Package 'thamesmix'

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Type Package

Title Truncated Harmonic Mean Estimator of the Marginal Likelihood for Mixtures

Version 0.1.3

Description Implements the truncated harmonic mean estimator (THAMES) of the reciprocal marginal likelihood for uni- and multivariate mixture models using posterior samples and unnormalized log posterior values via reciprocal importance sampling.
Metodiev, Irons, Perrot-Dockès, Latouche & Raftery (2025) <doi:10.48550/arXiv.2504.21812>.

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Imports stats, sparsediscrim, quadprog, igraph, gor, Rfast, mvtnorm, combinat, withr

VignetteBuilder knitr

Suggests multimode, knitr, bayesmix, label.switching, LaplacesDemon, markdown

NeedsCompilation no

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Contents

`alltopsorts_recursion` *all topological orderings of a DAG*

Description

This function computes all topological orderings of a graph using the recursive algorithm described in Knuth and Szwarcfiter (1974).

Usage

```
alltopsorts_recursion(n, adj_list)
```

Arguments

`n`	number of nodes in the DAG
`adj_list`	edges given as an adjacency list

Value

Returns a list of topological orderings.

References

Knuth, D. E. and J. L. Szwarcfiter (1974). A structured program to generate all topological sorting arrangements. Information Processing Letters 2(6), 153–157.

Examples

```
n = 4
alltopsorts_recursion(n, list(c(1,3),c(2,4)))
```

`compute_nobile_identity` *Nobile's identity for the marginal likelihood*

Description

This function uses the identity from Nobile (2004, 2007) to compute an estimate of the marginal likelihood for a mixture model with G components given an estimate of the marginal likelihood for a mixture model with G-1 components and an estimate of the proportion of empty components.

Usage

```
compute_nobile_identity(logZhatGminus1, p0hat_value, G, dirichlet_vec, n)
```

Arguments

`logZhatGminus1`	estimate of the marginal likelihood for G-1
`p0hat_value`	estimate of the proportion of empty components
`G`	number of components
`dirichlet_vec`	hyperparameter-vector of the dirichlet prior
`n`	size of the data

Value

estimate of the marginal likelihood for G

References

Nobile, A. (2004). On the posterior distribution of the number of components in a finite mixture. The Annals of Statistics 32(5), 2044–2073.

Nobile, A. (2007). Bayesian finite mixtures: a note on prior specification and posterior computation.arXiv preprint arXiv:0711.0458.

Martin Metodiev, Nicholas J. Irons, Marie Perrot-Dockès, Pierre Latouche, Adrian E. Raftery. "Easily Computed Marginal Likelihoods for Multivariate Mixture Models Using the THAMES Estimator." arXiv preprint arXiv:2504.21812.

Examples

```
# computes log marginal likelihood of the Swiss banknote dataset
# for G=4, given the settings in Metodiev et al. (2025)
compute_nobile_identity(logZhatGminus1 = -909.49,
p0hat_value = 1/4,
dirichlet_vec = rep(1,4),
n=200)
```

`overlapgraph` *Estimator of the overlap graph*

Description

This function computes the overlap graph for mixture models.

Usage

```
overlapgraph(sims)
```

Arguments

`sims`	n_simul x G x (u+1) array of parameters sampled from the posterior, where n_simul is the number of simulations from the posterior, G is the number of components, u is the number of mixture component parameters (parameter u+1 is the mixture weight)

Value

Returns a named list with the following elements:

graph, the overlap graph

co, the criterion of overlap

References

Martin Metodiev, Nicholas J. Irons, Marie Perrot-Dockès, Pierre Latouche, Adrian E. Raftery. "Easily Computed Marginal Likelihoods for Multivariate Mixture Models Using the THAMES Estimator." arXiv preprint arXiv:2504.21812.

Examples

```
# toy sample from the posterior
mus = rbind(c(17.67849, 21.46734),
            c(17.67849, 21.46734),
            c(16.98067, 21.11391),
            c(20.58628, 21.22104),
            c(17.38332, 21.37224),
            c(16.43644, 21.19085),
            c(19.49676, 21.28964),
            c(17.82287, 21.22475),
            c(18.06050, 21.36945),
            c(18.70759, 21.60244),
            c(15.93795, 21.04681),
            c(16.23184, 20.96049))
sigmasqus = rbind(c(46.75089, 3.660171),
                  c(58.44208, 3.026577),
                  c(63.19334, 4.090872),
```

```
                    c(87.02758, 2.856063),
                    c(82.34268, 3.760550),
                    c(50.92386, 2.380784),
                    c(49.51412, 3.605798),
                    c(38.67681, 3.362407),
                    c(49.59170, 3.130254),
                    c(63.41569, 2.475669),
                    c(65.95225, 3.927501),
                    c(47.22989, 5.465702))
taus = rbind(c(0.2653882, 0.7346118),
             c(0.2560075, 0.7439925),
             c(0.2371868, 0.7628132),
             c(0.2998265, 0.7001735),
             c(0.3518301, 0.6481699),
             c(0.2840316, 0.7159684),
             c(0.2060193, 0.7939807),
             c(0.2859257, 0.7140743),
             c(0.2420695, 0.7579305),
             c(0.2466622, 0.7533378),
             c(0.2726186, 0.7273814),
             c(0.2738916, 0.7261084))
sims = array(dim=c(12,2,3))
sims[,,1] = mus
sims[,,2] = sigmasqus
sims[,,3] = taus

overlapgraph(sims)$co
```

`thames_mixtures` *THAMES estimator of the reciprocal log marginal likelihood for mixture models*

Description

This function computes the THAMES estimate of the reciprocal log marginal likelihood for mixture models using posterior samples and unnormalized log posterior values.

Usage

```
thames_mixtures(
  logpost,
  sims,
  n_samples = NULL,
  c_opt = NULL,
  type = "simple",
  seed = NULL,
  lps = NULL,
  lps_unif = NULL,
  max_iters = Inf
)
```

Arguments

logpost	function logpost(sims,G) to compute lps with input "sims"
sims	n_simul x G x (u+1) array of parameters sampled from the posterior, where n_simul is the number of simulations from the posterior, G is the number of components, u is the number of mixture component parameters (parameter u+1 is the mixture weight)
n_samples	integer, number of posterior samples
c_opt	radius of the ellipsoid used to compute the THAMES
type	THAMES variant ("simple", "permutations", or "standard")
seed	a seed
lps	values of the unnormalized log posterior density
lps_unif	values of the unnormalized log posterior density, evaluated on a uniform sample on the posterior ellipsoid
max_iters	maximum number of shrinkage iterations

Value

Returns a named list with the following elements:

theta_hat, posterior mean

sigma_hat, posterior covariance matrix

log_det_sigma_hat, log-determinant of sigma_hat

logvolA, log-volume of the ellipsoid

log_zhat_inv, log-reciprocal-marginal likelihood

log_zhat_inv_L, lower bound

log_zhat_inv_U, upper bound

alpha, HPD-region correction

len_perms, number of permutations evaluated

log_cor, log-correction of the volume of the ellipsoid

etas, Monte-Carlo sample on the ellipsoid

graph, the overlap graph for G

se, standard_error

phi, ar(1) model parameter

c_opt, radius of the ellipsoid

d_par, dimension of the parameter

G, number of mixture components

scaling, list of fit of QDA (means, covariances)

co, the criterion of overlap

References

Martin Metodiev, Nicholas J. Irons, Marie Perrot-Dockès, Pierre Latouche, Adrian E. Raftery. "Easily Computed Marginal Likelihoods for Multivariate Mixture Models Using the THAMES Estimator." arXiv preprint arXiv:2504.21812.

Examples

```
y = c(9.172, 9.350, 9.483, 9.558, 9.775, 10.227, 10.406, 16.084, 16.170,
  18.419, 18.552, 18.600, 18.927, 19.052, 19.070, 19.330, 19.343, 19.349,
  19.440, 19.473, 19.529, 19.541, 19.547, 19.663, 19.846, 19.856, 19.863,
  19.914, 19.918, 19.973, 19.989, 20.166, 20.175, 20.179, 20.196, 20.215,
  20.221, 20.415, 20.629, 20.795, 20.821, 20.846, 20.875, 20.986, 21.137,
  21.492, 21.701, 21.814, 21.921, 21.960, 22.185, 22.209, 22.242, 22.249,
  22.314, 22.374, 22.495, 22.746, 22.747, 22.888, 22.914, 23.206, 23.241,
  23.263, 23.484, 23.538, 23.542, 23.666, 23.706, 23.711, 24.129, 24.285,
  24.289, 24.366, 24.717, 24.990, 25.633, 26.690, 26.995, 32.065, 32.789,
  34.279)

R <- diff(range(y))
m <- mean(range(y))

# likelihood
loglik_gmm <- function(sims,G){
  mus = sims[,,1]
  sigma_squs = sims[,,2]
  pis = sims[,,3]
  log_single_y = Vectorize(function(x)
    log(rowSums(sapply(1:G,
      function(g) pis[,g]*dnorm(x,mus[,g],sqrt(sigma_squs[,g]))))
    )
  )
  res = suppressWarnings(rowSums(log_single_y(y)))
  return(rowSums(log_single_y(y)))
}

# prior
logprior_gmm_marginal <- function(sims,G) {
  mus = sims[,,1]
  sigma_squs = sims[,,2]
  pis = sims[,,3]

  l_mus <- rowSums(sapply(1:G, function(g) dnorm(mus[,g], mean = m, sd = R,
                                                 log = TRUE)))
  l_pis <- LaplacesDemon::ddirichlet(1:G/G, rep(1,G),log=TRUE)
  l_sigma_squs <- lgamma(2*G+0.2) - lgamma(0.2) +
    0.2*log(10/R^2) - (2*G+0.2) * log(rowSums(sigma_squs^(-1))+10/R^2) -
    3*rowSums(log(sigma_squs))
  return(l_mus + l_pis + l_sigma_squs)
}
# unnormalized log-posterior density
logpost = function(sims){
  G = dim(sims)[2]
```

```
  mus = sims[,1:G,1]
  # apply exp transform
  sims[,1:G,2] = sims[,1:G,2]
  sigma_squs = sims[,1:G,2]
  pis = sims[,1:G,3]

  # set to 0 outside of support
  if(G>2){
    mask = (((pis > 0) & (rowSums(pis[,1:(G-1)])<=1)) & (sigma_squs>0))
  }else{
    mask = (((pis > 0) & (pis[,1]<=1)) & (sigma_squs>0))
  }
  l_total = suppressWarnings(loglik_gmm(sims,G)+
    logprior_gmm_marginal(sims,G))
  l_total[exp(rowSums(log(mask)))==0] = -Inf
  return(l_total)
}

# toy sample from the posterior
mus = rbind(c(17.67849, 21.46734),
            c(17.67849, 21.46734),
            c(16.98067, 21.11391),
            c(20.58628, 21.22104),
            c(17.38332, 21.37224),
            c(16.43644, 21.19085),
            c(19.49676, 21.28964),
            c(17.82287, 21.22475),
            c(18.06050, 21.36945),
            c(18.70759, 21.60244),
            c(15.93795, 21.04681),
            c(16.23184, 20.96049))
sigmasqus = rbind(c(46.75089, 3.660171),
                  c(58.44208, 3.026577),
                  c(63.19334, 4.090872),
                  c(87.02758, 2.856063),
                  c(82.34268, 3.760550),
                  c(50.92386, 2.380784),
                  c(49.51412, 3.605798),
                  c(38.67681, 3.362407),
                  c(49.59170, 3.130254),
                  c(63.41569, 2.475669),
                  c(65.95225, 3.927501),
                  c(47.22989, 5.465702))
taus = rbind(c(0.2653882, 0.7346118),
             c(0.2560075, 0.7439925),
             c(0.2371868, 0.7628132),
             c(0.2998265, 0.7001735),
             c(0.3518301, 0.6481699),
             c(0.2840316, 0.7159684),
             c(0.2060193, 0.7939807),
             c(0.2859257, 0.7140743),
             c(0.2420695, 0.7579305),
             c(0.2466622, 0.7533378),
```

```
              c(0.2726186, 0.7273814),
              c(0.2738916, 0.7261084))
sims = array(dim=c(12,2,3))
sims[,,1] = mus
sims[,,2] = sigmasqus
sims[,,3] = taus

# estimate of the log marginal likelihood
-thames_mixtures(logpost,sims)$log_zhat_inv
```

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