

# Package ‘khaos’

May 9, 2026

**Type** Package

**Title** Bayesian Sparse Polynomial Chaos Expansion

**Version** 2.1.1

**Description** Implements Bayesian polynomial chaos expansion methods for surrogate modeling, uncertainty quantification, and sensitivity analysis. Includes sparse regression-based approaches and adaptive Bayesian models based on reversible-jump Markov chain Monte Carlo. Optional screening and basis-enrichment strategies are provided to improve scalability in moderate to high dimensions.

**Imports** glmnet, mvtnorm

**Suggests** knitr, rmarkdown, lhs, testthat (>= 2.1.0)

**License** BSD\_3\_clause + file LICENSE

**Encoding** UTF-8

**NeedsCompilation** no

**RoxygenNote** 7.3.2

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**Repository** CRAN

**Date/Publication** 2026-04-23 20:30:03 UTC

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adaptive_khaos	<i>Bayesian Adaptive Polynomial Chaos Expansion</i>
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## Description

A wrapper for adaptive Bayesian polynomial chaos expansion models with different coefficient prior formulations.

## Usage

```
adaptive_khaos(
  X,
  y,
  prior_type = "ridge",
  nmcmc = 10000,
  nburn = 9000,
  thin = 1,
  legacy = TRUE,
  verbose = TRUE,
  ...
)
```

## Arguments

X	A data frame or matrix of predictors scaled to lie between 0 and 1.
y	A numeric response vector of length <code>nrow(X)</code> .
prior_type	Character string specifying the coefficient-prior formulation. Currently one of "ridge" or "gprior".
nmcmc	Number of MCMC iterations.
nburn	Number of initial MCMC iterations to discard.
thin	Keep every thin-th retained MCMC sample.
legacy	Logical. If TRUE, reproduces the historical storage behavior of earlier implementations, which may retain stale values in unused portions of the internal vars and degs arrays. If FALSE, these unused entries are cleared more carefully.
verbose	Logical; if TRUE, progress messages are printed.
...	Additional arguments passed to the prior-specific fitting routine.

## Details

Depending on `prior_type`, this function calls either `adaptive_khaos_ridge()` or `adaptive_khaos_gprior()`.

This function dispatches to one of the prior-specific adaptive KHAOS fitting routines:

`prior_type = "ridge"` Calls [adaptive\\_khaos\\_ridge](#).

`prior_type = "gprior"` Calls [adaptive\\_khaos\\_gprior](#).

The wrapper exposes only the most commonly used arguments. Additional prior-specific tuning parameters can be supplied through `...`; see [adaptive\\_khaos\\_ridge](#) and [adaptive\\_khaos\\_gprior](#) for full documentation.

## Value

An object of class `"adaptive_khaos"` containing the fitted model. The object is a list including sampled basis functions, coefficient samples, variance parameters, and additional MCMC output. The specific structure depends on the chosen `prior_type`.

## References

Francom, Devin, and Bruno Sanso. "BASS: An R package for fitting and performing sensitivity analysis of Bayesian adaptive spline surfaces." *Journal of Statistical Software* 94.LA-UR-20-23587 (2020).

Rumsey, K.N., Francom, D., Gibson, G., Tucker, J. D., and Huerta, G. (2026). Bayesian Adaptive Polynomial Chaos Expansions. *Stat*, 15(1), e70151.

## Examples

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391 * ((x[1] - 0.4) * (x[2] - 0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)

fit1 <- adaptive_khaos(X, y)
fit2 <- adaptive_khaos(X, y, prior_type = "gprior")
```

---

adaptive\_khaos\_gprior *Bayesian Adaptive Polynomial Chaos Expansion (Modified g-Prior)*

---

## Description

Adaptive Bayesian polynomial chaos expansion using a modified g-prior. This implementation corresponds to the adaptive Bayesian PCE methodology described in Rumsey et al. (2026)

**Usage**

```

adaptive_khaos_gprior(
  X,
  y,
  degree = 15,
  order = 5,
  nmcmc = 10000,
  nburn = 9000,
  thin = 1,
  max_basis = 1000,
  a_g = 0.001,
  b_g = 1000,
  zeta = 1,
  g2_sample = "mh",
  g2_init = NULL,
  s2_lower = 0,
  a_sigma = 0,
  b_sigma = 0,
  a_M = 4,
  b_M = 4/length(y),
  move_probs = rep(1/3, 3),
  coin_pars = list(function(j) 1/j, 1, 2, 3),
  degree_penalty = 0,
  legacy = TRUE,
  verbose = TRUE
)

adaptive_khaos2(...)

```

**Arguments**

<code>X</code>	A data frame or matrix of predictors scaled to be between 0 and 1
<code>y</code>	a response vector
<code>degree</code>	Maximum polynomial degree for each basis function.
<code>order</code>	Maximum order of interaction for each basis function.
<code>nmcmc</code>	Number of MCMC iterations.
<code>nburn</code>	Number of initial MCMC iterations to discard.
<code>thin</code>	Keep every thin samples.
<code>max_basis</code>	Maximum number of basis functions.
<code>a_g, b_g</code>	Prior parameters for global g-prior term (on precision scale)
<code>zeta</code>	Hyperparameter for modified g-prior. Setting $zeta = 0$ reduces to the usual g-prior.
<code>g2_sample</code>	Character string specifying the method used to sample or update the prior scaling parameter $g\theta^2$ .

<code>g2_init</code>	Initial value of $g_2$ (global precision for g-prior). Becomes the only value when <code>g2_sample = "fixed"</code> .
<code>s2_lower</code>	Lower bound on process variance (numerically useful for deterministic functions).
<code>a_sigma, b_sigma</code>	Shape/rate parameters for the IG prior on process variance (default is Jeffrey's prior)
<code>a_M, b_M</code>	Shape/rate parameters for the Gamma prior on expected number of basis functions.
<code>move_probs</code>	A 3-vector with probabilities for (i) birth, (ii) death, and (iii) mutation.
<code>coin_pars</code>	A list of control parameters for coinflip proposal
<code>degree_penalty</code>	Increasing this value encourages lower order polynomial terms (0 is no penalization).
<code>legacy</code>	Logical. If TRUE, mimics original implementation behavior (from the emulator comparison paper), which may retain invalid basis function structures across iterations. Defaults to FALSE.
<code>verbose</code>	Logical. Should progress information be printed?
<code>...</code>	additional arguments passed to <code>adaptive_khaos</code>

## Details

Implements the RJMCMC algorithm described by Francom & Sanso (2020) for BMARS, modifying it for polynomial chaos basis functions. As an alternative the NKD procedure of Nott et al. (2005), we use a coinflipping procedure to identify useful variables. See writeup (coming soon) for details. The `coin_pars` argument is an ordered list with elements:

1. a function giving proposal probability for  $q_0$ , the expected order of interaction,
2. `epsilon`, the base weight for each variable (`epsilon=Inf` corresponds to uniform sampling),
3. `alpha`, the exponent-learning rate,
4. `num_passes` a numerical parameter only.

Sampling method for  $g_0^2$  depends on `g2_sample`

"f" Fixed: Do not update  $g_0^2$ ; carry forward the previous value (`g2[i] <- g2[i-1]`).

"1f" Laplace-Full: Use a Laplace approximation to sample  $g_0^2$  under the full marginal likelihood (no orthogonality assumption).

"1o" Laplace-Orthogonal: Use a Laplace approximation to sample  $g_0^2$  assuming the orthogonality approximation applies.

"mh" Metropolis-Hastings with full Laplace approximation as proposal. Target is the full posterior density of  $g_0^2$ .

"mho" Metropolis-Hastings with orthogonal Laplace approximation as proposal. Target is the full posterior density of  $g_0^2$ . under the orthogonality assumption.

"mhoo" Metropolis-Hastings with orthogonal Laplace approximation as proposal. Target is the posterior density of  $g_0^2$  under the orthogonality assumption.

Other proposal notes: Expected order  $q_0$  is chosen from  $1:order$  with weights `coin_pars[[1]](1:order)`  
 Degree is chosen from  $q_0:degree$  with weights  $(1:(degree-q_0+1))^{(-degree\_penalty)}$  and a random partition is created (see helper function).

Two types of change steps are possible (and equally likely) A re-ordering of the degrees A single variable is swapped out with another one (only used when  $ncol(X) > 3$ )

## Value

An object of class "adaptive\_khaos". The object is a list containing:

**B** Matrix of basis functions evaluated at the training inputs.

**vars, degs** Arrays encoding the variables and polynomial degrees for each basis function across MCMC iterations.

**nint, dtot** Interaction order and total degree for each basis function.

**nbasis** Number of basis functions per MCMC iteration.

**beta** Posterior samples of regression coefficients.

**s2** Posterior samples of the noise variance.

**lam** Posterior samples of the Poisson rate parameter controlling model size.

**g2** Posterior samples of the global g-prior scaling parameter.

**sum\_sq** Residual sum of squares at each iteration.

**eta** Variable inclusion counts used in the proposal distribution.

**count\_accept, count\_propose** Acceptance and proposal counts for RJMCMC moves.

**prior\_type** Character string indicating the g-prior formulation.

**X, y** Training data.

## References

Francom, Devin, and Bruno Sanso. "BASS: An R package for fitting and performing sensitivity analysis of Bayesian adaptive spline surfaces." *Journal of Statistical Software* 94.LA-UR-20-23587 (2020).

Nott, David J., Anthony YC Kuk, and Hiep Duc. "Efficient sampling schemes for Bayesian MARS models with many predictors." *Statistics and Computing* 15 (2005): 93-101.

Rumsey, K.N., Francom, D., Gibson, G., Derek Tucker, J. and Huerta, G., 2026. Bayesian Adaptive Polynomial Chaos Expansions. *Stat*, 15(1), p.e70151.

## Examples

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391*((x[1]-0.4)*(x[2]-0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)
fit <- adaptive_khaos(X, y)
```

---

adaptive\_khaos\_ridge *Bayesian Adaptive Polynomial Chaos Expansion (Ridge Prior)*

---

## Description

Adaptive Bayesian polynomial chaos expansion using a fixed Gaussian (ridge) prior on coefficients. This implementation corresponds to a simplified version of the adaptive Bayesian PCE methodology described in Rumsey et al. (2026)

## Usage

```
adaptive_khaos_ridge(  
  X,  
  y,  
  degree = 15,  
  order = 5,  
  nmcmc = 10000,  
  nburn = 9000,  
  thin = 1,  
  max_basis = 1000,  
  tau2 = 10^5,  
  s2_lower = 0,  
  g1 = 0,  
  g2 = 0,  
  h1 = 4,  
  h2 = 40/length(y),  
  move_probs = rep(1/3, 3),  
  coin_pars = list(function(j) 1/j, 1, 2, 3),  
  degree_penalty = 0,  
  legacy = TRUE,  
  verbose = TRUE  
)
```

## Arguments

X	A data frame or matrix of predictors scaled to be between 0 and 1
y	a response vector
degree	Maximum polynomial degree for each basis function.
order	Maximum order of interaction for each basis function.
nmcmc	Number of MCMC iterations.
nburn	Number of initial MCMC iterations to discard.
thin	Keep every thin samples.
max_basis	Maximum number of basis functions.
tau2	Prior variance for coefficients

s2_lower	Lower bound on process variance (numerically useful for deterministic functions).
g1, g2	Shape/rate parameters for the IG prior on process variance (default is Jeffrey's prior)
h1, h2	Shape/rate parameters for the Gamma prior on expected number of basis functions.
move_probs	A 3-vector with probabilities for (i) birth, (ii) death, and (iii) mutation.
coin_pars	A list of control parameters for coinflip proposal
degree_penalty	Increasing this value encourages lower order polynomial terms (0 is no penalization).
legacy	Logical. If TRUE, mimics original implementation behavior (from the emulator comparison paper), which may retain invalid basis function structures across iterations. Defaults to FALSE.
verbose	Logical. Should progress information be printed?

### Details

Implements the RJMCMC algorithm described by Francom & Sanso (2020) for BMARS, modifying it for polynomial chaos basis functions. As an alternative the NKD procedure of Nott et al. (2005), we use a coinflipping procedure to identify useful variables. See writeup (coming soon) for details. The coin\_pars argument is an ordered list with elements:

1. a function giving proposal probability for  $q_0$ , the expected order of interaction,
2. epsilon, the base weight for each variable (epsilon=Inf corresponds to uniform sampling),
3. alpha, the exponent-learning rate,
4. num\_passes a numerical parameter only.

Other proposal notes: Expected order  $q_0$  is chosen from  $1:order$  with weights `coin_pars[[1]](1:order)`  
Degree is chosen from  $q_0:degree$  with weights  $(1:(degree-q_0+1))^{(-degree\_penalty)}$  and a random partition is created (see helper function).

Two types of change steps are possible (and equally likely) A re-ordering of the degrees A single variable is swapped out with another one

### Value

An object of class "adaptive\_khaos". The object is a list containing:

**B** Matrix of basis functions evaluated at the training inputs.

**vars, degs** Arrays encoding the variables and polynomial degrees for each basis function across MCMC iterations.

**nint, dtot** Interaction order and total degree for each basis function.

**nbasis** Number of basis functions per MCMC iteration.

**beta** Posterior samples of regression coefficients.

**s2** Posterior samples of the noise variance.

**lam** Posterior samples of the Poisson rate parameter controlling model size.

**sum\_sq** Residual sum of squares at each iteration.  
**eta** Variable inclusion counts used in the proposal distribution.  
**count\_accept, count\_propose** Acceptance and proposal counts for RJMCMC moves.  
**prior\_type** Character string indicating the ridge prior.  
**X, y** Training data.

## References

Francom, Devin, and Bruno Sanso. "BASS: An R package for fitting and performing sensitivity analysis of Bayesian adaptive spline surfaces." *Journal of Statistical Software* 94.LA-UR-20-23587 (2020).

Nott, David J., Anthony YC Kuk, and Hiep Duc. "Efficient sampling schemes for Bayesian MARS models with many predictors." *Statistics and Computing* 15 (2005): 93-101.

Rumsey, K.N., Francom, D., Gibson, G., Derek Tucker, J. and Huerta, G., 2026. Bayesian Adaptive Polynomial Chaos Expansions. *Stat*, 15(1), p.e70151.

## Examples

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391*((x[1]-0.4)*(x[2]-0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)
fit <- adaptive_khaos(X, y)
```

---

 ordinal\_khaos

---

*Ordinal Probit Regression with BA-PCE*


---

## Description

The emulation approach of Francom et al. (2020) for BMARS, modified for polynomial chaos.

## Usage

```
ordinal_khaos(
  X,
  y,
  degree = 15,
  order = 5,
  nmcmc = 10000,
  nburn = 9000,
  thin = 1,
  max_basis = 1000,
  tau2 = 10^5,
  sigma_thresh = 10,
  h1 = 4,
  h2 = 40/length(y),
```

```

move_probs = rep(1/3, 3),
coin_pars = list(function(j) 1/j, 1, 2, 3),
degree_penalty = 0,
verbose = TRUE
)

```

### Arguments

<code>x</code>	A data frame or matrix of predictors scaled to be between 0 and 1
<code>y</code>	a response vector
<code>degree</code>	Maximum polynomial degree for each basis function.
<code>order</code>	Maximum order of interaction for each basis function.
<code>nmcmc</code>	Number of MCMC iterations.
<code>nburn</code>	Number of initial MCMC iterations to discard.
<code>thin</code>	Keep every thin samples.
<code>max_basis</code>	Maximum number of basis functions.
<code>tau2</code>	Prior variance for coefficients
<code>sigma_thresh</code>	Prior variance for the threshold parameters.
<code>h1, h2</code>	Shape/rate parameters for the Gamma prior on expected number of basis functions.
<code>move_probs</code>	A 3-vector with probabilities for (i) birth, (ii) death, and (iii) mutation.
<code>coin_pars</code>	A list of control parameters for coinflip proposal
<code>degree_penalty</code>	Increasing this value encourages lower order polynomial terms (0 is no penalization).
<code>verbose</code>	Logical. Should progress information be printed?

### Details

Implements the RJMCMC algorithm described by Francom & Sanso (2020) for BMARS, modifying it for polynomial chaos basis functions. As an alternative the NKD procedure of Nott et al. (2005), we use a coinflipping procedure to identify useful variables. See writeup (coming soon) for details. The `coin_pars` argument is an ordered list with elements:

1. a function giving proposal probability for  $q_0$ , the expected order of interaction,
2. `epsilon`, the base weight for each variable (`epsilon=Inf` corresponds to uniform sampling),
3. `alpha`, the exponent-learning rate,
4. `num_passes` a numerical parameter only.

Other proposal notes: Expected order  $q_0$  is chosen from  $1:order$  with weights `coin_pars[[1]](1:order)` Degree is chosen from  $q_0:degree$  with weights  $(1:(degree-q_0+1))^{(-degree\_penalty)}$  and a random partition is created (see helper function).

Two types of change steps are possible (and equally likely) A re-ordering of the degrees A single variable is swapped out with another one

**Value**

An object of class "ordinal\_khaos". The object is a list containing:

**B** Matrix of basis functions evaluated at the training inputs.

**vars, degs** Arrays encoding the variables and polynomial degrees for each basis function across MCMC iterations.

**nint, dtot** Interaction order and total degree for each basis function.

**nbasis** Number of basis functions per MCMC iteration.

**beta** Posterior samples of regression coefficients.

**thresh** Posterior samples of the ordinal threshold parameters.

**s2z** Estimated latent variance across iterations.

**lam** Posterior samples of the Poisson rate parameter controlling model size.

**eta** Variable inclusion counts used in the proposal distribution.

**count\_accept, count\_propose** Acceptance and proposal counts for RJMCMC moves.

**X, y** Training data.

**References**

Francom, Devin, and Bruno Sanso. "BASS: An R package for fitting and performing sensitivity analysis of Bayesian adaptive spline surfaces." *Journal of Statistical Software* 94.LA-UR-20-23587 (2020).

Nott, David J., Anthony YC Kuk, and Hiep Duc. "Efficient sampling schemes for Bayesian MARS models with many predictors." *Statistics and Computing* 15 (2005): 93-101.

**Examples**

```
set.seed(1)
X <- matrix(runif(200), ncol = 1)
y <- sample(1:4, 200, replace = TRUE)
fit <- ordinal_khaos(X, y, nmcmc = 2000, nburn = 1000, thin = 2, verbose = FALSE)
plot(fit)
```

---

plot.adaptive\_khaos     *Plot Method for class adaptive\_khaos*

---

**Description**

See adaptive\_khaos() for details.

**Usage**

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

**Arguments**

`x` An object returned by the `adaptive_khaos()` function.  
`...` Additional arguments for plotting

**Details**

Plot function for `adaptive_khaos` object.

**Value**

No return value; called for its side effects (plotting).

**References**

Francom, Devin, and Bruno Sanso. "BASS: An R package for fitting and performing sensitivity analysis of Bayesian adaptive spline surfaces." *Journal of Statistical Software* 94.LA-UR-20-23587 (2020).

**Examples**

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391*((x[1]-0.4)*(x[2]-0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)
fit <- adaptive_khaos(X, y)
plot(fit)
```

---

plot.ordinal\_khaos *Plot Method for class ordinal\_khaos*

---

**Description**

Produces a 2x2 diagnostic plot: (1) trace of the number of basis functions; (2) jittered predicted vs. actual classes with point size indicating posterior support; (3) posterior mean class probabilities on `x$X` (lines if 1D, otherwise barplot of averages); (4) histogram of latent means  $f(x)$  with posterior-average thresholds overlaid.

**Usage**

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

**Arguments**

`x` An object of class `ordinal_khaos`.  
`...` additional arguments passed to `plot`

**Details**

Panel (2) uses `predict(x, type="class", aggregate=FALSE)` to compute per-draw MAP classes, plotting the modal class vs. observed class; point size reflects the fraction of draws supporting the modal class. Panel (3) uses `predict(x, type="prob")` to plot posterior mean class probabilities. Panel (4) uses `predict(x, type="latent", aggregate=FALSE)` to pool latent means across draws and overlays posterior-average cutpoints (handles either stored  $\gamma_1, \dots, \gamma_{K-1}$  or  $\gamma_2, \dots, \gamma_{K-1}$  with  $\gamma_1 \equiv 0$ ).

**Value**

Invisibly returns NULL.

**Examples**

```
set.seed(1)
X <- matrix(runif(200), ncol = 1)
y <- sample(1:4, 200, replace = TRUE)
fit <- ordinal_khaos(X, y, nmc = 2000, nburn = 1000, thin = 2, verbose = FALSE)
plot(fit)
```

---

plot.sparse\_khaos      *Plot Method for class sparse\_khaos*

---

**Description**

See `sparse_khaos()` for details.

**Usage**

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

**Arguments**

`x`                    An object returned by the `sparse_khaos()` function.  
`...`                additional arguments passed to `plot`

**Details**

Plot function for `sparse_khaos` object.

**Value**

returns `invisible(x)`

## References

Shao, Q., Younes, A., Fahs, M., & Mara, T. A. (2017). Bayesian sparse polynomial chaos expansion for global sensitivity analysis. *Computer Methods in Applied Mechanics and Engineering*, 318, 474-496.

## Examples

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391*((x[1]-0.4)*(x[2]-0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)
fit <- sparse_khaos(X, y)
plot(fit)
```

---

predict.adaptive\_khaos

*Predict Method for class adaptive\_khaos*

---

## Description

See adaptive\_khaos() for details.

## Usage

```
## S3 method for class 'adaptive_khaos'
predict(
  object,
  newdata = NULL,
  mcmc.use = NULL,
  nugget = FALSE,
  nreps = 1,
  ...
)
```

## Arguments

object	An object returned by the adaptive_khaos() function.
newdata	A dataframe of the same dimension as the training data.
mcmc.use	Which posterior samples should be used for prediction?
nugget	Logical. Should predictions include error?
nreps	How many predictions should be taken for each mcmc sample (ignored when nugget = FALSE).
...	Additional arguments to predict

## Details

Predict function for adaptive\_khaos object.

**Value**

A numeric matrix of posterior predictive samples, with rows corresponding to samples and columns corresponding to observations.

**References**

Francom, Devin, and Bruno Sanso. "BASS: An R package for fitting and performing sensitivity analysis of Bayesian adaptive spline surfaces." *Journal of Statistical Software* 94.LA-UR-20-23587 (2020).

**Examples**

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391*((x[1]-0.4)*(x[2]-0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)
fit <- adaptive_khaos(X, y)
predict(fit)
```

---

predict.ordinal\_khaos *Predict Method for class ordinal\_khaos*

---

**Description**

Compute posterior predictive quantities for an ordinal probit BA-PCE model. For each selected MCMC draw, the method builds the polynomial chaos basis, forms the linear predictor  $f(x) = B(x)\beta$ , reconstructs the ordered cutpoints, and returns either category probabilities, MAP classes, or latent means. Results can be averaged across draws or returned per-draw.

**Usage**

```
## S3 method for class 'ordinal_khaos'
predict(
  object,
  newdata = NULL,
  mcmc.use = NULL,
  type = c("class", "prob", "latent"),
  aggregate = FALSE,
  ...
)
```

**Arguments**

object	An object of class <code>ordinal_khaos</code> returned by <code>ordinal_khaos()</code> .
newdata	A data frame or matrix of predictors on the same scale and with the same columns as used for fitting. If <code>NULL</code> , uses <code>object\$X</code> .

mcmc.use	Integer vector of posterior draw indices to use. If NULL, uses all stored draws (i.e., seq_along(object\$nbasis)).
type	Character; one of "prob", "class", or "latent". "prob" returns category probabilities $P(Y = k   x)$ for $k = 1, \dots, K$ . "class" returns MAP classes. "latent" returns the latent mean $f(x)$ (i.e., $B(x)\beta$ ) for each draw.
aggregate	Logical (default FALSE); if TRUE, averages results across the selected MCMC draws (probabilities are averaged; classes are aggregated by simple voting; latent means are averaged). If FALSE, returns per-draw arrays.
...	Unused; included for method compatibility.

### Details

Let  $Z = f_\beta(X) + \varepsilon$  with  $\varepsilon \sim \mathcal{N}(0, 1)$  and ordered cutpoints  $\gamma_0 = -\infty < \gamma_1 < \dots < \gamma_{K-1} < \gamma_K = \infty$ . For a new input  $x$ , the category probabilities are

$$P(Y = k | x) = \Phi(\gamma_k - f(x)) - \Phi(\gamma_{k-1} - f(x)).$$

The function reconstructs the full cutpoint vector internally. If the fitted object stored  $\gamma_1, \dots, \gamma_{K-1}$  then these are used directly; if it stored only  $\gamma_2, \dots, \gamma_{K-1}$  (with  $\gamma_1 \equiv 0$ ) the missing fixed cutpoint is inserted automatically.

### Value

If type = "prob" and aggregate = TRUE, an  $\text{nrow}(\text{newdata}) \times K$  numeric matrix of posterior mean category probabilities. If aggregate = FALSE, a 3-D array of dimension  $(\#\text{draws}) \times \text{nrow}(\text{newdata}) \times K$ .

If type = "class" and aggregate = TRUE, an integer vector of length  $\text{nrow}(\text{newdata})$  with MAP classes aggregated by voting across draws. If aggregate = FALSE, a  $(\#\text{draws}) \times \text{nrow}(\text{newdata})$  integer matrix of per-draw MAP classes.

If type = "latent", returns the latent mean(s)  $f(x)$ : a numeric vector of length  $\text{nrow}(\text{newdata})$  if aggregate = TRUE, or a  $(\#\text{draws}) \times \text{nrow}(\text{newdata})$  numeric matrix otherwise.

A numeric matrix of posterior predictive samples, with rows corresponding to samples and columns corresponding to observations.

### References

Hoff, Peter D. (2009). *A First Course in Bayesian Statistical Methods*. Springer. (See ordinal probit data augmentation.)

Francom, Devin, and Bruno Sanso (2020). "BASS: An R package for fitting and performing sensitivity analysis of Bayesian adaptive spline surfaces." *Journal of Statistical Software* 94. LA-UR-20-23587.

### See Also

[ordinal\\_khaos](#) for model fitting.

**Examples**

```

# Toy example (X scaled to [0,1])
set.seed(1)
X <- lhs::maximinLHS(200, 3)
# Suppose y has K=4 ordered categories:
fit <- ordinal_khaos(X, sample(1:4, 200, replace=TRUE),
                    nmc = 2000, nburn = 1000, thin = 2, verbose = FALSE)

# Posterior mean probabilities for each class
p_hat <- predict(fit, newdata = X, type = "prob", aggregate = TRUE)

# MAP classes (aggregated across draws)
y_hat <- predict(fit, newdata = X, type = "class")

# Latent mean f(x)
f_hat <- predict(fit, newdata = X, type = "latent")

```

---

predict.sparse\_khaos *Predict Method for class sparse\_khaos*

---

**Description**

See sparse\_khaos() for details.

**Usage**

```

## S3 method for class 'sparse_khaos'
predict(object, newdata = NULL, samples = 1000, nugget = FALSE, ...)

```

**Arguments**

object	An object returned by the sparse_khaos() function.
newdata	A dataframe of the same dimension as the training data.
samples	How many posterior samples should be taken at each test point? If 0 or FALSE, then the MAP estimate is returned.
nugget	logical; should predictions include error? If FALSE, predictions will be for mean.
...	Additional arguments to predict

**Details**

Predict function for sparse\_khaos object.

**Value**

A numeric matrix of predictive samples (or a vector if `samples = FALSE`), with rows corresponding to samples and columns corresponding to observations.

**References**

Shao, Q., Younes, A., Fahs, M., & Mara, T. A. (2017). Bayesian sparse polynomial chaos expansion for global sensitivity analysis. *Computer Methods in Applied Mechanics and Engineering*, 318, 474-496.

**Examples**

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391*((x[1]-0.4)*(x[2]-0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)
fit <- sparse_khaos(X, y)
predict(fit)
```

---

`print.sparse_khaos`      *Print Method for class sparse\_khaos*

---

**Description**

See `sparse_khaos()` for details.

**Usage**

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

**Arguments**

`x`                      An object returned by the `sparse_khaos()` function.  
`...`                    additional arguments passed to or from other methods.

**Details**

Print function for `sparse_khaos` object.

**Value**

The input object `x`, invisibly.

**References**

Shao, Q., Younes, A., Fahs, M., & Mara, T. A. (2017). Bayesian sparse polynomial chaos expansion for global sensitivity analysis. *Computer Methods in Applied Mechanics and Engineering*, 318, 474-496.

**Examples**

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391*((x[1]-0.4)*(x[2]-0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)
fit <- sparse_khaos(X, y)
print(fit)
```

sobol\_khaos

*Compute Sobol Sensitivity Indices for khaos Models***Description**

Computes first-order, total-effect, and full interaction Sobol indices from an adaptive KHAOS model fit. Returns MCMC samples of sensitivity indices, including all active interaction terms used in the model.

**Usage**

```
sobol_khaos(obj, plot_it = TRUE, samples = 1000)
```

**Arguments**

obj	An object of class "adaptive_khaos" returned by adaptive_khaos() or of class "sparse_khaos" returned by sparse_khaos().
plot_it	Logical; if TRUE, boxplots of the sensitivity indices are shown.
samples	How many samples from the posterior (only used for sparse class).

**Value**

A list with the following components:

**S** A data frame of Sobol indices for all main effects and interactions (MCMC samples).

**T** A data frame of total-effect Sobol indices (MCMC samples).

**leftover** A numeric vector of unexplained variance proportions (residuals).

**Examples**

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391*((x[1]-0.4)*(x[2]-0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)
fit <- adaptive_khaos(X, y)
sob <- sobol_khaos(fit)
head(sob$S)
```

sparse\_khaos

*Bayesian Sparse Polynomial Chaos Expansion***Description**

A Bayesian sparse polynomial chaos expansion (PCE) method based on the forward-selection framework of Shao et al. (2017), with optional enrichment strategies that adapt the candidate basis set across degree and interaction-order expansions.

**Usage**

```
sparse_khaos(
  X,
  y,
  degree = c(2, 2, 16),
  order = c(1, 1, 5),
  prior = c(1, 1, 1),
  lambda = 1,
  rho = 0,
  regularize = TRUE,
  max_basis = 1e+06,
  enrichment = "adaptive",
  adaptive_ladder = c(10000, 1e+05),
  verbose = TRUE
)
```

**Arguments**

<code>X</code>	A data frame or matrix of predictors scaled to lie between 0 and 1.
<code>y</code>	A numeric response vector of length <code>nrow(X)</code> .
<code>degree</code>	Integer vector of length 3 giving the polynomial-degree schedule: <code>c(d_init, d_increment, d_max)</code> .
<code>order</code>	Integer vector of length 3 giving the interaction-order schedule: <code>c(q_init, q_increment, q_max)</code> .
<code>prior</code>	Numeric vector of prior hyperparameters <code>c(n0, v0, s0)</code> , where <code>n0</code> controls shrinkage of the regression coefficients, <code>v0</code> is the degrees-of-freedom parameter for the inverse-gamma prior on $\sigma^2$ , and <code>s0</code> is the scale parameter for that prior.
<code>lambda</code>	Nonnegative penalty parameter used in the KIC calculation. Larger values favor sparser models.
<code>rho</code>	Basis functions are discarded after partial-correlation screening if their squared partial correlation is smaller than <code>rho</code> .
<code>regularize</code>	Logical; if TRUE, a weighted LASSO pre-screen is used to reduce the candidate basis set before partial-correlation ranking.

max_basis	Maximum number of candidate basis functions allowed in any fitting round. This acts as a hard cap on computational cost.
enrichment	Either an integer in 0:4 specifying a fixed enrichment strategy, or the character string "adaptive", which allows the strategy to become more restrictive when the next candidate set would otherwise be too large. See Details.
adaptive_ladder	Numeric vector of candidate-size thresholds used only when enrichment = "adaptive". The ladder should have length between 1 and 4, be sorted in increasing order, and satisfy $\max(\text{adaptive\_ladder}) \leq \text{max\_basis}$ . Internally, the ladder is used to determine when the algorithm should fall back to a more restrictive enrichment strategy before attempting the next recursion step.
verbose	Logical; if TRUE, progress messages are printed.

## Details

For fixed maximum degree and interaction order, the method constructs a candidate library of polynomial basis functions, ranks them using marginal correlations and sequential partial correlations, and evaluates nested models using the Kashyap information criterion (KIC). The best-ranked model is retained at that stage.

If the selected model contains a basis function at the current maximum degree or interaction order, the algorithm attempts another fitting round with increased degree and/or interaction order. In later rounds, the candidate basis set can be rebuilt using one of several enrichment strategies rather than constructing the full basis library from scratch.

The enrichment argument controls how the candidate set is generated after the first fitting round:

**0 (local enrichment)** Starts from the previously selected basis functions and applies local modifications to each term. These include deletion, simplification, complication, and promotion moves. This is typically the fastest strategy, but it is also the most local.

**1 (active-variable rebuild)** Rebuilds the full candidate library using only variables that were active in the previously selected model. This is computationally efficient, but inactive variables cannot re-enter once dropped.

**2 (full active rebuild plus sparse inactive enrichment)** Rebuilds the candidate library on the currently active variables, then enriches around the previously selected basis functions by allowing inactive variables to re-enter through complication and promotion moves. This is a compromise between speed and flexibility.

**3 (full active rebuild plus inactive enrichment)** Rebuilds the candidate library on the active variables, then enriches that larger active-variable library by allowing inactive variables to re-enter through complication and promotion moves. This is more expansive than enrichment = 2, but can be substantially more expensive.

**4 (full rebuild)** Rebuilds the full candidate library over all variables at each enrichment step. This is the most exhaustive strategy.

"adaptive" Begins with a relatively expansive enrichment strategy and, before the next recursion step, uses an upper bound on the candidate-set size to decide whether a more restrictive strategy should be used instead. This recovers the computational benefit of avoiding construction of candidate sets that are known in advance to be too large.

When `enrichment = "adaptive"`, the function uses `adaptive_ladder` together with an upper bound on the next candidate-set size. If the current enrichment choice appears too expensive, the algorithm steps down to a more restrictive enrichment rule before proceeding. If even the most restrictive admissible next step is predicted to exceed the allowed budget, the current fitted model is returned.

Strategies 2, 3, and "adaptive" are designed to address a limitation of active-variable-only rebuilds: variables that are inactive in one round are allowed to re-enter the model in later rounds.

### Value

An object of class "sparse\_khaos". The object is a list containing:

**B** Matrix of selected basis functions evaluated at the training inputs.

**nbasis** Number of selected basis functions (including intercept).

**vars** Matrix encoding the polynomial multi-indices for each basis function.

**beta\_hat** MAP estimates of the regression coefficients.

**s2** Estimated noise variance.

**X, y** Training data (with `y` on the original scale).

**mu\_y, sigma\_y** Centering and scaling constants used for `y`.

**BtB, BtBi** Cross-product matrix and its inverse.

**G** Prior scaling factors for coefficients.

**prior** Prior hyperparameters.

**KIC** Kashyap information criterion values for candidate models.

### References

Shao, Q., Younes, A., Fahs, M., and Mara, T. A. (2017). Bayesian sparse polynomial chaos expansion for global sensitivity analysis. *Computer Methods in Applied Mechanics and Engineering*, **318**, 474–496.

Rumsey, K. N., Francom, D., Gibson, G., Tucker, J. D., and Huerta, G. (2026). Bayesian adaptive polynomial chaos expansions. *Stat*, **15**(1), e70151.

### Examples

```
X <- lhs::maximinLHS(100, 2)
f <- function(x) 10.391 * ((x[1] - 0.4) * (x[2] - 0.6) + 0.36)
y <- apply(X, 1, f) + stats::rnorm(100, 0, 0.1)

fit <- sparse_khaos(X, y)
```

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