Package 'vbayesGP'

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Type Package

Title Gaussian Variational Approximation to Gaussian Process Regression

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Description Implements Gaussian variational approximation to
Bayesian semiparametric regression with Gaussian process prior based on
the Radial basis function (RBF) kernel. Consider the normal prior,
the independent normal priors, or the horseshoe prior on
the positive real number for the lengthscale parameters of the RBF kernel.

License GPL-2

Imports Rcpp (>= 1.0.8), fields, ggplot2, MASS

LinkingTo Rcpp, RcppArmadillo

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extractELBO *Extract ELBO from VGPR model fits*

Description

Compute the expected lower bound (ELBO) using the posterior samples for class "gpr"

Usage

```
extractELBO(object, nsamples = 1000)
```

Arguments

object	an object of class gpr.
nsamples	(positive integer), number of posterior samples to draw and save, defaults to 1000.

Author(s)

Seongil Jo

See Also

gvagpr

extractPostSamps *Extract Posterior Samples from VGPR model fits*

Description

Generate the posterior samples for class "gpr"

Usage

```
extractPostSamps(object, nsamples = 1000)
```

Arguments

object	an object of class gpr.
nsamples	(positive integer), number of posterior samples to draw and save, defaults to 1000.

Value

a data frame including posterior samples for β, σ^2, λ_f, and γ. If `object$id` is not `NULL`, the data frame also includes $b_i, i = 1, \ldots, N$.

Author(s)

Seongil Jo

See Also

gvagpr

`fitted.gpr` *Extract GPR Model Fitted Values*

Description

fitted is a generic function which extracts fitted values of nonparametric part from an object of class "gpr"

Usage

```
## S3 method for class 'gpr'
fitted(object, nsamples = 1000, ...)
```

Arguments

`object`	an object of class `gpr`.
`nsamples`	(positive integer) number of posterior samples. Default value is 1000.

Value

`fmean`

posterior mean of nonparametric part.

`fcov`

posterior variance of nonparametric part. an object of class "gprfit", which has the associated method:

* plot (i.e., plot.gprfit)

Author(s)

Seongil Jo

See Also

gvagpr

gvagpr *Gaussian Variational Approximation to Gaussian Process Regression*

Description

Fits the Bayesian kernel machine regression using Gaussian variational approximation algorithm.

Usage

```
gvagpr(
  y,
  X,
  Z,
  id = NULL,
  random.slope = NULL,
  priors = list(),
  covstr = c("diagonal", "fullrank"),
  control = list(),
  minibatch = FALSE,
  verbose = TRUE,
  seed = 1
)
```

Arguments

y	a vector of response of length n.
X	an n-by-p matrix of covariates for parametric term. Should not contain an intercept.
Z	an n-by-M matrix of predictor variables to be included in nonparametric part.
id	optional vector (of length n) of grouping factors for fitting a model with random effects (including both a random intercept and a random slope). If NULL then no random effects will be included.
random.slope	a column index of the matrix (X) including covariates for random slope. If NULL and id is given, the model considers the random intercept only.
priors	a list giving the prior information. The list includes the following parameters (with default values in parentheses): asig (0.001) and bsig (0.001) giving the hyper parameters for σ^2, alam (0.1) and blam (0.01) giving the hyper parameters for λ_f, lam0 (1) and tau0 (1) giving the hyper parameters of the horseshoe prior.
covstr	Either "diagonal" (the default) or "fullrank", indicating which covariance structure of variational distribution is used. The "diagonal" option uses a fully factorized Gaussian for the approximation whereas the fullrank option uses a Gaussian with a full-rank covariance matrix for the approximation.
control	a named list of parameters to control the algorithm's behavior. The list includes the following parameters (with default values in parentheses): max_iter (100000) giving the maximum number of iterations, rho (0.95) giving the decaying constant, eps (1e-6) giving the small positive constant added to ensure the denominator of the step size is positive and the initial step size is nonzero, nws (2500) giving rolling window size for calculating the moving average of the lower bounds, nsp (100) giving the maximum patience parameter.

`minibatch`	TRUE or FALSE: If `TRUE`, `nbatch` (the number of batch size) should be given in `control` argument. Default value is $n/100$.
`verbose`	TRUE or FALSE: flag indicating whether to print intermediate diagnostic information during the model fitting.
`seed`	The seed for random number generation. The default is generated from 1 to the maximum integer supported by **R** on the machine.

Details

Jo, and Lee (2023+) proposed the Bayesian semiparametric regression model with Gaussian process prior based on the Radial basis function (RBF) kernel:

$$y_i = x_i^\top \beta + f(z_i) + \epsilon_i, \;\; \epsilon_i \overset{iid}{\sim} N(0, \sigma^2),$$

$$f = (f(z_1), \ldots, f(z_D))^\top \sim GP(0, \sigma^2 \lambda_f K_D), \; z_i = (z_{i1}, \ldots, z_{iM})^\top,$$

where K_D denotes the RBF kernel given as

1) Equal lengthscale parameter:

$$K_D = \left(\exp\left(-\gamma \sum_{m=1}^{M} \|z_i - z_j\|^2 \right) \right)_{i,j=1}^{D}$$

2) Varying lengthscale parameters:

$$K_D = \left(\exp\left(-\sum_{m=1}^{M} \gamma_m \|z_i - z_j\|^2 \right) \right)_{i,j=1}^{D}$$

For the parameters, the following priors are used:

$$\pi(\beta) \propto 1,$$

$$\pi(\sigma^{-2}) = Gamma(a_\sigma, b_\sigma),$$

$$\pi(\lambda_f) = Gamma(a_\lambda, b_\lambda),$$

1) Normal prior:

$$\pi(\gamma) = N_+(0, \tau_0^2)$$

2) Independent Normal priors:

$$\pi(\gamma_m) = N_+(0, \tau_0^2), \; m = 1, \ldots, M$$

3) Horseshoe prior:

$$\pi(\gamma_m \mid \lambda_m, \tau_\gamma) = N_+(0, \lambda_m^2 \tau_\gamma^2), \; m = 1, \ldots, M$$

$$\pi(\lambda_m) = C_+(0, \lambda_0), \; m = 1, \ldots, M$$

$$\pi(\tau_\gamma) = C_+(0, \tau_0),$$

where $a_\sigma, b_\sigma, a_\lambda, b_\lambda, \lambda_0$ and τ_0 are positive constants specified by users.

For more details, see Jo and Lee (2023+).

Value

an object of class "gpr", which has the associated methods:

* extractELBO

* fitted (i.e., fitted.gpr)

* summary (i.e., summary.gpr)

* predict (i.e., predict.gpr)

* plot (i.e., plot.gpr)

Author(s)

Seongil Jo and Woojoo Lee

References

Jo, S., and Lee, W. (2023+), "Gaussian variational inference for Bayesian kernel machine regression with Horseshoe prior for estimating high-dimensional exposures", *preprint*.

Titsias, M. K. and L\'azaro-Gredilla, M. (2014), "Doubly stochastic variational Bayes for non-conjugate inference", *Proceedings of the 31st ICML*.

Bobb, J. F., Valeri, L., Claus, H. B., Christiani, D. C., Wright, R. O., Mazumdar, M., Godleski, J. J., and Coull, B. A. (2015). "Bayesian Kernel Machine Regression for Estimating the Health Effects of Multi-Pollutant Mixtures", *Biostatistics*, 16, 493-508.

Chen, H., Zheng, L., Kontai, R. A., and Raskutti, G. (2022), "Gaussian process parameter estimation using mini-batch stochastic gradient descent: convergence guarantees and empirical benefits", *Journal of Machine Learning Research*, 23, 1-59.

See Also

extractELBO, fitted.gpr, predict.gpr, plot.gpr, summary.gpr

Examples

```
## Not run:
sdat <- bkmr::SimData()
y <- sdat$y
X <- sdat$X
Z <- sdat$Z

fout <- vbayesGP::gvagpr(y, X, Z, priors = list(lengthscale = 'normal'), covstr = 'diagonal')
plot(fout)
summary(fout)
vbayesGP::extractELBO(fout)  # ELBO
## End(Not run)
```

plot.gpr *Plot Diagnostics for a gpr Object*

Description

Provides a plot of the smoothed evidence lower bound (ELBO) against iterations for checking the convergence.

Usage

```
## S3 method for class 'gpr'
plot(object, nsamples = 1000, ...)
```

Arguments

object	gpr object, result of **gvagpr**.

Author(s)

Seongil Jo

See Also

gvagpr

predict.gpr *Extract GPR Model Predicted Values*

Description

predicted is a generic function which extracts predicted values for nonparametric part from an object of class "gpr"

Usage

```
## S3 method for class 'gpr'
predict(object, Z_new, ...)
```

Arguments

object	an object of class gpr.
Z_new	a matrix of new predictor values at which to predict new f, where each row represents a new observation.

Value

`fmean`

posterior mean of nonparametric part.

`fcov`

posterior variance of nonparametric part. an object of class "gprfit", which has the associated method:

* plot (i.e., plot.gprfit)

Author(s)

Seongil Jo

See Also

gvagpr

`print.gpr` *Print basic summary of gpr model fit*

Description

print method for class "gpr"

Usage

```
## S3 method for class 'gpr'
print(object, ...)
```

Arguments

`object`	an object of class `gpr`.

Author(s)

Seongil Jo

See Also

gvagpr

summary.gpr *Summarizing gpr model fits*

Description

summary method for class "gpr"

Usage

```
## S3 method for class 'gpr'
summary(object, q = c(0.025, 0.975), digits = 5, nsamples = 1000, ...)
```

Arguments

object	an object of class gpr.
q	quantiles of posterior distribution (credible interval) to show.
digits	the number of digits to show when printing.
nsamples	(positive integer), number of posterior samples to draw and save, defaults to 1000.

Author(s)

Seongil Jo

See Also

gvagpr

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