

Package ‘bhetGP’

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Type Package

Title Bayesian Heteroskedastic Gaussian Processes

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Description Performs Bayesian posterior inference for heteroskedastic Gaussian processes. Models are trained through MCMC including elliptical slice sampling (ESS) of latent noise processes and Metropolis-Hastings sampling of kernel hyperparameters. Replicates are handled efficiently through a Woodbury formulation of the joint likelihood for the mean and noise process (Binois, M., Gramacy, R., Ludkovski, M. (2018) <[doi:10.1080/10618600.2018.1458625](https://doi.org/10.1080/10618600.2018.1458625)>) For large data, Vecchia-approximation for faster computation is leveraged (Sauer, A., Cooper, A., and Gramacy, R., (2023), <[doi:10.1080/10618600.2022.2129662](https://doi.org/10.1080/10618600.2022.2129662)>). Incorporates 'OpenMP' and SNOW parallelization and utilizes 'C'/C++' under the hood.

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Contents

bhetgp-package	2
bhetGP	3
bhomGP	7

plot	11
predict	12
trim	15
Index	16

bhetgp-package	Package bhetGP
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Description

Performs Bayesian posterior inference for heteroskedastic Gaussian processes (hetGP; Binois, M., Gramacy, R., Ludkovski, M. (2018) <doi:10.48550/arXiv.1611.05902>) Models are trained through MCMC including elliptical slice sampling (ESS) of latent noise processes and Metropolis-Hastings sampling of kernel hyperparameters. For large data, Vecchia-approximation for faster computation is leveraged (Sauer, A., Cooper, A., and Gramacy, R., (2023), <doi:10.48550/arXiv.2204.02904>). Incorporates 'OpenMP' and SNOW parallelization and utilizes 'C'/'C++' under the hood.

Important Functions

- **bhetGP**: conducts MCMC sampling of hyperparameters and latent noise layer for a heteroskedatic GP.
- **bhomGP**: conducts MCMC sampling of hyperparameters for a homoskedastic GP.
- **trim**: cuts off burn-in and optionally thins samples
- **predict**: calculates posterior mean and variance over a set of input locations (optionally calculates EI or entropy)
- **plot**: produces trace plots, hidden layer plots, and posterior predictive plots

Author(s)

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References

M. Binois, Robert B. Gramacy, M. Ludkovski (2018), Practical heteroskedastic Gaussian process modeling for large simulation experiments, Journal of Computational and Graphical Statistics, 27(4), 808–821.

Katzfuss, Matthias, Joseph Guinness, and Earl Lawrence. Scaled Vecchia approximation for fast computer-model emulation. SIAM/ASA Journal on Uncertainty Quantification 10.2 (2022): 537-554.

Sauer, A., Cooper, A., & Gramacy, R. B. (2023). Vecchia-approximated deep Gaussian processes for computer experiments. Journal of Computational and Graphical Statistics, 32(3), 824-837.

Examples

More examples including real-world computer experiments are available at:
<https://bitbucket.org/gramacylab/bhgp/src/main/examples>

bhetGP

*MCMC sampling for Heteroskedastic GP***Description**

Conducts MCMC sampling of hyperparameters and latent noise process $\mathbf{l}_{lam}$ for a hetGP. Separate length scale parameters θ_{lam} and θ_y govern the correlation strength of the hidden layer and outer layer respectively. $\mathbf{l}_{lam}$ layer may have a non-zero nugget g which governs noise for the latent noise layer. τ_{2_y} and $\tau_{2_{lam}}$ control the amplitude of the mean and noise process respectively. In Matern covariance, ν governs smoothness.

Usage

```
bhetGP(
  x = NULL,
  y = NULL,
  reps_list = NULL,
  nmcmc = 1000,
  sep = TRUE,
  inits = NULL,
  priors = NULL,
  reps = TRUE,
  cov = c("exp2", "matern", "ARD matern"),
  v = 2.5,
  strategy = c("default", "flat"),
  vecchia = FALSE,
  m = min(25, length(y) - 1),
  ordering = NULL,
  verb = TRUE,
  cores = 4
)
```

Arguments

<code>x</code>	vector or matrix of input locations
<code>y</code>	vector of response values
<code>reps_list</code>	list object from <code>hetGP::find_reps</code>
<code>nmcmc</code>	number of MCMC iterations
<code>sep</code>	logical indicating whether to fit isotropic GP (<code>sep = FALSE</code>) or seperable GP (<code>sep = TRUE</code>)
<code>inits</code>	set initial values for hyparameters: $\mathbf{l}_{lam}$, θ_y , θ_{lam} , g , μ_y , μ_{lam} , σ_y , σ_{lam} . Additionally, set initial conditions for tuning: <code>theta_check</code>: logical; if <code>theta_check = TRUE</code>, then ensures that $\theta_{lam} > \theta_y$ i.e., decay of correlation for noise process is slower than mean process.

	• <code>prof_ll_lam</code>: logical; if <code>prof_ll_lam = TRUE</code>, infers <code>tau2_lam</code> i.e., scale parameter for latent noise process • <code>noise</code>: logical; if <code>noise = TRUE</code>, infers nugget <code>g</code> through M-H for latent noise process.
<code>priors</code>	hyperparameters for priors and proposals (see details)
<code>reps</code>	logical; if <code>reps = TRUE</code> uses Woodbury inference adjusting for replication of design points and <code>reps = FALSE</code> does not use Woodbury inference
<code>cov</code>	covariance kernel, either Matern, ARD Matern or squared exponential ("exp2")
<code>v</code>	Matern smoothness parameter (only used if <code>cov = "matern"</code>)
<code>strategy</code>	choose initialization strategy; "default" uses hetGP for <code>vecchia = FALSE</code> settings and sVecchia for <code>vecchia = TRUE</code> . See details.
<code>vecchia</code>	logical indicating whether to use Vecchia approximation
<code>m</code>	size of Vecchia conditioning sets (only used if <code>vecchia = TRUE</code>)
<code>ordering</code>	optional ordering for Vecchia approximation, must correspond to rows of <code>x</code> , defaults to random, is applied to <code>x</code> (only used if <code>vecchia = TRUE</code>)
<code>verb</code>	logical indicating whether to print progress
<code>cores</code>	logical; if <code>vecchia = TRUE</code> , user may specify the number of cores to use for OpenMP parallelization. Defaults to $\min(2, \text{maxcores} - 1)$ where <code>maxcores</code> is the number of detectable available cores.

Details

Maps inputs `x` to mean response `y` and noise levels `llam`. Conducts sampling of the latent noise process using Elliptical Slice sampling. Utilizes Metropolis Hastings sampling of the length scale and nugget parameters with proposals and priors controlled by `priors`. `g` for the noise process is set to a specific value, and by default, is not estimated. When `vecchia = TRUE`, all calculations leverage the Vecchia approximation with specified conditioning set size `m`. `tau2_y` is always inferred from likelihood; `tau2_lam` is inferred by default but may be pre-specified and fixed.

NOTE on OpenMP: The Vecchia implementation relies on OpenMP parallelization for efficient computation. This function will produce a warning message if the package was installed without OpenMP (this is the default for CRAN packages installed on Apple machines). To set up OpenMP parallelization, download the package source code and install using the `gcc/g++` compiler.

Proposals for `g` and `theta` follow a uniform sliding window scheme, e.g.

```
theta_star <- runif(1, 1 * theta_t / u, u * theta_t / 1),
```

with defaults `l = 1` and `u = 2` provided in `priors`. To adjust these, set `priors = list(l = new_l, u = new_u)`. Priors on `g`, `theta_y`, and `theta_lam` follow Gamma distributions with shape parameters (`alpha`) and rate parameters (`beta`) controlled within the `priors` list object. Defaults are

- `priors$alpha$theta_lam <- 1.5`
- `priors$beta$theta_lam <- 4`
- `priors$alpha$theta_y <- 1.5`
- `priors$beta$theta_y <- 4`
- `priors$alpha$g <- 1.5`

- `priors$beta$g <- 4`

`tau2_y` and `tau2_lam` are not sampled; rather directly inferred under conjugate Inverse Gamma prior with shape (alpha) and scale parameters (beta) within the `priors` list object

- `priors$a$tau2_y <- 10`
- `priors$a$tau2_y <- 4`
- `priors$a$tau2_lam <- 10`
- `priors$a$tau2_lam <- 4`

These priors are designed for x scaled to $[0, 1]$ and y having mean `mean_y`. These may be adjusted using the `priors` input.

Initial values for `theta_y`, `theta_lam`, `llam` may be specified by the user. If no initial values are specified, `stratery` will determine the initialization method. `stratery = "default"` leverages `mleHetGP` for initial values of hyper-parameters if `vecchia = FALSE` and Scaled-Vecchia with Stochastic Kriging (Sk-Vec) hybrid approach if `vecchia = TRUE`.

For SK-Vec hybrid approach, scaled Vecchia code from https://github.com/katzfuss-group/scaledVecchia/blob/master/vecchia_scaled.R is used to fit two GPs using the Vecchia approximation. The first for (x, y) pairs, which result in estimated residual sums of squares based on predicted y values. Another GP on (x, s) to obtain latent noise estimates which are smoothed. A script is leveraged internally within this package that fits this method.

Optionally, choose `stratery = "flat"` which will start at uninformative initial values; `llam = log(var(y) * 0.1)` or specify initial values.

The output object of class `bhetgp` or `bhetgp_vec` is designed for use with `trim`, `predict`, and `plot`.

Value

a list of the S3 class `bhetgp` or `bhetgp_vec` with elements:

- `x`: copy of input matrix
- `y`: copy of response mean at inputs (x)
- `Ylist`: list of all responses observed per location (x)
- `A`: number of replicates at each location
- `nmcmc`: number of MCMC iterations
- `priors`: copy of proposal/priors
- `settings`: setting for predictions using `bhetgp` or `bhetgp_vec` object
- `theta_y`: vector of MCMC samples for `theta_y` (length scale of mean process)
- `theta_lam`: matrix of MCMC samples for `theta_lam` (length scale of latent noise process)
- `llam_samples`: matrix of ESS samples for `log lambda` (latent noise process samples)
- `g`: vector of MCMC samples for `g` if inferred
- `tau2`: vector of MAP estimates for `tau2` (scale parameter of mean process)
- `tau2_lam`: vector of MAP estimates for `tau2_lam` (scale parameter of latent noise process)
- `llik_y`: vector of MVN log likelihood of Y for each Gibbs iteration

- `llik_lam`: vector of MVN log likelihood of `llam` i.e. the latent noise process for each Gibbs iteration
- `x_approx`: conditioning set, NN and ordering for `vecchia = TRUE`
- `m`: copy of size of conditioning set for `vecchia = TRUE`
- `time`: computation time in seconds

References

Binois, Mickael, Robert B. Gramacy, and Mike Ludkovski. "Practical heteroscedastic Gaussian process modeling for large simulation experiments." *Journal of Computational and Graphical Statistics* 27.4 (2018): 808-821.

Katzfuss, Matthias, Joseph Guinness, and Earl Lawrence. "Scaled Vecchia approximation for fast computer-model emulation." *SIAM/ASA Journal on Uncertainty Quantification* 10.2 (2022): 537-554.

Sauer, Annie Elizabeth. "Deep Gaussian process surrogates for computer experiments." (2023).

Examples

```
#' @examples
# Additional examples including real-world computer experiments are available at:
# https://bitbucket.org/gramacylab/bhgp/src/main/examples

fx <- function(x){
  result <- (6 * x - 2)^2 * sin(12 * x - 4)
}
rx <- function(x){
  result <- (1.1 + sin(2 * pi * x))^2
  return(result)
}

# Training data
r <- 10
xn <- seq(0, 1, length = 25)
x <- rep(xn, r)

rn <- drop(rx(x))
noise <- as.numeric(t(mvtnorm::rmvnorm(r, sigma = diag(rn, length(xn)))))

f <- fx(x)
y <- f + noise

# Testing data
xx <- seq(0, 1, length = 100)
yy <- fx(xx)

# Example 1: Full model, no Vecchia
fit <- bhetGP(x, y, nmcmc = 100)
fit <- trim(fit, 50, 10)
fit <- predict(fit, xx, cores = 2)
plot(fit) # can run with trace = TRUE to view trace plots
```

```
# Example 2: Vecchia approximated model

fit <- bhetGP(x, y, nmcmc = 100, vecchia = TRUE, m = 5)
fit <- trim(fit, 50, 10)
fit <- predict(fit, xx, cores = 2, vecchia = TRUE)
plot(fit)

# Example 3: Vecchia inference, non-vecchia predictions
fit <- bhetGP(x, y, nmcmc = 200, vecchia = TRUE, m = 5)
fit <- trim(fit, 100, 10)
fit <- predict(fit, xx, cores = 2, vecchia = FALSE)
plot(fit)
```

bhomGP

MCMC sampling for Homoskedastic GP

Description

Conducts MCMC sampling of hyperparameters for a homGP. Separate length scale parameters θ_y govern the correlation strength of the response. g governs noise for the noise. τ_{y^2} control the amplitude of the mean process. In Matern covariance, ν governs smoothness.

Usage

```
bhomGP(
  x = NULL,
  y = NULL,
  reps_list = NULL,
  nmcmc = 1000,
  sep = TRUE,
  inits = NULL,
  priors = NULL,
  cov = c("exp2", "matern", "ARD matern"),
  v = 2.5,
  strategy = c("default", "flat"),
  vecchia = FALSE,
  m = min(25, length(y) - 1),
  ordering = NULL,
  reps = TRUE,
  verb = TRUE,
  cores = 4
)
```

Arguments

<code>x</code>	vector or matrix of input locations
<code>y</code>	vector of response values
<code>reps_list</code>	list object from <code>hetGP::find_reps</code>
<code>nmc</code>	number of MCMC iterations
<code>sep</code>	logical indicating whether to fit isotropic GP (<code>sep = FALSE</code>) or separable GP (<code>sep = TRUE</code>)
<code>inits</code>	set initial values for hyperparameters: <code>theta_y</code> , <code>g</code> , <code>mean_y</code> , <code>scale_y</code> . Additionally, set initial conditions for tuning: <code>prof_ll</code>: logical; if <code>prof_ll = TRUE</code>, infers <code>tau2_y</code> i.e., scale parameter for <code>homGP</code>. <code>noise</code>: logical; if <code>noise = TRUE</code>, infers nugget <code>g</code> through M-H for latent noise process.
<code>priors</code>	hyperparameters for priors and proposals (see details)
<code>cov</code>	covariance kernel, either Matern, ARD Matern or squared exponential ("exp2")
<code>v</code>	Matern smoothness parameter (only used if <code>cov = "matern"</code>)
<code>strategy</code>	choose initialization strategy; "default" uses <code>hetGP</code> for <code>vecchia = FALSE</code> settings and <code>sVecchia</code> for <code>vecchia = TRUE</code> . See details.
<code>vecchia</code>	logical indicating whether to use Vecchia approximation
<code>m</code>	size of Vecchia conditioning sets (only used if <code>vecchia = TRUE</code>)
<code>ordering</code>	optional ordering for Vecchia approximation, must correspond to rows of <code>x</code> , defaults to random, is applied to <code>x</code>
<code>reps</code>	logical; if <code>reps = TRUE</code> uses Woodbury inference adjusting for replication of design points and <code>reps = FALSE</code> does not use Woodbury inference
<code>verb</code>	logical indicating whether to print progress
<code>cores</code>	if <code>vecchia = TRUE</code> , user may specify the number of cores to use for OpenMP parallelization. Defaults to <code>min(2, maxcores - 1)</code> where <code>maxcores</code> is the number of detectable available cores.

Details

Maps inputs `x` to mean response `y`. Utilizes Metropolis Hastings sampling of the length scale and nugget parameters with proposals and priors controlled by `priors`. `g` is estimated by default but may be specified and fixed. When `vecchia = TRUE`, all calculations leverage the Vecchia approximation with specified conditioning set size `m`. `tau2_y` is inferred by default but may be pre-specified and fixed.

NOTE on OpenMP: The Vecchia implementation relies on OpenMP parallelization for efficient computation. This function will produce a warning message if the package was installed without OpenMP (this is the default for CRAN packages installed on Apple machines). To set up OpenMP parallelization, download the package source code and install using the `gcc/g++` compiler.

Proposals for `g` and `theta` follow a uniform sliding window scheme, e.g.

```
theta_star <- runif(1, 1 * theta_t / u, u * theta_t / 1),
```


with defaults $l = 1$ and $u = 2$ provided in priors. To adjust these, set `priors = list(l = new_l, u = new_u)`. Priors on g , θ_{y} follow Gamma distributions with shape parameters (α) and rate parameters (β) controlled within the priors list object. Defaults are

- `priors$alpha$theta_lam <- 1.5`
- `priors$beta$theta_lam <- 4`
- `priors$alpha$theta_y <- 1.5`
- `priors$beta$theta_y <- 4`
- `priors$alpha$g <- 1.5`
- `priors$beta$g <- 4`

$\tau_{2\text{y}}$ is not sampled; rather directly inferred under conjugate Inverse Gamma prior with shape (α) and scale parameters (β) within the priors list object

- `priors$a$tau2_y <- 10`
- `priors$a$tau2_y <- 4`

These priors are designed for x scaled to $[0, 1]$ and y having mean mean_y . These may be adjusted using the priors input.

Initial values for θ_{y} , and g may be specified by the user. If no initial values are specified, strategy will determine the initialization method. `strategy = "default"` leverages `mle-HomGP` for initial values of hyper-parameters if `vecchia = FALSE` and scaled `vecchia` approach if `vecchia = TRUE`.

For scaled `Vecchia` code from https://github.com/katzfuss-group/scaledVecchia/blob/master/vecchia_scaled.R is used to fit a `vecchia` approximated GP to (x, y) . A script is leveraged internally within this package that fits this method.

Optionally, choose `strategy = "flat"` which will start at uninformative initial values or specify initial values.

The output object of class `bhomgp` or `bhomgp_vec` is designed for use with `trim`, `predict`, and `plot`.

Value

a list of the S3 class `bhomgp` or `bhomgp_vec` with elements:

- `x`: copy of input matrix
- `y`: copy of response vector
- `Ylist`: list of all responses observed per location (x)
- `A`: number of replicates at each location
- `nmcmc`: number of MCMC iterations
- `priors`: copy of proposal/prior settings
- `settings`: setting for predictions using `bhetgp` or `bhetgp_vec` object
- `g_y`: vector of MCMC samples for g_y
- `theta_y`: vector of MCMC samples for θ_{y} (length scale of mean process)
- `tau2`: vector of MAP estimates for $\tau_{2\text{y}}$ (scale parameter of outer layer)

- `llik_y`: vector of MVN log likelihood of Y for each Gibbs iteration
- `time`: computation time in seconds
- `x_approx`: conditioning set, NN and ordering for `vecchia = TRUE`
- `m`: copy of size of conditioning set for `vecchia = TRUE`

References

Binois, Mickael, Robert B. Gramacy, and Mike Ludkovski. "Practical heteroscedastic Gaussian process modeling for large simulation experiments." *Journal of Computational and Graphical Statistics* 27.4 (2018): 808-821.

Katzfuss, Matthias, Joseph Guinness, and Earl Lawrence. "Scaled Vecchia approximation for fast computer-model emulation." *SIAM/ASA Journal on Uncertainty Quantification* 10.2 (2022): 537-554.

Sauer, Annie Elizabeth. "Deep Gaussian process surrogates for computer experiments." (2023).

Examples

```
fx <- function(x){
  result <- (6 * x - 2)^2* sin(12 * x - 4)
}

# Training data
r <- 10
xn <- seq(0, 1, length = 25)
x <- rep(xn, r)

f <- fx(x)
y <- f + rnorm(length(x))

# Testing data
xx <- seq(0, 1, length = 100)
yy <- fx(xx)

# Example 1: Full model, no Vecchia
fit <- bhomGP(x, y, nmcmc = 100)
fit <- trim(fit, 50, 10)
fit <- predict(fit, xx)
plot(fit) # can run with trace = TRUE to view trace plots

# Example 2: Vecchia approximated model
fit <- bhomGP(x, y, nmcmc = 100, vecchia = TRUE, m = 5)
fit <- trim(fit, 50, 10)
fit <- predict(fit, xx, vecchia = TRUE)
plot(fit)
```

plot

Plots object from bhetGP package

Description

Acts on a bhetgp, bhetgp_vec, bhomgp or, bhomgp_vec object. Generates trace plots for log likelihood of mean and noise process, length scales of corresponding processes, scale parameters and the nuggets. Generates plots of hidden layers for one-dimensional inputs. Generates plots of the posterior mean and estimated 90% prediction intervals for one-dimensional inputs; generates heat maps of the posterior mean and point-wise variance for two-dimensional inputs.

Usage

```
## S3 method for class 'bhetgp'
plot(x, trace = NULL, predict = NULL, verb = TRUE, ...)

## S3 method for class 'bhomgp'
plot(x, trace = NULL, predict = NULL, verb = TRUE, ...)

## S3 method for class 'bhetgp_vec'
plot(x, trace = NULL, predict = NULL, verb = TRUE, ...)

## S3 method for class 'bhomgp_vec'
plot(x, trace = NULL, predict = NULL, verb = TRUE, ...)
```

Arguments

x	object of class bhetgp, bhetgp_vec, bhomgp, or bhomgp_vec
trace	logical indicating whether to generate trace plots (default is TRUE if the object has not been through predict)
predict	logical indicating whether to generate posterior predictive plot (default is TRUE if the object has been through predict)
verb	logical indicating whether to print plot.
...	N/A

Details

Trace plots are useful in assessing burn-in. If there are too many hyperparameters to plot them all, then it is most useful to visualize the log likelihood (e.g., `plot(fit$l1, type = "l")`).

Value

...N/A

predict	<i>Predict posterior mean and variance/covariance</i>
---------	---

Description

Acts on a `bhetgp`, `bhetgp_vec`, `bhomgp` or `bhomgp_vec` object. Calculates posterior mean and variance/covariance over specified input locations. Optionally utilizes SNOW parallelization.

Usage

```
## S3 method for class 'bhetgp'
predict(
  object,
  x_new,
  lite = TRUE,
  return_all = FALSE,
  interval = c("pi", "ci", "both"),
  lam_ub = TRUE,
  cores = 1,
  samples = TRUE,
  ...
)

## S3 method for class 'bhetgp_vec'
predict(
  object,
  x_new,
  lite = TRUE,
  return_all = FALSE,
  interval = c("pi", "ci", "both"),
  lam_ub = TRUE,
  vecchia = FALSE,
  m = object$m,
  ordering_new = NULL,
  cores = 1,
  samples = TRUE,
  ...
)

## S3 method for class 'bhomgp'
predict(
  object,
  x_new,
  lite = TRUE,
  return_all = FALSE,
  interval = c("pi", "ci", "both"),
  cores = 1,
```

```

    samples = TRUE,
    ...
)

## S3 method for class 'bhomgp_vec'
predict(
  object,
  x_new,
  lite = TRUE,
  return_all = FALSE,
  interval = c("pi", "ci", "both"),
  vecchia = FALSE,
  m = object$m,
  ordering_new = NULL,
  cores = 1,
  samples = TRUE,
  ...
)

```

Arguments

<code>object</code>	object from <code>bhetGP</code> or <code>bhomGP</code> , with burn-in already removed
<code>x_new</code>	matrix of predictive input locations
<code>lite</code>	logical indicating whether to calculate only point-wise variances (<code>lite = TRUE</code>) or full covariance (<code>lite = FALSE</code>)
<code>return_all</code>	logical indicating whether to return mean and point-wise variance prediction for ALL samples (only available for <code>lite = TRUE</code>)
<code>interval</code>	returns predictive variances by default <code>interval = "pi"</code> . <code>interval = "ci"</code> returns variances for only mean process and <code>interval = "both"</code> returns both variances.
<code>lam_ub</code>	logical uses upper 95 quantile for latent noise to obtain predictive variances for the response. If <code>lam_ub = FALSE</code> , the mean latent noise is used for inference.
<code>cores</code>	number of cores to utilize for SNOW parallelization
<code>samples</code>	logical indicating if you want all posterior samples returned including latent layer.
<code>...</code>	N/A
<code>vecchia</code>	logical uses <code>vecchia</code> approximation for prediction if <code>vecchia = TRUE</code> .
<code>m</code>	size of <code>Vecchia</code> conditioning sets (only for fits with <code>vecchia = TRUE</code>), defaults to the <code>m</code> used for MCMC
<code>ordering_new</code>	optional ordering for <code>Vecchia</code> approximation, must correspond to rows of <code>x_new</code> , defaults to random, is applied to all layers in deeper models.

Details

All iterations in the object are used for prediction, so samples should be burned-in. Thinning the samples using `trim` will speed up computation. Posterior moments are calculated using conditional

expectation and variance. As a default, only point-wise variance is calculated. Full covariance may be calculated using `lite = FALSE`.

The posterior predictive variances are returned by default. The variance for the mean process may be obtained by specifying `interval = "ci"`. `interval = "both"` will return both variances.

SNOW parallelization reduces computation time but requires more memory storage.

Value

object of the same class with the following additional elements:

- `x_new`: copy of predictive input locations
- `m_pred`: size of predictive conditioning set if `vecchia = TRUE`
- `mean_y`: predicted posterior mean, indices correspond to `x_new` locations
- `s2_y`: predicted point-wise variances, indices correspond to `x_new` locations (only returned when `lite = TRUE` & `interval = c("pi", "both")`)
- `s2_y_ci`: predicted point-wise variances for the mean process, indices correspond to `x_new` locations (only returned when `lite = TRUE` & `interval = c("ci", "both")`)
- `mean_all`: predicted posterior mean for each sample (column indices), only returned when `return_all = TRUE`
- `s2_all` predicted point-wise variances each sample (column indices), only returned when `return-all = TRUE` & `interval = c("pi", "both")`
- `s2_all_ci` predicted point-wise variances for each sample (column indices), only returned when `return-all = TRUE` & `interval = c("ci", "both")`
- `Sigma`: predicted posterior covariance, indices correspond to `x_new` locations (only returned when `lite = FALSE` & `interval = c("pi", "both")`)
- `Sigma_ci`: predicted posterior covariance for mean process, indices correspond to `x_new` locations (only returned when `lite = FALSE` & `interval = c("ci", "both")`)

Additionally, if object belongs to class `bhetGP` or `bhetGP_vec`, the log-noise process is also predicted for new locations `x_new`. The following are returned:

- `mean_lbugs`: predicted posterior mean for log noise process, indices correspond to `x_new` locations
- `s2_lbugs`: predicted point-wise variances for log noise process, indices correspond to `x_new` locations (only returned when `lite = TRUE` & `interval = c("pi", "both")`)
- `s2_lbugs_ci`: predicted point-wise variances for the log noise process, indices correspond to `x_new` locations (only returned when `lite = TRUE` & `interval = c("ci", "both")`)
- `mean_lbugs_all`: predicted posterior mean for each sample for log noise process (column indices), only returned when `return_all = TRUE`
- `s2_lbugs_all` predicted point-wise variances each sample (column indices) for log noise process, only returned when `return-all = TRUE` & `interval = c("pi", "both")`
- `s2_lbugs_all_ci` predicted point-wise variances for each sample (column indices) for log noise process, only returned when `return-all = TRUE` & `interval = c("ci", "both")`
- `Sigma_lbugs`: predicted posterior covariance for log noise process, indices correspond to `x_new` locations (only returned when `lite = FALSE` & `interval = c("pi", "both")`)

- `Sigma_lnugs_ci`: predicted posterior covariance for log noise process, indices correspond to `x_new` locations (only returned when `lite = FALSE` & `interval = c("ci", "both")`)

Computation time is added to the computation time of the existing object.

trim	<i>Trim/Thin MCMC iterations</i>
------	----------------------------------

Description

Acts on a `bhetgp`, `bhetgp_vec`, `bhomgp`, or `bhomgp_vec` object. Removes the specified number of MCMC iterations (starting at the first iteration). After these samples are removed, the remaining samples are optionally thinned.

Usage

```
trim(object, burn, thin)
```

Arguments

<code>object</code>	object from <code>bhetGP</code> , or <code>bhomGP</code>
<code>burn</code>	integer specifying number of iterations to cut off as burn-in
<code>thin</code>	integer specifying amount of thinning (<code>thin = 1</code> keeps all iterations, <code>thin = 2</code> keeps every other iteration, <code>thin = 10</code> keeps every tenth iteration, etc.)

Details

The resulting object will have `nmc` equal to the previous `nmc` minus `burn` divided by `thin`. Removing burn-ins are necessary following convergence. Thinning is recommended as it can eliminate highly correlated consecutive samples. Additionally, the size of the object reduces and ensures faster prediction.

Value

object of the same class with the selected iterations removed

Index

bhetGP, [2](#), [3](#)
bhetGP-package (bhetgp-package), [2](#)
bhetgp-package, [2](#)
bhomGP, [2](#), [7](#)

plot, [2](#), [11](#)
predict, [2](#), [12](#)

trim, [2](#), [15](#)