Package 'vbayesGP'

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Title Gaussian Variational Approximation to Gaussian Process Regression

Type Package

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Author Seongil Jo [aut, cre], Woojoo Lee [aut]	
Maintainer Seongil Jo <bstatsjo@gmail.com></bstatsjo@gmail.com>	
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.	
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computeOverallRisk

Calculate Overall Risk Summaries

Description

Compare estimated f function when all predictors are at a particular quantile to when all are at a second fixed quantile

Usage

```
computeOverallRisk(
  object,
  qs = seq(0.25, 0.75, by = 0.05),
  q.fixed = 0.5,
  nsamples = 1000,
  ...
)
```

Arguments

object an object of class gpr obtained from **gvagpr** function
qs vector of quantiles at which to calculate the overall risk summary
q.fixed a second quantile at which to compare the estimated f function
nsamples (positive integer), number of posterior samples to draw and save, defaults to
1000
.... unused argument

Value

a data frame containing the (posterior mean) estimate and posterior standard deviation of the overall risk measures

References

Bobb J (2023). _bkmr: Bayesian Kernel Machine Regression_. R package version 0.2.2, https://github.com/jenfb/bkmr.

See Also

computePPIPs 3

Examples

```
## Not run:
## First generate dataset
set.seed(111)
dat <- bkmr::SimData(n = 50, M = 4)
y <- dat$y
Z <- dat$Z
X <- dat$X

set.seed(111)
priors <- list(lengthscale = 'horseshoe')
fout <- vbayesGP::gvagpr(y = y, Z = Z, X = X, priors = priors, covstr = 'diagonal')
risks.overall <- vbayesGP::computeOverallRisk(fout, qs = seq(0.25, 0.75, by = 0.05), q.fixed = 0.5)
plot(risk.overall)
## End(Not run)</pre>
```

computePPIPs

Compute pseudo posterior inclusion probabilities (PPIPs) from VGPR

model fits

Description

Compute pseudo posterior inclusion probabilities (PPIPs) using Sequential-2-Means from Variational Gaussian Process Regression (VGPR) model fit

Usage

```
computePPIPs(object, nsamples = 1000, ntuning = 10)
```

Arguments

object an object of class gpr

nsamples (positive integer), number of posterior samples to draw and save, defaults to

1000

ntuning the number of chosen values of the tuning parameter for variable selection

Value

a data frame including the variable-specific PPIPs for VGPR fit with horseshoe prior

Author(s)

Seongil Jo

References

Li, H. and Pati, D. (2017). "Variable Selection Using Shrinkage Priors", Computational Statistics and Data Analysis, 107, 107-119.

See Also

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computeSingVarInt

Single Variable Interaction Summaries

Description

Compare the single-predictor health risks when all of the other predictors in Z are fixed to their a specific quantile to when all of the other predictors in Z are fixed to their a second specific quantile.

Usage

```
computeSingVarInt(
  object,
  which.z,
  qs.diff = c(0.25, 0.75),
  qs.fixed = c(0.25, 0.75),
  nsamples = 1000,
  ...
)
```

Arguments

object	an object of class gpr obtained from gyagpr function
which.z	vector indicating which variables (columns of Z) for which the summary should be computed
qs.diff	vector indicating the two quantiles at which to compute the single-predictor risk summary
qs.fixed	vector indicating the two quantiles at which to fix all of the remaining exposures in Z
nsamples	(positive integer), number of posterior samples to draw and save, defaults to 1000
	unused argument

Value

a data frame containing the (posterior mean) estimate and posterior standard deviation of the single-predictor risk measures

Examples

```
## Not run:
## First generate dataset
set.seed(111)
dat <- bkmr::SimData(n = 50, M = 4)
y <- dat$y
Z <- dat$Z
X <- dat$X

set.seed(111)
priors <- list(lengthscale = 'horseshoe')
fout <- vbayesGP::gvagpr(y = y, Z = Z, X = X, priors = priors, covstr = 'diagonal')
risks.int <- computeSingVarInt(fout)</pre>
```

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```
plot(risks.int)
## End(Not run)
```

computeSingVarRisk

Single Variable Risk Summaries

Description

Compute summaries of the risks associated with a change in a single variable in Z from a single level (quantile) to a second level (quantile), for the other variables in Z fixed to a specific level (quantile)

Usage

```
computeSingVarRisk(
  object,
  which.z,
  qs.diff = c(0.25, 0.75),
  q.fixed = c(0.25, 0.5, 0.75),
  nsamples = 1000,
  ...
)
```

Arguments

object	an object of class gpr obtained from gvagpr function.
which.z	vector indicating which variables (columns of Z) for which the summary should be computed
qs.diff	vector indicating the two quantiles q_1 and q_2 at which to compute $f(z_{q2}) - f(z_{q1})$
q.fixed	vector of quantiles at which to fix the remaining predictors in Z
nsamples	(positive integer), number of posterior samples to draw and save, defaults to 1000
	unused argument

Value

a data frame containing the (posterior mean) estimate and posterior standard deviation of the single-predictor risk measures

References

Bobb J (2023). _bkmr: Bayesian Kernel Machine Regression_. R package version 0.2.2, https://github.com/jenfb/bkmr:

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Examples

```
## Not run:
## First generate dataset
set.seed(111)
dat <- bkmr::SimData(n = 50, M = 4)
y <- dat$y
Z <- dat$Z
X <- dat$X

set.seed(111)
fout <- vbayesGP::gvagpr(y = y, Z = Z, X = X, priors = priors, covstr = 'diagonal')
risks.singvar <- computeSingVarRisk(fout)
plot(risk.singvar)
## End(Not run)</pre>
```

extractELB0

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

extractPostSamps 7

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.

... unused argument.

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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 = sample.int(.Machine$integer.max, 1)
)
```

Arguments

У	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.

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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.

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.

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.

TRUE or FALSE: If TRUE, nbatch (the number of batch) should be given in control argument and max_iter denotes the number of epoch. Default value is n/150.

TRUE or FALSE: flag indicating whether to print intermediate diagnostic information during the model fitting.

The seed for random number generation. The default is generated from 1 to the maximum integer supported by **R** on the machine.

Details

covstr

control

minibatch

verbose

seed

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

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

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

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:

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

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

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

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1) Normal prior:

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

2) Independent Normal priors:

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

3) Horseshoe prior:

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

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

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

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

plot.gpr 11

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)</pre>
```

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(x, ...)
```

Arguments

```
x gpr object, result of gvagpr.... unused argument.
```

Author(s)

Seongil Jo

See Also

12 plot.gprfitBivarLevels

plot.gprfitBivar

Plot bivariate predictor-response function on a new grid of points

Description

Provides a plot of bivariate predictor-response function on a new grid of points

Usage

```
## S3 method for class 'gprfitBivar' plot(x, ...)
```

Arguments

```
x gpr object, result of predictorResponseBivar.... unused argument.
```

Author(s)

Seongil Jo

See Also

gvagpr predictorResponseBivar

```
plot.gprfitBivarLevels
```

Plot interactions

Description

Provides a plot of the predictor-response function of a single predictor in Z for the second predictor in Z fixed at various quantiles

Usage

```
## S3 method for class 'gprfitBivarLevels' plot(x, ...)
```

Arguments

```
x gpr object, result of predictorResponseBivarLevels.... unused argument.
```

Author(s)

Seongil Jo

See Also

gvagpr predictorResponseBivar

plot.gprfitUnivar 13

plot.gprfitUnivar

Plot univariate predictor-response function on a new grid of points

Description

Provides a plot of univariate predictor-response function on a new grid of points

Usage

```
## S3 method for class 'gprfitUnivar' plot(x, ...)
```

Arguments

x gpr object, result of **predictorResponseUnivar**.

... unused argument.

Author(s)

Seongil Jo

See Also

gvagpr predictorResponseUnivar

plot.risks

Plot Risk Summaries

Description

Provides a plot of risk summaries

Usage

```
## S3 method for class 'risks'
plot(x, ...)
```

Arguments

x risks object, result of computeOverallRisk, computeSingVarRisk, or computeSingVarInt unused argument

Author(s)

Seongil Jo

See Also

gvagpr computeOverallRisk computeSingVarRisk computeSingVarInt

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, nsamples = 1000, ...)
```

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.

nsamples (positive integer) number of posterior samples. Default value is 1000.

... additional arguments affecting the predictions produced.

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

predictorResponseBivar

Predict the exposure-response function at a new grid of points

Description

Predict the exposure-response function at a new grid of points

predictorResponseBivar

Usage

```
predictorResponseBivar(
   fit,
   z.pairs = NULL,
   ngrid = 50,
   q.fixed = 0.5,
   nsamples = 1000,
   min.plot.dist = 0.5,
   center = TRUE,
   verbose = TRUE,
   ...
)
```

Arguments

fit	an object of class gpr
z.pairs	data frame showing which pairs of predictors to plot
ngrid	number of grid points in each dimension
q.fixed	a second quantile at which to compare the estimated f function
nsamples	(positive integer) number of posterior samples. Default value is 1000
min.plot.dist	specifies a minimum distance that a new grid point needs to be from an observed data point in order to compute the prediction; points further than this will not be computed
center	flag for whether to scale the exposure-response function to have mean zero
verbose	TRUE or FALSE: flag of whether to print intermediate output to the screen
	additional arguments affecting the predictions produced

Value

a long data frame with the name of the first predictor, the name of the second predictor, the value of the first predictor, the value of the second predictor, the posterior mean estimate, and the posterior standard deviation of the estimated exposure response function

References

Bobb J (2023). _bkmr: Bayesian Kernel Machine Regression_. R package version 0.2.2, https://github.com/jenfb/bkmr

Examples

```
## Not run:
## First generate dataset
set.seed(111)
dat <- bkmr::SimData(n = 50, M = 4)
y <- dat$y
Z <- dat$Z
X <- dat$X

set.seed(111)
priors = list(lengthscale = 'horseshoe')
fout <- vbayesGP::gvagpr(y = y, Z = Z, X = X, priors = priors, covstr = 'diagonal')</pre>
```

```
## Obtain predicted value on new grid of points for each pair of predictors
## Using only a 10-by-10 point grid to make example run quickly
pred.resp.bivar <- vbayesGP::predictorResponseBivar(fit = fout, min.plot.dist = 1, ngrid = 10)
## End(Not run)</pre>
```

predictorResponseBivarLevels

Plot cross-sections of the bivariate predictor-response function

Description

Function to plot the f function of a particular variable at different levels (quantiles) of a second variable

Usage

```
predictorResponseBivarLevels(
  object,
  Z = NULL,
  qs = c(0.25, 0.5, 0.75),
  both_pairs = TRUE
)
```

Arguments

object obtained from running the function predictorResponseBivar

Z an n-by-M matrix of predictor variables to be included in nonparametric part.

qs vector of quantiles at which to fix the second variable

both_pairs flag indicating whether, if h(z1) is being plotted for z2 fixed at different levels, that they should be plotted in the reverse order as well (for h(z2) at different levels of z1)

Value

a long data frame with the name of the first predictor, the name of the second predictor, the value of the first predictor, the quantile at which the second predictor is fixed, the posterior mean estimate, and the posterior standard deviation of the estimated exposure response function

References

Bobb J (2023). _bkmr: Bayesian Kernel Machine Regression_. R package version 0.2.2, https://github.com/jenfb/bkmr

Examples

```
## Not run:
## First generate dataset
set.seed(111)
dat <- bkmr::SimData(n = 50, M = 4)
y <- dat$y
Z <- dat$Z
X <- dat$X</pre>
```

```
set.seed(111)
priors = list(lengthscale = 'horseshoe')
fout <- vbayesGP::gvagpr(y = y, Z = Z, X = X, priors = priors, covstr = 'diagonal')
## Obtain predicted value on new grid of points for each pair of predictors
## Using only a 10-by-10 point grid to make example run quickly
pred.resp.bivar <- vbayesGP::predictorResponseBivar(fit = fout, min.plot.dist = 1, ngrid = 10)
pred.resp.bivar.levels <- vbayesGP::predictorResponseBivarLevels(pred.resp.df = pred.resp.bivar,
Z = Z, qs = c(0.1, 0.5, 0.9))
## End(Not run)</pre>
```

predictorResponseBivarPair

Predict bivariate predictor-response function on a new grid of points

Description

Predict bivariate predictor-response function on a new grid of points

Usage

```
predictorResponseBivarPair(
   fit,
   whichz1 = 1,
   whichz2 = 2,
   whichz3 = NULL,
   prob = 0.5,
   q.fixed = 0.5,
   nsamples = 1000,
   ngrid = 50,
   min.plot.dist = 0.5,
   center = TRUE,
   ...
)
```

Arguments

fit	an object of class gpr
whichz1	vector identifying the first predictor that (column of Z) should be plotted
whichz2	vector identifying the second predictor that (column of Z) should be plotted
whichz3	vector identifying the third predictor that will be set to a pre-specified fixed quantile (determined by prob)
prob	pre-specified quantile to set the third predictor (determined by whichz3); defaults to 0.5 (50th percentile)
q.fixed	a second quantile at which to compare the estimated f function
nsamples	(positive integer) number of posterior samples. Default value is 1000
ngrid	number of grid points in each dimension

min.plot.dist specifies a minimum distance that a new grid point needs to be from an observed data point in order to compute the prediction; points further than this will not be computed

center flag for whether to scale the exposure-response function to have mean zero additional arguments affecting the predictions produced

Value

a data frame with value of the first predictor, the value of the second predictor, the posterior mean estimate, and the posterior standard deviation

References

Bobb J (2023). _bkmr: Bayesian Kernel Machine Regression_. R package version 0.2.2, https://github.com/jenfb/bkmr

Examples

```
## Not run:
## First generate dataset
set.seed(111)
dat <- bkmr::SimData(n = 50, M = 4)
y <- dat$y
Z <- dat$Z
X <- dat$X

set.seed(111)
priors = list(lengthscale = 'horseshoe')
fout <- vbayesGP::gvagpr(y = y, Z = Z, X = X, priors = priors, covstr = 'diagonal')
## Obtain predicted value on new grid of points
## Using only a 10-by-10 point grid to make example run quickly
pred.resp.bivar12 <- vbayesGP::predictorResponseBivarPair(fit = fout, min.plot.dist = 1, ngrid = 10)
## End(Not run)</pre>
```

predictorResponseUnivar

Predict univariate predictor-response function on a new grid of points

Description

Predict univariate predictor-response function on a new grid of points

Usage

```
predictorResponseUnivar(
   fit,
   which.z = 1:ncol(Z),
   ngrid = 50,
   q.fixed = 0.5,
   nsamples = 1000,
   min.plot.dist = Inf,
   center = TRUE,
```

```
z.names = colnames(Z),
...
)
```

Arguments

fit	an object of class gpr
which.z	vector identifying which predictors (columns of Z) should be plotted
ngrid	number of grid points to cover the range of each predictor (column in Z)
q.fixed	a second quantile at which to compare the estimated f function
nsamples	(positive integer) number of posterior samples. Default value is 1000
min.plot.dist	specifies a minimum distance that a new grid point needs to be from an observed data point in order to compute the prediction; points further than this will not be computed
center	flag for whether to scale the exposure-response function to have mean zero
z.names	a vector of names of predictors Z. Default values are colnames(Z).
	additional arguments affecting the predictions produced.

Value

a long data frame with the predictor name, predictor value, posterior mean estimate, and posterior standard deviation

References

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.

Bobb J (2023). _bkmr: Bayesian Kernel Machine Regression_. R package version 0.2.2, https://github.com/jenfb/bkmr

Examples

```
## Not run:
## First generate dataset
set.seed(111)
dat <- bkmr::SimData(n = 50, M = 4)
y <- dat$y
Z <- dat$Z
X <- dat$X

set.seed(111)
priors <- list(lengthscale = 'horseshoe')
fout <- vbayesGP::gvagpr(y = y, Z = Z, X = X, priors = priors, covstr = 'diagonal')
pred.resp.univar <- vbayesGP::predictorResponseUnivar(fout)
## End(Not run)</pre>
```

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print.gpr

Print basic summary of gpr model fit

Description

```
print method for class "gpr"
```

Usage

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

Arguments

```
x an object of class gpr.... unused argument.
```

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,
   ntuning = 10,
   ...
)
```

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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

ntuning the number of chosen values of the tuning parameter for variable selection, de-

faults to 10

... unused argument.

Author(s)

Seongil Jo

See Also

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