Package 'oHMMed'

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Type Package

Title HMMs with Ordered Hidden States and Emission Densities

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Description Inference using a class of Hidden Markov models (HMMs) called 'oHMMed' (ordered HMM with emission densities doi:10.1186/s12859-024-05751-4): The 'oHMMed' algorithms identify the number of comparably homogeneous regions within observed sequences with autocorrelation patterns. These are modelled as discrete hidden states; the observed data points are then realisations of continuous probability distributions with state-specific means that enable ordering of these distributions. The observed sequence is labelled according to the hidden states, permitting only neighbouring states that are also neighbours within the ordering of their associated distributions. The parameters that characterise these state-specific distributions are then inferred. Relevant for application to genomic sequences, time series, or any other sequence data with serial autocorrelation.

```
License GPL-3
```

```
URL https://github.com/LynetteCaitlin/oHMMed,
    https://lynettecaitlin.github.io/oHMMed/
```

BugReports https://github.com/LynetteCaitlin/oHMMed/issues

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oHMMed-package

oHMMed: HMMs with Ordered Hidden States and Emission Densities

Description

Inference using a class of Hidden Markov models (HMMs) called 'oHMMed' (ordered HMM with emission densities doi:10.1186/s12859024057514): The 'oHMMed' algorithms identify the number of comparably homogeneous regions within observed sequences with autocorrelation patterns. These are modelled as discrete hidden states; the observed data points are then realisations of continuous probability distributions with state-specific means that enable ordering of these distributions. The observed sequence is labelled according to the hidden states, permitting only neighbouring states that are also neighbours within the ordering of their associated distributions. The parameters that characterise these state-specific distributions are then inferred. Relevant for application to genomic sequences, time series, or any other sequence data with serial autocorrelation.

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References

Claus Vogl, Mariia Karapetiants, Burçin Yıldırım, Hrönn Kjartansdóttir, Carolin Kosiol, Juraj Bergman, Michal Majka, Lynette Caitlin Mikula. Inference of genomic landscapes using ordered Hidden Markov Models with emission densities (oHMMed). BMC Bioinformatics 25, 151 (2024). doi:10.1186/s12859024057514

See Also

Useful links:

- https://github.com/LynetteCaitlin/oHMMed
- https://lynettecaitlin.github.io/oHMMed/
- Report bugs at https://github.com/LynetteCaitlin/oHMMed/issues

coef.hmm_mcmc_normal Extract Model Estimates

Description

coef is a generic function which extracts model estimates from mcmc_hmm_* objects

Usage

```
## S3 method for class 'hmm_mcmc_normal'
coef(object, ...)
## S3 method for class 'hmm_mcmc_gamma_poisson'
coef(object, ...)
```

Arguments

```
object an object of class inheriting from "mcmc_hmm_*"
... not used
```

Value

Estimates extracted from MCMC HMM objects

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Examples

```
coef(example_hmm_mcmc_normal)
coef(example_hmm_mcmc_gamma_poisson)
```

conf_mat

Calculate and Visualise a Confusion Matrix

Description

A diagnostic function that tests the reliability of estimation procedures given the inferred transition rates

Usage

```
conf_mat(N, res, plot = TRUE)
```

Arguments

```
N (numeric) number of simulations

res (mcmc_hmm_*) simulated MCMC HMM model

plot (logical) plot confusion matrix. By default TRUE
```

Details

First the data is simulated given the inferred model parameters and transition rates. Then posterior probabilities are calculated and states are inferred. Finally, the inferred states and simulated states are compared via confusion_matrix function.

Value

```
confusion_matrix
```

```
if (interactive()) {
  res <- conf_mat(100, example_hmm_mcmc_normal, plot = TRUE)
}</pre>
```

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convert_to_ggmcmc

Converts MCMC Samples into ggmcmc Format

Description

This helper function converts MCMC samples into ggmcmc format

Usage

```
convert_to_ggmcmc(
   x,
   pattern = c("mean", "sigma", "beta", "alpha", "pois_means", "T"),
   include_warmup = FALSE
)
```

Arguments

```
x (mcmc_hmm_*) MCMC HMM object

pattern (character) pattern(s) with model parameters to be included in the output

include_warmup (logical) include warmup samples. By default FALSE
```

Details

By default, for a given model, all parameters are converted into ggmcmc format.

The parameter pattern can be used to extract specific parameters. For instance pattern="mean" extracts all mean parameters from a hmm_mcmc_normal model.

If a specific parameter is of interest it can be matched by an exact name: pattern=c("mean[1]", "T[1,1]").

Value

data.frame compatible with functions from the ggmcmc package

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eigen_system

Calculate Eigenvalues and Eigenvectors

Description

This helper function returns the eigenvalues in lambda and the left and right eigenvectors in forwards and backwards

Usage

```
eigen_system(mat)
```

Arguments

mat

(matrix) a square matrix

Value

a list with three elements:

• lambda: eigenvalues

• forwards: left eigenvector

• backwards: right eigenvector

```
\begin{array}{lll} \text{mat\_T0} & \leftarrow & \text{rbind}(c(1-0.01,0.01,0),\\ & & c(0.01,1-0.02,0.01),\\ & & c(0,0.01,1-0.01)) \\ \text{eigen\_system}(\text{mat\_T0}) \end{array}
```

```
{\it example\_hmm\_mcmc\_gamma\_poisson} \\ {\it Example of a Simulated Gamma-Poisson Model}
```

Description

Example of a Simulated Gamma-Poisson Model

Usage

```
example_hmm_mcmc_gamma_poisson
```

Format

hmm_mcmc_gamma_poisson object

Examples

```
example_hmm_mcmc_normal
```

Example of a Simulated Normal Model

Description

Example of a Simulated Normal Model

Usage

```
example_hmm_mcmc_normal
```

Format

hmm_mcmc_normal object

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Examples

```
# Data stored in the object
plot(density(example_hmm_mcmc_normal$data), main = "")
# Priors used in simulation
example_hmm_mcmc_normal$priors
# Model
example_hmm_mcmc_normal
summary(example_hmm_mcmc_normal)
```

generate_random_T

Generate a Random Transition Matrix

Description

This helper function generates a transition matrix at random for testing purposes

Usage

```
generate_random_T(n = 3)
```

Arguments

n

(integer) dimension of a transition matrix

Details

Uniform random numbers [0,1] are used to fill the matrix. Rows are then normalized.

Value

random n x n transition matrix

```
mat_T <- generate_random_T(3)
mat_T
rowSums(mat_T)</pre>
```

get_pi

get_pi

Get the Prior Probability of States

Description

Calculate the prior probability of states that correspond to the stationary distribution of the transition matrix T

Usage

```
get_pi(mat_T = NULL)
```

Arguments

```
mat_T (matrix) transition matrix
```

Details

It is assumed that the prior probability of states corresponds to the stationary distribution of the transition matrix T, denoted with π and its entries with $\pi_i = Pr(\theta_{l-1} = i)$.

Value

A numeric vector

Examples

```
\begin{array}{c} T_{\text{-}mat} < - \ rbind(c(1-0.01,0.01,0),\\ & c(0.01,1-0.02,0.01),\\ & c(0,0.01,1-0.01)) \\ T_{\text{-}mat} \\ get_{\text{-}pi(T_{\text{-}mat})} \end{array}
```

hmm_mcmc_gamma_poisson

MCMC Sampler sampler for the Hidden Markov with Gamma-Poisson emission densities

Description

MCMC Sampler sampler for the Hidden Markov with Gamma-Poisson emission densities

Usage

```
hmm_mcmc_gamma_poisson(
  data,
  prior_T,
  prior_betas,
  prior_alpha = 1,
  iter = 5000,
  warmup = floor(iter/1.5),
  thin = 1,
  seed = sample.int(.Machine$integer.max, 1),
  init_T = NULL,
  init_betas = NULL,
  init_alpha = NULL,
  print_params = TRUE,
  verbose = TRUE
)
```

Arguments

data	(numeric) data
prior_T	(matrix) prior transition matrix
prior_betas	(numeric) prior beta parameters
prior_alpha	(numeric) a single prior alpha parameter. By default, prior_alpha=1
iter	(integer) number of MCMC iterations
warmup	(integer) number of warmup iterations
thin	(integer) thinning parameter. By default, 1
seed	(integer) seed parameter
init_T	(matrix) optional parameter; initial transition matrix
init_betas	(numeric) optional parameter; initial beta parameters
init_alpha	(numeric) optional parameter; initial alpha parameter
print_params	(logical) optional parameter; print estimated parameters every iteration. By default, \ensuremath{TRUE}
verbose	(logical) optional parameter; print additional messages. By default, TRUE

Details

Please see supplementary information at doi:10.1186/s12859024057514 for more details on the algorithm.

For usage recommendations please see https://github.com/LynetteCaitlin/oHMMed/blob/main/UsageRecommendations.pdf.

List with following elements:

- data: data used for simulation
- samples: list with samples
- estimates: list with various estimates
- idx: indices with iterations after the warmup period
- priors: prior parameters
- inits: initial parameters
- last_iter: list with samples from the last MCMC iteration
- info: list with various meta information about the object

References

Claus Vogl, Mariia Karapetiants, Burçin Yıldırım, Hrönn Kjartansdóttir, Carolin Kosiol, Juraj Bergman, Michal Majka, Lynette Caitlin Mikula. Inference of genomic landscapes using ordered Hidden Markov Models with emission densities (oHMMed). BMC Bioinformatics 25, 151 (2024). doi:10.1186/s12859024057514

```
# Simulate Poisson-Gamma data
N <- 2<sup>1</sup>0
true_T \leftarrow rbind(c(0.95, 0.05, 0),
                 c(0.025, 0.95, 0.025),
                 c(0.0, 0.05, 0.95))
true_betas <- c(2, 1, 0.1)
true_alpha <- 1
simdata_full <- hmm_simulate_gamma_poisson_data(L = N,</pre>
                                                    mat_T = true_T,
                                                    betas = true_betas,
                                                    alpha = true_alpha)
simdata <- simdata_full$data</pre>
hist(simdata, breaks = 40, probability = TRUE,
     main = "Distribution of the simulated Poisson-Gamma data")
lines(density(simdata), col = "red")
# Set numbers of states to be inferred
n_states_inferred <- 3</pre>
# Set priors
prior_T <- generate_random_T(n_states_inferred)</pre>
prior_betas <- c(1, 0.5, 0.1)
prior_alpha <- 3</pre>
# Simmulation settings
iter <- 50
```

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```
warmup <- floor(iter / 5) # 20 percent</pre>
thin <- 1
seed <- sample.int(10000, 1)</pre>
print_params <- FALSE # if TRUE then parameters are printed in each iteration</pre>
verbose <- FALSE # if TRUE then the state of the simulation is printed
# Run MCMC sampler
res <- hmm_mcmc_gamma_poisson(data = simdata,</pre>
                               prior_T = prior_T,
                               prior_betas = prior_betas,
                               prior_alpha = prior_alpha,
                               iter = iter,
                               warmup = warmup,
                               thin = thin,
                               seed = seed,
                               print_params = print_params,
                               verbose = verbose)
res
summary(res)# summary output can be also assigned to a variable
coef(res) # extract model estimates
# plot(res) # MCMC diagnostics
```

hmm_mcmc_normal

MCMC Sampler for the Hidden Markov Model with Normal emission densities

Description

MCMC Sampler for the Hidden Markov Model with Normal emission densities

Usage

```
hmm_mcmc_normal(
  data,
  prior_T,
  prior_means,
  prior_sd,
  iter = 600,
  warmup = floor(iter/5),
  thin = 1,
  seed = sample.int(.Machine$integer.max, 1),
  init_T = NULL,
  init_means = NULL,
  init_sd = NULL,
  print_params = TRUE,
  verbose = TRUE
)
```

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Arguments

data (numeric) normal data

prior_T (matrix) prior transition matrix

prior_means (numeric) prior means

prior_sd (numeric) a single prior standard deviation
iter (integer) number of MCMC iterations
warmup (integer) number of warmup iterations
thin (integer) thinning parameter. By default, 1
seed (integer) optional parameter; seed parameter

init_T (matrix) optional parameter; initial transition matrix

init_sd (numeric) optional parameter; initial standard deviation

print_params (logical) optional parameter; print parameters every iteration. By default,

TRUE

verbose (logical) optional parameter; print additional messages. By default, TRUE

Details

Please see supplementary information at doi:10.1186/s12859024057514 for more details on the algorithm.

For usage recommendations please see https://github.com/LynetteCaitlin/oHMMed/blob/main/UsageRecommendations.pdf.

Value

List with following elements:

- data: data used for simulation
- samples: list with samples
- estimates: list with various estimates
- idx: indices with iterations after the warmup period
- priors: prior parameters
- inits: initial parameters
- last_iter: list with samples from the last MCMC iteration
- info: list with various meta information about the object

References

Claus Vogl, Mariia Karapetiants, Burçin Yıldırım, Hrönn Kjartansdóttir, Carolin Kosiol, Juraj Bergman, Michal Majka, Lynette Caitlin Mikula. Inference of genomic landscapes using ordered Hidden Markov Models with emission densities (oHMMed). BMC Bioinformatics 25, 151 (2024). doi:10.1186/s12859024057514

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```
# Simulate normal data
N <- 2<sup>1</sup>0
true_T \leftarrow rbind(c(0.95, 0.05, 0),
                 c(0.025, 0.95, 0.025),
                 c(0.0, 0.05, 0.95))
true_means <- c(-5, 0, 5)
true_sd <- 1.5
simdata_full <- hmm_simulate_normal_data(L = N,</pre>
                                            mat_T = true_T,
                                            means = true_means,
                                            sigma = true_sd)
simdata <- simdata_full$data</pre>
hist(simdata,
     breaks = 40,
     probability = TRUE,
     main = "Distribution of the simulated normal data")
lines(density(simdata), col = "red")
# Set numbers of states to be inferred
n_states_inferred <- 3</pre>
# Set priors
prior_T <- generate_random_T(n_states_inferred)</pre>
prior_means <- c(-18, -1, 12)
prior_sd <- 3</pre>
# Simmulation settings
iter <- 50
warmup <- floor(iter / 5) # 20 percent</pre>
thin <- 1
seed <- sample.int(10000, 1)</pre>
print_params <- FALSE # if TRUE then parameters are printed in each iteration</pre>
verbose <- FALSE # if TRUE then the state of the simulation is printed
# Run MCMC sampler
res <- hmm_mcmc_normal(data = simdata,</pre>
                        prior_T = prior_T,
                        prior_means = prior_means,
                        prior_sd = prior_sd,
                        iter = iter,
                        warmup = warmup,
                        seed = seed,
                        print_params = print_params,
                        verbose = verbose)
res
summary(res) # summary output can be also assigned to a variable
coef(res) # extract model estimates
```

```
# plot(res) # MCMC diagnostics
```

```
hmm_simulate_gamma_poisson_data
```

Simulate data distributed according to oHMMed with gamma-poisson emission densities

Description

Simulate data distributed according to oHMMed with gamma-poisson emission densities

Usage

```
hmm_simulate_gamma_poisson_data(L, mat_T, betas, alpha)
```

Arguments

```
L (integer) number of simulations

mat_T (matrix) a square matrix with the initial state

betas (numeric) rate parameter in rgamma for emission probabilities

alpha (numeric) shape parameter in rgamma for emission probabilities
```

Value

Returns a list with the following elements:

- data: numeric vector with data
- states: an integer vector with "true" hidden states used to generate the data vector
- pi: numeric vector with prior probability of states

```
hmm_simulate_normal_data
```

Simulate data distributed according to oHMMed with normal emission densities

Description

Simulate data distributed according to oHMMed with normal emission densities

Usage

```
hmm_simulate_normal_data(L, mat_T, means, sigma)
```

Arguments

```
L (integer) number of simulations

mat_T (matrix) a square matrix with the initial state

means (numeric) mean parameter in rnorm for emission probabilities

sigma (numeric) sd parameter in rnorm for emission probabilities
```

Value

Returns a list with the following elements:

- data: numeric vector with data
- states: an integer vector with "true" hidden states used to generate the data vector
- pi: numeric vector with prior probability of states

```
kullback_leibler_cont_appr
```

Calculate a Continuous Approximation of the Kullback-Leibler Divergence

Description

Calculate a Continuous Approximation of the Kullback-Leibler Divergence

Usage

```
kullback_leibler_cont_appr(p, q)
```

Arguments

p (numeric) probabilities q (numeric) probabilities

Details

The continuous approximation of the Kullback-Leibler divergence is calculated as follows:

$$\frac{1}{n}\sum_{i=1}^{n} \left[\log(p_i)p_i - \log(q_i)p_i \right]$$

Value

Numeric vector

```
# Simulate n normally distributed variates
n <- 1000
dist1 <- rnorm(n)
dist2 <- rnorm(n, mean = 0, sd = 2)
dist3 <- rnorm(n, mean = 2, sd = 2)

# Estimate probability density functions
pdf1 <- density(dist1)
pdf2 <- density(dist2)
pdf3 <- density(dist3)

# Visualise PDFs
plot(pdf1, main = "PDFs", col = "red", xlim = range(dist3))
lines(pdf2, col = "blue")
lines(pdf3, col = "green")

# PDF 1 vs PDF 2</pre>
```

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```
kullback_leibler_cont_appr(pdf1$y, pdf2$y)
# PDF 1 vs PDF 3
kullback_leibler_cont_appr(pdf1$y, pdf3$y)
# PDF 2 vs PDF 2
kullback_leibler_cont_appr(pdf2$y, pdf3$y)
```

kullback_leibler_disc Calculate a Kullback-Leibler Divergence for a Discrete Distribution

Description

Calculate a Kullback-Leibler Divergence for a Discrete Distribution

Usage

```
kullback_leibler_disc(p, q)
```

Arguments

p (numeric) probabilitiesq (numeric) probabilities

Details

The Kullback-Leibler divergence for a discrete distribution is calculated as follows:

$$\sum_{i=1}^{n} p_i \log \left(\frac{p_i}{q_i} \right)$$

Value

Numeric vector

```
# Simulate n Poisson distributed variates
n <- 1000
dist1 <- rpois(n, lambda = 1)
dist2 <- rpois(n, lambda = 5)
dist3 <- rpois(n, lambda = 20)

# Generate common factor levels
x_max <- max(c(dist1, dist2, dist3))
all_levels <- 0:x_max
# Estimate probability mass functions</pre>
```

```
pmf_dist1 <- table(factor(dist1, levels = all_levels)) / n
pmf_dist2 <- table(factor(dist2, levels = all_levels)) / n
pmf_dist3 <- table(factor(dist3, levels = all_levels)) / n

# Visualise PMFs
barplot(pmf_dist1, col = "green", xlim = c(0, x_max))
barplot(pmf_dist2, col = "red", add = TRUE)
barplot(pmf_dist3, col = "blue", add = TRUE)

# Calculate distances
kullback_leibler_disc(pmf_dist1, pmf_dist2)
kullback_leibler_disc(pmf_dist2, pmf_dist3)
kullback_leibler_disc(pmf_dist2, pmf_dist3)</pre>
```

plot.hmm_mcmc_gamma_poisson

 $Plot\ Diagnostics\ for\ hmm_mcmc_gamma_poisson\ Objects$

Description

This function creates a variety of diagnostic plots that can be useful when conducting Markov Chain Monte Carlo (MCMC) simulation of a gamma-poisson hidden Markov model (HMM). These plots will help to assess convergence, fit, and performance of the MCMC simulation

Usage

```
## $3 method for class 'hmm_mcmc_gamma_poisson'
plot(
    X,
    simulation = FALSE,
    true_betas = NULL,
    true_alpha = NULL,
    true_mat_T = NULL,
    true_states = NULL,
    show_titles = TRUE,
    log_statesplot = FALSE,
    ...
)
```

Arguments

```
true_states (integer) optional parameter; true states. To be used if simulation=TRUE show_titles (logical) if TRUE then titles are shown for all graphs. By default, TRUE log_statesplot (logical) if TRUE then log-statesplots are shown. By default, FALSE ... not used
```

Several diagnostic plots that can be used to evaluate the MCMC simulation of the gamma-poisson HMM

Examples

```
plot(example_hmm_mcmc_gamma_poisson)
```

Description

This function creates a variety of diagnostic plots that can be useful when conducting Markov Chain Monte Carlo (MCMC) simulation of a normal hidden Markov model (HMM). These plots will help to assess convergence, fit, and performance of the MCMC simulation

Usage

```
## $3 method for class 'hmm_mcmc_normal'
plot(
    X,
    simulation = FALSE,
    true_means = NULL,
    true_sd = NULL,
    true_mat_T = NULL,
    true_states = NULL,
    show_titles = TRUE,
    ...
)
```

Arguments

```
x (hmm_mcmc_normal) HMM MCMC normal object
simulation (logical) optional parameter; default is simulation=FALSE, so the input data
was empirical. If the input data was simulated, it must be set simulation=TRUE.

true_means (numeric) optional parameter; true means. To be used if simulation=TRUE
true_sd (numeric) optional parameter; true standard deviation. To be used if simulation=TRUE
```

true_mat_T	(matrix) optional parameter; true transition matrix. To be used if simulation = TRUE
true_states	$(integer)\ optional\ parameter;\ true\ states.\ To\ be\ used\ if\ simulation = TRUE$
show_titles	(logical) optional parameter; if TRUE then titles are shown for all graphs. By default, $TRUE$
	not used

Several diagnostic plots that can be used to evaluate the MCMC simulation of the normal HMM

Examples

```
plot(example_hmm_mcmc_normal)
```

```
posterior_prob_gamma_poisson
```

Forward-Backward Algorithm to Calculate the Posterior Probabilities of Hidden States in Poisson-Gamma Model

Description

Forward-Backward Algorithm to Calculate the Posterior Probabilities of Hidden States in Poisson-Gamma Model

Usage

```
posterior_prob_gamma_poisson(data, pi, mat_T, betas, alpha)
```

Arguments

data	(numeric) Poisson data
pi	(numeric) prior probability of states
mat_T	(matrix) transition probability matrix
betas	(numeric) vector with prior rates
alpha	(numeric) prior scale

Details

Please see supplementary information at doi:10.1186/s12859024057514 for more details on the algorithm.

List with the following elements:

- F: auxiliary forward variables
- B: auxiliary backward variables
- s: weights

Examples

```
mat_T \leftarrow rbind(c(1-0.01,0.01,0),
                c(0.01,1-0.02,0.01),
                c(0,0.01,1-0.01))
L <- 2^10
betas <- c(0.1, 0.3, 0.5)
alpha <- 1
sim_data <- hmm_simulate_gamma_poisson_data(L = L,</pre>
                                               mat_T = mat_T,
                                               betas = betas,
                                               alpha = alpha)
pi <- sim_data$pi
hmm_poison_data <- sim_data$data</pre>
hist(hmm_poison_data, breaks = 100)
# Calculate posterior probabilities of hidden states
post_prob <- posterior_prob_gamma_poisson(data = hmm_poison_data,</pre>
                                             pi = pi,
                                             mat_T = mat_T,
                                             betas = betas,
                                             alpha = alpha)
str(post_prob)
```

 $posterior_prob_normal \quad \textit{Forward-Backward Algorithm to Calculate the Posterior Probabilities} \\ \quad of \textit{Hidden States in Normal Model}$

Description

Forward-Backward Algorithm to Calculate the Posterior Probabilities of Hidden States in Normal Model

Usage

```
posterior_prob_normal(data, pi, mat_T, means, sdev)
```

Arguments

data	(numeric) normal data
pi	(numeric) prior probability of states
mat_T	(matrix) transition probability matrix
means	(numeric) vector with prior means
sdev	(numeric) prior standard deviation

Details

Please see supplementary information at doi:10.1186/s12859024057514 for more details on the algorithm.

Value

List with the following elements:

- F: auxiliary forward variables
- B: auxiliary backward variables
- s: weights

```
prior_mat <- rbind(c(1-0.05, 0.05, 0),</pre>
                   c(0.05, 1-0.1, 0.05),
                   c(0, 0.05, 1-0.05))
prior_means <- c(-0.1, 0.0, 0.1)
prior_sd <- sqrt(0.1)</pre>
L <- 100
# Simulate HMM model based on normal data based on prior information
sim_data_normal <- hmm_simulate_normal_data(L = L,</pre>
                                               mat_T = prior_mat,
                                               means = prior_means,
                                               sigma = prior_sd)
pi <- sim_data_normal$pi</pre>
# pi <- get_pi(prior_mat)</pre>
hmm_norm_data <- sim_data_normal$data</pre>
# Calculate posterior probabilities of hidden states
post_prob <- posterior_prob_normal(data = hmm_norm_data,</pre>
                                      pi = pi,
                                      mat_T = prior_mat,
                                      means = prior_means,
                                       sdev = prior_sd)
str(post_prob)
```

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