Package 'stan4bart'

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Title Bayesian Additive Regression Trees with Stan-Sampled Parametric
      Extensions
Depends R (>= 3.5-0), methods, dbarts (>= 0.9-21)
Imports stats, Matrix, parallel, RcppParallel (>= 5.1.1)
LinkingTo BH (>= 1.72.0.3), Rcpp (>= 1.0.5), RcppEigen (>= 0.3.3.7.0),
      RcppParallel (>= 5.1.1), dbarts (>= 0.9-20)
Suggests testthat (>= 2.0-0), lme4
Description Fits semiparametric linear and multilevel models with non-parametric addi-
      tive Bayesian additive regression tree (BART; Chipman, George, and McCul-
      loch (2010) <doi:10.1214/09-AOAS285>) components and Stan (Stan Develop-
      ment Team (2021) <a href="https://mc-stan.org/">https://mc-stan.org/</a>) sampled parametric ones. Multilevel mod-
      els can be expressed using 'lme4' syntax (Bates, Maech-
      ler, Bolker, and Walker (2015) <doi:10.18637/jss.v067.i01>).
License GPL (>= 3)
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UseLTO true
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Author Vincent Dorie [aut, cre] (ORCID:
       <a href="https://orcid.org/0000-0002-9576-3064">https://orcid.org/0000-0002-9576-3064</a>),
      Ben Goodrich [ctb] (rstanarm_functions.R, StanHeaders),
      Jonah Gabry [ctb] (rstanarm_functions.R, StanHeaders),
      Imad Ali [ctb] (rstanarm_functions.R),
      Sam Brilleman [ctb] (rstanarm_functions.R),
      Paul-Christian Burkner [ctb] (rstanarm functions.R, ORCID:
       <https://orcid.org/0000-0001-5765-8995>),
      Joshua Pritikin [ctb] (StanHeaders, ORCID:
       <https://orcid.org/0000-0002-9862-5484>),
```

```
Andrew Gelman [ctb] (StanHeaders, ORCID:
 <https://orcid.org/0000-0002-6975-2601>),
Bob Carpenter [ctb] (StanHeaders),
Matt Hoffman [ctb] (StanHeaders),
Daniel Lee [ctb] (StanHeaders),
Michael Betancourt [ctb] (StanHeaders, ORCID:
 <a href="https://orcid.org/0000-0002-2900-0931">),</a>
Marcus Brubaker [ctb] (StanHeaders, ORCID:
 <a href="https://orcid.org/0000-0002-7892-9026">https://orcid.org/0000-0002-7892-9026</a>),
Jiqiang Guo [ctb] (StanHeaders),
Peter Li [ctb] (StanHeaders),
Allen Riddell [ctb] (StanHeaders),
Marco Inacio [ctb] (StanHeaders, ORCID:
 <a href="https://orcid.org/0000-0002-6865-5404">https://orcid.org/0000-0002-6865-5404</a>),
Mitzi Morris [ctb] (StanHeaders),
Jeffrey Arnold [ctb] (StanHeaders, ORCID:
 <https://orcid.org/0000-0001-9953-3904>),
Rob Goedman [ctb] (StanHeaders),
Brian Lau [ctb] (StanHeaders),
Rob Trangucci [ctb] (StanHeaders),
Alp Kucukelbir [ctb] (StanHeaders),
Robert Grant [ctb] (StanHeaders),
Dustin Tran [ctb] (StanHeaders),
Michael Malecki [ctb] (StanHeaders),
Yuanjun Gao [ctb] (StanHeaders),
Trustees of Columbia University [cph] (rstanarm functions.R,
 StanHeaders),
Lawrence Livermore National Security [cph] (CVODES),
The Regents of the University of California [cph] (CVODES),
Southern Methodist University [cph] (CVODES),
Douglas Bates [ctb] (lme4_functions.R, ORCID:
 <a href="https://orcid.org/0000-0001-8316-9503">https://orcid.org/0000-0001-8316-9503</a>),
Martin Maechler [ctb] (lme4_functions.R, ORCID:
 <https://orcid.org/0000-0002-8685-9910>),
Ben Bolker [ctb] (lme4_functions.R, ORCID:
 <https://orcid.org/0000-0002-2127-0443>),
Steve Walker [ctb] (lme4 functions.R, ORCID:
 <https://orcid.org/0000-0002-4394-9078>),
Armon Dadgar [ctb] (adaptive radix tree),
Bothner Per [ctb] (config.guess),
Elliston Ben [ctb] (config.guess),
Free Software Foundation [cph] (config.sub),
Guido U Draheim [ctb] (ax check compile flag.m4),
Maarten Bosmans [ctb] (ax_check_compile_flag.m4),
Christophe Tournayre [ctb] (ax_ext.m4),
Michael Petch [ctb] (ax_ext.m4, ax_gcc_x86_avx_xgetbv.m4,
 ax_gcc_x86_cpuid.m4),
Rafael de Lucena Valle [ctb] (ax_ext.m4),
```

Contents 3

Contents

stan4bart		Semiparametric Models Using Stan and BART			
Index	stan4bart-generics .			9 12	
	stan4bart			3	

Description

This function fits semi-parametric linear and probit models that have a non-parametric, BART component and one or more of a parametric fixed effect (unmodeled coefficients), or a parametric random effect (modeled coefficients). If f(x) is a BART "sum-of-trees" model, fits:

• For continuous response variables:

$$Y \mid b \sim N\left(f(X^b) + X^f\beta + Zb, \sigma^2\right)b \sim N(0, \Sigma_b)$$

• For binary response variables:

$$P(Y = 1 \mid b) = \Phi \left(f(X^b) + X^f \beta + Zb \right) b \sim \mathcal{N}(0, \Sigma_b)$$

Usage

```
warmup = iter %/% 2L,
skip = 1L,
chains = 4L,
cores = getOption("mc.cores", 1L),
refresh = max(iter %/% 10L, 1L),
offset_type = c("default", "fixef", "ranef", "bart", "parametric"),
seed = NA_integer_,
keep_fits = TRUE,
callback = NULL,
stan_args = NULL,
bart_args = NULL)
```

Arguments

formula a formula object, or one that can be coerced to that type. Terms on the right-

hand-side of the formula that are encased in a symbolic call to bart() will be used to create the non-parametric component. Terms that use the lmer-style grouping syntax will be added as parametric, hierarchical varying intercepts and

slopes. All other terms will be added as fixed effects.

data an optional data frame containing the variables in the formula. Its use is strongly

encouraged.

subset, weights, na.action, offset, contrasts

optional components adjusting the constructed model matrices and otherwise changing the linear predictor. na.action cannot be "na.pass". See 1m and

model.matrix.default.

test an optional data frame to be used as test data. If present, the test predictions will

be stored as the sampler runs and can be extracted later.

treatment an optional symbol, that when present and refers to a binary variable, will be

used to create a test data frame with the treatment variable set to its counterfac-

tual. Only one of test and treatment can be supplied.

offset_test optional vector which will be added to the test predictions.

verbose a logical or integer. If FALSE or non-positive, runs quietly. Additional levels

of information may be displayed for increasingly positive numbers, however a large number of diagnostics are suppressed when running multi-threaded. If

negative, all diagnostic information is ignored.

iter positive integer indicating the number of posterior samples to draw and return.

Includes warmup samples.

warmup non-negative integer indicating number of posterior samples to draw and throw

away. Also controls the number of iterations for which adaptation is run.

skip one or two positive integers. Every skip sample will be kept, while every other

sample will be discarded. If argument is length two, an attempt will be made to use he named element "bart" for BART and "stan" for Stan. If not named, BART is the first skip element and Stan is the second. This argument does not impact the number of iters returned, unlike a conventional "thinning" parame-

ter.

chains positive integer giving the number of Markov Chains to sample.

cores	positive integer giving the number of units of parallelization. Computation for each chain will be divide among the cores available. When greater than one, verbose output within chains will not be available.
refresh	positive integer giving the frequency with which diagnostic information should be printed as the sampler runs. Only applies with cores (or chains) equal to 1.
offset_type	character; an experimental/testing feature that controls how offset is to be interpreted. When one of "fixef", "ranef", or "bart", the offset is used to replace that part of the model. When "parametric", it replaces both of the fixed and random parametric components. Sampling is still done for these components and their draws are stored, however whenever they were present in the fit the supplied value is used instead.
seed	Optional integer specifying the desired pRNG seed. It should not be needed when running single-threaded - calling set.seed will suffice. The primary use of seed is to obtain reproducible results when multi-threaded. See Reproducibility section below.
keep_fits	Logical that, when false, prevents the sampler from storing each draw. Intended to be used with callback.
callback	A function that will be called at each iteration, accepting three arguments: yhat.train, yhat.test, stan_pars. See details for more information.
stan_args	optional list, specifying further arguments to Stan. See details below.
bart_args	optional list, specifying further arguments to BART. See details below.

Details

Fits a Bayesian "mixed effect" model with a non-parametric Bayesian Additive Regression Trees (BART) component. For continuous responses:

•
$$Y_i \mid b \sim \mathcal{N}\left(f(X_i^b) + X_i^f \beta + Z_i b_{g[i]}, \sigma^2\right)$$

• $b_i \sim \mathcal{N}(0, \Sigma_b)$

where b_j are the "random effects" - random intercepts and slopes - that correspond to group j,g[i] is a mapping from individual i to its group index, f - a BART sum-of-trees model, X^b are predictors used in the BART model, X^f are predictors in a parametric, linear "fixed effect" component, Z is the design matrix for the random intercept and slopes, and sigma and $Sigma_b$ are variance components.

Binary outcome models are obtained by assuming a latent variable that has the above distribution, and that the observed response is 1 when that variable is positive and 0 otherwise. The response variable marginally has the distribution:

$$P(Y_i = 1 \mid b) = \Phi\left(f(X_i^b) + X_i^f \beta + Z_i b_{g[i]}\right)$$

where Φ is the cumulative distribution function of the standard normal distribution.

Terminology: As stan4bart fits a Bayesian model, essentially all components are "modeled". Furthermore, as it has two first-level, non-hierarchical components, "fixed" effects are ambiguous. Thus we adopt:

• "fixed" - refers only to the parametric, linear, individual level mean component, $X^f\beta$; these are "unmodeled coefficients" in other contexts

- "random" refers only to the parametric, linear, hierarchical mean component, Zb; these are "modeled coefficients" in other contexts
- "bart" refers only to the nonparametric, individual level mean component, $f(X^b)$

Model Specification: Model specification occurs in the formula object, according to the following rules:

- variables or terms specified inside a pseudo-call to bart are used for the "bart" component,
 e.g. y ~ bart(x_1 + x_2)
- variables or terms specified according to lmer syntax are used for the "random" effect component, e.g. y ~ (1 | g_1) + (1 + x_3 | g_1)
- remaining variables not inside a bart or "bars" construct are used for the "fixed" effect component; e.g. $y \sim x_4$

All three components can be present in a single model, however are bart part must present. If you wish to fit a model without one, use stan_glmer in the rstanarm package instead.

Additional Arguments: The stan_args and bart_args arguments to stan4bart can be used to pass further arguments to stan and bart respectively. These are similar to the functions stan in the rstan package and bart, but not identical as stan4bart constructs its own model internally. Stan arguments include:

- prior_covariance
- prior, prior_intercept, prior_aux, QR
- init_r, adapt_gamma, adapt_delta, adapt_kappa see the help page for stan in the rstan package.

For reference on the first two sets of options, see the help page for stan_glmer in the rstanarm package; for reference on the third set, see the help page for stan in the rstan package.

BART arguments include:

• further arguments to dbartsControl that are not specified by stan4bart, such as keepTrees or n. trees; keeping trees can be costly in terms of memory, but is required to use predict

Reproducibility: Behavior differs when running multi- and single-threaded, as the pseudo random number generators (pRNG) used by R are not thread safe. When single-threaded, R's built-in generator is used; if set at the start, .Random.seed will be used and its value updated as samples are drawn. When multi-threaded, the default behavior is draw new random seeds for each thread using the clock and use thread-specific pRNGs.

This behavior can be modified by setting seed. For the single-threaded case, that seed will be installed and the existing seed replaced at the end, if applicable. For multi-threaded runs, the seeds for threads are drawn sequentially using the supplied seed, and will not change the state of R's built-in generator.

Consequently, the seed argument should not be needed when running single-threaded - set. seed will suffice. When multi-threaded, seed can be used to obtain reproducible results.

Callbacks: Callbacks can be used to avoid expensive memory allocation, aggregating results as the sampler proceeds instead of waiting until the end. A callback funtion must accept the arguments:

• yhat.train - BART predictions of the expected value of the training data, conditioned on the Stan parameters

- yhat.test when applicable, the same values as above but for the test data; NULL otherwise
- stan_pars named vector of Stan samples, including fixed and random effects and variance parameters

It is expected that the callback will return a vector of the same length each time. If not, invalid memory writes will likely result. If the result of the callback has names, they will be added to the result.

Serialization: At present, stan4bart models cannot be safely saved and loaded in a way that the sampler can be restarted. This feature may be added in the future.

Value

Returns a list assigned class stan4bartFit. Has components below, some of which will be NULL if not applicable.

Input values:

y response vector

weights weights vector or null offset offset vector or null

frame joint model frame for all components formula formula used to specify the model

na.action supplied na.action call original call

Stored data:

bartData data object used for BART component X fixed effect design matrix or NULL

X_means column means of fixed effect design matrix when appropriate random effect "terms" object when applicable, as used by lmer

named list when applicable, having components X and reTrms; test data for

BART is added to the bartData result

treatment treatment vector, when applicable

Results, better accessed using extract:

bart_train samples of individual posterior predictions for BART component bart_test predicted test values for BART component, when applicable

bart_varcount BART variable counts

sigma samples of residual standard error; not present for binary outcomes

k samples of the end-node sensitivity parameter; only present when it is modeled ranef samples of random effects, or modeled coefficients; will be a named list, with

effects for each grouping factor

samples of covariance of random effects; also a named list with one element for Sigma each grouping factor fixef samples of the fixed effects, or unmodeled coefficients callback samples returned by an optional callback function Other items: warmup a list of warmup samples, containing the same objects in the results subsection diagnostics Stan sampler produced diagnostic information, include tree depth and divergent transitions sampler.bart external points to BART samplers; used only for predict when keepTrees is

range.bart internal scale used by BART samplers, used by predict when keepTrees is

TRUE

Author(s)

Vincent Dorie: <vdorie@gmail.com>.

See Also

bart, lmer, and stan_glmer in the rstanarm package

Examples

```
# simulate data (extension of Friedman MARS paper)
# x consists of 10 variables, only first 5 matter
# x_4 is linear
f <- function(x)</pre>
  10 * \sin(pi * x[,1] * x[,2]) + 20 * (x[,3] - 0.5)^2 +
      10 * x[,4] + 5 * x[,5]
set.seed(99)
sigma <- 1.0
n <- 100
n.g.1 < -5L
n.g.2 < - 8L
# sample observation level covariates and calculate marginal mean
x \leftarrow matrix(runif(n * 10), n, 10)
mu.bart <- f(x) - 10 * x[,4]
mu.fixef <- 10 * x[,4]
# varying intercepts and slopes for first grouping factor
g.1 <- sample(n.g.1, n, replace = TRUE)
Sigma.b.1 <- matrix(c(1.5^2, .2, .2, 1^2), 2)
b.1 <- matrix(rnorm(2 * n.g.1), n.g.1) %*% chol(Sigma.b.1)
# varying intercepts for second grouping factor
g.2 <- sample(n.g.2, n, replace = TRUE)
```

stan4bart-generics 9

```
Sigma.b.2 \leftarrow as.matrix(1.2)
b.2 <- rnorm(n.g.2, 0, sqrt(Sigma.b.2))</pre>
mu.ranef <- b.1[g.1,1] + x[,4] * b.1[g.1,2] + b.2[g.2]
y <- mu.bart + mu.fixef + mu.ranef + rnorm(n, 0, sigma)
df \leftarrow data.frame(y, x, g.1, g.2)
fit <- stan4bart(</pre>
    formula = y ~
                                       # linear component ("fixef")
        X4 +
        (1 + X4 | g.1) + (1 | g.2) + # multilevel ("ranef")
        bart(. - g.1 - g.2 - X4), # use bart for other variables
    verbose = −1, # suppress ALL output
    # low numbers for illustration
    data = df,
    chains = 1, iter = 10, bart_args = list(n.trees = 5))
# posterior means of individual expected values
y.hat <- fitted(fit)</pre>
# posterior means of the random effects
ranef.hat <- fitted(fit, type = "ranef")</pre>
```

stan4bart-generics

Generic Functions for stan4bart Model Fits

Description

Commonly expected utility functions to derive useful quantities from fitted models.

Usage

10 stan4bart-generics

Arguments

object a fitted model resulting from a call to stan4bart.

type a character vector; one of the options listed below.

sample one of "train" or "test", indicating if the training or test data frames should

be used.

combine_chains logical controlling if chain information should be discarded and the result re-

turned as a matrix instead of an array.

sample_new_levels

logical; if TRUE, levels out of the training sample will have random effects drawn from their posterior predictive distribution. If FALSE, their random effects will

be fixed to 0.

include_warmup logical or "only"; when TRUE/FALSE, warmup samples will or will not be in-

cluded in the result respectively. When "only", only the warmup samples will

be returned.

newdata data frame for making out of sample predictions.

offset optional vector which will be added to test predictors.

... not currently in use, but provided to match signatures of other generics.

Details

extract is used to obtain raw samples using the training or test data, fitted averages those samples, and predict operates on data not available at the time of fitting. Note: predict requires that the model be fit with args_bart = list(keepTrees = TRUE).

Return type: The type argument accepts:

- "ev" the individual level expected value, that is draws from $E[Y \mid X^b, X^f, Z] \mid Y = f(X^b) + X^f \beta + Zb \mid Y$ where the expectation is with respect to the posterior distribution of the parameters given the data
- "ppd" draws from the individual level posterior predictive distribution, generally speaking adding noise to the result for "ev" or simulating new Bernoulli trials.

stan4bart-generics 11

• "fixef" - draws from the posterior of the fixed effects (also known as the "unmodeled" coefficients), $\beta \mid Y$

- "indiv.fixef" draws from the posterior distribution of the individual level mean component deriving from the fixed effects, $X^f\beta$
- "ranef" the random effects, varying intercepts and slopes, or "modeled" coefficients, b;
 b has substantial structure that is represented as the returned value, where coefficients are reported within their grouping factors
- "indiv.ranef" individual level mean component deriving from the random effects, Zb
- "indiv.bart" individual level mean component deriving from the BART model, $f(X^b)$
- "sigma" for continuous responses, the residual standard error
- "Sigma" when applicable, the covariance matrices of the random effects
- "stan" raw matrix or array of Stan sampled transformed parameters.
- "trees" a data frame of flatted trees; see the subsection on extracted trees in bart and note that stan4bart variable names can be found in the bartData@x element of a fitted stan4bart model
- "callback" if a callback function was provided while fitting, the results of that for each sample

Value

extract and predict return either arrays of dimensions equal to n. observations x n. samples x n. chains when combine_chains is FALSE, or matrices of dimensions equal to n. observations x (n. samples x n. chains) when combine_chains is TRUE.

fitted returns a vector of the appropriate length by averaging the result of a call to extract.

Author(s)

Vincent Dorie: <vdorie@gmail.com>.

Index

```
.Random.seed, \boldsymbol{6}
bart, 6, 8, 11
data, 7
dbartsControl, 6
extract, 7
extract (stan4bart-generics), 9
fitted.stan4bartFit
         (stan4bart-generics), 9
formula, 4
1m, 4
1mer, 4, 6-8
load, 7
model, 3
model.matrix.default, 4
predict, 6, 8
predict.stan4bartFit
         (stan4bart-generics), 9
save, 7
seed, 5
set.seed, 5, 6
\mathtt{stan4bart}, 3, \textcolor{red}{10}
stan4bart-generics, 9
```