# Package 'lgpr'

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```
Title Longitudinal Gaussian Process Regression
```

Andrew Johnson [ctb]

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Description Interpretable nonparametric modeling of longitudinal data using additive Gaussian process regression. Contains functionality for inferring covariate effects and assessing covariate relevances.

Models are specified using a convenient formula syntax, and can include shared, group-specific, non-stationary, heterogeneous and temporally uncertain effects. Bayesian inference for model parameters is performed using 'Stan'. The modeling approach and methods are described in detail in Timonen et al. (2021) <doi:10.1093/bioinformatics/btab021>.

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# **Description**

Interpretable nonparametric modeling of longitudinal data using additive Gaussian process regression. Contains functionality for inferring covariate effects and assessing covariate relevances. Models are specified using a convenient formula syntax, and can include shared, group-specific, nonstationary, heterogeneous and temporally uncertain effects. Bayesian inference for model parameters is performed using 'Stan' (rstan). The modeling approach and methods are described in detail in Timonen et al. (2021).

# **Core functions**

Main functionality of the package consists of creating and fitting an additive GP model:

- 1gp: Specify and fit an additive GP model with one command.
- create\_model: Define an lgpmodel object.

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- sample\_model: Fit a model by sampling the posterior distribution of its parameters and create an lgpfit object.
- pred: Computing model predictions and inferred covariate effects after fitting a model.
- relevances: Assessing covariate relevances after fitting a model.
- prior\_pred: Prior predictive sampling to check if your prior makes sense.

#### Visualization

- plot\_pred: Plot model predictions.
- plot\_components: Visualize inferred model components.
- plot\_draws: Visualize parameter draws.
- plot\_data: Visualize longitudinal data.

#### Data

The data that you wish to analyze with 'lgpr' should be in an R data.frame where columns correspond to measured variables and rows correspond to observations. Some functions that can help working with such data frames are:

- new\_x: Creating new test points where the posterior distribution of any function component
  or sum of all components, or the posterior predictive distribution can be computed after model
  fitting.
- Other functions: add\_factor, add\_factor\_crossing, add\_dis\_age, adjusted\_c\_hat.

#### Vignettes and tutorials

See https://jtimonen.github.io/lgpr-usage/index.html. The tutorials focus on code and use cases, whereas the Mathematical description of lgpr models vignette describes the statistical models and how they can be customized in 'lgpr'.

#### Citation

Run citation("lgpr") to get citation information.

## Feedback

Bug reports, PRs, enhancement ideas or user experiences in general are welcome and appreciated. Create an issue in Github or email the author.

# Author(s)

Juho Timonen (first.last at iki.fi)

#### References

- 1. Timonen, J. et al. (2021). *lgpr: an interpretable non-parametric method for inferring covariate effects from longitudinal data.* Bioinformatics, url.
- 2. Carpenter, B. et al. (2017). *Stan: A probabilistic programming language*. Journal of Statistical Software 76(1).

add\_dis\_age 5

# Description

Creates the disease-related age covariate vector based on the disease initiation times and adds it to the data frame

# Usage

```
add_dis_age(data, t_init, id_var = "id", time_var = "age")
```

# **Arguments**

data	the original data frame
t_init	A named vector containing the observed initiation or onset time for each individual. The names, i.e. names(t_init), should specify the individual id.
id_var	name of the id variable in data
time_var	name of the time variable in data

#### Value

A data frame with one column added. The new column will be called dis\_age. For controls, its value will be NaN.

# See Also

```
Other data frame handling functions: add_factor_crossing(), add_factor(), adjusted_c_hat(), new_x(), split()
```

add_factor	Easily add a categorical covariate to a data frame

# Description

Easily add a categorical covariate to a data frame

# Usage

```
add_factor(data, x, id_var = "id")
```

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# **Arguments**

data the original data frame

x A named vector containing the category for each individual. The names should

specify the individual id.

id\_var name of the id variable in data

#### Value

A data frame with one column added. The new column will have same name as the variable passed as input x.

#### See Also

```
Other data frame handling functions: add_dis_age(), add_factor_crossing(), adjusted_c_hat(), new_x(), split()
```

add\_factor\_crossing

Add a crossing of two factors to a data frame

# **Description**

Add a crossing of two factors to a data frame

#### Usage

```
add_factor_crossing(data, fac1, fac2, new_name)
```

## **Arguments**

data a data frame

fac1 name of first factor, must be found in df fac2 name of second factor, must be found in df

new\_name name of the new factor

# Value

a data frame

#### See Also

```
Other data frame handling functions: add_dis_age(), add_factor(), adjusted_c_hat(), new_x(), split()
```

adjusted\_c\_hat 7

adjusted_c_hat	Set the GP mean vector, taking TMM or other normalization into ac-
	count

# **Description**

Creates the c\_hat input for lgp, so that it accounts for normalization between data points in the "poisson" or "nb" observation model

# Usage

```
adjusted_c_hat(y, norm_factors)
```

# Arguments

```
y response variable, vector of length n
norm_factors normalization factors, vector of length n
```

#### Value

a vector of length n, which can be used as the c\_hat input to the lgp function

#### See Also

```
Other data frame handling functions: add_dis_age(), add_factor_crossing(), add_factor(), new_x(), split()
```

appry_scarring Appry variable scaling	apply_scaling	Apply variable scaling
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# **Description**

Apply variable scaling

# Usage

```
apply_scaling(scaling, x, inverse = FALSE)
```

#### **Arguments**

scaling an object of class lgpscaling

x object to which apply the scaling (numeric)

inverse whether scaling should be done in inverse direction

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# Value

```
a similar object as x
```

#### See Also

Other variable scaling functions: create\_scaling()

 $as\_character$ 

Character representations of different formula objects

# Description

Character representations of different formula objects

# Usage

```
## S4 method for signature 'lgpexpr'
as.character(x)

## S4 method for signature 'lgpterm'
as.character(x)

## S4 method for signature 'lgpformula'
as.character(x)
```

# **Arguments**

Х

an object of some S4 class

# Value

a character representation of the object

create\_model

Create a model

# Description

See the Mathematical description of lgpr models vignette for more information about the connection between different options and the created statistical model.

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#### Usage

```
create_model(
  formula,
  data,
  likelihood = "gaussian",
  prior = NULL,
  c_hat = NULL
  num trials = NULL.
  options = NULL,
  prior_only = FALSE,
  verbose = FALSE,
  sample_f = !(likelihood == "gaussian")
)
```

#### **Arguments**

formula

The model formula, where

• it must contain exactly one tilde (~), with response variable on the left-hand side and model terms on the right-hand side

- terms are be separated by a plus (+) sign
- all variables appearing in formula must be found in data

See the "Model formula syntax" section below (1gp) for instructions on how to specify the model terms.

data

A data. frame where each column corresponds to one variable, and each row is one observation. Continuous covariates and the response variable must have type "numeric" and categorical covariates must have type "factor". Missing values should be indicated with NaN or NA. The response variable cannot contain missing values. Column names should not contain trailing or leading under-

likelihood

Determines the observation model. Must be either "gaussian" (default), "poisson", "nb" (negative binomial), "binomial" or "bb" (beta binomial).

prior

A named list, defining the prior distribution of model (hyper)parameters. See the "Defining priors" section below (lgp).

c\_hat

The GP mean. This should only be given if sample\_f is TRUE, otherwise the GP will always have zero mean. If sample\_f is TRUE, the given c\_hat can be a vector of length dim(data)[1], or a real number defining a constant GP mean. If not specified and sample\_f is TRUE, c\_hat is set to

- c\_hat = mean(y), if likelihood is "gaussian",
- c\_hat = log(mean(y)) if likelihood is "poisson" or "nb",
- c\_hat = log(p/(1-p)), where p = mean(y/num\_trials) if likelihood is "binomial" or "bb",

where y denotes the response variable measurements.

num\_trials

This argument (number of trials) is only needed when likelihood is "binomial" or "bb". Must have length one or equal to the number of data points. Setting num\_trials=1 and likelihood="binomial" corresponds to Bernoulli observation model.

options A named list with the following possible fields:

delta Amount of added jitter to ensure positive definite covariance matrices.

vm\_params Variance mask function parameters (numeric vector of length
 2)

If options is NULL, default options are used. The defaults are equivalent to options = list(delta = 1e-8,  $vm_params = c(0.025, 1)$ ).

prior\_only Should likelihood be ignored? See also sample\_param\_prior which can be

used for any lgpmodel, and whose runtime is independent of the number of

observations.

verbose Should some informative messages be printed?

sample\_f Determines if the latent function values are sampled (must be TRUE if likelihood

is not "gaussian"). If this is TRUE, the response variable will be normalized to

have zero mean and unit variance.

#### Value

An object of class lgpmodel, containing the Stan input created based on parsing the specified formula, prior, and other options.

#### See Also

Other main functions: draw\_pred(), get\_draws(), lgp(), pred(), prior\_pred(), sample\_model()

create\_model.covs\_and\_comps

Parse the covariates and model components from given data and formula

#### **Description**

Parse the covariates and model components from given data and formula

## Usage

```
create_model.covs_and_comps(data, model_formula, x_cont_scl, verbose)
```

#### **Arguments**

data A data. frame where each column corresponds to one variable, and each row

is one observation. Continuous covariates and the response variable must have type "numeric" and categorical covariates must have type "factor". Missing values should be indicated with NaN or NA. The response variable cannot contain missing values. Column names should not contain trailing or leading under-

scores.

model\_formula an object of class lgpformula

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x\_cont\_scl Information on how to scale the continuous covariates. This can either be

- an existing list of objects with class lgpscaling, or
- NA, in which case such list is created by computing mean and standard deviation from data

verbose Should some informative messages be printed?

#### Value

parsed input to Stan and covariate scaling, and other info

#### See Also

Other internal model creation functions: create\_model.formula(), create\_model.likelihood(), create\_model.prior()

## **Description**

Checks if formula is in advanced format and translates if not.

#### Usage

```
create_model.formula(formula, data, verbose = FALSE)
```

#### **Arguments**

formula The model formula, where

- it must contain exatly one tilde (~), with response variable on the left-hand side and model terms on the right-hand side
- terms are be separated by a plus (+) sign
- all variables appearing in formula must be found in data

See the "Model formula syntax" section below (1gp) for instructions on how to specify the model terms.

data

verbose

A data.frame where each column corresponds to one variable, and each row is one observation. Continuous covariates and the response variable must have type "numeric" and categorical covariates must have type "factor". Missing values should be indicated with NaN or NA. The response variable cannot contain missing values. Column names should not contain trailing or leading underscores.

Should some informative messages be printed?

#### Value

an object of class lgpformula

#### See Also

Other internal model creation functions: create\_model.covs\_and\_comps(), create\_model.likelihood(), create\_model.prior()

```
create_model.likelihood
```

Parse the response variable and its likelihood model

# **Description**

Parse the response variable and its likelihood model

# Usage

```
create_model.likelihood(
  data,
  likelihood,
  c_hat,
  num_trials,
  y_name,
  sample_f,
  verbose
)
```

## **Arguments**

data

A data.frame where each column corresponds to one variable, and each row is one observation. Continuous covariates and the response variable must have type "numeric" and categorical covariates must have type "factor". Missing values should be indicated with NaN or NA. The response variable cannot contain missing values. Column names should not contain trailing or leading underscores.

likelihood

Determines the observation model. Must be either "gaussian" (default), "poisson", "nb" (negative binomial), "binomial" or "bb" (beta binomial).

c\_hat

The GP mean. This should only be given if sample\_f is TRUE, otherwise the GP will always have zero mean. If sample\_f is TRUE, the given c\_hat can be a vector of length dim(data)[1], or a real number defining a constant GP mean. If not specified and sample\_f is TRUE, c\_hat is set to

- c\_hat = mean(y), if likelihood is "gaussian",
- c\_hat = log(mean(y)) if likelihood is "poisson" or "nb",
- c\_hat = log(p/(1-p)), where p = mean(y/num\_trials) if likelihood is "binomial" or "bb",

where y denotes the response variable measurements.

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num\_trials This argument (number of trials) is only needed when likelihood is "binomial"

or "bb". Must have length one or equal to the number of data points. Setting num\_trials=1 and likelihood="binomial" corresponds to Bernoulli obser-

vation model.

y\_name Name of response variable

sample\_f Determines if the latent function values are sampled (must be TRUE if likelihood

is not "gaussian"). If this is TRUE, the response variable will be normalized to

have zero mean and unit variance.

verbose Should some informative messages be printed?

#### Value

a list of parsed options

#### See Also

Other internal model creation functions: create\_model.covs\_and\_comps(), create\_model.formula(), create\_model.prior()

create\_model.options Parse the given modeling options

# **Description**

Parse the given modeling options

#### Usage

```
create_model.options(options, verbose)
```

## **Arguments**

options

A named list with the following possible fields:

- delta Amount of added jitter to ensure positive definite covariance matrices.
- vm\_params Variance mask function parameters (numeric vector of length 2).

If options is NULL, default options are used. The defaults are equivalent to options = list(delta = 1e-8,  $vm_params = c(0.025, 1)$ ).

verbose

Should some informative messages be printed?

#### Value

a named list of parsed options

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create\_model.prior

Parse given prior

# Description

Parse given prior

# Usage

```
create_model.prior(prior, stan_input, verbose)
```

# **Arguments**

prior A named list, defining the prior distribution of model (hyper)parameters. See

the "Defining priors" section below (lgp).

stan\_input a list of stan input fields

verbose Should some informative messages be printed?

#### Value

a named list of parsed options

#### See Also

Other internal model creation functions: create\_model.covs\_and\_comps(), create\_model.formula(), create\_model.likelihood()

create\_plot\_df

Helper function for plots

# Description

Helper function for plots

# Usage

```
create_plot_df(object, x = "age", group_by = "id")
```

# **Arguments**

object model or fit

x x-axis variable name

group\_by grouping variable name (use NULL for no grouping)

## Value

a data frame

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create\_scaling

Create a standardizing transform

# Description

Create a standardizing transform

# Usage

```
create_scaling(x, name)
```

# **Arguments**

x variable measurements (might contain NA or NaN)

name variable name

### Value

an object of class lgpscaling

# See Also

Other variable scaling functions: apply\_scaling()

dinvgamma\_stanlike

Density and quantile functions of the inverse gamma distribution

# **Description**

Using the same parametrization as Stan. More info here.

# Usage

```
dinvgamma_stanlike(x, alpha, beta, log = FALSE)
qinvgamma_stanlike(p, alpha, beta)
```

# **Arguments**

x point where to compute the density

alpha positive real number beta positive real number log is log-scale used?

p quantile (must be between 0 and 1)

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#### Value

density/quantile value

# See Also

Other functions related to the inverse-gamma distribution: plot\_invgamma(), priors

draw_pred	Draw pseudo-observations from posterior or prior predictive distribu-
	tion

# Description

Draw pseudo-observations from predictive distribution. If pred contains draws from the component posterior (prior) distributions, then the output is draws from the posterior (prior) predictive distribution. If pred is not specified, then whether output draws are from prior or posterior predictive distribution depends on whether fit is created using the lgp option prior\_only=TRUE or not.

# Usage

```
draw_pred(fit, pred = NULL)
```

#### **Arguments**

fit	An object of class lgpfit that has been created using the lgp option sample_f=TRUE.
pred	An object of class Prediction, containing draws of each model component. If
	NULL, this is obtained using get_pred(fit).

## Value

An array with shape SxP, where S is the number of draws that pred contains and P is the length of each function draw. Each row  $s=1,\ldots,S$  of the output is one vector drawn from the predictive distribution, given parameter draw s.

#### See Also

```
Other main functions: create_model(), get_draws(), lgp(), pred(), prior_pred(), sample_model()
```

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example\_fit

Quick way to create an example lgpfit, useful for debugging

# **Description**

Quick way to create an example lgpfit, useful for debugging

# Usage

```
example_fit(
  formula = y ~ id + age + age | SEX + age | LOC,
  likelihood = "gaussian",
  chains = 1,
  iter = 30,
  num_indiv = 6,
  num_timepoints = 5,
  ...
)
```

# **Arguments**

```
formula model formula

likelihood observation model

chains number of chains to run

iter number of iterations to run

num_indiv number of individuals (data simulation)

num_timepoints number of time points (data simulation)

additional arguments to lgp
```

#### Value

An lgpfit object created by fitting the example model.

fit\_summary

Print a fit summary.

# **Description**

Print a fit summary.

# Usage

```
fit_summary(fit, ignore_pars = c("f_latent", "eta", "teff_raw", "lp__"))
```

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#### **Arguments**

fit an object of class lgpfit

ignore\_pars parameters and generated quantities to ignore from output

#### Value

object invisibly.

GaussianPrediction-class

An S4 class to represent analytically computed predictive distributions (conditional on hyperparameters) of an additive GP model

## **Description**

An S4 class to represent analytically computed predictive distributions (conditional on hyperparameters) of an additive GP model

#### Usage

```
## S4 method for signature 'GaussianPrediction'
show(object)

## S4 method for signature 'GaussianPrediction'
component_names(object)

## S4 method for signature 'GaussianPrediction'
num_components(object)

## S4 method for signature 'GaussianPrediction'
num_paramsets(object)

## S4 method for signature 'GaussianPrediction'
num_evalpoints(object)
```

# **Arguments**

object GaussianPrediction object for which to apply a class method.

#### Methods (by generic)

- show(GaussianPrediction): Print a summary about the object.
- component\_names(GaussianPrediction): Get names of components.
- num\_components(GaussianPrediction): Get number of components.
- num\_paramsets(GaussianPrediction): Get number of parameter combinations (different parameter vectors) using which predictions were computed.
- num\_evalpoints(GaussianPrediction): Get number of points where predictions were computed.

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# **Slots**

```
f_comp_mean component means
```

f\_comp\_std component standard deviations

f\_mean signal mean (on normalized scale)

f\_std signal standard deviation (on normalized scale)

y\_mean predictive mean (on original data scale)

y\_std predictive standard deviation (on original data scale)

x a data frame of points (covariate values) where the function posteriors or predictive distributions have been evaluated

#### See Also

#### Prediction

get	draws	

Extract parameter draws from lgpfit or stanfit

# **Description**

Uses extract with permuted = FALSE and inc\_warmup = FALSE.

#### Usage

```
get_draws(object, draws = NULL, reduce = NULL, ...)
```

# Arguments

object	An object of class lgpfit or stanfit.
draws	Indices of the parameter draws. NULL corresponds to all post-warmup draws.
reduce	Function used to reduce all parameter draws into one set of parameters. Ignored if NULL, or if draws is not NULL.
	Additional arguments to rstan::extract().

#### Value

The return value is always a 2-dimensional array of shape num\_param\_sets x num\_params.

#### See Also

```
Other main functions: create_model(), draw_pred(), lgp(), pred(), prior_pred(), sample_model()
```

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get_	nred
get_	preu

Extract model predictions and function posteriors

## **Description**

*NOTE*: It is not recommended for users to call this. Use pred instead.

## Usage

```
get_pred(fit, draws = NULL, reduce = NULL, verbose = TRUE)
```

## **Arguments**

fit An object of class lgpfit.

draws Indices of parameter draws to use, or NULL to use all draws.

reduce Reduction for parameters draws. Can be a function that is applied to reduce all

parameter draws into one parameter set, or NULL (no reduction). Has no effect if

draws is specified.

verbose Should more information and a possible progress bar be printed?

#### Value

an object of class GaussianPrediction or Prediction

kernel

Compute a kernel matrix (covariance matrix)

# **Description**

These have STAN\_kernel\_\* counterparts. These R versions are provided for reference and are not optimized for speed. These are used when generating simulated data, and not during model inference.

#### Usage

```
kernel_eq(x1, x2, alpha = 1, ell)
kernel_ns(x1, x2, alpha = 1, ell, a)
kernel_zerosum(x1, x2, M)
kernel_bin(x1, x2, pos_class = 0)
kernel_cat(x1, x2)
```

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```
kernel_varmask(x1, x2, a, vm_params)
kernel_beta(beta, idx1_expand, idx2_expand)
```

#### **Arguments**

x1vector of length n x2vector of length m

alpha marginal std (default = 1)

ell lengthscale

a steepness of the warping function rise

M number of categories

pos\_class binary (mask) kernel function has value one if both inputs have this value, other

wise it is zero

vm\_params vector of two mask function parameters.

beta a parameter vector (row vector) of length N\_cases

idx1\_expand integer vector of length nidx2\_expand integer vector of length m

#### Value

A matrix of size  $n \times m$ .

#### **Functions**

- kernel\_eq(): Uses the exponentiated quadratic kernel.
- kernel\_ns(): Uses the non-stationary kernel (input warping + squared exponential).
- kernel\_zerosum(): Uses the zero-sum kernel. Here, x1 and x2 must be integer vectors (integers denoting different categories). Returns a binary matrix.
- kernel\_bin(): Uses the binary (mask) kernel. Here, x1 and x2 must be integer vectors (integers denoting different categories). Returns a binary matrix.
- kernel\_cat(): Uses the categorical kernel. Here, x1 and x2 must be integer vectors (integers denoting different categories). Returns a binary matrix.
- kernel\_varmask(): Computes variance mask multiplier matrix. NaN's in x1 and x2 will be replaced by 0.
- kernel\_beta(): Computes the heterogeneity multiplier matrix. *NOTE:* idx\_expand needs to be given so that idx\_expand[j]-1 tells the index of the beta parameter that should be used for the *j*th observation. If observation *j* doesn't correspond to any beta parameter, then idx\_expand[j] should be 1.

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KernelComputer-class An S4 class to represent input for kernel matrix computations

#### **Description**

An S4 class to represent input for kernel matrix computations

# Usage

```
## S4 method for signature 'KernelComputer'
show(object)

## S4 method for signature 'KernelComputer'
num_components(object)

## S4 method for signature 'KernelComputer'
num_evalpoints(object)

## S4 method for signature 'KernelComputer'
num_paramsets(object)

## S4 method for signature 'KernelComputer'
component_names(object)
```

# Arguments

object

The object for which to call a class method.

## Methods (by generic)

- show(KernelComputer): Print a summary about the object.
- num\_components(KernelComputer): Get number of components.
- num\_evalpoints(KernelComputer): Get number of evaluation points.
- num\_paramsets(KernelComputer): Get number of parameter sets.
- component\_names(KernelComputer): Get component names.

#### **Slots**

input Common input (for example parameter values).

K\_input Input for computing kernel matrices between data points (N x N). A list.

Ks\_input Input for computing kernel matrices between data and output points (P x N). A list.

Kss\_input Input for computing kernel matrices between output points (P x P). A list, empty if full\_covariance=FALSE.

comp\_names Component names (character vector).

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full\_covariance Boolean value determining if this can compute full predictive covariance matrices (or just marginal variance at each point).

no\_separate\_output\_points Boolean value determining if Ks\_input and Kss\_input are the same thing. Using this knowledge can reduce unnecessary computations of kernel matrices.

STREAM external pointer (for calling 'Stan' functions)

lgp

lgp

Main function of the 'lgpr' package

## **Description**

Creates an additive Gaussian process model using create\_model and fits it using sample\_model. See the Mathematical description of lgpr models vignette for more information about the connection between different options and the created statistical model.

#### Usage

```
lgp(
  formula,
  data,
  likelihood = "gaussian",
  prior = NULL,
  c_hat = NULL,
  num_trials = NULL,
  options = NULL,
  prior_only = FALSE,
  verbose = FALSE,
  sample_f = !(likelihood == "gaussian"),
  quiet = FALSE,
  skip_postproc = sample_f,
  ...
)
```

# Arguments

formula

The model formula, where

- it must contain exatly one tilde (~), with response variable on the left-hand side and model terms on the right-hand side
- terms are be separated by a plus (+) sign
- all variables appearing in formula must be found in data

See the "Model formula syntax" section below (1gp) for instructions on how to specify the model terms.

data

A data.frame where each column corresponds to one variable, and each row is one observation. Continuous covariates and the response variable must have type "numeric" and categorical covariates must have type "factor". Missing

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values should be indicated with NaN or NA. The response variable cannot contain missing values. Column names should not contain trailing or leading underscores.

likelihood

Determines the observation model. Must be either "gaussian" (default), "poisson", "nb" (negative binomial), "binomial" or "bb" (beta binomial).

prior

A named list, defining the prior distribution of model (hyper)parameters. See the "Defining priors" section below (lgp).

c\_hat

The GP mean. This should only be given if sample\_f is TRUE, otherwise the GP will always have zero mean. If sample\_f is TRUE, the given c\_hat can be a vector of length dim(data)[1], or a real number defining a constant GP mean. If not specified and sample\_f is TRUE, c\_hat is set to

- c\_hat = mean(y), if likelihood is "gaussian",
- c\_hat = log(mean(y)) if likelihood is "poisson" or "nb",
- c\_hat = log(p/(1-p)), where p = mean(y/num\_trials) if likelihood is "binomial" or "bb".

where y denotes the response variable measurements.

num\_trials

This argument (number of trials) is only needed when likelihood is "binomial" or "bb". Must have length one or equal to the number of data points. Setting num\_trials=1 and likelihood="binomial" corresponds to Bernoulli observation model.

options

A named list with the following possible fields:

- delta Amount of added jitter to ensure positive definite covariance matrices
- vm\_params Variance mask function parameters (numeric vector of length 2).

If options is NULL, default options are used. The defaults are equivalent to options = list(delta = 1e-8,  $vm_params = c(0.025, 1)$ ).

prior\_only

Should likelihood be ignored? See also sample\_param\_prior which can be used for any lgpmodel, and whose runtime is independent of the number of observations.

verbose

Can messages be printed during model creation? Has no effect if quiet=TRUE.

sample\_f

Determines if the latent function values are sampled (must be TRUE if likelihood is not "gaussian"). If this is TRUE, the response variable will be normalized to have zero mean and unit variance.

quiet

Should all output messages be suppressed? You need to set also refresh=0 if you want to suppress also the progress update messages from sampling.

skip\_postproc

Should all postprocessing be skipped? If this is TRUE, the returned lgpfit object will likely be much smaller (if sample\_f=FALSE).

Optional arguments passed to sampling or optimizing.

#### Value

Returns an object of the S4 class lgpfit.

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#### Model formula syntax

There are two ways to define the model formula:

1. Using a common formula-like syntax, like in y ~ age + age | id + sex. Terms can consist of a single variable, such as age, or an interaction of two variables, such as age | id. In single-variable terms, the variable can be either continuous (numeric) or categorical (factor), whereas in interaction terms the variable on the left-hand side of the vertical bar (|) has to be continuous and the one on the right-hand side has to be categorical. Formulae specified using this syntax are translated to the advanced format so that

- single-variable terms become gp(x) if variable x is numeric and zs(x) if x is a factor
- interaction terms x | z become gp(x)\*zs(z)
- 2. Using the advanced syntax, like in y ~ gp(age) + gp(age)\*zs(id) + het(id)\*gp\_vm(disAge). This creates lgprhs objects, which consist of lgpterms, which consist of lgpexprs. This approach must be used if creating nonstationary, heterogeneous or temporally uncertain components.

Either one of the approaches should be used and they should not be mixed.

# **Defining priors**

The prior argument must be a named list, like list(alpha=student\_t(4), wrp=igam(30,10)). See examples in tutorials. Possible allowed names are

- "alpha" = component magnitude parameters
- "ell" = component lengthscale parameters
- "wrp" = input warping steepness parameters
- "sigma" = noise magnitude (Gaussian obs. model)
- "phi" = inv. overdispersion (negative binomial obs. model)
- "gamma" = overdispersion (beta-binomial obs. model)
- "beta" = heterogeneity parameters
- "effect\_time" = uncertain effect time parameters
- "effect\_time\_info" = additional options for the above

See priors for functions that can be used to define the list elements. If a parameter of a model is not given in this list, a default prior will be used for it.

# When to not use default priors

It is not recommended to use default priors blindly. Rather, priors should be specified according to the knowledge about the problem at hand, as in any Bayesian analysis. In 1gpr this is especially important when

1. Using a non-Gaussian likelihood or otherwise setting sample\_f = TRUE. In this case the response variable is not normalized, so the scale on which the data varies must be taken into account when defining priors of the signal magnitude parameters alpha and possible noise parameters (sigma, phi, gamma). Also it should be checked if c\_hat is set in a sensible way.

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2. Using a model that contains a gp\_ns(x) or gp\_vm(x) expression in its formula. In this case the corresponding covariate x is not normalized, and the prior for the input warping steepness parameter wrp must be set according to the expected width of the window in which the non-stationary effect of x occurs. By default, the width of this window is about 36, which has been set assuming that the unit of x is months.

#### See Also

```
Other main functions: create_model(), draw_pred(), get_draws(), pred(), prior_pred(), sample_model()
```

lgpexpr-class

An S4 class to represent an lgp expression

# Description

An S4 class to represent an lgp expression

#### **Slots**

```
covariate name of a covariate fun function name
```

# See Also

See operations for performing arithmetics on lgprhs, lgpterm and lgpexpr objects.

lgpfit-class

An S4 class to represent the output of the 1gp function

# Description

An S4 class to represent the output of the 1gp function

#### Usage

```
## S4 method for signature 'lgpfit'
show(object)

## S4 method for signature 'lgpfit'
component_names(object)

## S4 method for signature 'lgpfit'
num_components(object)

## S4 method for signature 'lgpfit'
```

lgpfit-class 27

```
postproc(object, verbose = TRUE)

## S4 method for signature 'lgpfit'
contains_postproc(object)

## S4 method for signature 'lgpfit'
clear_postproc(object)

## S4 method for signature 'lgpfit'
get_model(object)

## S4 method for signature 'lgpfit'
get_stanfit(object)

## S4 method for signature 'lgpfit'
is_f_sampled(object)

## S4 method for signature 'lgpfit'
is_f_sampled(object)
```

## **Arguments**

object The object for which to apply a class method.

verbose Can the method print any messages?

x an lgpfit object to visualize

y unused argument

## Methods (by generic)

- show(lgpfit): Print information and summary about the fit object.
- component\_names(lgpfit): Get names of model components.
- num\_components(lgpfit): Get number of model components. Returns a positive integer.
- postproc(lgpfit): Apply postprocessing. Returns an updated lgpfit object (copies data).
- contains\_postproc(lgpfit): Check if object contains postprocessing information.
- clear\_postproc(lgpfit): Returns an updated (copies data) lgpfit object without any post-processing information.
- get\_model(lgpfit): Get the stored lgpmodel object. Various properties of the returned object can be accessed as explained in the documentation of lgpmodel.
- get\_stanfit(lgpfit): Get the stored stanfit object. Various properties of the returned object can be accessed or plotted as explained here or in the documentation of stanfit.
- is\_f\_sampled(lgpfit): Determine if inference was done by sampling the latent signal f (and its components).
- plot(x = lgpfit, y = missing): Visualize parameter draws using plot\_draws.

28 lgpmodel-class

# **Slots**

```
stan_fit An object of class stanfit.
model An object of class lgpmodel.
num_draws Total number of parameter draws.
postproc_results A named list containing possible postprocessing results.
```

#### See Also

For extracting parameter draws, see get\_draws, or the rstan methods for stanfit objects.

For more detailed plotting functions, see plot\_draws, plot\_beta, plot\_warp, plot\_effect\_times

lgpformula-class

An S4 class to represent an lgp formula

# Description

An S4 class to represent an lgp formula

#### **Slots**

```
terms an object of class lgprhs
y_name name of the response variable
call original formula call
```

## See Also

See operations for performing arithmetics on lgprhs, lgpterm and lgpexpr objects.

lgpmodel-class

An S4 class to represent an additive GP model

# **Description**

An S4 class to represent an additive GP model

lgpmodel-class 29

#### Usage

```
## S4 method for signature 'lgpmodel'
show(object)

## S4 method for signature 'lgpmodel'
parameter_info(object, digits = 3)

## S4 method for signature 'lgpmodel'
component_info(object)

## S4 method for signature 'lgpmodel'
num_components(object)

## S4 method for signature 'lgpmodel'
covariate_info(object)

## S4 method for signature 'lgpmodel'
component_names(object)

## S4 method for signature 'lgpmodel'
is_f_sampled(object)
```

#### **Arguments**

object The object for which to apply a class method.

digits number of digits to show for floating point numbers

# Methods (by generic)

- show(lgpmodel): Print information and summary about the object. Returns object invisibly.
- parameter\_info(lgpmodel): Get a parameter summary (bounds and priors). Returns a data.frame.
- component\_info(lgpmodel): Get a data frame with information about each model component.
- num\_components(lgpmodel): Get number of model components. Returns a positive integer.
- covariate\_info(lgpmodel): Get covariate information.
- component\_names(lgpmodel): Get names of model components.
- is\_f\_sampled(lgpmodel): Determine if inference of the model requires sampling the latent signal f (and its components).

## **Slots**

```
formula An object of class <a href="legistranger">Igpformula</a>
data The original unmodified data.
stan_input The data to be given as input to rstan::sampling
var_names List of variable names grouped by type.
```

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var\_scalings A named list with fields

• y - Response variable normalization function and its inverse operation. Must be an lgp-scaling object.

• x\_cont - Continuous covariate normalization functions and their inverse operations. Must be a named list with each element is an lgpscaling object.

var\_info A named list with fields

• x\_cat\_levels - Names of the levels of categorical covariates before converting from factor to numeric.

info Other info in text format.

sample\_f Whether the signal f is sampled or marginalized.

full\_prior Complete prior information.

lgprhs-class

An S4 class to represent the right-hand side of an lgp formula

## **Description**

An S4 class to represent the right-hand side of an lgp formula

#### **Slots**

summands a list of one or more lgpterms

#### See Also

See operations for performing arithmetics on lgprhs, lgpterm and lgpexpr objects.

lgpscaling-class

An S4 class to represent variable scaling

# **Description**

An S4 class to represent variable scaling

# Slots

```
loc original location (mean)
scale original scale (standard deviation)
var_name variable name
```

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lgpsim-class	An S4 class to represent a data set simulated using the additive GP formalism
	jornansin

# Description

An S4 class to represent a data set simulated using the additive GP formalism

#### **Usage**

```
## S4 method for signature 'lgpsim'
show(object)
## S4 method for signature 'lgpsim,missing'
plot(x, y, ...)
```

# **Arguments**

```
object an lgpsim object

x an lgpsim object to plot

y not used

... optional arguments passed to plot_sim
```

#### Methods (by generic)

- show(lgpsim): Show summary of object.
- plot(x = lgpsim, y = missing): Plot the data and generating process. For more information see plot\_sim.

# Slots

data the actual data

response name of the response variable in the data

components the drawn function components

kernel\_matrices the covariance matrices for each gp

info A list with fields

- par\_ell the used lengthscale parameters
- par\_cont the parameters used to generate the continuous covariates
- p\_signal signal proportion

effect\_times A list with fields

- true possible true effect times that generate the disease effect
- observed possible observed effect times

32 model\_summary

lgpterm-class

An S4 class to represent one formula term

# Description

An S4 class to represent one formula term

# **Slots**

factors a list of at most two lgpexprs

# See Also

See operations for performing arithmetics on lgprhs, lgpterm and lgpexpr objects.

model\_summary

Print a model summary.

# Description

Print a model summary.

# Usage

```
model_summary(object, digits = 3)
param_summary(object, digits = 3)
```

# Arguments

object a model or fit

digits number of digits to round floats to

# Value

object invisibly.

new\_x

new	X

Create test input points for prediction

# Description

Replaces a continuous variable x in the data frame, and possibly another continuous variable x\_ns derived from it, with new values, for each level of a grouping factor (usually id)

# Usage

```
new_x(data, x_values, group_by = "id", x = "age", x_ns = NULL)
```

# Arguments

data	A data frame. Can also be an lgpfit or lgpmodel object, in which case data is extracted from it.
x_values	the values of x to set for each individual
group_by	name of the grouping variable, must be a factor in data (or use group_by=NA to create a dummy grouping factor which has only one value)
X	of the variable along which to extend, must be a numeric in data
x_ns	of a nonstationary variable derived from x, must be a numeric in data

#### Value

a data frame containing the following columns

- all factors in the original data
- X
- x\_ns (unless it is NULL)

#### See Also

```
Other data frame handling functions: add_dis_age(), add_factor_crossing(), add_factor(), adjusted_c_hat(), split()
```

plot\_api\_c

operations

Operations on formula terms and expressions

# Description

Operations on formula terms and expressions

#### Usage

```
## S4 method for signature 'lgprhs,lgprhs'
e1 + e2

## S4 method for signature 'lgpterm,lgpterm'
e1 + e2

## S4 method for signature 'lgprhs,lgpterm'
e1 + e2

## S4 method for signature 'lgpterm,lgpterm'
e1 * e2
```

# **Arguments**

- e1 The first sum, term or expression
- e2 The second sum, term or expression

# Value

The behaviour and return type depend on the types of e1 and e2. You can

- sum (+) two lgprhs's to yield an lgprhs
- sum (+) two lgpterm's to yield an lgprhs
- sum (+) an lgprhs and an lgpterm to yield an lgprhs
- multiply (\*) two lgpterm's to yield an lgpterm

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## **Description**

Data frames specified in arguments df, and df\_err must have a format where

- The first column is the grouping factor (usually id).
- The second column is the x-axis variable (usually age).
- The third column is the coloring factor. If name of the third column is NA, coloring is not done.
- A column named y must contain the y-axis variable (not for df\_err).
- A column named lower (upper) must contain the lower (upper) bound of error bar (only for df\_err).
- The posterior draw using which the fit has been computed can be specified with a factor named \_draw\_ (only for df).

# Usage

```
plot_api_c(
   df,
   df_err = NULL,
   alpha = 1,
   alpha_err = 0.2,
   no_err = FALSE,
   no_line = FALSE
)
```

# Arguments

```
df a data frame

df_err a data frame

alpha line opacity

alpha_err ribbon opacity

no_err hide error bar even when it would normally be plotted?

no_line hide line even when it would normally be plotted?
```

#### Value

```
A ggplot object.
```

## See Also

```
Other internal plot API functions: plot_api_g()
```

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plot\_api\_g

Plot longitudinal data and/or model fit so that each subject/group has their own panel

#### **Description**

Data frames specified in arguments df\_data, df\_signal, df\_fit, and df\_fit\_err must have a format where

- the first column is the grouping factor (usually id)
- the second column is the x-axis variable (usually age)
- a column named y must contain the y-axis variable (not for df\_fit\_err)
- a column named lower (upper) must contain the lower (upper) bound of error bar (only for df\_fit\_err)
- a column named draw must be a factor that specifies the posterior draw using which the fit has been computed (only for df\_fit)

# Usage

```
plot_api_g(
  df_data,
  df_signal = NULL,
  df = NULL,
  df_{err} = NULL
  teff_signal = NULL,
  teff_obs = NULL,
  i_test = NULL,
  color_signal = color_palette(2)[1],
  color = color_palette(2)[2],
  color_err = colorset("red", "light_highlight"),
  color_vlines = colorset("gray", "mid_highlight"),
  alpha = 1,
  alpha_err = 0.5,
  nrow = NULL,
 ncol = NULL,
  y_{transform} = function(x) x
)
```

# **Arguments**

df

df\_data A data frame containing the observations.

df\_signal A data frame containing the true signal. Omitted if NULL.

A data frame containing the model fit, or a list of data frames. The list version can be used for example so that each list element corresponds to the fit computed using one parameter draw. Omitted if NULL.

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df\_err A data frame containing error bars. Omitted if NULL. Must be NULL if df\_fit is

a list.

teff\_signal A named vector containing true effect times used to generate the signal. Omitted

if NULL.

teff\_obs A named vector containing observed effect times. Omitted if NULL.

color\_vlines Two line colors for vertical lines (true and obs. effect time).

alpha Line opacity for model fit.
alpha\_err Opacity of the error ribbon.

nrow number of rows, an argument for facet\_wrap

ncol number of columns, an argument for facet\_wrap

y\_transform A function to be applied to the third column of df\_data.

#### Value

A ggplot object.

#### See Also

Other internal plot API functions: plot\_api\_c()

plot\_components

Visualize all model components

### Description

This calls plot\_f for all model components.

# Usage

```
plot_components(
   fit,
   pred = NULL,
   group_by = "id",
   t_name = "age",
   MULT_STD = 2,
   verbose = TRUE,
   draws = NULL,
   reduce = function(x) base::mean(x),
   color_by = NA,
   no_err = FALSE,
```

38 plot\_components

```
ylim = NULL,
draw = TRUE,
nrow = NULL,
ncol = NULL,
gg_add = NULL,
x = NULL,
...
)
```

#### **Arguments**

fit An object of class lgpfit.

An object of class Coussian Production or Production

pred An object of class GaussianPrediction or Prediction. If pred=NULL, the pred

function is called with the given reduce and draws arguments.

group\_by name of the grouping variable (use group\_by=NA to avoid grouping)

t\_name name of the x-axis variable

MULT\_STD a multiplier for standard deviation verbose Can this print any messages?

draws
Only has effect if pred=NULL.
reduce
Only has effect if pred=NULL.

color\_by Names of coloring factors. Can have length 1 or equal to the number of compo-

nents. See the color\_by argument of plot\_f.

no\_err Should the error ribbons be skipped even though they otherwise would be shown?

Can have length 1 or equal to number of components + 1. See the no\_err argu-

ment of plot\_api\_c.

ylim a vector of length 2 (upper and lower y-axis limits), or NULL

draw if this is TRUE, the plot grid is drawn using arrangeGrob

nrow number of grid rows ncol number of grid columns

gg\_add additional ggplot obejct to add to each plot

x Deprecated argument. This is now taken from the pred object to ensure com-

patibility.

... additional arguments to plot\_api\_c

#### Value

a list of ggplot objects invisibly

### See Also

Other main plot functions: plot\_draws(), plot\_pred()

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plot\_data

Vizualizing longitudinal data

# Description

Vizualizing longitudinal data

# Usage

```
plot_data(
    data,
    x_name = "age",
    y_name = "y",
    group_by = "id",
    facet_by = NULL,
    color_by = NULL,
    highlight = NULL,
    sub = NULL
)
```

# Arguments

data	A data frame.
x_name	Name of x-axis variable.
y_name	Name of the y-axis variable.
group_by	Name of grouping variable (must be a factor).
facet_by	Name of the faceting variable (must be a factor).
color_by	Name of coloring variable (must be a factor).
highlight	Value of category of the group_by variable that is highlighted. Can only be used if color_by is NULL.
main	main plot title
sub	plot subtitle

```
a ggplot object
```

40 plot\_draws

plot\_draws

Visualize the distribution of parameter draws

### **Description**

Visualize the distribution of parameter draws

# Usage

```
plot_draws(
    fit,
    type = "intervals",
    regex_pars = c("alpha", "ell", "wrp", "sigma", "phi", "gamma"),
    ...
)

plot_beta(fit, type = "dens", verbose = TRUE, ...)

plot_warp(
    fit,
    num_points = 300,
    window_size = 48,
    color = colorset("red", "dark"),
    alpha = 0.5
)

plot_effect_times(fit, type = "areas", verbose = TRUE, ...)
```

# **Arguments**

```
fit
                  an object of class lgpfit
                  plot type, allowed options are "intervals", "dens", "areas", and "trace"
type
                  regex for parameter names to plot
regex_pars
                  additional arguments for the bayesplot function mcmc_intervals, mcmc_dens,
                  mcmc_areas or mcmc_trace
verbose
                  Can any output be printed?
                  number of plot points
num_points
window_size
                  width of time window
color
                  line color
alpha
                  line alpha
```

```
a ggplot object or list of them
```

plot\_inputwarp 41

# **Functions**

• plot\_draws(): visualizes the distribution of any set of model parameters (defaults to kernel hyperparameters and possible observation model parameters)

- plot\_beta(): visualizes the distribution of the individual-specific disease effect magnitude parameter draws
- plot\_warp(): visualizes the input warping function for different draws of the warping steepness parameter
- plot\_effect\_times(): visualizes the input warping function for different parameter draws

#### See Also

Other main plot functions: plot\_components(), plot\_pred()

plot_inputwarp	Visualize input warping function with several steepness parameter val-
	ues

### **Description**

Visualize input warping function with several steepness parameter values

### Usage

```
plot_inputwarp(wrp, x, color = colorset("red", "dark"), alpha = 0.5)
```

# **Arguments**

wrp a vector of values of the warping steepness parameter

x a vector of input values

color line color alpha line alpha

```
a ggplot object
```

42 plot\_invgamma

plot\_invgamma

Plot the inverse gamma-distribution pdf

# Description

Plot the inverse gamma-distribution pdf

# Usage

```
plot_invgamma(
   alpha,
   beta,
   by = 0.01,
   log = FALSE,
   IQR = 0.95,
   return_quantiles = FALSE,
   linecolor = colorset("red", "dark"),
   fillcolor = colorset("red", "mid")
)
```

# **Arguments**

alpha positive real number beta positive real number

by grid size

log is log-scale used?

IQR inter-quantile range width

return\_quantiles

should this return a list

linecolor line color fillcolor fill color

# Value

a ggplot object

# See Also

Other functions related to the inverse-gamma distribution: dinvgamma\_stanlike(), priors

plot\_pred 43

plot\_pred

Visualizing model predictions or inferred covariate effects

# **Description**

- Function draws at data points can be visualized using plot\_pred. If the pred argument is NULL, it is computed using the pred function with x=NULL.
- The total signal f or any of its additive components can be plotted using plot\_f.

# Usage

```
plot_pred(
  fit,
  pred = NULL,
  group_by = "id",
  t_name = "age",
 MULT_STD = 2,
  verbose = TRUE,
  draws = NULL,
  reduce = function(x) base::mean(x),
  x = NULL
)
plot_f(
  fit,
  pred = NULL,
  group_by = "id",
  t_name = "age",
 MULT_STD = 2,
  verbose = TRUE,
  draws = NULL,
  reduce = function(x) base::mean(x),
  comp_idx = NULL,
  color_by = NA,
  x = NULL,
)
```

# Arguments

fit	An object of class lgpfit.
pred	An object of class GaussianPrediction or Prediction. If pred=NULL, the pred function is called with the given reduce and draws arguments.
group_by	name of the grouping variable (use group_by=NA to avoid grouping)
t_name	name of the x-axis variable

plot\_sim

```
MULT_STD a multiplier for standard deviation

verbose Can this print any messages?

draws Only has effect if pred=NULL.

reduce Only has effect if pred=NULL.

x Deprecated argument. This is now taken from the pred object to ensure compatibility.

... additional arguments to plot_api_g or plot_api_c

comp_idx Index of component to plot. The total sum is plotted if this is NULL.

color_by name of coloring factor
```

# Value

```
a ggplot object
```

# See Also

Other main plot functions: plot\_components(), plot\_draws()

plot\_sim

Visualize an lgpsim object (simulated data)

# Description

Visualize an lgpsim object (simulated data)

# Usage

```
plot_sim(
    simdata,
    group_by = "id",
    x_name = "age",
    h_name = "h",
    y_name = "y",
    comp_idx = NULL,
    color_by = NA,
    verbose = TRUE,
    ...
)
```

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#### **Arguments**

simdata an object of class lgpsim

group\_by grouping factor

x\_name name of x-axis variable

h\_name name of the signal in simdata\$components ("h" or "f")

y\_name name of response variable

comp\_idx Possible index of a component to be shown. If this is NULL, the data and total

signal are shown.

color\_by coloring factor

verbose should some information be printed?

additional arguments to plot\_api\_g or plot\_api\_c

#### Value

a ggplot object

ррс

Graphical posterior predictive checks

# **Description**

Graphical posterior predictive checks

# Usage

```
ppc(fit, data = NULL, fun = default_ppc_fun(fit), verbose = TRUE, ...)
```

# **Arguments**

fit An object of class lgpfit that can been created with sample\_f=TRUE.

data the original data frame (deprecated argument with no effect, now obtained from

fit object)

fun bayesplot function name verbose Can this print any messages?

... additional arguments passed to the default pp\_check method in bayesplot

#### Value

a ggplot object

#### See Also

Introduction to graphical posterior predictive checks: here. Prior predictive check can be done by calling prior\_pred and then bayesplot::pp\_check().

46 pred

pred

Posterior predictions and function posteriors

### Description

- If fit is for a model that marginalizes the latent signal f (i.e. is\_f\_sampled(fit) is FALSE), this computes the analytic conditional posterior distributions of each model component, their sum, and the conditional predictive distribution. All these are computed for each (hyper)parameter draw (defined by draws), or other parameter set (obtained by a reduction defined by reduce). Results are stored in a GaussianPrediction object which is then returned.
- If fit is for a model that samples the latent signal f (i.e. is\_f\_sampled(fit) is TRUE), this will extract these function samples, compute their sum, and a version of the sum f that is transformed through the inverse link function. If x is not NULL, the function draws are extrapolated to the points specified by x using kernel regression. Results are stored in a Prediction object which is then returned.

# Usage

```
pred(
   fit,
   x = NULL,
   reduce = function(x) base::mean(x),
   draws = NULL,
   verbose = TRUE,
   STREAM = get_stream(),
   c_hat_pred = NULL,
   force = FALSE,
   debug_kc = FALSE
)
```

# Arguments

fit	An object of class lgpfit.
x	A data frame of points where function posterior distributions and predictions should be computed or sampled. The function <a href="new_x">new_x</a> provides an easy way to create it. If this is NULL, the data points are used.
reduce	Reduction for parameters draws. Can be a function that is applied to reduce all parameter draws into one parameter set, or NULL (no reduction). Has no effect if draws is specified.
draws	Indices of parameter draws to use, or NULL to use all draws.
verbose	Should more information and a possible progress bar be printed?
STREAM	External pointer. By default obtained with rstan::get_stream().
c_hat_pred	This is only used if the latent signal f was sampled. This input contains the values added to the sum f before passing through inverse link function. Must be a vector with length equal to the number of prediction points. If original

Prediction-class 47

<pre>c_hat was constant,</pre>	then c_hat_pred	can be ignored, in	which case this will

by default use the same constant.

force This is by default FALSE to prevent unintended large computations that might

crash R or take forever. Set it to TRUE try computing no matter what.

debug\_kc If this is TRUE, this only returns a KernelComputer object that is created inter-

nally. Meant for debugging.

#### Value

An object of class GaussianPrediction or Prediction.

#### See Also

```
Other main functions: create_model(), draw_pred(), get_draws(), lgp(), prior_pred(), sample_model()
```

Prediction-class

An S4 class to represent prior or posterior draws from an additive function distribution.

# **Description**

An S4 class to represent prior or posterior draws from an additive function distribution.

#### Usage

```
## S4 method for signature 'Prediction'
show(object)

## S4 method for signature 'Prediction'
component_names(object)

## S4 method for signature 'Prediction'
num_components(object)

## S4 method for signature 'Prediction'
num_paramsets(object)

## S4 method for signature 'Prediction'
num_evalpoints(object)
```

### **Arguments**

object Prediction object for which to apply a class method.

48 priors

#### Methods (by generic)

- show(Prediction): Print a summary about the object.
- component\_names(Prediction): Get names of components.
- num\_components(Prediction): Get number of components.
- num\_paramsets(Prediction): Get number of parameter combinations (different parameter vectors) using which predictions were computed.
- num\_evalpoints(Prediction): Get number of points where predictions were computed.

#### **Slots**

- f\_comp component draws
- f signal draws
- h predictions (signal draws + scaling factor c\_hat, transformed through inverse link function)
- x a data frame of points (covariate values) where the functions/predictions have been evaluated/sampled extrapolated Boolean value telling if the function draws are original MCMC draws or if they have been created by extrapolating such draws.

#### See Also

GaussianPrediction

priors

Prior definitions

# **Description**

These use the same parametrizations as defined in the 'Stan' documentation. See the docs for gamma and inverse gamma distributions.

# Usage

```
uniform(square = FALSE)
normal(mu, sigma, square = FALSE)
student_t(nu, square = FALSE)
gam(shape, inv_scale, square = FALSE)
igam(shape, scale, square = FALSE)
log_normal(mu, sigma, square = FALSE)
bet(a, b)
```

prior\_pred 49

# Arguments

is prior for a square-transformed parameter? square mean mu standard deviation sigma degrees of freedom nu shape shape parameter (alpha) inv\_scale inverse scale parameter (beta) scale scale parameter (beta) shape parameter а b shape parameter

#### Value

a named list

#### See Also

Other functions related to the inverse-gamma distribution: dinvgamma\_stanlike(), plot\_invgamma()

# **Examples**

```
# Log-normal prior
log_normal(mu = 1, sigma = 1)

# Cauchy prior
student_t(nu = 1)

# Exponential prior with rate = 0.1
gam(shape = 1, inv_scale = 0.1)

# Create a similar priors as in LonGP (Cheng et al., 2019)
# Not recommended, because a lengthscale close to 0 is possible.
a <- log(1) - log(0.1)
log_normal(mu = 0, sigma = a / 2) # for continuous lengthscale
student_t(nu = 4) # for interaction lengthscale
igam(shape = 0.5, scale = 0.005, square = TRUE) # for sigma</pre>
```

prior\_pred

Prior (predictive) sampling

#### **Description**

These functions take an lgpmodel object, and

- prior\_pred samples from the prior predictive distribution of the model
- sample\_param\_prior samples only its parameter prior using sampling

50 prior\_to\_num

#### Usage

```
prior_pred(
  model,
  verbose = TRUE,
  quiet = FALSE,
  refresh = 0,
  STREAM = get_stream(),
  ...
)
sample_param_prior(model, verbose = TRUE, quiet = FALSE, ...)
```

### **Arguments**

model An object of class lgpmodel.

verbose Should more information and a possible progress bar be printed?

quiet This forces verbose to be FALSE. If you want to suppress also the output from Stan, give the additional argument refresh=0.

refresh Argument for sampling.

STREAM External pointer. By default obtained with rstan::get\_stream().

Additional arguments for sampling.

#### Value

- prior\_pred returns a list with components
  - y\_draws: A matrix containing the prior predictive draws as rows. Can be passed to bayesplot::pp\_check() for graphical prior predictive checking.
  - pred\_draws: an object of class Prediction, containing prior draws of each model component and their sum
  - param\_draws: a stanfit object of prior parameter draws (obtained by calling sample\_param\_prior internally)
- sample\_param\_prior returns an object of class stanfit

### See Also

Other main functions: create\_model(), draw\_pred(), get\_draws(), lgp(), pred(), sample\_model()

prior\_to\_num Convert given prior to numeric format

# **Description**

Convert given prior to numeric format

read\_proteomics\_data 51

# Usage

```
prior_to_num(desc)
```

# Arguments

desc

Prior description as a named list, containing fields

- dist Distribution name. Must be one of 'uniform', 'normal', 'student-t', 'gamma', 'inv-gamma', 'log-normal' (case-insensitive)
- square Is the prior for a square-transformed parameter.

Other list fields are interpreted as hyperparameters.

#### Value

a named list of parsed options

read\_proteomics\_data

Function for reading the built-in proteomics data

# **Description**

Function for reading the built-in proteomics data

#### Usage

```
read_proteomics_data(parentDir = NULL, protein = NULL, verbose = TRUE)
```

# Arguments

parentDir Path to local parent directory for the data. If this is NULL, data is downloaded

from https://github.com/jtimonen/lgpr-usage/tree/master/data/proteomics.

protein Index or name of protein.

verbose Can this print some output?

```
a data.frame
```

52 s4\_generics

relevances

Assess component relevances

# **Description**

Assess component relevances

#### Usage

```
relevances(fit, reduce = function(x) base::mean(x), verbose = TRUE, ...)
```

# **Arguments**

fit an object of class lgpfit

reduce a function to apply to reduce the relevances given each parameter draw into one

value

verbose Can this print any messages? ... currently has no effect

#### Value

a named vector with length equal to num\_comps + 1

s4\_generics

S4 generics for lgpfit, lgpmodel, and other objects

# **Description**

S4 generics for lgpfit, lgpmodel, and other objects

# Usage

```
parameter_info(object, digits)
component_info(object)
covariate_info(object)
component_names(object)
get_model(object)
is_f_sampled(object)
get_stanfit(object)
```

s4\_generics 53

```
postproc(object, ...)
contains_postproc(object)
clear_postproc(object)
num_paramsets(object)
num_evalpoints(object)
num_components(object)
```

#### **Arguments**

object object for which to apply the generic digits number of digits to show additional optional arguments to pass

#### Value

- parameter\_info returns a data frame with one row for each parameter and columns for parameter name, parameter bounds, and the assigned prior
- component\_info returns a data frame with one row for each model component, and columns encoding information about model components
- covariate\_info returns a list with names continuous and categorical, with information about both continuous and categorical covariates
- component\_names returns a character vector with component names
- get\_model for lgpfit objects returns an lgpmodel
- is\_f\_sampled returns a logical value
- get\_stanfit returns a stanfit (rstan)
- postproc applies postprocessing and returns an updated lgpfit
- clear\_postproc removes postprocessing information and returns an updated lgpfit
- num\_paramsets, num\_evalpoints and num\_components return an integer

#### **Functions**

- parameter\_info(): Get parameter information (priors etc.).
- component\_info(): Get component information.
- covariate\_info(): Get covariate information.
- component\_names(): Get component names.
- get\_model(): Get lgpmodel object.
- is\_f\_sampled(): Determine if signal f is sampled or marginalized.
- get\_stanfit(): Extract stanfit object.

54 sample\_model

- postproc(): Perform postprocessing.
- contains\_postproc(): Determine if object contains postprocessing information.
- clear\_postproc(): Clear postprocessing information (to reduce size of object).
- num\_paramsets(): Get number of parameter sets.
- num\_evalpoints(): Get number of points where posterior is evaluated.
- num\_components(): Get number of model components.

#### See Also

To find out which methods have been implemented for which classes, see lgpfit, lgpmodel, Prediction and GaussianPrediction.

sample\_model

Fitting a model

### **Description**

- sample\_model takes an lgpmodel object and fits it using sampling.
- optimize\_model takes an lgpmodel object and fits it using optimizing.

#### Usage

```
sample_model(
  model,
  verbose = TRUE,
  quiet = FALSE,
  skip_postproc = is_f_sampled(model),
  ...
)
optimize_model(model, ...)
```

### **Arguments**

model An object of class lgpmodel.

verbose Can messages be printed?

quiet Should all output messages be suppressed? You need to set also refresh=0 if you want to suppress also the progress update messages from sampling.

skip\_postproc Should all postprocessing be skipped? If this is TRUE, the returned lgpfit object will likely be much smaller (if sample\_f=FALSE).

Optional arguments passed to sampling or optimizing.

select 55

#### Value

 sample\_model returns an object of class lgpfit containing the parameter draws, the original model object, and possible postprocessing results. See documentation of lgpfit for more information.

 optimize\_model directly returns the list returned by optimizing. See its documentation for more information.

#### See Also

Other main functions: create\_model(), draw\_pred(), get\_draws(), lgp(), pred(), prior\_pred()

select

Select relevant components

# **Description**

- select performs strict selection, returning either TRUE or FALSE for each component.
- select.integrate is like select, but instead of a fixed threshold, computes probabilistic selection by integrating over a threshold density.
- select\_freq performs the selection separately using each parameter draw and returns the frequency at which each component was selected.
- select\_freq.integrate is like select\_freq, but instead of a fixed threshold, computes probabilistic selection frequencies by integrating over a threshold density.

### Usage

```
select(fit, reduce = function(x) base::mean(x), threshold = 0.95, ...)

select_freq(fit, threshold = 0.95, ...)

select.integrate(
    fit,
    reduce = function(x) base::mean(x),
    p = function(x) stats::dbeta(x, 100, 5),
    h = 0.01,
    verbose = TRUE,
    ...
)

select_freq.integrate(
    fit,
    p = function(x) stats::dbeta(x, 100, 5),
    h = 0.01,
    verbose = TRUE,
    ...
)
```

56 show

### **Arguments**

fit An object of class lgpfit.

reduce The reduce argument for relevances.

threshold Threshold for relevance sum. Must be a value between 0 and 1.

... Additional arguments to relevances.

p A threshold density over interval [0,1].

h A discretization parameter for computing a quadrature.

verbose Should this show a progress bar?

#### Value

See description.

show

Printing formula object info using the show generic

# **Description**

Printing formula object info using the show generic

# Usage

```
## S4 method for signature 'lgpformula'
show(object)

## S4 method for signature 'lgprhs'
show(object)

## S4 method for signature 'lgpterm'
show(object)
```

# **Arguments**

object an object of some S4 class

#### Value

the object invisibly

sim.create\_f 57

sim.create\_f

Simulate latent function components for longitudinal data analysis

#### **Description**

Simulate latent function components for longitudinal data analysis

# Usage

```
sim.create_f(
   X,
   covariates,
   relevances,
   lengthscales,
   X_affected,
   dis_fun,
   bin_kernel,
   steepness,
   vm_params,
   force_zeromean
)
```

# **Arguments**

Χ

input data matrix (generated by sim.create\_x)

covariates

Integer vector that defines the types of covariates (other than id and age). Different integers correspond to the following covariate types:

- 0 = disease-related age
- 1 = other continuous covariate
- 2 = a categorical covariate that interacts with age
- 3 = a categorical covariate that acts as a group offset
- 4 = a categorical covariate that that acts as a group offset AND is restricted to have value 0 for controls and 1 for cases

relevances

Relative relevance of each component. Must have be a vector so that

length(relevances) = 2 + length(covariates).

First two values define the relevance of the individual-specific age and shared age component, respectively.

lengthscales

A vector so that

length(lengthscales) = 2 + sum(covariates %in% c(0,1,2)).

X\_affected

which individuals are affected by the disease

dis\_fun

A function or a string that defines the disease effect. If this is a function, that function is used to generate the effect. If dis\_fun is "gp\_vm" or "gp\_ns", the disease component is drawn from a nonstationary GP prior ("vm" is the variance

masked version of it).

58 sim.create\_x

Should the binary kernel be used for categorical covariates? If this is TRUE, the bin\_kernel

effect will exist only for group 1.

Steepness of the input warping function. This is only used if the disease composteepness

nent is in the model.

vm\_params Parameters of the variance mask function. This is only needed if useMaskedVarianceKernel

= TRUE.

force\_zeromean Should each component (excluding the disease age component) be forced to

have a zero mean?

#### Value

a data frame FFF where one column corresponds to one additive component

sim.create\_x

Create an input data frame X for simulated data

# **Description**

Create an input data frame X for simulated data

### Usage

```
sim.create_x(
 N,
  covariates,
  names,
  n_categs,
  t_data,
  t_jitter,
  t_effect_range,
  continuous_info
)
```

# Arguments Ν

Number of individuals.

covariates

Integer vector that defines the types of covariates (other than id and age). If not given, only the id and age covariates are created. Different integers correspond to the following covariate types:

- 0 = disease-related age
- 1 = other continuous covariate
- 2 = a categorical covariate that interacts with age
- 3 = a categorical covariate that acts as a group offset
- 4 = a categorical covariate that that acts as a group offset AND is restricted to have value 0 for controls and 1 for cases

59 sim.create\_y

Covariate names. names

An integer vector defining the number of categories for each categorical con\_categs

variate, so that length(n\_categs) equals to the number of 2's and 3's in the

covariates vector.

t\_data Measurement times (same for each individual, unless  $t_{jitter} > 0$  in which

case they are perturbed).

Standard deviation of the jitter added to the given measurement times. t\_jitter

t\_effect\_range Time interval from which the disease effect times are sampled uniformly. Alter-

natively, This can any function that returns the (possibly randomly generated)

real disease effect time for one individual.

continuous\_info

Info for generating continuous covariates. Must be a list containing fields lambda and mu, which have length 3. The continuous covariates are generated so that x <- sin(a\*t + b) + c, where

• t <- seq(0, 2\*pi, length.out = k)

• a <- mu[1] + lambda[1]\*stats::runif(1)

• b <- mu[2] + lambda[2]\*stats::runif(1)

• c <- mu[3] + lambda[3]\*stats::runif(1)

#### Value

a list

sim.create\_y Simulate noisy observations

# **Description**

Simulate noisy observations

#### **Usage**

```
sim.create_y(noise_type, f, snr, phi, gamma, N_trials)
```

### **Arguments**

noise_type	Either "gaussian", "poisson", "nb" (negative binomial), "binomial", or "bb" (beta-binomial).
f	The underlying signal.
snr	The desired signal-to-noise ratio. This argument is valid only when noise_type is "gaussian".
phi	The inverse overdispersion parameter for negative binomial data. The variance is $g + g^2/phi$ .
gamma	The dispersion parameter for beta-binomial data.
N_trials	The number of trials parameter for binomial data.

60 sim.kernels

#### Value

A list out, where

• out\$h is f mapped through an inverse link function (times N\_trials if noise\_type is binomial or beta-binomial)

• out\$y is the noisy response variable.

sim.kernels

Compute all kernel matrices when simulating data

### **Description**

Compute all kernel matrices when simulating data

# Usage

```
sim.kernels(
   X,
   types,
   lengthscales,
   X_affected,
   bin_kernel,
   useMaskedVarianceKernel,
   steepness,
   vm_params
)
```

### **Arguments**

X covariates

types vector of covariate types, so that

- 1 = ID
- 2 = age
- 3 = diseaseAge
- 4 = other continuous covariate
- 5 = a categorical covariate that interacts with age
- 6 = a categorical covariate that acts as an offset

lengthscales vector of lengthscales

X\_affected which individuals are affected by the disease

bin\_kernel whether or not binary (mask) kernel should be used for categorical covariates (if

not, the zerosum kernel is used)

useMaskedVarianceKernel

should the masked variance kernel be used for drawing the disease component

steepness steepness of the input warping function vm\_params parameters of the variance mask function

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#### Value

a 3D array

simulate\_data

Generate an artificial longitudinal data set

# **Description**

Generate an artificial longitudinal data set.

### Usage

```
simulate_data(
 Ν,
  t_data,
  covariates = c(),
  names = NULL,
  relevances = c(1, 1, rep(1, length(covariates))),
 n_categs = rep(2, sum(covariates %in% c(2, 3))),
  t_{jitter} = 0,
  lengthscales = rep(12, 2 + sum(covariates %in% c(0, 1, 2))),
  f_{var} = 1,
  noise_type = "gaussian",
  snr = 3,
  phi = 1,
  gamma = 0.2,
 N_{affected} = round(N/2),
  t_effect_range = "auto",
  t_observed = "after_0",
  c_hat = 0,
  dis_fun = "gp_warp_vm",
  bin_kernel = FALSE,
  steepness = 0.5,
  vm_params = c(0.025, 1),
  continuous_info = list(mu = c(pi/8, pi, -0.5), lambda = c(pi/8, pi, 1)),
 N_{trials} = 1,
  force_zeromean = TRUE
)
```

# Arguments

Ν Number of individuals.

t\_data Measurement times (same for each individual, unless  $t_{jitter} > 0$  in which

case they are perturbed).

covariates Integer vector that defines the types of covariates (other than id and age). If not given, only the id and age covariates are created. Different integers correspond

to the following covariate types:

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• 0 = disease-related age

• 1 = other continuous covariate

• 2 = a categorical covariate that interacts with age

• 3 = a categorical covariate that acts as a group offset

• 4 = a categorical covariate that that acts as a group offset AND is restricted to have value 0 for controls and 1 for cases

names Covariate names.

relevances Relative relevance of each component. Must have be a vector so that

length(relevances) = 2 + length(covariates).

First two values define the relevance of the individual-specific age and shared

age component, respectively.

n\_categs An integer vector defining the number of categories for each categorical co-

variate, so that length(n\_categs) equals to the number of 2's and 3's in the

covariates vector.

t\_jitter Standard deviation of the jitter added to the given measurement times.

lengthscales A vector so that

length(lengthscales) = 2 + sum(covariates %in% c(0,1,2)).

f\_var variance of f

noise\_type Either "gaussian", "poisson", "nb" (negative binomial), "binomial", or "bb" (beta-

binomial).

snr The desired signal-to-noise ratio. This argument is valid only when noise\_type

is "gaussian".

phi The inverse overdispersion parameter for negative binomial data. The variance

is  $g + g^2/phi$ .

gamma The dispersion parameter for beta-binomial data.

N\_affected Number of diseased individuals that are affected by the disease. This defaults

to the number of diseased individuals. This argument can only be given if

covariates contains a zero.

t\_effect\_range Time interval from which the disease effect times are sampled uniformly. Alter-

natively, This can any function that returns the (possibly randomly generated)

real disease effect time for one individual.

t\_observed Determines how the disease effect time is observed. This can be any function

that takes the real disease effect time as an argument and returns the (possibly randomly generated) observed onset/initiation time. Alternatively, this can be a

string of the form "after\_n" or "random\_p" or "exact".

c\_hat a constant added to f

dis\_fun A function or a string that defines the disease effect. If this is a function, that

function is used to generate the effect. If dis\_fun is "gp\_vm" or "gp\_ns", the disease component is drawn from a nonstationary GP prior ("vm" is the variance

masked version of it).

bin\_kernel Should the binary kernel be used for categorical covariates? If this is TRUE, the

effect will exist only for group 1.

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steepness Steepness of the input warping function. This is only used if the disease compo-

nent is in the model.

vm\_params Parameters of the variance mask function. This is only needed if useMaskedVarianceKernel

= TRUE.

continuous\_info

Info for generating continuous covariates. Must be a list containing fields lambda and mu, which have length 3. The continuous covariates are generated so that  $x < -\sin(a t + b) + c$ , where

• t <- seq(0, 2\*pi, length.out = k)

• a <- mu[1] + lambda[1]\*stats::runif(1)

• b <- mu[2] + lambda[2]\*stats::runif(1)

• c <- mu[3] + lambda[3]\*stats::runif(1)

N\_trials The number of trials parameter for binomial data.

force\_zeromean Should each component (excluding the disease age component) be forced to have a zero mean?

#### Value

An object of class lgpsim.

# **Examples**

```
# Generate Gaussian data
dat <- simulate_data(N = 4, t_data = c(6, 12, 24, 36, 48), snr = 3)
# Generate negative binomially (NB) distributed count data
dat <- simulate_data(
  N = 6, t_data = seq(2, 10, by = 2), noise_type = "nb",
  phi = 2
)</pre>
```

split

Split data into training and test sets

# Description

- split\_by\_factor splits according to given factor
- split\_within\_factor splits according to given data point indices within the same level of a factor
- split\_within\_factor\_random selects k points from each level of a factor uniformly at random as test data
- split\_random splits uniformly at random
- split\_data splits according to given data rows

64 testdata\_001

#### Usage

```
split_by_factor(data, test, var_name = "id")
split_within_factor(data, idx_test, var_name = "id")
split_within_factor_random(data, k_test = 1, var_name = "id")
split_random(data, p_test = 0.2, n_test = NULL)
split_data(data, i_test, sort_ids = TRUE)
```

# **Arguments**

data	a data frame
test	the levels of the factor that will be used as test data
var_name	name of a factor in the data
idx_test	indices point indices with the factor
k_test	desired number of test data points per each level of the factor
p_test	desired proportion of test data
n_test	desired number of test data points (if NULL, p_test is used to compute this)
i_test	test data row indices
sort_ids	should the test indices be sorted into increasing order

#### Value

```
a named list with names train, test, i_train and i_test
```

# See Also

```
Other data frame handling functions: add_dis_age(), add_factor_crossing(), add_factor(), adjusted_c_hat(), new_x()
```

testdata\_001

A very small artificial test data, used mostly for unit tests

# **Description**

A very small artificial test data, used mostly for unit tests

# Usage

```
testdata_001
```

testdata\_002 65

# **Format**

A data frame with 24 rows and 6 variables:

id individual id, a factor with levels: 1, 2, 3, 4

age age

dis\_age disease-related age

blood a continuous variable

sex a factor with 2 levels: Male, Female

y a continuous variable

#### See Also

Other built-in datasets: testdata\_002

testdata\_002

Medium-size artificial test data, used mostly for tutorials

# **Description**

Medium-size artificial test data, used mostly for tutorials

# Usage

testdata\_002

#### **Format**

A data frame with 96 rows and 6 variables:

id individual id, a factor with levels: 01-12

age age

diseaseAge disease-related age

**sex** a factor with 2 levels: Male, Female

group a factor with 2 levels: Case, Control

y a continuous variable

# See Also

read\_proteomics\_data

Other built-in datasets: testdata\_001

66 var\_mask

validate

Validate S4 class objects

# Description

Validate S4 class objects

# Usage

```
validate_lgpexpr(object)
validate_lgpformula(object)
validate_lgpscaling(object)
validate_lgpfit(object)
validate_GaussianPrediction(object)
validate_Prediction(object)
```

# Arguments

object

an object to validate

# Value

TRUE if valid, otherwise reasons for invalidity

var\_mask

Variance masking function

# Description

Variance masking function

# Usage

```
var_mask(x, stp)
```

# Arguments

x a vector of length n

stp a positive real number (steepness of mask function)

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# Value

```
a vector of length \boldsymbol{n}
```

# See Also

Other kernel utility functions: warp\_input()

warp\_input

Input warping function

# Description

Input warping function

# Usage

```
warp_input(x, a)
```

# Arguments

 ${\sf x}$  a vector of length n

a steepness of the warping function rise

# Value

```
a vector of warped inputs w(x), length n
```

# See Also

Other kernel utility functions: var\_mask()

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