix necessarily has diagonal entries all equal to zero as self-transitions are impossible.

This function builds such an embedded/ conditional transition probability matrix from an unconstrained parameter vector. For each row of the matrix, the inverse multinomial logistic link is applied.

For a matrix of dimension  $c(nStates, nStates)$ , the number of free off-diagonal elements is  $nStates * (nStates-2)$ , hence also the length of param. This means, for 2 states, the function needs to be called without any arguments, for 3-states with a vector of length 3, for 4 states with a vector of length 8, etc.

Compatible with automatic differentiation by RTMB

### Usage

```
tpm_emb(param = NULL)
```

**Arguments**

`param` unconstrained parameter vector of length  $nStates * (nStates - 2)$   
 If the function is called without `param`, it will return the conditional transition probability matrix for a 2-state HSMM, which is fixed with 0 diagonal entries and off-diagonal entries equal to 1.

**Value**

embedded/ conditional transition probability matrix of dimension  $c(nStates, nStates)$

**See Also**

Other transition probability matrix functions: [generator\(\)](#), [generator\\_g\(\)](#), [tpm\(\)](#), [tpm\\_ct\(\)](#), [tpm\\_emb\\_g\(\)](#), [tpm\\_g\(\)](#), [tpm\\_g2\(\)](#), [tpm\\_p\(\)](#)

**Examples**

```
# 2 states: no free off-diagonal elements
omega = tpm_emb()

# 3 states: 3 free off-diagonal elements
param = rep(0, 3)
omega = tpm_emb(param)

# 4 states: 8 free off-diagonal elements
param = rep(0, 8)
omega = tpm_emb(param)
```

---

|                        |                                                                                    |
|------------------------|------------------------------------------------------------------------------------|
| <code>tpm_emb_g</code> | <i>Build all embedded transition probability matrices of an inhomogeneous HSMM</i> |
|------------------------|------------------------------------------------------------------------------------|

---

**Description**

Hidden semi-Markov models are defined in terms of state durations and an **embedded** transition probability matrix that contains the conditional transition probabilities given that the **current state is left**. This matrix necessarily has diagonal entries all equal to zero as self-transitions are impossible. We can allow this matrix to vary with covariates, which is the purpose of this function.

It builds all embedded/ conditional transition probability matrices based on a design and parameter matrix. For each row of the matrix, the inverse multinomial logistic link is applied.

For a matrix of dimension  $c(nStates, nStates)$ , the number of free off-diagonal elements is  $nStates * (nStates - 2)$  which determines the number of rows of the parameter matrix.

Compatible with automatic differentiation by RTMB

**Usage**

```
tpm_emb_g(Z, beta, report = TRUE)
```

**Arguments**

|        |                                                                                                                                                                                                                                                                      |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Z      | covariate design matrix with or without intercept column, i.e. of dimension $c(nObs, p)$ or $c(nObs, p+1)$<br>If Z has only p columns, an intercept column of ones will be added automatically.                                                                      |
| beta   | matrix of coefficients for the off-diagonal elements of the embedded transition probability matrix<br>Needs to be of dimension $c(nStates * (nStates-2), p+1)$ , where the first column contains the intercepts. p can be 0, in which case the model is homogeneous. |
| report | logical, indicating whether the coefficient matrix beta should be reported from the fitted model. Defaults to TRUE.                                                                                                                                                  |

**Value**

array of embedded/ conditional transition probability matrices of dimension  $c(nStates, nStates, nObs)$

**See Also**

Other transition probability matrix functions: [generator\(\)](#), [generator\\_g\(\)](#), [tpm\(\)](#), [tpm\\_ct\(\)](#), [tpm\\_emb\(\)](#), [tpm\\_g\(\)](#), [tpm\\_g2\(\)](#), [tpm\\_p\(\)](#)

**Examples**

```
## parameter matrix for 3-state HSMM
beta = matrix(c(rep(0, 3), -0.2, 0.2, 0.1), nrow = 3)
# no intercept
Z = rnorm(100)
omega = tpm_emb_g(Z, beta)
# intercept
Z = cbind(1, Z)
omega = tpm_emb_g(Z, beta)
```

---

tpm\_g

---

*Build all transition probability matrices of an inhomogeneous HMM*


---

**Description**

In an HMM, we often model the influence of covariates on the state process by linking them to the transition probability matrix. Most commonly, this is done by specifying a linear predictor

$$\eta_{ij}^{(t)} = \beta_0^{(ij)} + \beta_1^{(ij)} z_{t1} + \dots + \beta_p^{(ij)} z_{tp}$$

for each off-diagonal element ( $i \neq j$ ) of the transition probability matrix and then applying the inverse multinomial logistic link (also known as softmax) to each row. This function efficiently calculates all transition probability matrices for a given design matrix Z and parameter matrix beta.

**Usage**

```
tpm_g(Z, beta, Eta = NULL, byrow = FALSE, ref = NULL, ad = NULL, report = TRUE)
```

**Arguments**

|        |                                                                                                                                                                                                                                                            |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Z      | Covariate design matrix with or without intercept column, i.e. of dimension $c(nObs, p)$ or $c(nObs, p+1)$ . If not provided, intercept column is added automatically.                                                                                     |
| beta   | Matrix of coefficients for the off-diagonal elements of the transition probability matrix of dimension $c(nStates * (nStates-1), p+1)$ . First columns contains the intercepts.                                                                            |
| Eta    | optional pre-calculated matrix of linear predictors of dimension $c(nObs, nStates * (nStates-1))$ . If provided, no Z and beta are necessary and will be ignored.                                                                                          |
| byrow  | logical indicating if each transition probability matrix should be filled by row. Defaults to FALSE, but should be set to TRUE if one wants to work with a matrix of beta parameters returned by popular HMM packages like moveHMM, momentuHMM, or hmmTMB. |
| ref    | optional integer vector of length nStates giving, for each row, the column index of the reference state (its predictor is fixed to 0). Defaults to the diagonal ( $ref = 1:nStates$ ).                                                                     |
| ad     | logical; whether to use automatic differentiation. Determined automatically — for debugging only.                                                                                                                                                          |
| report | logical; if TRUE (default), delta, Gamma, allprobs, and trackID are reported from the fitted model. Requires $ad = TRUE$ .                                                                                                                                 |

**Details**

**Deprecated:** please use [tpm\(beta, Z\)](#) for all model types instead.

**Value**

array of transition probability matrices of dimension  $c(nStates, nStates, nObs)$

**See Also**

Other transition probability matrix functions: [generator\(\)](#), [generator\\_g\(\)](#), [tpm\(\)](#), [tpm\\_ct\(\)](#), [tpm\\_emb\(\)](#), [tpm\\_emb\\_g\(\)](#), [tpm\\_g2\(\)](#), [tpm\\_p\(\)](#)

**Examples**

```
## inhomogeneous Markov chain
# t.p.m. depends on covariates
z1 <- runif(100); z2 <- runif(100) # 2 covariates
Z <- cbind(1, z1, z2) # design matrix
beta0 <- c(-2, -2); beta1 = c(1, -2); beta2 = c(2, -1) # coefficients for intercept and covariates
beta <- cbind(beta0, beta1, beta2) # coefficient matrix; with intercepts!
#' Gamma <- tpm(beta, Z) # array with 100 slices
```

tpm\_g2

*Build all transition probability matrices of an inhomogeneous HMM***Description**

In an HMM, we often model the influence of covariates on the state process by linking them to the transition probability matrix. Most commonly, this is done by specifying linear predictors

$$\eta_{ij}^{(t)} = \beta_0^{(ij)} + \beta_1^{(ij)} z_{t1} + \dots + \beta_p^{(ij)} z_{tp}$$

for each off-diagonal element ( $i \neq j$ ) of the transition probability matrix and then applying the inverse multinomial logistic link (also known as softmax) to each row. This function efficiently calculates all transition probability matrices for a given design matrix Z and parameter matrix beta.

**Usage**

```
tpm_g2(Z, beta, byrow = FALSE, ad = NULL, report = TRUE, ref = NULL)
```

**Arguments**

|        |                                                                                                                                                                                                                                                                                                                                                                                     |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Z      | covariate design matrix with or without intercept column, i.e. of dimension c(n, p) or c(n, p+1)<br>If Z has only p columns, an intercept column of ones will be added automatically.<br>Can also be a list of N*(N-1) design matrices with different number of columns but the same number of rows. In that case, no intercept column will be added.                               |
| beta   | matrix of coefficients for the off-diagonal elements of the transition probability matrix<br>Needs to be of dimension c(N*(N-1), p+1), where the first column contains the intercepts.<br>If Z is a list, beta can also be a list of length N*(N-1) with each entry being a vector or a (long) matrix of coefficients, each matching the dimension of the corresponding entry in Z. |
| byrow  | logical indicating if each transition probability matrix should be filled by row<br>Defaults to FALSE, but should be set to TRUE if one wants to work with a matrix of beta parameters returned by popular HMM packages like moveHMM, momentuHMM, or hmmTMB.                                                                                                                        |
| ad     | optional logical, indicating whether automatic differentiation with RTMB should be used. By default, the function determines this itself.                                                                                                                                                                                                                                           |
| report | logical, indicating whether the coefficient matrix beta should be reported from the fitted model. Defaults to TRUE, but only works if ad = TRUE.                                                                                                                                                                                                                                    |
| ref    | optional vector of length N with the reference state indices for each column of the transition probability matrix. Each row in the transition matrix corresponds to a multinomial regression, hence one state needs to be the reference category. Defaults to off-diagonal elements (ref = 1:N).                                                                                    |

**Value**

array of transition probability matrices of dimension  $c(N,N,n)$

**See Also**

Other transition probability matrix functions: [generator\(\)](#), [generator\\_g\(\)](#), [tpm\(\)](#), [tpm\\_ct\(\)](#), [tpm\\_emb\(\)](#), [tpm\\_emb\\_g\(\)](#), [tpm\\_g\(\)](#), [tpm\\_p\(\)](#)

**Examples**

```
Z = matrix(runif(200), ncol = 2)
beta = matrix(c(-1, 1, 2, -2, 1, -2), nrow = 2, byrow = TRUE)
Gamma = tpm_g(Z, beta)
```

---

|          |                                                                              |
|----------|------------------------------------------------------------------------------|
| tpm_hsmm | <i>Builds the transition probability matrix of an HSMM-approximating HMM</i> |
|----------|------------------------------------------------------------------------------|

---

**Description**

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs, where the state duration distribution is explicitly modelled. For direct numerical maximum likelihood estimation, HSMMs can be represented as HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities.

This function computes the transition matrix to approximate a given HSMM by an HMM with a larger state space.

**Usage**

```
tpm_hsmm(omega, dm, Fm = NULL, sparse = TRUE, eps = 1e-10)
```

**Arguments**

|        |                                                                                                                                                                                                            |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| omega  | embedded transition probability matrix of dimension $c(nStates, nStates)$ as computed by <a href="#">tpm_emb</a> .                                                                                         |
| dm     | state dwell-time distributions arranged in a list of length <code>nStates</code> . Each list element needs to be a vector of length <code>N_i</code> , where <code>N_i</code> is the state aggregate size. |
| Fm     | optional list of length <code>nStates</code> containing the cumulative distribution functions of the dwell-time distributions.                                                                             |
| sparse | logical, indicating whether the output should be a <b>sparse</b> matrix. Defaults to <code>TRUE</code> .                                                                                                   |
| eps    | rounding value: If an entry of the transition probability matrix is smaller, than it is rounded to zero. Usually, this should not be changed.                                                              |

**Value**

extended-state-space transition probability matrix of the approximating HMM

**Examples**

```
# building the t.p.m. of the embedded Markov chain
omega = matrix(c(0,1,1,0), nrow = 2, byrow = TRUE)
# defining state aggregate sizes
sizes = c(20, 30)
# defining state dwell-time distributions
lambda = c(5, 11)
dm = list(dpois(1:sizes[1]-1, lambda[1]), dpois(1:sizes[2]-1, lambda[2]))
# calculating extended-state-space t.p.m.
Gamma = tpm_hsmm(omega, dm)
```

---

|           |                                                                             |
|-----------|-----------------------------------------------------------------------------|
| tpm_hsmm2 | <i>Build the transition probability matrix of an HSMM-approximating HMM</i> |
|-----------|-----------------------------------------------------------------------------|

---

**Description**

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs. For direct numerical maximum likelihood estimation, HSMMs can be represented as HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities. This function computes the transition matrix of an HSMM.

**Usage**

```
tpm_hsmm2(omega, dm, eps = 1e-10)
```

**Arguments**

|       |                                                                                                                                                                       |
|-------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| omega | embedded transition probability matrix of dimension $c(N,N)$                                                                                                          |
| dm    | state dwell-time distributions arranged in a list of length $(N)$ . Each list element needs to be a vector of length $N_i$ , where $N_i$ is the state aggregate size. |
| eps   | rounding value: If an entry of the transition probability matrix is smaller, than it is rounded to zero.                                                              |

**Value**

extended-state-space transition probability matrix of the approximating HMM

## Examples

```
# building the t.p.m. of the embedded Markov chain
omega = matrix(c(0,1,1,0), nrow = 2, byrow = TRUE)
# defining state aggregate sizes
sizes = c(20, 30)
# defining state dwell-time distributions
lambda = c(5, 11)
dm = list(dpois(1:sizes[1]-1, lambda[1]), dpois(1:sizes[2]-1, lambda[2]))
# calculating extended-state-space t.p.m.
Gamma = tpm_ihsmm(omega, dm)
```

---

|           |                                                                                              |
|-----------|----------------------------------------------------------------------------------------------|
| tpm_ihsmm | <i>Builds all transition probability matrices of an inhomogeneous-HSMM-approximating HMM</i> |
|-----------|----------------------------------------------------------------------------------------------|

---

## Description

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs. For direct numerical maximum likelihood estimation, HSMMs can be represented as HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities.

This function computes the transition matrices of a periodically inhomogeneous HSMMs.

## Usage

```
tpm_ihsmm(omega, dm, eps = 1e-10)
```

## Arguments

|       |                                                                                                                                                                                                                                                                                                                                                       |
|-------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| omega | embedded transition probability matrix<br>Either a matrix of dimension $c(nStates, nStates)$ for homogeneous conditional transition probabilities (as computed by <a href="#">tpm_emb</a> ), or an array of dimension $c(nStates, nStates, nObs)$ for inhomogeneous conditional transition probabilities (as computed by <a href="#">tpm_emb_g</a> ). |
| dm    | state dwell-time distributions arranged in a list of length $nStates$<br>Each list element needs to be a matrix of dimension $c(n, N_i)$ , where each row $t$ is the (approximate) probability mass function of state $i$ at time $t$ .                                                                                                               |
| eps   | rounding value: If an entry of the transition probability matrix is smaller, than it is rounded to zero. Usually, this should not be changed.                                                                                                                                                                                                         |

## Value

list of dimension length  $n - \max(\text{sapply}(dm, \text{ncol}))$ , containing sparse extended-state-space transition probability matrices for each time point (except the first  $\max(\text{sapply}(dm, \text{ncol})) - 1$ ).

## Examples

```

N = 2
# time-varying mean dwell times
n = 100
z = runif(n)
beta = matrix(c(2, 2, 0.1, -0.1), nrow = 2)
Lambda = exp(cbind(1, z) %*% t(beta))
sizes = c(15, 15) # approximating chain with 30 states
# state dwell-time distributions
dm = lapply(1:N, function(i) sapply(1:sizes[i]-1, dpois, lambda = Lambda[,i]))

## homogeneous conditional transition probabilities
# diagonal elements are zero, rowsums are one
omega = matrix(c(0,1,1,0), nrow = N, byrow = TRUE)

# calculating extended-state-space t.p.m.s
Gamma = tpm_ihsmm(omega, dm)

## inhomogeneous conditional transition probabilities
# omega can be an array
omega = array(omega, dim = c(N,N,n))

# calculating extended-state-space t.p.m.s
Gamma = tpm_ihsmm(omega, dm)

```

---

tpm\_p

---

*Build all transition probability matrices of a periodically inhomogeneous HMM*


---

## Description

Given a periodically varying variable such as time of day or day of year and the associated cycle length, this function calculates the transition probability matrices by applying the inverse multinomial logistic link (also known as softmax) to linear predictors of the form

$$\eta_{ij}^{(t)} = \beta_0^{(ij)} + \sum_{k=1}^K (\beta_{1k}^{(ij)} \sin(\frac{2\pi kt}{L}) + \beta_{2k}^{(ij)} \cos(\frac{2\pi kt}{L}))$$

for the off-diagonal elements ( $i \neq j$ ) of the transition probability matrix. This is relevant for modeling e.g. diurnal variation and the flexibility can be increased by adding smaller frequencies (i.e. increasing  $K$ ).

## Usage

```

tpm_p(
  tod = 1:24,
  L = 24,
  beta,

```

```

degree = 1,
Z = NULL,
byrow = FALSE,
ad = NULL,
report = TRUE
)

```

## Arguments

|                     |                                                                                                                                                                                                                                                                                                                                            |
|---------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>tod</code>    | equidistant sequence of a cyclic variable<br>For time of day and e.g. half-hourly data, this could be 1, ..., L and L = 48, or 0.5, 1, 1.5, ..., 24 and L = 24.                                                                                                                                                                            |
| <code>L</code>      | length of one full cycle, on the scale of <code>tod</code>                                                                                                                                                                                                                                                                                 |
| <code>beta</code>   | matrix of coefficients for the off-diagonal elements of the transition probability matrix<br>Needs to be of dimension $c(nStates * (nStates - 1), 2 * degree + 1)$ , where the first column contains the intercepts.                                                                                                                       |
| <code>degree</code> | degree of the trigonometric link function<br>For each additional degree, one sine and one cosine frequency are added.                                                                                                                                                                                                                      |
| <code>Z</code>      | pre-calculated design matrix (excluding intercept column)<br>Defaults to NULL if trigonometric link should be calculated. From an efficiency perspective, Z should be pre-calculated within the likelihood function, as the basis expansion should not be redundantly calculated. This can be done by using <a href="#">trigBasisExp</a> . |
| <code>byrow</code>  | logical indicating if each transition probability matrix should be filled by row<br>Defaults to FALSE, but should be set to TRUE if one wants to work with a matrix of beta parameters returned by popular HMM packages like <code>moveHMM</code> , <code>momentuHMM</code> , or <code>hmmTMB</code> .                                     |
| <code>ad</code>     | optional logical, indicating whether automatic differentiation with RTMB should be used. By default, the function determines this itself.                                                                                                                                                                                                  |
| <code>report</code> | logical, indicating whether the coefficient matrix <code>beta</code> should be reported from the fitted model. Defaults to TRUE, but only works if <code>ad</code> = TRUE.                                                                                                                                                                 |

## Details

Note that using this function inside the negative log-likelihood function is convenient, but it performs the basis expansion into sine and cosine terms each time it is called. As these do not change during the optimisation, using [tpm\\_g](#) with a pre-calculated (by [trigBasisExp](#)) design matrix would be more efficient.

## Value

array of transition probability matrices of dimension  $c(nStates, nStates, length(tod))$

## See Also

Other transition probability matrix functions: [generator\(\)](#), [generator\\_g\(\)](#), [tpm\(\)](#), [tpm\\_ct\(\)](#), [tpm\\_emb\(\)](#), [tpm\\_emb\\_g\(\)](#), [tpm\\_g\(\)](#), [tpm\\_g2\(\)](#)

## Examples

```
# hourly data
tod = seq(1, 24, by = 1)
L = 24
beta = matrix(c(-1, 2, -1, -2, 1, -1), nrow = 2, byrow = TRUE)
Gamma = tpm_p(tod, L, beta, degree = 1)

# half-hourly data
## integer tod sequence
tod = seq(1, 48, by = 1)
L = 48
beta = matrix(c(-1, 2, -1, -2, 1, -1), nrow = 2, byrow = TRUE)
Gamma1 = tpm_p(tod, L, beta, degree = 1)

## equivalent specification
tod = seq(0.5, 24, by = 0.5)
L = 24
beta = matrix(c(-1, 2, -1, -2, 1, -1), nrow = 2, byrow = TRUE)
Gamma2 = tpm_p(tod, L, beta, degree = 1)

all(Gamma1 == Gamma2) # same result
```

---

|           |                                                                                         |
|-----------|-----------------------------------------------------------------------------------------|
| tpm_phsmm | <i>Builds all transition probability matrices of an periodic-HSMM-approximating HMM</i> |
|-----------|-----------------------------------------------------------------------------------------|

---

## Description

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs. For direct numerical maximum likelihood estimation, HSMMs can be represented as HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities.

This function computes the transition matrices of a periodically inhomogeneous HSMMs.

## Usage

```
tpm_phsmm(omega, dm, eps = 1e-10)
```

## Arguments

|       |                                                                                                                                                                                                                                                                                                                                                    |
|-------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| omega | embedded transition probability matrix<br>Either a matrix of dimension $c(nStates, nStates)$ for homogeneous conditional transition probabilities (as computed by <a href="#">tpm_emb</a> ), or an array of dimension $c(nStates, nStates, L)$ for inhomogeneous conditional transition probabilities (as computed by <a href="#">tpm_emb_g</a> ). |
| dm    | state dwell-time distributions arranged in a list of length $nStates$<br>Each list element needs to be a matrix of dimension $c(L, N_i)$ , where each row $t$ is the (approximate) probability mass function of state $i$ at time $t$ .                                                                                                            |
| eps   | rounding value: If an entry of the transition probability matrix is smaller, than it is rounded to zero. Usually, this should not be changed.                                                                                                                                                                                                      |

**Value**

list of dimension length  $L$ , containing sparse extended-state-space transition probability matrices of the approximating HMM for each time point of the cycle.

**Examples**

```

N = 2 # number of states
L = 24 # cycle length
# time-varying mean dwell times
Z = cosinor(1:L, period = L) # trigonometric basis functions design matrix
beta = matrix(c(2, 2, 0.1, -0.1, -0.2, 0.2), nrow = 2)
Lambda = exp(cbind(1, Z) %*% t(beta))
sizes = c(20, 20) # approximating chain with 40 states
# state dwell-time distributions
dm = lapply(1:N, function(i) sapply(1:sizes[i]-1, dpois, lambda = Lambda[,i]))

## homogeneous conditional transition probabilities
# diagonal elements are zero, rowsums are one
omega = matrix(c(0,1,1,0), nrow = N, byrow = TRUE)

# calculating extended-state-space t.p.m.s
Gamma = tpm_phsmm(omega, dm)

## inhomogeneous conditional transition probabilities
# omega can be an array
omega = array(omega, dim = c(N,N,L))

# calculating extended-state-space t.p.m.s
Gamma = tpm_phsmm(omega, dm)

```

---

tpm\_phsmm2

---

*Build all transition probability matrices of an periodic-HSMM-approximating HMM*


---

**Description**

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs. For direct numerical maximum likelihood estimation, HSMMs can be represented as HMMs on an enlarged state space (of size  $M$ ) and with structured transition probabilities. This function computes the transition matrices of a periodically inhomogeneous HSMMs.

**Usage**

```
tpm_phsmm2(omega, dm, eps = 1e-10)
```

**Arguments**

|       |                                                                                                                                                                                                                                                                                       |
|-------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| omega | <p>embedded transition probability matrix</p> <p>Either a matrix of dimension <math>c(N,N)</math> for homogeneous conditional transition probabilities, or an array of dimension <math>c(N,N,L)</math> for inhomogeneous conditional transition probabilities.</p>                    |
| dm    | <p>state dwell-time distributions arranged in a list of length(N)</p> <p>Each list element needs to be a matrix of dimension <math>c(L, N_i)</math>, where each row <math>t</math> is the (approximate) probability mass function of state <math>i</math> at time <math>t</math>.</p> |
| eps   | <p>rounding value: If an entry of the transition probability matrix is smaller, than it is rounded to zero.</p>                                                                                                                                                                       |

**Value**

array of dimension  $c(N,N,L)$ , containing the extended-state-space transition probability matrices of the approximating HMM for each time point of the cycle.

**Examples**

```

N = 3
L = 24
# time-varying mean dwell times
Lambda = exp(matrix(rnorm(L*N, 2, 0.5), nrow = L))
sizes = c(25, 25, 25) # approximating chain with 75 states
# state dwell-time distributions
dm = list()
for(i in 1:3){
  dmi = matrix(nrow = L, ncol = sizes[i])
  for(t in 1:L){
    dmi[t,] = dpois(1:sizes[i]-1, Lambda[t,i])
  }
  dm[[i]] = dmi
}

## homogeneous conditional transition probabilities
# diagonal elements are zero, rowsums are one
omega = matrix(c(0,0.5,0.5,0.2,0,0.8,0.7,0.3,0), nrow = N, byrow = TRUE)

# calculating extended-state-space t.p.m.s
Gamma = tpm_phsmm(omega, dm)

## inhomogeneous conditional transition probabilities
# omega can be an array
omega = array(rep(omega,L), dim = c(N,N,L))
omega[1,,4] = c(0, 0.2, 0.8) # small change for inhomogeneity

# calculating extended-state-space t.p.m.s
Gamma = tpm_phsmm(omega, dm)

```

---

|             |                                                                                                        |
|-------------|--------------------------------------------------------------------------------------------------------|
| tpm_thinned | <i>Compute the transition probability matrix of a thinned periodically inhomogeneous Markov chain.</i> |
|-------------|--------------------------------------------------------------------------------------------------------|

---

## Description

If the transition probability matrix of an inhomogeneous Markov chain varies only periodically (with period length  $L$ ), it converges to a so-called periodically stationary distribution. This happens, because the thinned Markov chain, which has a full cycle as each time step, has homogeneous transition probability matrix

$$\Gamma_t = \Gamma^{(t)} \Gamma^{(t+1)} \dots \Gamma^{(t+L-1)}$$

for all  $t = 1, \dots, L$ . This function calculates the matrix above efficiently as a preliminary step to calculating the periodically stationary distribution.

## Usage

```
tpm_thinned(Gamma, t)
```

## Arguments

|       |                                                                                                                |
|-------|----------------------------------------------------------------------------------------------------------------|
| Gamma | array of transition probability matrices of dimension $c(nStates, nStates, L)$ .                               |
| t     | integer index of the time point in the cycle, for which to calculate the thinned transition probability matrix |

## Value

thinned transition probability matrix of dimension  $c(nStates, nStates)$

## Examples

```
# setting parameters for trigonometric link
beta = matrix(c(-1, -2, 2, -1, 2, -4), nrow = 2, byrow = TRUE)
# calculating periodically varying t.p.m. array (of length 24 here)
Gamma = tpm_p(beta = beta)
# calculating t.p.m. of thinned Markov chain
tpm_thinned(Gamma, 4)
```

---

|      |                            |
|------|----------------------------|
| trex | <i>T-Rex Movement Data</i> |
|------|----------------------------|

---

**Description**

Hourly step lengths and turning angles of a Tyrannosaurus rex, living 66 million years ago.

**Usage**

trex

**Format**

A data frame with 10.000 rows and 4 variables:

**tod** time of day variable ranging from 1 to 24

**step** hourly step lengths in kilometres

**angle** hourly turning angles in radians

**state** hidden state variable

**Source**

Generated for example purposes.

---

|              |                                                                      |
|--------------|----------------------------------------------------------------------|
| trigBasisExp | <i>Compute the design matrix for a trigonometric basis expansion</i> |
|--------------|----------------------------------------------------------------------|

---

**Description**

Given a periodically varying variable such as time of day or day of year and the associated cycle length, this function performs a basis expansion to efficiently calculate a linear predictor of the form

$$\eta^{(t)} = \beta_0 + \sum_{k=1}^K (\beta_{1k} \sin(\frac{2\pi kt}{L}) + \beta_{2k} \cos(\frac{2\pi kt}{L})).$$

This is relevant for modeling e.g. diurnal variation and the flexibility can be increased by adding smaller frequencies (i.e. increasing  $K$ ).

**Usage**

trigBasisExp(tod, L = 24, degree = 1)

**Arguments**

|        |                                                                                                                                                                 |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| tod    | equidistant sequence of a cyclic variable<br>For time of day and e.g. half-hourly data, this could be 1, ..., L and L = 48, or 0.5, 1, 1.5, ..., 24 and L = 24. |
| L      | length of one cycle on the scale of the time variable. For time of day, this would be 24.                                                                       |
| degree | degree K of the trigonometric link above. Increasing K increases the flexibility.                                                                               |

**Value**

design matrix (without intercept column), ordered as sin1, cos1, sin2, cos2, ...

**Examples**

```
# no examples
```

---

|         |                                                     |
|---------|-----------------------------------------------------|
| viterbi | <i>Viterbi algorithm for state decoding in HMMs</i> |
|---------|-----------------------------------------------------|

---

**Description**

The Viterbi algorithm decodes the most probable state sequence of an HMM.

**Usage**

```
viterbi(delta, Gamma, allprobs, trackID = NULL, mod = NULL, tod = NULL)
```

**Arguments**

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial distribution; either <ul style="list-style-type: none"> <li>• a vector of length nStates,</li> <li>• a matrix of dimension c(nTracks, nStates) if trackID is provided, or</li> <li>• a model object as for mod, so that mod can be passed as the first argument</li> </ul>                                                                                                                                                                    |
| Gamma    | transition probability matrix; either <ul style="list-style-type: none"> <li>• a matrix of dimension c(nStates, nStates),</li> <li>• an array of dimension c(nStates, nStates, nTracks) if trackID is provided,</li> <li>• an array of dimension c(nStates, nStates, nObs) for time-varying transition probabilities, or</li> <li>• an array of dimension c(nStates, nStates, L) for periodic transition probabilities, if tod is provided</li> </ul> |
| allprobs | matrix of state-dependent probabilities or density values of dimension c(nObs, nStates)                                                                                                                                                                                                                                                                                                                                                               |

|         |                                                                                                                                                                                                                                                                                                                                                                          |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| trackID | optional vector of length nObs containing nTracks unique IDs that separate tracks. The observations of each track need to be consecutive.                                                                                                                                                                                                                                |
| mod     | optional model object containing delta, Gamma, allprobs, and optionally trackID. When using RTMB: :MakeADFun or <a href="#">qrem1</a> with <a href="#">forward</a> in the likelihood, these are reported automatically after model fitting and the object returned by <code>obj\$report()</code> , <a href="#">lama</a> or <a href="#">qrem1</a> can be passed directly. |
| tod     | optional integer vector of length nObs with values in 1, ..., L, indexing the slices of Gamma for periodic models                                                                                                                                                                                                                                                        |

**Value**

vector of decoded states of length nObs

**See Also**

Other decoding functions: [stateprobs\(\)](#), [stateprobs\\_g\(\)](#), [stateprobs\\_p\(\)](#), [viterbi\\_g\(\)](#), [viterbi\\_p\(\)](#)

**Examples**

```
delta = c(0.5, 0.5)
Gamma = matrix(c(0.9, 0.1, 0.2, 0.8), nrow = 2, byrow = TRUE)
allprobs = matrix(runif(200), nrow = 100, ncol = 2)
states = viterbi(delta, Gamma, allprobs)
```

viterbi\_g

*Viterbi algorithm for state decoding in inhomogeneous HMMs***Description**

The Viterbi algorithm decodes the most probable state sequence of an HMM.

**Usage**

```
viterbi_g(delta, Gamma, allprobs, trackID = NULL, mod = NULL)
```

**Arguments**

|          |                                                                                                                                                                                                                                                                              |
|----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial distribution; either <ul style="list-style-type: none"> <li>• a vector of length nStates, or</li> <li>• a matrix of dimension c(nTracks, nStates) if trackID is provided</li> </ul>                                                                                  |
| Gamma    | array of transition probability matrices of dimension c(nStates, nStates, nObs), where the first slice of each track is ignored as there is no transition into the start of a track. For a single track, an array of dimension c(nStates, nStates, nObs-1) is also accepted. |
| allprobs | matrix of state-dependent probabilities or density values of dimension c(nObs, nStates)                                                                                                                                                                                      |

|         |                                                                                                                                                                                                                                                                                             |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| trackID | optional vector of length nObs containing nTracks unique IDs that separate tracks. The observations of each track need to be consecutive.                                                                                                                                                   |
| mod     | optional model object containing delta, Gamma, allprobs, and optionally trackID. When using RTMB::MakeADFun or qrem1 with forward_g in the likelihood, these are reported automatically after model fitting and the object returned by obj\$report(), lama or qrem1 can be passed directly. |

### Details

**Deprecated:** please use [viterbi](#) for all model types instead.

### Value

vector of decoded states of length nObs

### See Also

Other decoding functions: [stateprobs\(\)](#), [stateprobs\\_g\(\)](#), [stateprobs\\_p\(\)](#), [viterbi\(\)](#), [viterbi\\_p\(\)](#)

### Examples

```
delta = c(0.5, 0.5)
Gamma = tpm_g(runif(10), matrix(c(-2,-2,1,-1), nrow = 2))
allprobs = matrix(runif(20), nrow = 10, ncol = 2)
states = viterbi_g(delta, Gamma[,,-1], allprobs)
```

---

|           |                                                                                |
|-----------|--------------------------------------------------------------------------------|
| viterbi_p | <i>Viterbi algorithm for state decoding in periodically inhomogeneous HMMs</i> |
|-----------|--------------------------------------------------------------------------------|

---

### Description

The Viterbi algorithm allows one to decode the most probable state sequence of an HMM.

### Usage

```
viterbi_p(delta, Gamma, allprobs, tod, trackID = NULL, mod = NULL)
```

### Arguments

|          |                                                                                                                                                                                                   |
|----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| delta    | initial distribution of length N, or matrix of dimension c(k,N) for k independent tracks, if trackID is provided<br>This could e.g. be the periodically stationary distribution (for each track). |
| Gamma    | array of transition probability matrices for each time point in the cycle of dimension c(N,N,L), where L is the length of the cycle                                                               |
| allprobs | matrix of state-dependent probabilities/ density values of dimension c(n, N)                                                                                                                      |

|         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| tod     | (Integer valued) variable for cycle indexing in 1, ..., L, mapping the data index to a generalised time of day (length n)<br>For half-hourly data L = 48. It could, however, also be day of year for daily data and L = 365.                                                                                                                                                                                                                                                                                                                                                                                     |
| trackID | optional vector of k track IDs, if multiple tracks need to be decoded separately. The observations of each track need to be consecutive.                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| mod     | optional model object containing initial distribution delta, transition probability matrix Gamma, matrix of state-dependent probabilities allprobs, and potentially a trackID variable<br><br>If you are using automatic differentiation either with RTMB: :MakeADFun or <a href="#">qrem1</a> and include <a href="#">forward_p</a> in your likelihood function, the objects needed for state decoding are automatically reported after model fitting. Hence, you can pass the model object obtained from <code>obj\$report()</code> , <a href="#">lama</a> or <a href="#">qrem1</a> directly to this function. |

### Details

**Deprecated:** please use [viterbi](#) with argument tod instead.

### Value

vector of decoded states of length n

### See Also

Other decoding functions: [stateprobs\(\)](#), [stateprobs\\_g\(\)](#), [stateprobs\\_p\(\)](#), [viterbi\(\)](#), [viterbi\\_g\(\)](#)

### Examples

```
delta = c(0.5, 0.5)
beta = matrix(c(-2, 1, -1,
                -2, -1, 1), nrow = 2, byrow = TRUE)
Gamma = tpm_p(1:24, 24, beta)

tod = rep(1:24, 5)
n = length(tod)

allprobs = matrix(runif(2*n), nrow = n, ncol = 2)
states = viterbi_p(delta, Gamma, allprobs, tod)
```

### Description

Density, distribution function and random generation for the von Mises distribution.

**Usage**

```
dvm(x, mu = 0, kappa = 1, log = FALSE)

pvm(q, mu = 0, kappa = 1, from = NULL, tol = 1e-20)

rvm(n, mu = 0, kappa = 1, wrap = TRUE)
```

**Arguments**

|       |                                                                                                    |
|-------|----------------------------------------------------------------------------------------------------|
| x, q  | vector of angles measured in radians at which to evaluate the density function.                    |
| mu    | mean direction of the distribution measured in radians.                                            |
| kappa | non-negative numeric value for the concentration parameter of the distribution.                    |
| log   | logical; if TRUE, densities are returned on the log scale.                                         |
| from  | value from which the integration for CDF starts. If NULL, is set to $\mu - \pi$ .                  |
| tol   | the precision in evaluating the distribution function                                              |
| n     | number of observations. If $\text{length}(n) > 1$ , the length is taken to be the number required. |
| wrap  | logical; if TRUE, generated angles are wrapped to the interval $[-\pi, \pi]$ .                     |

**Details**

This implementation of `dvm` allows for automatic differentiation with RTMB. `rvm` and `pvm` are simply wrappers of the corresponding functions from `circular`.

**Value**

`dvm` gives the density, `pvm` gives the distribution function, and `rvm` generates random deviates.

**Examples**

```
set.seed(1)
x = rvm(10, 0, 1)
d = dvm(x, 0, 1)
p = pvm(x, 0, 1)
```

---

wrpcauchy

*Wrapped Cauchy distribution*


---

**Description**

Density and random generation for the wrapped Cauchy distribution.

**Usage**

```
dwrpcauchy(x, mu = 0, rho, log = FALSE)

rwrpcauchy(n, mu = 0, rho, wrap = TRUE)
```

**Arguments**

|      |                                                                                                           |
|------|-----------------------------------------------------------------------------------------------------------|
| x    | vector of angles measured in radians at which to evaluate the density function.                           |
| mu   | mean direction of the distribution measured in radians.                                                   |
| rho  | concentration parameter of the distribution, must be in the interval from 0 to 1.                         |
| log  | logical; if TRUE, densities are returned on the log scale.                                                |
| n    | number of observations. If <code>length(n) &gt; 1</code> , the length is taken to be the number required. |
| wrap | logical; if TRUE, generated angles are wrapped to the interval $[-\pi, \pi]$ .                            |

**Details**

This implementation of `dwrpcauchy` allows for automatic differentiation with RTMB. `rwrpcauchy` is simply a wrapper for `rwrappedcauchy` imported from `circular`.

**Value**

`dwrpcauchy` gives the density and `rwrpcauchy` generates random deviates.

**Examples**

```
set.seed(1)
x = rwrpcauchy(10, 0, 0.3)
d = dwrpcauchy(x, 0, 0.3)
```

---

|              |                                          |
|--------------|------------------------------------------|
| zero_inflate | <i>Zero-inflated density constructor</i> |
|--------------|------------------------------------------|

---

**Description**

Constructs a zero-inflated density function from a given probability density function

**Usage**

```
zero_inflate(dist, discrete = NULL)
```

**Arguments**

|          |                                                                                                                                                                                                                                                                                                                                 |
|----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dist     | either a probability density function or a probability mass function                                                                                                                                                                                                                                                            |
| discrete | logical; if TRUE, the density for $x = 0$ will be <code>zeroprob + (1-zeroprob) * dist(0, ...)</code> . Otherwise it will just be <code>zeroprob</code> . In standard cases, this will be determined automatically. For non-standard cases, set this to TRUE or FALSE depending on the type of <code>dist</code> . See details. |

### Details

The definition of zero-inflation is different for discrete and continuous distributions. For discrete distributions with p.m.f.  $f$  and zero-inflation probability  $p$ , we have

$$\Pr(X = 0) = p + (1 - p) \cdot f(0),$$

and

$$\Pr(X = x) = (1 - p) \cdot f(x), \quad x > 0.$$

For continuous distributions with p.d.f.  $f$ , we have

$$f_{\text{zinfl}}(x) = p \cdot \delta_0(x) + (1 - p) \cdot f(x),$$

where  $\delta_0$  is the Dirac delta function at zero.

### Value

zero-inflated density function with first argument  $x$ , second argument `zeroprob`, and additional arguments ... that will be passed to `dist`.

### Examples

```
dzinorm <- zero_inflate(dnorm)
dzinorm(c(NA, 0, 2), 0.5, mean = 1, sd = 1)

zipois <- zero_inflate(dpois)
zipois(c(NA, 0, 1), 0.5, 1)
```

---

%sp%

*Sparsity-retaining matrix multiplication*

---

### Description

Standard matrix multiplication destroys automatic sparsity detection by RTMB which is essential for models with high-dimensional random effects. This can be mitigated by changing to "plain" with `TapeConfig`, but this can make AD tape construction very slow. Here, we provide a different version that retains sparsity. It may be slightly slower than the standard method when constructing the AD tape.

### Usage

```
A %sp% B
```

### Arguments

|   |                                  |
|---|----------------------------------|
| A | matrix of dimension $n \times p$ |
| B | matrix of dimension $p \times m$ |

**Value**

the matrix product of A and B, which is of dimension n x m

**Examples**

```
A <- matrix(1:6, nrow = 2, ncol = 3)
B <- matrix(7:12, nrow = 3, ncol = 2)
A %sp% B
```

# Index

- \* **datasets**
  - nessi, [40](#)
  - trex, [105](#)
- \* **decoding functions**
  - stateprobs, [78](#)
  - stateprobs\_g, [79](#)
  - stateprobs\_p, [81](#)
  - viterbi, [106](#)
  - viterbi\_g, [107](#)
  - viterbi\_p, [108](#)
- \* **forward algorithms**
  - forward, [8](#)
  - forward\_g, [10](#)
  - forward\_hsmm, [13](#)
  - forward\_ihsmm, [14](#)
  - forward\_p, [17](#)
  - forward\_phsmm, [19](#)
- \* **stationary distribution functions**
  - stationary, [82](#)
  - stationary\_ct, [83](#)
  - stationary\_p, [84](#)
- \* **transition probability matrix functions**
  - generator, [25](#)
  - generator\_g, [27](#)
  - tpm, [88](#)
  - tpm\_ct, [90](#)
  - tpm\_emb, [91](#)
  - tpm\_emb\_g, [92](#)
  - tpm\_g, [93](#)
  - tpm\_g2, [95](#)
  - tpm\_p, [99](#)
- %sp%, [112](#)
- calc\_trackInd, [4](#)
- cosinor, [4](#), [6](#)
- ddwell, [5](#)
- dgamma2, [76](#)
- dgamma2 (gamma2), [24](#)
- dgmrf2, [6](#)
- dskewnorm (skewnorm), [73](#)
- dvm, [76](#)
- dvm (vm), [109](#)
- dwrpcauchy (wrpcauchy), [110](#)
- forward, [8](#), [11](#), [12](#), [14](#), [16](#), [18](#), [20](#), [28](#), [55](#), [56](#),  
[67](#), [71](#), [72](#), [76–78](#), [84](#), [107](#)
- forward\_g, [10](#), [10](#), [14](#), [16](#), [18](#), [20](#), [80](#), [108](#)
- forward\_hsmm, [10](#), [12](#), [13](#), [16](#), [18](#), [20](#)
- forward\_ihsmm, [10](#), [12](#), [14](#), [14](#), [18–20](#)
- forward\_p, [10](#), [12](#), [14](#), [16](#), [17](#), [20](#), [81](#), [109](#)
- forward\_phsmm, [10](#), [12](#), [14](#), [16](#), [18](#), [19](#)
- forward\_s, [21](#)
- forward\_sp, [22](#)
- gamma2, [24](#)
- gdeterminant, [25](#)
- generator, [25](#), [27](#), [83](#), [89](#), [91–94](#), [96](#), [100](#)
- generator\_g, [26](#), [27](#), [89](#), [91–94](#), [96](#), [100](#)
- initial.sp, [36](#)
- lama, [9](#), [28](#), [32](#), [37](#), [46](#), [52](#), [55](#), [56](#), [61](#), [67](#), [71](#),  
[78](#), [80](#), [81](#), [87](#), [107–109](#)
- LaMaColors, [29](#), [47](#)
- logLik.LaMaModel, [30](#)
- make\_matrices (modmat), [35](#)
- make\_matrices\_dens, [31](#), [75](#)
- MakeADFun, [32](#), [33](#), [67](#)
- max0\_smooth (minmax0\_smooth), [35](#)
- max2 (minmax), [34](#)
- MCreport, [28](#), [32](#)
- min0\_smooth (minmax0\_smooth), [35](#)
- min2 (minmax), [34](#)
- minmax, [34](#)
- minmax0\_smooth, [35](#)
- modmat, [35](#), [49–51](#), [53](#), [66](#)
- multistart, [37](#)
- nessi, [40](#)

- nlminb, 38
- optim, 38, 59, 64
- optimHess, 60
- penalty, 36, 40, 43, 58, 61–63, 65, 66
- penalty2, 36, 42, 58, 61, 65, 66
- penalty\_uni, 45
- pgamma2 (gamma2), 24
- plot.LaMaModel, 46
- plot.LaMaResiduals, 46, 47, 56
- pred\_matrix, 51
- predict, 51, 52, 76
- predict.LaMa\_matrices, 37, 49
- predict.smoothdens, 50
- print.LaMa\_matrices, 52
- print.LaMaModel, 52
- print.summary.LaMaModel  
(summary.LaMaModel), 87
- print.summary.qrem1Model  
(summary.qrem1Model), 88
- process\_hid\_formulas, 53
- pseudo\_res, 9, 11, 18, 46–48, 54
- pskewnorm (skewnorm), 73
- pvm (vm), 109
- qgamma2 (gamma2), 24
- qrem1, 32, 40, 41, 43, 44, 46, 52, 55, 56, 57,  
62, 67, 68, 70, 71, 78, 80, 81, 87, 88,  
107–109
- qrem1\_old, 61, 62
- qskewnorm (skewnorm), 73
- rep\_sp, 36, 66
- report (lama), 28
- rgamma2 (gamma2), 24
- rskewnorm (skewnorm), 73
- rvm (vm), 109
- rwrpcauchy (wrpcauchy), 110
- scores, 28, 67
- sdreport, 32, 33
- sdreport\_outer, 60, 61, 70
- sdreportMC, 68
- simulate.LaMaModel, 71, 77
- skewnorm, 73
- smoothdens, 50, 74
- statedens, 46, 71, 72, 76
- stateprobs, 9, 47, 54, 55, 78, 80, 82, 107–109
- stateprobs\_g, 11, 79, 79, 82, 107–109
- stateprobs\_p, 18, 79, 80, 81, 107–109
- stationary, 82, 83, 85, 86
- stationary\_cont (stationary\_ct), 83
- stationary\_ct, 83, 83, 85
- stationary\_p, 9, 81, 83, 84, 85
- stationary\_p\_sparse, 85
- stationary\_sparse, 86
- summary(), 28
- summary.LaMaModel, 87, 88
- summary.qrem1Model, 61, 88
- tpm, 26, 27, 83, 88, 91–94, 96, 100
- tpm\_cont (tpm\_ct), 90
- tpm\_ct, 26, 27, 87, 89, 90, 92–94, 96, 100
- tpm\_emb, 13, 15, 20, 26, 27, 89, 91, 91, 93, 94,  
96, 98, 100, 101
- tpm\_emb\_g, 15, 20, 26, 27, 89, 91, 92, 92, 94,  
96, 98, 100, 101
- tpm\_g, 26, 27, 85, 89, 91–93, 93, 96, 100
- tpm\_g2, 26, 27, 89, 91–94, 95, 100
- tpm\_hsmm, 96
- tpm\_hsmm2, 97
- tpm\_ihsmm, 98
- tpm\_p, 6, 26, 27, 85, 89, 91–94, 96, 99
- tpm\_phsmm, 101
- tpm\_phsmm2, 102
- tpm\_thinned, 104
- trex, 105
- trigBasisExp, 100, 105
- viterbi, 9, 47, 79, 80, 82, 106, 108, 109
- viterbi\_g, 11, 79, 80, 82, 107, 107, 109
- viterbi\_p, 18, 79, 80, 82, 107, 108, 108
- vm, 109
- wrpcauchy, 110
- zero\_inflate, 71, 77, 111