# Package 'LaMa'

### November 13, 2024

Type Package

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

Version 2.0.1

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 esti-

mated 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 in-

cluded that show how to simulate data from and estimate all the above model classes.

URL https://janoleko.github.io/LaMa/

**License** GPL-3 **Encoding** UTF-8

Imports Rcpp, mgcv, Matrix, stats, utils, MASS, mvtnorm, splines,

methods, CircStats, circular

LinkingTo Rcpp, RcppArmadillo

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

RoxygenNote 7.3.2

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

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# Description

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

### Usage

```
buildSmoothDens(data, type = "real", par, k = 20, degree = 3, diff_order = 2)
```

### **Arguments**

data	named data frame of different data streams
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. Needs to be a vector corresponding to the number of data streams in data.
par	nested named list of initial means and sds/concentrations for each data stream
k	number of basis functions for each data stream
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.

#### **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. buildSmoothDens 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.

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### Value

a nested list containing the design matrices Z, the penalty matrices S, the initial coefficients coef the prediction design matrices Z\_predict, the prediction grids xseq, and details for the basis expansion for each data stream.

### **Examples**

```
## 3 data streams, each with one distribution
# normal data with mean 0 and sd 1
x1 = rnorm(100, mean = 0, sd = 1)
# gamma data with mean 5 and sd 3
x2 = rgamma2(100, mean = 5, sd = 3)
# circular data
x3 = rvm(100, mu = 0, kappa = 2)
data = data.frame(x1 = x1, x2 = x2, x3 = x3)
par = list(x1 = list(mean = 0, sd = 1),
           x2 = list(mean = 5, sd = 3),
           x3 = list(mean = 0, concentration = 2))
SmoothDens = buildSmoothDens(data,
                             type = c("real", "positive", "circular"),
# extracting objects for x1
Z1 = SmoothDens$Z$x1
S1 = SmoothDens$S$x1
coefs1 = SmoothDens$coef$x1
## one data stream, but mixture of two distributions
# normal data with mean 0 and sd 1
x = rnorm(100, mean = 0, sd = 1)
data = data.frame(x = x)
# now parameters for mixture of two normals
par = list(x = list(mean = c(0, 5), sd = c(1,1)))
SmoothDens = buildSmoothDens(data, par = par)
# extracting objects
Z = SmoothDens$Z$x
S = SmoothDens$S$x
coefs = SmoothDens$coef$x
```

calc\_trackInd

Calculate the index of the first observation of each track based on an ID variable

dgmrf2 5

### **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)
```

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

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lambda precision scaling parameter

Can be a vector if x is a matrix. Then each row of x is evaluated with the corresponding lambda. This is benefitial 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

Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrockForward algorithm with homogeneous transition probability matrix

### **Description**

Calculates the log-likelihood of a sequence of observations under a homogeneous hidden Markov model using the **forward algorithm**.

### Usage

```
forward(delta, Gamma, allprobs, trackID = NULL, ad = NULL, report = TRUE)
```

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### **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(N,N), or array of k transition prob-

ability matrices of dimension c(N,N,k), if trackID is provided

allprobs matrix of state-dependent probabilities/ density values of dimension c(n, N)

trackID optional vector of length n containing IDs

If provided, the total log-likelihood will be the sum of each track's likelihood contribution. In this case, Gamma can be a matrix, leading to the same transition probabilities for each track, or an array of dimension c(N,N,k), with one (homogeneous) 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(k,N), 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 and allprobs should be reported from

the fitted model. Defaults to TRUE, but only works if ad = TRUE.

#### Value

log-likelihood for given data and parameters

#### See Also

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

```
## 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])
```

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forward\_g

General Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hiddenmarkov-models-time-series-walter-zucchini-iain-macdonald-rolandlangrockforward 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**.

### Usage

```
forward_g(delta, Gamma, allprobs, trackID = NULL, ad = NULL, report = TRUE)
```

#### **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(N,N,n-1), as in a time series of length n, there are only n-1 transitions.

If an array of dimension c(N,N,n) for a single track is provided, the first slice will be ignored.

If the elements of  $\Gamma^{(t)}$  depend on covariate values at t or covariates t+1 is your choice in the calculation of the array, prior to using this function. When conducting the calculation by using tpm\_g(), the choice comes down to including the covariate matrix Z[-1,] oder Z[-n,].

If trackInd is provided, Gamma needs to be an array of dimension c(N,N,n), matching the number of rows of all probs. For each track, the transition matrix at the beginning will be ignored. If the parameters for Gamma are pooled across tracks or not, depends on your calculation of Gamma. If pooled, you can use tpm\_g(Z, beta) to calculate the entire array of transition matrices when Z is of dimension c(n,p).

This function can also be used to fit continuous-time HMMs, where each array entry is the Markov semigroup  $\Gamma(\Delta t) = \exp(Q\Delta t)$  and Q is the generator of the continuous-time Markov chain.

trackID

matrix of state-dependent probabilities/ density values of dimension c(n, N) optional vector of length n containing IDs

If provided, the total log-likelihood will be the sum of each track's likelihood contribution. In this case, Gamma needs to be an array of dimension c(N,N,n), 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). Furthermore, instead of a single vector delta corresponding to the initial distribution, a delta matrix of initial distributions, of dimension c(k,N), can be provided, such that each track starts with it's own initial distribution.

allprobs

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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 and allprobs should be reported from

the fitted model. Defaults to TRUE, but only works if ad = TRUE.

#### Value

log-likelihood for given data and parameters

### See Also

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

### **Examples**

```
## 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
                         # initial tpm intercepts (logit-scale)
par = c(-2, -2,
        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$step[1:500], Z = trigBasisExp(trex$tod[1:500]))
```

forward\_hsmm

Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrockForward algorithm for homogeneous hidden semi-Markov models

# Description

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

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### Usage

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

#### Arguments

dm list of length N 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 probablity mass not covered

by these.

omega matrix of dimension c(N,N) of conditional transition probabilities, also called

embedded transition probability matrix.

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 tpm\_emb.

allprobs matrix of state-dependent probabilities/ density values of dimension c(n, N)

which will automatically be converted to the appropriate dimension.

trackID optional vector of length n containing IDs

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(N,N,k) 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(k,N), can be

provided, such that each track starts with it's own initial distribution.

delta optional vector of initial state probabilities of length N

By default, the stationary distribution is computed (which is typically recom-

mended).

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 prob-

ability 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

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maximum likelhood 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

log-likelihood for given data and parameters

### See Also

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

# Examples

```
# currently no examples
```

forward\_ihsmm

Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrockForward algorithm for hidden semi-Markov models with inhomogeneous state durations and/ or conditional transition probabilities

# 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
)
```

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#### **Arguments**

dm

list of length N 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 probablity mass not covered by these.

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 correponds to the size of the approximating state aggregates.

In the latter case, the first max(sapply(dm, ncol)) - 1 observations will not be used because the first approximating transition probability matrix needs to be computed based on the first max(sapply(dm, ncol)) covariate values (represented by dm).

omega

matrix of dimension c(N,N) or array of dimension c(N,N,n) of conditional transition probabilites, also called embedded transition probability matrix.

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 tpm\_emb and an array using tpm\_emb\_g.

allprobs

matrix of state-dependent probabilities/ density values of dimension c(n, N)

trackID

trackID optional vector of length n containing IDs

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(k,N), can be provided, such that each track starts with it's own initial distribution.

delta

optional vector of initial state probabilities of length N

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.

startInd

optional integer index at which the forward algorithm starts.

When approximating inhomogeneous HSMMs by inhomogeneous HMMs, the first transition probability matrix that can be constructed is at time max(sapply(dm, ncol)) (as it depends on the previous covariate values). Hence, when not provided, startInd is chosen to be max(sapply(dm, ncol)). Fixing startInd at a value larger than max(aggregate sizes) 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.

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.

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### **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 likelhood 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

log-likelihood for given data and parameters

### See Also

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

### **Examples**

```
# currently no examples
```

forward\_p

Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrockForward 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
)
```

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### Arguments

Gamma array of transition probability matrices of dimension $c(N,N,L)$ .	
Here we use the definition $\Pr(S_t = j \mid S_{t-1} = i) = \gamma_{ij}^{(t)}$ such that the transiti probabilities between time point $t-1$ and $t$ are an element of $\Gamma^{(t)}$ .	on
all probs $\mbox{matrix of state-dependent probabilities/ density values of dimension } c(n, N)$	
tod (Integer valued) variable for cycle indexing in 1,, L, mapping the data ind to a generalised time of day (length n)	ex
For half-hourly data $L = 48$ . It could, however, also be day of year for daily data $L = 365$ .	ıta
trackID optional vector of length n containing IDs	
If provided, the total log-likelihood will be the sum of each track's likeliho contribution. Instead of a single vector delta corresponding to the initial d tribution, a delta matrix of initial distributions of dimension c(k,N), can provided, such that each track starts with it's own initial distribution.	is-
ad optional logical, indicating whether automatic differentiation with RTMB show	ld

be used. By default, the function determines this itself.

logical, indicating whether delta, Gamma and allprobs should be reported from

#### **Details**

report

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  $(1, \ldots, L)$  time variable that maps the data index to the according time.

the fitted model. Defaults to TRUE, but only works if ad = TRUE.

#### Value

log-likelihood for given data and parameters

### See Also

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

```
## 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]) # stationary HMM
```

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```
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

Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrockForward 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 likelhood 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 <code>forward\_ihsmm</code> 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,
```

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```
delta = NULL,
  eps = 1e-10,
  report = TRUE
)
```

### Arguments

dm

list of length N 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 probablity mass not covered by these.

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 correpond to the size of the approximating state aggregates.

omega

matrix of dimension c(N,N) or array of dimension c(N,N,L) of conditional transition probabilites, also called embedded transition probability matrix

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 tpm\_emb and an array using tpm\_emb\_g.

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 length n containing IDs 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(k,N), can be provided, such that each track starts with it's own initial distribution.

delta

Optional vector of initial state probabilities of length N. 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 allprobs 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**.

forward\_s 17

### Value

log-likelihood for given data and parameters

# See Also

Other forward algorithms: forward(), forward\_g(), forward\_hsmm(), forward\_ihsmm(), forward\_p()

# Examples

# currently no examples

forward	Physilitans //www.touloufususis com/hocks/wows/10 1201/h20700/hiddon
forward_s	Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-
	markov-models-time-series-walter-zucchini-iain-macdonald-roland-
	langrockForward algorithm for hidden semi-Markov models with
	homogeneous transition probability matrix

# 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

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### **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

Rhrefhttps://www.taylorfrancis.com/books/mono/10.1201/b20790/hidden-markov-models-time-series-walter-zucchini-iain-macdonald-roland-langrockForward 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

forward\_sp 19

matrix for each time point in a period, and an integer valued  $(1, \ldots, L)$  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).
	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,, 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

```
## 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, trigBasisExp(1:24, 24, 1))%*%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){
```

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```
# 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, trigBasisExp(1:24, 24, 1))%*%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
 mean
 mean parameter, must be positive scalar.
 sd
 standard deviation parameter, must be positive scalar.

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log, log.p	logical; if TRUE, probabilities/ densities $p$ are returned as $\log(p)$ .
lower.tail	logical; if TRUE, probabilities are $P[X \le x]$ , otherwise, $P[X > x]$ .
р	vector of probabilities
n	number of observations. If $length(n) > 1$ , 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)
```

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(param, byrow = FALSE, report = TRUE)
```

# Arguments

param	unconstrained parameter vector of length $N*(N-1)$ where N is the number of states of the Markov chain
byrow	logical indicating if the transition probability 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.

### Value

infinitesimal generator matrix of dimension c(N,N)

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### See Also

```
Other transition probability matrix functions: tpm(), tpm_cont(), tpm_emb(), tpm_emb_g(), tpm_g(), 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))
```

make\_matrices

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

# Description

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

# Usage

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

### **Arguments**

formula right side of a formula as used in mgcv

data frame containing the variables in the formula

knots optional list containing user specified knot values to be used for basis construc-

tion

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.

### Value

a list containing the design matrix Z, the penalty matrix S, the formula, the data and the knots

```
modmat = make_matrices(~s(x), data.frame(x = 1:10))
```

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# 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,
    npoints = 10000,
    diff_order = 2,
    pow = 0.5
)
```

### **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
npoints	number of points used in the numerical integration for normalizing the B-spline basis functions
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
	Such non-equidistant knot spacing is only used for type = "positive".

# Value

list containing the design matrix Z, the penalty matrix S, the prediction design matrix Z\_predict, the prediction grid xseq, and details for the basis expansion.

```
\label{eq:modmat} modmat = make\_matrices\_dens(x = (-50):50, k = 20) \\ modmat = make\_matrices\_dens(x = 1:100, k = 20, type = "positive") \\ modmat = make\_matrices\_dens(x = seq(-pi,pi), k = 20, type = "circular") \\
```

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nessi

Loch Ness Monster Acceleration Data

### **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

Computes penalty based on quadratic form

### **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 qreml function. For qreml to work, the likelihood function needs to be compatible with the RTMB R package to enable automatic differentiation.

### Usage

penalty(re\_coef, S, lambda)

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### **Arguments**

re\_coef coefficient vector/ matrix or list of coefficient vectors/ matrices

> 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

lambda penalty strength parameter vector that has a length corresponding to the total

**number** of random effects/ spline coefficients in re\_coef

E.g. if re\_coef contains one vector and one matrix with 4 rows, then lambda

needs to be of length 5.

#### **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 seperate 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 greml.

# Value

returns the penalty value and reports to greml.

### See Also

```
qreml for the qREML algorithm
```

```
# Example with a single random effect
re = rep(0, 5)
S = diag(5)
lambda = 1
penalty(re, S, lambda)
# 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))
lambda = c(1,1,2) # length = total number of random effects
penalty(re, S, lambda)
# Full model-fitting example
data = trex[1:1000,] # subset
```

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```
# initial parameter list
par = list(logmu = log(c(0.3, 1)), # step mean
          logsigma = log(c(0.2, 0.7)), # 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 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 = make_matrices(~ 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 = 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, ad = TRUE) +
      penalty(betaspline, S, lambda) # this does all the penalization work
}
# model fitting
mod = qreml(pnll, par, dat, random = "betaspline")
```

pred\_matrix

Build the prediction design matrix based on new data and model\_matrices object created by make\_matrices

#### **Description**

Build the prediction design matrix based on new data and model\_matrices object created by make\_matrices

### Usage

```
pred_matrix(model_matrices, newdata)
```

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### **Arguments**

model\_matrices model\_matrices object as returned from make\_matrices

newdata

data frame containing the variables in the formula and new data for which to evaluate the basis

### Value

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

### **Examples**

```
modmat = make_matrices(\sim s(x), data.frame(x = 1:10))
Z_predict = pred_matrix(modmat, data.frame(x = 1:10 - 0.5))
```

pseudo\_res

Calculate pseudo-residuals

### **Description**

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

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

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

This function calculates such residuals via probability integral transform, based on the local state probabilities obtained by stateprobs or stateprobs\_g and the respective parametric family.

### Usage

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

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#### **Arguments**

obs vector of continuous-valued observations (of length n)

dist character string specifying which parametric CDF to use (e.g., "norm" for nor-

mal or "pois" for Poisson)

par named parameter list for the parametric CDF

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(n,N),

where N is the number of states) as computed by stateprobs, stateprobs\_g

or stateprobs\_p

mod optional model object containing initial distribution delta, transition probabil-

ity matrix Gamma, matrix of state-dependent probabilities allprobs, and poten-

tially a trackID variable

If you are using automatic differentiation either with RTMB::MakeADFun or qreml and include forward, forward\_g or forward\_p 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 running RTMB::report() or from qreml directly to this function and avoid calculating local state proabilities manually. In this case, a call should look like pseudo\_res(obs, "norm",

par, mod = mod).

normal logical, if TRUE, returns Gaussian pseudo residuals

These will be approximately standard normally distributed if the model is cor-

rect.

discrete logical, if TRUE, computes discrete pseudo residuals (which slightly differ in

their definition)

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. See pseudo\_res\_discrete for details.

randomise for discrete pseudo residuals only. Logical, if TRUE, return randomised pseudo

residuals. Recommended for discrete observations.

seed for discrete pseudo residuals only. Integer, seed for random number generation

### Details

When used for discrete pseudo-residuals, this function is just a wrapper for pseudo\_res\_discrete.

#### Value

vector of pseudo residuals

pseudo\_res\_discrete 29

### **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)
stateprobs = matrix(0.5, nrow = 100, ncol = 2)
par = list(lambda = c(1,2))
pres = pseudo_res(obs, "pois", par, stateprobs)
```

pseudo\_res\_discrete

Calculate pseudo-residuals for discrete-valued observations

### **Description**

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

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

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

This function calculates such residuals for **discrete-valued** observations, based on the local state probabilities obtained by **stateprobs** or **stateprobs**\_g and the respective parametric family.

### Usage

```
pseudo_res_discrete(
  obs,
  dist,
  par,
  stateprobs,
  normal = TRUE,
  randomise = TRUE,
  seed = NULL
)
```

#### **Arguments**

obs vector of discrete-valued observations (of length n)

dist character string specifying which parametric CDF to use (e.g., "norm" for normal or "pois" for Poisson)

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par named parameter list for the parametric CDF

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(n,N),

where N is the number of states)

normal logical, if TRUE, returns Gaussian pseudo residuals

These will be approximately standard normally distributed if the model is cor-

rect.

randomise logical, if TRUE, return randomised pseudo residuals. Recommended for discrete

observations.

seed integer, seed for random number generation

#### **Details**

For discrete observations, calculating pseudo residuals is slightly more involved, as the CDF is a step function. Therefore, one can calculate the lower and upper CDF values for each observation. By default, this function does exactly that and then randomly samples the interval in between to give approximately Gaussian psuedo-residuals. If randomise is set to FALSE, the lower, upper and mean pseudo-residuals are returned.

#### Value

vector of pseudo residuals

### **Examples**

```
obs = rpois(100, lambda = 1)
stateprobs = matrix(0.5, nrow = 100, ncol = 2)
par = list(lambda = c(1,2))
pres = pseudo_res_discrete(obs, "pois", par, stateprobs)
```

greml

Quasi restricted maximum likelihood (qREML) algorithm for models with penalised splines or simple i.i.d. random effects

# 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  $S_i$ .

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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.

Under the hood, qreml 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(
  pnll,
  par,
  dat,
  random,
  psname = "lambda",
  alpha = 0,
  smoothing = 1,
  maxiter = 100,
  tol = 1e-04,
  control = list(reltol = 1e-10, maxit = 1000),
  silent = 1,
  joint_unc = TRUE,
  saveall = FALSE
)
```

### Arguments

pnll	penalised negative log-likelihood function that is structured as dictated by RTMB
nnıı	nenglised negative log-likelingod tilnetion that is striletilted as dictated by RTMR
DIIII	behalised hegalive log-inclinioud function that is structured as dictated by Nirib

and uses the penalty function from LaMa to compute the penalty

Needs to be a function of the named list of initial parameters par only.

par named list of initial parameters

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.

dat initial data list that contains the data used in the likelihood function, hyperpa-

rameters, and the initial penalty strength vector

If the initial penalty strength vector is **not** called lambda, the name it has in dat needs to be specified using the penalty argument below. Its length needs to

match the to the total number of random effects.

random vector of names of the random effects/ penalised parameters in par

Caution: The ordering of random needs to match the order of the random effects

passed to penalty inside the likelihood function.

psname optional name given to the penalty strength parameter in dat. Defaults to "lambda".

alpha optional hyperparamater for exponential smoothing of the penalty strengths

For larger values smoother convergence is to be expected but the algorithm may

need more iterations.

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smoothing	optional scaling factor for the final penalty strength parameters
	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.
maxiter	maximum number of iterations in the outer optimisation over the penalty strength parameters.
tol	Convergence tolerance for the penalty strength parameters.
control	list of control parameters for optim to use in the inner optimisation. Here, optim uses the BFGS method which cannot be changed.
	We advise against changing the default values of reltol and maxit as this can decrease the accuracy of the Laplace approximation.
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.
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

returns a model list influenced by the users report statements in pnll

### See Also

penalty to compute the penalty inside the likelihood function

```
data = trex[1:1000,] # subset
# initial parameter list
par = list(logmu = log(c(0.3, 1)), # step mean
           logsigma = log(c(0.2, 0.7)), # 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 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 = make_matrices(~ 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
```

sdreportMC 33

```
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 = 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, ad = TRUE) +
        penalty(betaspline, S, lambda) # this does all the penalization work
}
# model fitting
mod = qreml(pnll, par, dat, random = "betaspline")
```

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,
   Hessian = NULL,
   CI = FALSE,
   n = 1000,
   probs = c(0.025, 0.975)
)
```

# Arguments

obj	object returned by MakeADFun() after optimisation
what	vector of strings with names of parameters and REPORT()ed quantities to be reported $% \left( 1\right) =\left( 1\right) \left( 1$
Hessian	optional Hessian matrix. If not provided, it will be computed from the object
CI	logical. If TRUE, only confidence intervals instead of samples will be returned
n	number of samples to draw from the multivariate normal distribution of the MLE
probs	vector of probabilities for the confidence intervals (ignored if no CIs are computed)

34 sdreportMC

#### **Details**

**Caution:** Currently does not work for models with fixed parameters (i.e. that use the map argument of MakeADFun.)

#### 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.

```
# 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)
                               # initial t.p.m. parameters (on logit scale)
 eta = rep(-2, 2)
)
## data and hyperparameters
dat = list(
                            # hourly step lengths
 step = trex$step[1:500],
 angle = trex$angle[1:500], # hourly turning angles
 N = 2
)
## creating AD function
obj = MakeADFun(nll, par, silent = TRUE) # creating the objective function
```

stateprobs 35

stateprobs

Calculate conditional local state probabilities for homogeneous HMMs

#### **Description**

Computes

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

for homogeneous HMMs

### Usage

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

### **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(N,N), or array of k transition prob-

ability matrices of dimension c(N,N,k), if trackID is provided

allprobs matrix of state-dependent probabilities/ density values of dimension c(n, N)

trackID optional vector of length n containing IDs

If provided, the total log-likelihood will be the sum of each track's likelihood contribution. In this case, Gamma can be a matrix, leading to the same transition probabilities for each track, or an array of dimension c(N,N,k), with one (homogeneous) 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(k,N), can be provided, such that each track

starts with it's own initial distribution.

optional model object containing initial distribution delta, transition probability matrix Gamma, matrix of state-dependent probabilities allprobs, and poten-

tially a trackID variable

If you are using automatic differentiation either with RTMB::MakeADFun or qreml and include forward 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 running RTMB::report() or from qreml directly to this function.

mod

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### Value

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

### 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(200), nrow = 100, ncol = 2)
probs = stateprobs(delta, Gamma, allprobs)
```

 $stateprobs_g$ 

Calculate conditional local state probabilities for inhomogeneous HMMs

# **Description**

Computes

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

for inhomogeneous HMMs

### Usage

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

### Arguments

trackID

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 $c(N,N,n-1)$ , as in a time series of length n, there are only n-1 transitions
	If an array of dimension $c(N,N,n)$ for a single track is provided, the first slice will be ignored.
	If trackID is provided, Gamma needs to be an array of dimension $c(N,N,n)$ , where n is the number of rows in allprobs. Then for each track the first transition matrix will be ignored.
allprobs	matrix of state-dependent probabilities/ density values of dimension c(n, N)

optional vector of k track IDs, if multiple tracks need to be decoded separately

stateprobs\_p 37

mod

optional model object containing initial distribution delta, transition probability matrix Gamma, matrix of state-dependent probabilities allprobs, and potentially a trackID variable

If you are using automatic differentiation either with RTMB::MakeADFun or qreml and include forward\_g 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 running RTMB::report() or from qreml directly to this function.

#### Value

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

## See Also

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

## **Examples**

```
Gamma = tpm_g(runif(99), matrix(c(-1,-1,1,-2), nrow = 2, byrow = TRUE)) delta = c(0.5, 0.5) allprobs = matrix(runif(200), nrow = 100, ncol = 2) probs = stateprobs_g(delta, Gamma, allprobs)
```

stateprobs\_p

Calculate conditional local state probabilities for periodically inhomogeneous HMMs

## Description

Computes

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

for periodically inhomogeneous HMMs

## Usage

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

# **Arguments**

delta initial or stationary distribution of length N, or matrix of dimension c(k,N) for k

independent tracks, if trackID is provided

This could e.g. be the periodically stationary distribution (for each track) as

computed by stationary\_p.

Gamma array of transition probability matrices for each time point in the cycle of dimen-

sion c(N,N,L), where L is the length of the cycle.

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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 mod optional vector of k track IDs, if multiple tracks need to be decoded separately optional model object containing initial distribution delta, transition probability matrix Gamma, matrix of state-dependent probabilities allprobs, and potentially a trackID variable

If you are using automatic differentiation either with RTMB::MakeADFun or qreml and include forward\_p 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 running RTMB::report() or from qreml directly to this function.

#### 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, 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)
```

stationary\_cont 39

## Arguments

Gamma

transition probability matrix of dimension c(N,N)

#### Value

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

## See Also

```
tpm to create a transition probability matrix using the multinomial logistic link (softmax)

Other stationary distribution functions: stationary_cont(), stationary_p()
```

## **Examples**

```
Gamma = tpm(c(rep(-2,3), rep(-3,3)))
delta = stationary(Gamma)
```

stationary\_cont

Compute the stationary distribution of a continuous-time Markov chain

# 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_cont(Q)
```

## **Arguments**

Q

infinitesimal generator matrix of dimension c(N,N)

#### Value

stationary distribution of the continuous-time Markov chain with given generator matrix

#### See Also

```
generator to create a generator matrix
Other stationary distribution functions: stationary(), stationary_p()
```

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## **Examples**

```
Q = generator(c(-2,-2))
Pi = stationary_cont(Q)
```

stationary\_p

Compute the periodically stationary distribution of a periodically inhomogeneous Markov chain

# 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, ..., L. The stationary distribution for time t satisfies  $\delta^{(t)}\Gamma_t = \delta^{(t)}$ .

This function calculates said periodically stationary distribution.

## 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
	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.

# Value

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

## 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\_cont()

stationary\_p\_sparse 41

## **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)
```

## Description

This is 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 distribu-

tions for each time point in the cycle.

#### Value

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

```
## periodic HSMM example (here the approximating tpm is sparse)
N = 2 # number of states
L = 24 # cycle length
# time-varying mean dwell times
Z = trigBasisExp(1: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)
```

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```
# Periodically stationary distribution for specific time point
delta = stationary_p_sparse(Gamma, 4)

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

stationary\_sparse

Sparse version of stationary

# 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

```
## 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)
```

tpm 43

tpm	Build the transition probability matrix from unconstrained parameter vector
	vector

## **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 parametrise 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(param, byrow = FALSE)
```

## **Arguments**

param unconstrained parameter vector of length N\*(N-1) where N is the number of

states of the Markov chain

byrow logical indicating if the 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.

## Value

Transition probability matrix of dimension c(N,N)

## See Also

```
Other transition probability matrix functions: generator(), tpm_cont(), tpm_emb(), tpm_emb_g(), tpm_g(), tpm_p()
```

```
# 2 states: 2 free off-diagonal elements
par1 = rep(-1, 2)
Gamma1 = tpm(par1)

# 3 states: 6 free off-diagonal elements
par2 = rep(-2, 6)
Gamma2 = tpm(par2)
```

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tpm\_cont

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  $t_1, \ldots, t_n$  the transition probabilites between  $t_i$  and  $t_{i+1}$  are caluclated 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_cont(Q, timediff, ad = NULL, report = TRUE)
```

## **Arguments**

Q	infinitesimal generator matrix of the continuous-time Markov chain of dimen-
	sion c(N,N)

timediff time differences between observations of length n-1 when based on n observa-

tions

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(N,N,n-1)

## See Also

```
Other transition probability matrix functions: generator(), tpm(), tpm_emb(), tpm_emb_g(), tpm_g(), tpm_p()
```

```
# 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 45

tpm_emb	Build the embedded transition probability matrix of an HSMM from
	unconstrained parameter vector

#### **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(N,N), the number of free off-diagonal elements is N\*(N-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 N\*(N-2) where N is the number of

states of the Markov chain

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(N,N)

#### See Also

```
Other transition probability matrix functions: generator(), tpm(), tpm_cont(), tpm_emb_g(), tpm_g(), tpm_p()
```

```
# 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)
```

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

tpm\_emb\_g

Build all embedded transition probability matrices of an inhomogeneous HSMM

# **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(N,N), the number of free off-diagonal elements is N\*(N-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 $c(n, p)$ or $c(n, p+1)$
	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
	Needs to be of dimension $c(N^*(N-2), p+1)$ , 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

## Value

array of embedded/ conditional transition probability matrices of dimension c(N,N,n)

the fitted model. Defaults to TRUE.

## See Also

```
Other transition probability matrix functions: generator(), tpm(), tpm_cont(), tpm_emb(), tpm_g(), tpm_p()
```

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## **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, byrow = FALSE, ad = NULL, report = TRUE)
```

## **Arguments**

Z	covariate design matrix with or without intercept column, i.e. of dimension $c(n,p)$ or $c(n,p+1)$ 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 transition probability matrix
	Needs to be of dimension $c(N^*(N-1),p+1)$ , where the first column contains the intercepts.
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.
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.

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## Value

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

#### See Also

```
Other transition probability matrix functions: generator(), tpm(), tpm_cont(), tpm_emb(), tpm_emb_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

Builds the transition probability matrix of an HSMM-approximating HMM

## **Description**

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs, where the state duration distribution is explicitly modelled. For direct numerical maximum likelhood 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 $c(N,N)$ as computed by $tpm\_emb$ .
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.
Fm	optional list of length N 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 TRUE.
eps	rounding value: If an entry of the transition probabily 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

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## **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

Build the transition probability matrix of an HSMM-approximating HMM

# Description

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs. For direct numerical maximum likelhood 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 probabily matrix is smaller, than it

is rounded to zero.

## Value

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

```
# 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)
```

50 tpm\_ihsmm

tpm_ihsmm	Builds all transition probability matrices of an inhomogeneous- HSMM-approximating HMM
	Homin approximating Hintin

## **Description**

Hidden semi-Markov models (HSMMs) are a flexible extension of HMMs. For direct numerical maximum likelhood 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 inhomogeneos HSMMs.

## Usage

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

## **Arguments**

omega	embedded transition probability matrix
	Either a matrix of dimension $c(N,N)$ for homogeneous conditional transition probabilities (as computed by $tpm\_emb$ ), or an array of dimension $c(N,N,n)$ for inhomogeneous conditional transition probabilities (as computed by $tpm\_emb\_g$ ).
dm	state dwell-time distributions arranged in a list of length N
	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 probabily matrix is smaller, than it is rounded to zero. Usually, this should not be changed.

## Value

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

```
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 probabilites
# diagonal elements are zero, rowsums are one
omega = matrix(c(0,1,1,0), nrow = N, byrow = TRUE)
```

tpm\_p 51

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

## inhomogeneous conditional transition probabilites
# 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

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

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**

tod equidistant sequence of a cyclic variable 
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.

52 tpm\_p

beta matrix of coefficients for the off-diagonal elements of the transition probability

matrix

Needs to be of dimension c(N \*(N-1), 2\*degree+1), where the first column con-

tains the intercepts.

degree degree of the trigonometric link function

For each additional degree, one sine and one cosine frequency are added.

Z pre-calculated design matrix (excluding intercept column)

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 trigBasisExp.

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.

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.

#### **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(N,N,length(tod))

#### See Also

```
Other transition probability matrix functions: generator(), tpm(), tpm_cont(), tpm_emb(), tpm_emb_g(), tpm_g()
```

```
# 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
```

tpm\_phsmm 53

```
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

Builds 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 likelhood 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 inhomogeneos HSMMs.

# Usage

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

# Arguments

omega	embedded transition probability matrix
	Either a matrix of dimension $c(N,N)$ for homogeneous conditional transition probabilities (as computed by $tpm\_emb$ ), or an array of dimension $c(N,N,L)$ for inhomogeneous conditional transition probabilities (as computed by $tpm\_emb\_g$ ).
dm	state dwell-time distributions arranged in a list of length N
	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 probabily 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.

54 tpm\_phsmm2

## **Examples**

```
N = 2 \# number of states
L = 24 # cycle length
# time-varying mean dwell times
Z = trigBasisExp(1: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 probabilites
# 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 probabilites
# 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 likelhood 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 inhomogeneos HSMMs.

#### Usage

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

## **Arguments**

omega embedded transition probability matrix

Either a matrix of dimension c(N,N) for homogeneous conditional transition probabilities, or an array of dimension c(N,N,L) for inhomogeneous conditional

transition probabilities.

dm state dwell-time distributions arranged in a list of length(N)

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.

tpm\_thinned 55

eps

rounding value: If an entry of the transition probabily matrix is smaller, than it is rounded to zero.

#### 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 probabilites
# 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 probabilites
# 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

Compute the transition probability matrix of a thinned periodically inhomogeneous Markov chain.

## **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,

56 trex

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, ..., L. This function calculates the matrix above efficiently as a preliminery step to calculating the periodically stationary distribution.

#### Usage

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

## **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 thinned

transition probility matrix

#### Value

thinned transition probabilty matrix of dimension c(N,N)

## **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

T-Rex Movement Data

## **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 24step hourly step lengths in kilometresangle hourly turning angles in radians

state hidden state variable

trigBasisExp 57

## **Source**

Generated for example purposes.

trigBasisExp

Compute the design matrix for a trigonometric basis expansion

## 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

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 K of the trigonometric link above. Increasing K increases the flexibility.

## Value

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

```
## hourly data
tod = rep(1:24, 10)
Z = trigBasisExp(tod, L = 24, degree = 2)
## half-hourly data
tod = rep(1:48/2, 10) # in [0,24] -> L = 24
Z1 = trigBasisExp(tod, L = 24, degree = 3)

tod = rep(1:48, 10) # in [1,48] -> L = 48
Z2 = trigBasisExp(tod, L = 48, degree = 3)

all(Z1 == Z2)
# The latter two are equivalent specifications!
```

58 viterbi

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Viterbi algorithm for state decoding in homogeneous HMMs

## Description

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

## Usage

```
viterbi(delta, Gamma, allprobs, 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
Gamma	transition probability matrix of dimension $c(N,N)$ or array of transition probability matrices of dimension $c(N,N,k)$ if trackID is provided
allprobs	matrix of state-dependent probabilities/ density values of dimension $c(n,N)$
trackID	optional vector of k track IDs, if multiple tracks need to be decoded separately
mod	optional model object containing initial distribution delta, transition probability matrix Gamma, matrix of state-dependent probabilities allprobs, and potentially a trackID variable
	If you are using automatic differentiation either with RTMB::MakeADFun or qreml and include forward 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 running RTMB::report() or from qreml directly to

## Value

vector of decoded states of length n

this function.

# See Also

```
Other decoding functions: stateprobs(), stateprobs_g(), stateprobs_p(), viterbi_g(), viterbi_p()
```

```
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 59

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Viterbi algorithm for state decoding in inhomogeneous HMMs

# Description

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

# Usage

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

## **Arguments**

rguments	
delta	initial 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 $c(N,N,n-1)$ , as in a time series of length n, there are only n-1 transitions
	If an array of dimension $c(N,N,n)$ is provided for a single track, the first slice will be ignored.
	If trackID is provided, Gamma needs to be an array of dimension $c(N,N,n)$ , where n is the number of rows in allprobs. Then for each track the first transition matrix will be ignored.
allprobs	matrix of state-dependent probabilities/ density values of dimension $c(n,N)$
trackID	optional vector of k track IDs, if multiple tracks need to be decoded separately
mod	optional model object containing initial distribution delta, transition probability matrix Gamma, matrix of state-dependent probabilities allprobs, and potentially a trackID variable
	If you are using automatic differentiation either with RTMB::MakeADFun or qreml and include forward_g in your likelihood function, the objects needed for state decoding are automatically reported after model fitting. Hence, you can pass the

## Value

vector of decoded states of length n

this function.

## See Also

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

model object obtained from running RTMB::report() or from qreml directly to

60 viterbi\_p

## **Examples**

viterbi\_p

Viterbi algorithm for state decoding in periodically inhomogeneous HMMs

## **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

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)

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 optional model object containing initial distribution delta, transition probabiles.

optional model object containing initial distribution delta, transition probability matrix Gamma, matrix of state-dependent probabilities allprobs, and potentially a trackID variable

If you are using automatic differentiation either with RTMB::MakeADFun or qreml and include forward\_p 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 running RTMB::report() or from qreml directly to

this function.

*vm* 61

## Value

vector of decoded states of length n

#### See Also

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

## **Examples**

 $\vee m$ 

von Mises distribution

# 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 $length(n) > 1$ , the length is taken to be the number required.
wrap	logical; if TRUE, generated angles are wrapped to the interval [-pi, pi].

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# **Details**

The implementation of dvm allows for automatic differentiation with RTMB. rvm and pvm are imported from CircStats and circular respectively.

# Value

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

```
set.seed(1)
x = rvm(1000, 0, 1)
d = dvm(x, 0, 1)
p = pvm(x, 0, 1)
```

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