Package 'lgpr'

September 30, 2019

Title Longitudinal Gaussian Process Regression

Version 0.24.2

Description Implements interpretable nonparametric analysis and covariate selection for longitudinal data using additive
Gaussian process regression. Includes specialized non-stationary disease effect modeling features for biomedical studies. Bayesian inference for model parameters is performed using Stan.

```
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Description

lgpr-package

Longitudinal Gaussian Process regression. The package features

- Additive Gaussian process modeling of longitudinal data
- Posterior inference of the model (hyper)parameters using Stan

The 'lgpr' package.

- Computation of covariate relevances, i.e. how much each covariate explains the target variable
- Specialized modeling of a non-stationary disease effect
- Functions for visualizing longitudinal data, posterior samples and model predictions
- Gaussian, Poisson or Negative Binomial observation models

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Basic usage

- See the main function 1gp for creating and fitting additive longitudinal GP models.
- Predictions outside the data can be computed using the function lgp_predict.
- See documentation of the function simulate_data for generating artificial data.
- For visualizing the data and results, see for example the functions
 - plot_data
 - plot_samples
 - plot_components
 - plot_posterior_y
 - plot_simdata

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References

- 1. Carpenter, B. et al. (2017). *Stan: A probabilistic programming language*. Journal of Statistical Software 76(1).
- 2. Gabry, J. and Goodrich, B. (2018). rstantools: Tools for Developing R Packages Interfacing with 'Stan'. R package version 1.5.1.
- 3. Gabry, J. and Mahr, T. (2018). *bayesplot: Plotting for Bayesian Models*. R package version 1.6.0.
- 4. Stan Development Team (2018). *RStan: the R interface to Stan.* R package version 2.17.4. http://mc-stan.org

add_test_caseIDs

Add case IDs to test data frame

Description

Add case IDs to test data frame

Usage

```
add_test_caseIDs(X_test, X_data)
```

Arguments

X_test test data frame X_data data frame

Value

Updated X_test data frame.

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affected

Select the affected individuals

Description

Select the affected individuals

Usage

```
affected(object, medians.return = FALSE, threshold = 0.5)
```

Arguments

object An object of class lgpfit.

medians.return Should the medians of beta parameters also be returned?

threshold A value that the median of beta has to exceed

Value

A binary vector indicating the individuals for which the disease effect is inferred to exist.

assess_convergence

Assess convergence of the chains

Description

Assess convergence of the chains

Usage

```
assess_convergence(fit, verbose = TRUE, recompute = F)
```

Arguments

fit An (incomplete) object of class lgpfit.

verbose should convergence info be printed?

recompute Should the Rhat statistics be recomputed?

Value

Potential scale reduction factors (R_hat).

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average_predictions

Average predictions over samples

Description

Average predictions over samples

Usage

```
average_predictions(LIST)
```

Arguments

LIST

a list over samples

Value

a list

check_data

Validate the 'data' input to 1gp and resolve covariate types

Description

Validate the 'data' input to 1gp and resolve covariate types

Usage

```
check_data(data, varInfo, verbose)
```

Arguments

data the data frame that was passed to 1gp

varInfo variable type info

verbose can this print some info?

Value

a list

check_formula

Validate the formula of 1gp

Description

Checks if the input 'formula' to lgp_model are valid with the given data

Usage

```
check_formula(formula, data)
```

Arguments

formula the formula that was passed to lgp_model data the data frame that was passed to lgp_model

Value

nothing

check_hyperparameter_names

An error message for wrong hyperparameter naming

Description

An error message for wrong hyperparameter naming

Usage

```
check_hyperparameter_names(dist, correct)
```

Arguments

dist the distribution

correct the allowed hyperparameter names

Value

nothing

```
compute_kernel_matrices
```

Evaluate kernel matrices for each component

Description

Used by compute_predictions.

Usage

```
compute_kernel_matrices(X1, X2, kernel_info)
```

Arguments

X1 Covariate matrix of size n1 x sum(D).X2 Covariate matrix of size n2 x sum(D).kernel_info A list of parameters and other kernel info.

Value

An array of size $n1 \times n2 \times sum(D)$.

compute_K_beta

Compute the multiplier matrix K_{beta} (to eneable heterogeneous disease effect)

Description

Compute the multiplier matrix K_beta (to eneable heterogeneous disease effect)

Usage

```
compute_K_beta(beta, row_to_caseID_1, row_to_caseID_2)
```

Arguments

```
beta a row vector of length N_cases
row_to_caseID_1
mapping from row index to case ID
row_to_caseID_2
mapping from row index to case ID
```

Value

a matrix

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compute_K_var_mask

Compute the variance mask kernel matrix

Description

Compute the variance mask kernel matrix

Usage

```
compute_K_var_mask(disAge1, disAge2, vm_params, stp, nan_replace = 0)
```

Arguments

disAge1 disease-related age covariate vector of length n1 disAge2 disease-related age covariate vector of length n2

vm_params vector of two mask function parameters

stp input warping steepness

nan_replace value to replace nans in disAge vectors

Value

a matrix of size n1 x n2

 $compute_lppd$

Compute log-posterior predictive density at test points

Description

Compute log-posterior predictive density at test points

Usage

```
compute_lppd(PRED, y_test)
```

Arguments

PRED predictions

y_test values of the response variable at the test points

Value

```
a matrix with size n_samples x n_data
```

 $compute_predicted_components$

Compute component-wise predictions at test points

Description

Used by compute_predictions.

Usage

```
compute_predicted_components(KK, KKs, KKss, y_data, sigma_n, DELTA)
```

Arguments

KK	Kernel matrices data vs. data.
KKs	Kernel matrices test vs. data.
KKss	Kernel matrices test vs. test.

y_data Response variable.

sigma_n Noise standard deviation parameter.

DELTA Diagonal jitter that ensures pos. def. kernel.

Value

A list containing predicted means and variances.

 $compute_predictions$

Compute component-wise predictions at test points

Description

```
Used by lgp_predict.
```

Usage

```
compute_predictions(X_data, y_data, X_test, params, D, info, cnames, TSCL,
handle_extra = "warning")
```

12 compute_relevances

Arguments

X_data Covariate matrix (data points).y_data Response variable (data points).X_test Covariate matrix (test points).

params Kernel function and other hyperparameters

D a vector of length 6 info other model info

cnames Names of the model components.

TSCL time scaling function and its inverse

handle_extra What to do if test data contains individuals that are not in the training data? Must

be 'silent', 'warning' or 'error'.

Value

A list.

compute_relevances

Covariate and component relevance calculations

Description

Covariate and component relevance calculations

Usage

```
compute_relevances(FFF, y_data, info, D, ell_smooth, x_age)
```

Arguments

FFF a data frame of size n_data x n_components+2 y_data (scaled) measurements of the response variable

info model info

D a vector of length 6

ell_smooth lengthscale for kernel smoothing

x_age (scaled) age covariate

Value

a list

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```
create_covariates_stan
```

Create the covariate matrix that is given to stan

Description

Create the covariate matrix that is given to stan

Usage

```
create_covariates_stan(data, varInfo, types, formula, verbose)
```

Arguments

data the data frame that was passed to lgp

varInfo original variable type info

types the types returned by check_data

formula the model formula

verbose can this print some info?

Value

a list

```
{\tt create\_data\_plot\_df} \qquad {\tt \it Create\ a\ plotting\ data\ frame\ for\ ggplot}
```

Description

A helper function for plot_data.

Usage

```
create_data_plot_df(data, hl_1, hl_2, hl_cont)
```

Arguments

data a data frame

hl_1 highlighting by color hl_2 highlighting by linestyle hl_cont highlighting continuous

Value

an extended data frame

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create_F

Simulate latent function components for longitudinal data analysis

Description

Simulate latent function components for longitudinal data analysis

Usage

```
create_F(X, covariates, relevances, lengthscales, X_affected, dis_fun,
  useBinKernel, steepness, vm_params)
```

Arguments

Χ

input data matrix (generated by 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 infividual-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).

useBinKernel

Should the binary kernel be used for categorical covariates? If this is TRUE, the effect will exist only for group 1.

steepness

Steepness of the input warping function. This is only used if the disease component is in the model.

vm_params

Parameters of the variance mask function. This is only needed if useMaskedVarianceKernel = TRUE.

Value

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

```
create_predictions_plot_df1
```

Create a plotting data frame for ggplot

Description

A helper function for plot_predictions.

Usage

```
create_predictions_plot_df1(fit, scale_f = TRUE, n_sds)
```

Arguments

fit An object of class lgpfit.

scale_f Should the predictions be scaled back to the original data scale?

n_sds number of standard deviations for the uncertainty band width

Value

a data frame

```
create_predictions_plot_df2
```

Create a plotting data frame for ggplot

Description

A helper function for plot_predictions.

Usage

```
create_predictions_plot_df2(model, PRED, scale_f = TRUE,
  componentwise = FALSE, mode, n_sds)
```

Arguments

model An object of class 1gpmodel.

PRED Predictions computed using lgp_predict.

scale_f Should the predictions be scaled back to the original data scale?

componentwise Should the predictions be plotted componentwise?

mode mode

n_sds number of standard deviations for the uncertainty band width

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Value

a data frame

create_simdata_plot_df

Create a plotting data frame for ggplot

Description

A helper function for plot_simdata_by_component.

Usage

```
create_simdata_plot_df(simData)
```

Arguments

simData

An object created using simulate_data.

Value

a data frame

create_stan_input

Create input for Stan

Description

Parses the formula and data input to lgp_model. Also performs many input checks.

Usage

```
create_stan_input(formula, data, prior, likelihood, varInfo, standardize,
  uncertain_diagnosis, equal_effect, C_hat, DELTA, sample_F, t_test,
  verbose, variance_mask, cat_interact_kernel_type)
```

Arguments

formul	la A	A formula of the form y ~	x1 +	x2 +	x3 defining the	he response	variable y and
--------	------	---------------------------	------	------	-----------------	-------------	----------------

covariates xi. All variables that appear in the formula must exist as columns of

data.

data A data frame containing (at least) the variables given in formula.

prior Prior distribution. Can be created for example using the function prior_default.

likelihood Either "Gaussian" (default), "Poisson" or "NB".

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varInfo Variable type info.

standardize Should the response variable be standardized?

uncertain_diagnosis

Do we wish to model uncertainty in the disease effect time?

C_hat This can only be given if likelihood is not Gaussian. The signal f will the

be transformed so that $g = \exp(C_hat + f)$. If NULL, it will be set to

 $C_{hat} = log(mean(y))$, where y is the response variable.

DELTA the amount of added jitter to ensure positive definiteness of the kernel

sample_F Determines if the function values are be sampled (must be TRUE if likelihood is

not Gaussian).

t_test Optional test time points. Should only be used if sample_F = TRUE. Otherwise

use lgp_predict after fitting the model.

verbose Can this print some info?

variance_mask Should a variance mask be used to force disease component variance to zero

before disease onset?

cat_interact_kernel_type

Kernel type for categorical variables (other than id). Possible options are "categorical"

(default) and "binary" (mask kernel where only category "1" will have an ef-

fect).

Value

A list containing the data to be given to rstan::sampling, some info about preprocessing and all the information about scaling the inputs and response, and updated variable type info.

create_test_points

Create a matrix of test points

Description

Create a matrix of test points

Usage

```
create_test_points(object, t_test)
```

Arguments

object An object of class lgpmodel or lgpfit

t_test Test time points (will be same for each individual).

Value

A data frame.

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create_X

Simulate an input data frame X

Description

Simulate an input data frame X

Usage

```
create_X(N, covariates, names, n_categs, t_data, t_jitter, onset_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

names

Covariate names.

n_categs

An integer vector defining the number of categories for each categorical covariate, so that length(n_categs) equals to the number of 2's and 3's in the covariates vector.

t_data

Measurement times.

t_jitter

Standard deviation of the jitter added to the given measurement times.

onset_range

Time interval from which the disease effect times are sampled uniformly. Alternatively, 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 $x \leftarrow \sin(a*t + b) + c$, where

```
• t \leftarrow 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

```
list(X, onsets, par_cont)
```

create_X_star 19

create_X_star	Create X_star
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Description

Create X_star

Usage

```
create_X_star(X, D, t_test, SCL, X_notnan)
```

Arguments

X covariate matrix

D covariate type information

t_test Test time points (will be same for each individual).

SCL time scaling function and its inverse

X_notnan indicates where X_diseaseAge is not NaN

Value

A data frame.

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Generate noisy observations

Description

Generate noisy observations

Usage

```
create_y(noise_type, f, snr, phi)
```

Arguments

noise_type	Either '	"Gaussian".	"Poisson"	or "NB"	(negative binomial).
110100_0,00	Litter	Caabbian	, 10100011	01 112	(megative omomun).

f The underlying signal.

snr The desired signal-to-noise ratio. This argument is valid only with

noise_type = "Gaussian".

phi The dispersion parameter for negative binomial noise.

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Value

A list out, where

- out\$g is f mapped through an inverse link function and
- out\$y is the noisy response variable.

disease_effect

Draw disease component from a parameteric form

Description

Draw disease component from a parameteric form

Usage

```
disease_effect(X_id, X_disAge, dis_fun)
```

Arguments

X_id the id covariate

X_disAge the diseaseAge covariate dis_fun the disease age effect function

Value

a vector

 ${\tt drawCategorical}$

Indepedently draw categorical variables for each individual

Description

Indepedently draw categorical variables for each individual

Usage

```
drawCategorical(N, k, v)
```

Arguments

N number of individuals k number of timepoints

v vector of numbers of different categories

Value

```
a matrix of size N x D, where D <- length(v)
```

drawContinuous 21

drawContinuous

Indepedently draw continuous variables for each individual

Description

Indepedently draw continuous variables for each individual

Usage

```
drawContinuous(N, k, D, mu, lambda)
```

Arguments

N	number of individuals
k	number of timepoints
D	number of variables
mu	a vector of length 3
lambda	a vector of length 3

Value

```
a matrix of size N x D
```

 ${\tt drawLatentComponents} \quad \textit{Draw realizations of multivariate normals}$

Description

Draw realizations of multivariate normals

Usage

```
drawLatentComponents(KK)
```

Arguments

KK

3D matrix where KK[,,j] is the jth kernel matrix

Value

```
a matrix FFF
```

Description

Draw the age covariate

Usage

```
drawMeasurementTimes(N, t_data, t_jitter)
```

Arguments

N number of individuals t_data a vector of length k

t_jitter Standard deviation of the jitter added to the given measurement times.

Value

```
a vector of length N*k
```

```
extract_components_onesample
```

Extract inferred components for one sample

Description

Extract inferred components for one sample

Usage

```
extract_components_onesample(fit, sample_idx)
```

Arguments

```
fit an object of class lgpfit
```

sample_idx sample index

Value

a list

extract_t_onset_samples

```
extract_t_onset_samples
```

Extract samples of T_onset

Description

Extract samples of T_onset

Usage

```
extract_t_onset_samples(fit)
```

Arguments

fit

an object of class lgpfit

Value

a matrix

get_case_ids

Get case ids in original data

Description

Get case ids in original data

Usage

```
get_case_ids(fit)
```

Arguments

fit

an object of class lgpfit

Value

a character vector

24 get_diseased_info

get_case_row_mappings Create case ID to rows and back mappings

Description

Create mappings

- from case ID to data rows (caseID_to_rows, caseID_nrows)
- from row number to case ID (row_to_caseID)

Usage

```
get_case_row_mappings(X_notnan, X_id, only_R2C = FALSE)
```

Arguments

X_notnan binary vector indicating if diseaseAge is available for that measurement

 X_id the id covariate in X

only_R2C should this return only the rows-to-caseID mapping

Value

a list

get_diseased_info

Get some variables related to diseased individuals

Description

Get some variables related to diseased individuals

Usage

```
get_diseased_info(D, X, X_notnan, uncertain_diagnosis, equal_effect, TSCL)
```

Arguments

D an integer vector of length 6

X the design matrix

X_notnan a binary vector of length n

uncertain_diagnosis

Boolean value

equal_effect Boolean value

TSCL time scaling function and its inverse

get_ell_smooth 25

Value

a list

get_ell_smooth

A convenience function used in postproc-main.R

Description

A convenience function used in postproc-main.R

Usage

```
get_ell_smooth(ell_smooth, ell_smooth_multip, ell_smp)
```

Arguments

Value

a number

```
get_function_component_samples
```

Get values of sampled function components at data points

Description

Get values of sampled function components at data points

Usage

```
get_function_component_samples(fit, only_at_datapoints)
```

Arguments

```
fit An (incomplete) object of class lgpfit. only_at_datapoints
```

Should the values be obtained only at data points or also test points?

Value

An array of size n_samples x n_data x n_components+2 if only_at_datapoints is TRUE, else the size is n_samples x n_total x n_components+2

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get_model_dims

Set a lot of generic variables that the Stan model needs as input

Description

Set a lot of generic variables that the Stan model needs as input

Usage

```
get_model_dims(X, D, likelihood)
```

Arguments

X the design matrix
D a vector of length 6

likelihood the 'likelihood' input to lgp

Value

a list

get_onset_info

Get disease onset info

Description

This returns

- a vector of observed onsets
- mapping from case ID to average sampling interval before the observed disease onset

Usage

```
get_onset_info(D, X, MAPS, TSCL)
```

Arguments

D an integer vector of length 6

X the design matrix

MAPS mappings created by get_case_row_mappings

TSCL time scaling function and its inverse

Value

two vectors of length N_cases

get_onset_times 27

get_onset_times

Extract observed disease onset times from diseaseAge covariate vector

Description

Extract observed disease onset times from diseaseAge covariate vector

Usage

```
get_onset_times(id, age, disAge)
```

Arguments

id the id covariate, vector of length nage the age covariate, vector of length n

disAge the observed disease-related age covariate, vector of length n

Value

vector of observed onset times

get_predicted

A helper function

Description

A helper function

Usage

```
get_predicted(fit)
```

Arguments

fit

An (incomplete) object of class lgpfit.

Value

a list

28 get_prior_type

get_prior_params

Get prior parameters

Description

Get prior parameters

Usage

```
get_prior_params(dist, add_correct)
```

Arguments

dist the distribution

add_correct additional correct parameter names

Value

a hyperparameter vector of length 2

get_prior_type

A dictionary from distribution names to integer encoding

Description

A dictionary from distribution names to integer encoding

Usage

```
get_prior_type(type)
```

Arguments

type

type of the distribution as a string

Value

an integer

get_response 29

get_response

Get the (scaled) response variable

Description

Gets and possibly scales the response variable.

Usage

```
get_response(data, varInfo, standardize, likelihood)
```

Arguments

data the data frame given as input to 1gp

varInfo variable type info

standardize should the response be standardized to unit variance and zero mean

likelihood the likelihood

Value

a list with the (scaled) response variable

get_runtime

Get average runtime of a chain

Description

Get average runtime of a chain

Usage

```
get_runtime(object)
```

Arguments

object

An object of class lgpfit.

Value

Average runtimes for warmup and sampling

30 hyperparam_estimate

get_transform_type

A dictionary from transform names to integer encoding

Description

A dictionary from transform names to integer encoding

Usage

Value

```
get_transform_type(type)
```

Arguments

type

Type of the transform as a string. Allowed arguments are "none" or "square". If NULL, "none" is used.

```
an integer (0, 1 \text{ or } 2)
```

hyperparam_estimate

Get a posterior estimate of model (hyper)parameters

Description

Get a posterior estimate of model (hyper)parameters

Usage

```
hyperparam_estimate(object, type = "mean")
```

Arguments

object An (incomplete) object of class lgpfit.
type Must be "mean", "median", or "map".

Value

a data frame

hyperparam_samples 31

hyperparam_samples

Get a set of model (hyper)parameter samples

Description

Get a set of model (hyper)parameter samples

Usage

```
hyperparam_samples(object, samples = NULL)
```

Arguments

object An (incomplete) object of class lgpfit.

samples Sample indices. If NULL, all samples are taken.

Value

a data frame

kernel_bin

Compute a binary kernel matrix

Description

Compute a binary kernel matrix

Usage

```
kernel_bin(x1, x2 = NULL, alpha = 1, pos_class = 1)
```

Arguments

x1 (integer) vector of length n
 x2 (integer) vector of length m
 alpha marginal std (default = 1)
 pos_class the positive class label

Value

A kernel matrix of size n x m

32 kernel_ns

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Compute a categorical kernel matrix

Description

Compute a categorical kernel matrix

Usage

```
kernel_cat(x1, x2, alpha = 1)
```

Arguments

x1	(integer) vector of length n
x2	(integer) vector of length m
alpha	marginal std ($default = 1$)

Value

A (binary) kernel matrix of size n x m

kernel_ns

Compute a nonstationary kernel matrix using input warping

Description

Compute a nonstationary kernel matrix using input warping

Usage

```
kernel_ns(x1, x2 = NULL, alpha = 1, ell, a, b, c, nan_replace = 0)
```

Arguments

x1	vector of length n
x2	vector of length m
alpha	marginal std (default = 1)
ell	lengthscale in the warped space
a	steepness of the warping function rise
b	location of the effective time window
С	maximum range

nan_replace the value to use for replacing NaN values

Value

A kernel matrix of size n x m

kernel_se 33

ker	ne l	_se

Compute a squared exponential kernel matrix

Description

Compute a squared exponential kernel matrix

Usage

```
kernel_se(x1, x2, alpha = 1, ell = 1)
```

Arguments

x1	vector of length n
x2	vector of length m
alpha	marginal std (default = 1)
ell	lengthscale (default $= 1$)

Value

A kernel matrix of size n x m

kernel_smoothing

Estimate conditional mean time profile using gaussian kernel smoothing

Description

Estimate conditional mean time profile using gaussian kernel smoothing

Usage

```
kernel_smoothing(v, t, t_out, ell)
```

Arguments

v a vector of length n to be smoothed
t vector of n time points corresponding to y

t_out the set of p time points where the smoothing should be evaluated

ell kernel lengthscale

Value

```
a vector of length p
```

34

lgp

The main function of the 'lgpr' package

Description

This is a wrapper for both lgp_model and lgp_fit. It first creates an lgpmodel object and then fits the model, finally returning an lgpfit object.

Usage

```
lgp(formula, data, likelihood = "Gaussian", prior = prior_default(),
  uncertain_diagnosis = FALSE, equal_effect = TRUE,
  id_variable = "id", time_variable = "age", disAge_variable = NULL,
  continuous_vars = NULL, categorical_vars = NULL,
  offset_vars = NULL, C_hat = NULL, DELTA = 1e-12,
  sample_F = (likelihood != "Gaussian"), parallel = FALSE,
  skip_postproc = FALSE, t_test = NULL, threshold = 0.95,
  variance_mask = TRUE, ell_smooth = "ell_shared",
  ell_smooth_multip = 1, cat_interact_kernel_type = "categorical", ...)
```

Arguments

formula A formula of the form $y \sim x1 + x2 + x3$ defining the response variable y and

covariates xi. All variables that appear in the formula must exist as columns of

data.

data A data frame containing (at least) the variables given in formula.

likelihood Either "Gaussian" (default), "Poisson" or "NB".

prior Prior distribution. Can be created for example using the function prior_default.

uncertain_diagnosis

Do we wish to model uncertainty in the disease effect time?

equal_effect Is the disease effect assumed to be equally strong for all diseased individuals?

id_variable Name of the unique subject identifier variable.

time_variable Name of the time variable.

disAge_variable

Name of the disease-related age variable. If NULL, this will be chosen to be

"diseaseAge", if such covariate is found in the data.

continuous_vars

Names of other continuous covariates. If NULL, the remaining covariates that

have floating point values are interpreted as continuous.

categorical_vars

Names of categorical covariates that interact with the time variable. If NULL, the

remaining covariates that have integer values are interpreted as categorical.

offset_vars Names of the categorical covariates that are treated as time-independent group

offsets. If NULL, no variables are interpreted as such covariates.

lgpfit-class 35

C_hat	This can only be given if likelihood is not Gaussian. The signal f will the be transformed so that $g = \exp(C_hat + f)$. If NULL, it will be set to $C_hat = \log(mean(y))$, where y is the response variable.	
DELTA	the amount of added jitter to ensure positive definiteness of the kernel	
sample_F	Determines if the function values are be sampled (must be TRUE if likelihood is not Gaussian).	
parallel	Determines if the chain will be run in parallel (default = FALSE). If TRUE, then Stan is run by first defining options(mc.cores = parallel::detectCores()).	
skip_postproc	In this mode the postprocessing after running Stan is skipped.	
t_test	Optional test time points. Should only be used if sample_F = TRUE. Otherwise use lgp_predict after fitting the model.	
threshold	Covariate selection threshold.	
variance_mask	Should a variance mask be used to force disease component variance to zero before disease onset?	
ell_smooth	Defines how to determine smoothing lengthscale for corrected shared age effect inference. Possible options are	
	 "ell_shared" (default) - the sampled lengthscale of the shared age com- ponent is used as ell_smooth 	
	2. "none" - no correction will be performed	
	3. A numeric argument that directly defines ell_smooth	
ell_smooth_mul	·	
	a multiplier for ell_smooth	
cat_interact_k		
	Kernel type for categorical variables (other than id). Possible options are "categorical" (default) and "binary" (mask kernel where only category "1" will have an effect).	
• • •	Optional arguments passed to rstan::sampling, for example iter, chains or control. See sampling for the possible arguments.	

Value

An object of class lgpfit.

lgpfit-class	An S4 class to represent the output of the lgp_fit function

Description

All slots that are lists contain fields 'samples' and 'average'.

Slots

```
stan_fit The stanfit object returned by rstan::sampling.
model The lgpmodel object returned by lgp_model.
components Inferred components.
components_corrected Covariate-effect corrected components.
component_relevances Inferred component relevances.
covariate_relevances Inferred covariate relevances.
covariate_selection Covariate selection info.
signal_variance Signal variance.
residual_variance Residual variance.
postproc_info Postprocessing information.
Rhat Split Rhat statistics.
```

lgpmodel-class

An S4 class to represent an lgp model

Description

An S4 class to represent an lgp model

Slots

```
data The original unmodified data frame.
stan_dat The data to be given as input to rstan::sampling.
scalings Preprocessing scaling functions and their inverse operations.
info Model info.
```

lgp_component_names

Get names of model components

Description

Get names of model components

Usage

```
lgp_component_names(stan_dat)
```

Arguments

stan_dat

The data that was passed to rstan::sampling

Value

names of model components

37 lgp_covariate_names

lgp_covariate_names Get names of model covariates

Description

Get names of model covariates

Usage

```
lgp_covariate_names(stan_dat)
```

Arguments

stan_dat The data that was passed to rstan::sampling

Value

names of model components

lgp_fit

Fit an lgp model

Description

Samples the posterior of an additive Gaussian process regression model using rstan.

Usage

```
lgp_fit(model, threshold, parallel = FALSE, skip_postproc = FALSE,
 ell_smooth = "ell_shared", ell_smooth_multip = 1, ...)
```

Arguments

mode1 An object of class 1gpmode1. threshold Covariate selection threshold. parallel Determines if the chain will be run in parallel (default = FALSE). If TRUE, then Stan is run by first defining options(mc.cores = parallel::detectCores()). skip_postproc In this mode the postprocessing after running Stan is skipped. ell_smooth Defines how to determine smoothing lengthscale for corrected shared age effect inference. Possible options are 1. "ell_shared" (default) - the sampled lengthscale of the shared age com-

- ponent is used as ell_smooth
- 2. "none" no correction will be performed
- 3. A numeric argument that directly defines ell_smooth

38 lgp_model

Value

An object of class lgpfit.

See Also

For the possible additional arguments, see sampling. For creating the lgpmodel input, see lgp_model.

|--|

Description

Creates an object of class 1gpmode1

Usage

```
lgp_model(formula, data, likelihood = "Gaussian",
    prior = prior_default(likelihood), uncertain_diagnosis = FALSE,
    equal_effect = TRUE, C_hat = NULL, DELTA = 1e-12,
    sample_F = (likelihood != "Gaussian"), t_test = NULL,
    id_variable = "id", time_variable = "age", disAge_variable = NULL,
    continuous_vars = NULL, categorical_vars = NULL,
    offset_vars = NULL, variance_mask = FALSE,
    cat_interact_kernel_type = "categorical")
```

Arguments

formula	A formula of the form $y \sim x1 + x2 + x3$ defining the response variable y and covariates xi. All variables that appear in the formula must exist as columns of data.	
data	A data frame containing (at least) the variables given in formula.	
likelihood	Either "Gaussian" (default), "Poisson" or "NB".	
prior	Prior distribution. Can be created for example using the function prior_default.	
uncertain_diag	nosis	
	Do we wish to model uncertainty in the disease effect time?	
equal_effect	Is the disease effect assumed to be equally strong for all diseased individuals?	
C_hat	This can only be given if likelihood is not Gaussian. The signal f will the be transformed so that $g = \exp(C_hat + f)$. If NULL, it will be set to	

 $C_{hat} = log(mean(y))$, where y is the response variable.

lgp_predict 39

DELTA the amount of added jitter to ensure positive definiteness of the kernel

sample_F Determines if the function values are be sampled (must be TRUE if likelihood is

not Gaussian).

t_test Optional test time points. Should only be used if sample_F = TRUE. Otherwise

use lgp_predict after fitting the model.

id_variable Name of the unique subject identifier variable.

time_variable Name of the time variable.

disAge_variable

Name of the disease-related age variable. If NULL, this will be chosen to be

"diseaseAge", if such covariate is found in the data.

continuous_vars

Names of other continuous covariates. If NULL, the remaining covariates that

have floating point values are interpreted as continuous.

categorical_vars

Names of categorical covariates that interact with the time variable. If NULL, the

remaining covariates that have integer values are interpreted as categorical.

offsets. If NULL, no variables are interpreted as such covariates.

variance_mask Should a variance mask be used to force disease component variance to zero

before disease onset?

cat_interact_kernel_type

Kernel type for categorical variables (other than id). Possible options are "categorical"

(default) and "binary" (mask kernel where only category "1" will have an ef-

fect).

Value

An object of class 1gpmodel.

See Also

For fitting the model, see lgp_fit.

lgp_predict

Compute predictions for a fitted model

Description

Compute predictions for a fitted model. Only possible for models with Gaussian likelihood.

Usage

```
lgp_predict(fit, X_test, samples = "mean", print_progress = TRUE,
    print_params = FALSE)
```

40 lgp_test

Arguments

fit An object of class lgpfit.

X_test The test points where the predictions should be computed.

samples The predictions can be computed either by using only the posterior mean

(samples="mean"), median (samples="median"), or MAP (samples="map") parameters, or for all parameter samples (samples="all"). This can also be a set of indices, for example samples=c(1:10) gives predictions for the parame-

ter samples 1...10.

print_progress Should progress be printed (if there is more than one sample)?

print_params Should the parameter values be printed? (only works if samples is mean or

median.)

Value

A list.

See Also

- For creating an lgpfit object, see lgp_fit.
- For creating an lgpmodel object, see lgp_model.

lgp_test

Compute predictions and log-posterior predictive density at test points

Description

This is a convenience function that wraps lgp_predict, compute_lppd and plot_posterior_y.

Usage

```
lgp_test(fit, test_data, plot = FALSE, verbose = TRUE,
  samples = "mean")
```

Arguments

fit an object of class lgpfit

test_data a test data matrix

should this return also a plot of the data and predictions?

verbose Should this print progress?

samples Sample indices or a keyword "mean", "median", "map", or "all".

Value

```
a ggplot object or lppd
```

likelihood_as_str 41

likelihood_as_str

Convert the Stan likelihood encoding to a string

Description

Convert the Stan likelihood encoding to a string

Usage

```
likelihood_as_str(LH)
```

Arguments

LH

an integer

Value

a string

log_gaussian_density Compute log-density for gaussian distribution

Description

Compute log-density for gaussian distribution

Usage

```
log_gaussian_density(x, mu, s2)
```

Arguments

x point x mu mean s2 variance

Value

a number

42 model_info

matrix_to_df

Matrix to data frame without editing column names

Description

Matrix to data frame without editing column names

Usage

```
matrix\_to\_df(M)
```

Arguments

M a matrix

Value

a data frame

model_info

Get model info

Description

Get model info

Usage

```
model_info(object, print = TRUE)
```

Arguments

object an object of class lgpmodel or lgpfit

print should this print the info?

Value

the info as a string

nameComponents 43

nameComponents

Create names for all components based on covariate names and types

Description

Create names for all components based on covariate names and types

Usage

```
nameComponents(types, names)
```

Arguments

types vector of covariate types names names of the covariates

Value

a vector of component names

 $\verb"onsetsToDiseaseAge"$

Compute the disease-related ages

Description

Compute the disease-related ages

Usage

```
onsetsToDiseaseAge(onsets, age, k)
```

Arguments

onsets true disease effect times, a vector of length N age the age covariate, a vector of length N*k number of measurements per individual

Value

the diseaseAge covariate, a vector of length N*k

parse_prior_onset

parse_prior_distribution

Turn a list describing a prior distribution into vectors to be given to Stan

Description

Turn a list describing a prior distribution into vectors to be given to Stan

Usage

```
parse_prior_distribution(dist, add_correct = NULL)
```

Arguments

dist a list with field type, and possibly others add_correct additional correct parameter names

Value

a list with two vectors to be given to Stan

parse_prior_onset Turn a list describing an onset prior distribution into things to be given

to Stan

Description

Turn a list describing an onset prior distribution into things to be given to Stan

Usage

```
parse_prior_onset(dist, N_cases, T_observed, T_last, UNCRT)
```

Arguments

dist This is prior\$onset, where prior is an argument of lgp_model

N_cases number of case individuals T_observed observed disease onsets

T_last last time point for each diseased individual

UNCRT 0 or 1

Value

a list with things to be given to Stan

```
plot, lgpfit, ANY-method
```

Visualize a fitted 'lgpfit' object

Description

Visualize a fitted 'lgpfit' object

Usage

```
## S4 method for signature 'lgpfit,ANY'
plot(fit, x = 1, y = 1, color_scheme = "red")
```

Arguments

fit an object of class lgpfit

x does nothing y does nothing

color_scheme bayesplot color scheme

Value

a ggplot object

plot_beta

Visualize posterior samples of individual-specific disease effect magnitude parameters

Description

Can only be used if the disease effect was modeled heterogeneously.

Usage

```
plot_beta(fit, color_scheme = "red", threshold = 0.5)
```

Arguments

fit An object of class lgpfit.

color_scheme Name of bayesplot color scheme.

threshold Threshold for median.

Value

a ggplot object

46 plot_data

plot_components	Visualize the (average) inferred components evaluated at data points
prot_components	visualize the (average) injerred components evaluated at data points

Description

Visualize the (average) inferred components evaluated at data points

Usage

```
plot_components(fit, corrected = TRUE, title = NULL,
   sample_idx = NULL, linealpha = 0.6)
```

Arguments

fit An object of class lgpfit.

corrected Should this plot the covariate-effect corrected components?

title optional prefix to plot title

samples.

linealpha line alpha

Value

a ggplot object

plot_data

A spaghetti plot of longitudinal data.

Description

A spaghetti plot of longitudinal data.

Usage

```
plot_data(data, highlight = NULL, response = "y", id_variable = "id",
   time_variable = "age", psize = 2, lwd = 0.5, title = NULL)
```

plot_data_hl_cat 47

Arguments

data A data frame.

highlight Name of a covariate to be highlighted with color, or id of a subject to be high-

lighted.

response Name of the response variable.

id_variable Name of id variable.time_variable Name of time variable.

psize point size lwd line width

title additional string added to title

Value

a ggplot object

plot_data_hl_cat A spaghetti plot of longitudinal data, highlighting a categorical co-

variate.

Description

A spaghetti plot of longitudinal data, highlighting a categorical covariate.

Usage

```
plot_data_hl_cat(data, highlight = NULL, response = "y",
   id_variable = "id", time_variable = "age", psize = 2, lwd = 0.5)
```

Arguments

data A data frame.

highlight Name of a categorical covariate to be highlighted with color.

response Name of the response variable.

id_variable Name of id variable.time_variable Name of time variable.

psize point size lwd line width

Value

a ggplot object

48 plot_data_hl_disease

plot_data_hl_cont	A spaghetti plot of longitudinal data, highlighting a continuous covariate.
-------------------	---

Description

A spaghetti plot of longitudinal data, highlighting a continuous covariate.

Usage

```
plot_data_hl_cont(data, highlight = NULL, response = "y",
  id_variable = "id", time_variable = "age", psize = 2, lwd = 0.5,
  colgrad = ggplot2::scale_colour_gradient2())
```

Arguments

data A data frame.

highlight Name of a continuous covariate to be highlighted with color.

response Name of the response variable.

id_variable Name of id variable.time_variable Name of time variable.

psize point size
lwd line width
colgrad color gradient

Value

a ggplot object

```
plot_data_hl_disease A spaghetti plot of longitudinal data, highlighting based on disease group.
```

Description

A spaghetti plot of longitudinal data, highlighting based on disease group.

Usage

```
plot_data_hl_disease(data, highlight = "diseaseAge", response = "y",
   id_variable = "id", time_variable = "age", psize = 2, lwd = 0.5)
```

plot_data_hl_individual

49

Arguments

data A data frame.

highlight Name of the disease-related age variable.

response Name of the response variable.

id_variable Name of id variable.time_variable Name of time variable.

psize point size lwd line width

Value

a ggplot object

```
plot_data_hl_individual
```

A spaghetti plot of longitudinal data, highlighting one individual.

Description

A spaghetti plot of longitudinal data, highlighting one individual.

Usage

```
plot_data_hl_individual(data, highlight = 1, response = "y",
   id_variable = "id", time_variable = "age", psize = 2, lwd = 0.5)
```

Arguments

data A data frame.

highlight Number indicating the individual to highlight.

response Name of the response variable.

id_variable Name of id variable.time_variable Name of time variable.

psize point size lwd line width

Value

a ggplot object

50 plot_inputwarp

$n \mid a \mid t$	data	plain
DIOL	uata	ртати

A spaghetti plot of longitudinal data without highlighting.

Description

A spaghetti plot of longitudinal data without highlighting.

Usage

```
plot_data_plain(data, response = "y", id_variable = "id",
    time_variable = "age", psize = 2, lwd = 0.5)
```

Arguments

data A data frame.

response Name of the response variable.

id_variable Name of id variable.time_variable Name of time variable.

psize point size lwd line width

Value

a ggplot object

plot_inputwarp

Visualize the input warping function for different parameter samples

Description

Visualize the input warping function for different parameter samples

Usage

```
plot_inputwarp(fit, p = 300, color_scheme = "red", b = 0, c = 1)
```

Arguments

fit An object of class 1gpfit.
p number of plot points

color_scheme Name of bayesplot color scheme.

b location of the effective time window (default = 0)

c maximum range (default = 1)

plot_onset 51

Value

a ggplot object

plot_onset

Visualize posterior uncertainty in the disease effect times

Description

Can only be used if the uncertainty of effect time was modeled.

Usage

```
plot_onset(fit, color_scheme = "red", prob = 1, prob_outer = 1,
    point_est = "none")
```

Arguments

fit An object of class lgpfit.

color_scheme Name of bayesplot color scheme.

prob Inner interval
prob_outer Outer interval

point_est Point estimate type

Value

a ggplot object

```
plot_posterior_components
```

Plot posterior of the components of f

Description

Plot posterior of the components of f

Usage

```
plot_posterior_components(fit, PRED = NULL, color_scheme = "red",
    alpha = 0.1, alpha_line = 1, plot_uncertainty = TRUE,
    title = NULL, ylim = NULL, n_sds = 2, original_y_scale = FALSE)
```

52 plot_posterior_f

Arguments

fit An object of class lgpfit.

PRED Predictions computed using lgp_predict.

color_scheme Name of bayesplot color scheme or a list with fieds 'dark' and 'light'.

alpha Ribbon fill opacity.
alpha_line Line opacity

plot_uncertainty

Should an uncertainty ribbon be plotted?

title optional prefix to plot title

ylim y axis limits

n_sds number of standard deviations for the uncertainty band width

original_y_scale

should the predictions be scaled back to original data scale

Value

a ggplot object

plot_posterior_f
Plot posterior of f

Description

This is a wrapper for plot_posterior_components. and plot_posterior_predictions.

Usage

```
plot_posterior_f(fit, PRED = NULL, componentwise = FALSE,
    plot_uncertainty = TRUE, n_sds = 2)
```

Arguments

fit An object of class lgpfit.

PRED Predictions computed using lgp_predict.

componentwise A boolean value.

plot_uncertainty

Should an uncertainty ribbon be plotted?

n_sds number of standard deviations for the uncertainty band width

Value

a ggplot object

```
plot_posterior_predictions
```

Plot posterior of f or predictive distribution for y

Description

Plot posterior of f or predictive distribution for y

Usage

```
plot_posterior_predictions(fit, mode, PRED = NULL,
   color_scheme = "red", color_scheme_onset = "gray", alpha = 0.5,
   alpha_line = 1, alpha2 = 0.5, plot_uncertainty = TRUE,
   title = NULL, ylim = NULL, plot_obs_onset = FALSE,
   plot_onset_samples = FALSE, ypos_dens = NULL, test_data = NULL,
   color_test = "deepskyblue2", pch_test = 21, size_test = 2,
   error_bar = FALSE, n_sds = 2, reference_onsets = NULL,
   post_onset_statistic = "none", original_y_scale = TRUE,
   data_color = "black", data_marker = 21, ons_linetypes = c(1, 2, 3),
   ons_linecolors = c("black", "red", "gray50"))
```

Arguments

fit An object of class lgpfit.

mode Must be either "posterior" or "predictive".

PRED Predictions computed using lgp_predict.

color_scheme_onset

color scheme name for effect time density plotting

alpha Ribbon fill opacity.

alpha_line Line opacity.

alpha2 alpha of t_onset density

plot_uncertainty

Should an uncertainty ribbon be plotted?

title optional prefix to plot title

ylim y axis limits

plot_obs_onset should the observed disease onset/initiation time be plotted by a vertical line plot_onset_samples

should a distribution of sampled effect times be plotted

ypos_dens y-position of the density plot

test_data Test data frame color_test test point color

54 plot_posterior_y

pch_test test point marker size_test test point size

error_bar should uncertainty be plotted using error bars instead of a ribbon n_sds number of standard deviations for the uncertainty band width

reference_onsets

reference onset times

post_onset_statistic

statistic computed from effect time samples (mean or median)

original_y_scale

should the predictions be scaled back to original data scale

data_color data marker color data_marker data marker type ons_linetypes onset line types ons_linecolors

Value

a ggplot object

plot_posterior_y

Plot posterior predictive distribution

Description

This is a wrapper for plot_posterior_predictions.

Usage

```
plot_posterior_y(fit, PRED, uncertainty = "ribbon", test_data = NULL,
    n_sds = 2)
```

Arguments

fit An object of class lgpfit.

PRED Predictions computed using 1gp_predict.
uncertainty Either "none", "ribbon" or "errorbar".

test_data Test data set.

n_sds number of standard deviations for the uncertainty band width

Value

a ggplot object

```
plot_predictions_add_onsets
```

Add disease onset / effect times to predictions plot

Description

NOTE: currently assumes that diseased individuals come first.

Usage

```
plot_predictions_add_onsets(fit, h, plot_obs_onset, plot_onset_samples,
  idvar, timevar, ypos_dens, color_scheme_onset, reference_onsets,
  post_onset_statistic, linetypes = c(1, 2, 3), linecolors = c("black",
  "red", "gray50"), alpha2 = 1)
```

Arguments

```
fit
                 An object of class lgpfit.
h
                 a ggplot object
plot_obs_onset a boolean value
plot_onset_samples
                 a boolean value
idvar
                 id variable name
timevar
                 time variable name
ypos_dens
                 y position of the estimated onset density
color_scheme_onset
                 color scheme
reference_onsets
```

reference onset times

post_onset_statistic

statistic computed from effect time samples

linetypes onset line types
linecolors onset line colors
alpha2 alpha parameter

Value

```
a modified ggplot object
```

56 plot_relevances

```
plot_predictions_options
```

Do input checks and set options for plotting predictions

Description

Do input checks and set options for plotting predictions

Usage

```
plot_predictions_options(fit, color_scheme, componentwise,
    original_y_scale, PRED, test_data, color_scheme_onset, mode, n_sds)
```

Arguments

fit An object of class lgpfit.

color_scheme Name of bayesplot color scheme.

componentwise Should the predictions be plotted componentwise?

original_y_scale

Boolean value.

PRED Predictions computed using lgp_predict.

Another color scheme.

mode mode

n_sds number of standard deviations for the uncertainty band width

Value

a list

plot_relevances Barplot of covariate relevances

Description

Barplot of covariate relevances

Usage

```
plot_relevances(object, color_scheme = "red")
```

plot_samples 57

Arguments

object an object of class lgpfit color_scheme bayesplot color scheme name

Value

a ggplot object

plot_samples

Visualize the distribution of the model parameter samples

Description

This is a wrapper for functions in the bayesplot package.

Usage

```
plot_samples(object, pars = character(), regex_pars = character(),
  type = "intervals", prob = 0.5, prob_outer = 0.9,
  color_scheme = "red", point_est = "median", binwidth = NULL,
  transformations = list(), off_diag_args = list(size = 1),
  facet_args = list())
```

Arguments

object An object of class lgpfit.

pars parameter names

regex_pars regex for parameter names

type Visualization type. Must be either "dens", "areas", "intervals" (default) or

"hist".

prob inner interval prob_outer outer interval

 ${\tt color_scheme}$ See different color schemes in the bayesplot package.

point_est the point estimate type

binwidth width of histogram bins if type = "hist"

transformations

the parameter transformations

off_diag_args Additional argument list for the pairs plot.

facet_args additional facetting arguments

Value

```
a ggplot object
```

plot_simdata

Visualize simulated data

Description

This is a wrapper for plot_simdata_by_individual and plot_simdata_by_component

Usage

```
plot_simdata(simData, componentwise = FALSE, nrow = NULL,
    ncol = NULL, i_test = NULL, color_test = "steelblue2")
```

Arguments

simData a list returned by simulate_data

componentwise should each component be plotted separately?

nrow an argument for ggplot2::facet_wrap

ncol an argument for ggplot2::facet_wrap

i_test test point indices color_test test point color

Value

a ggplot object

```
plot_simdata_by_component
```

Plot each component of a simulated longitudinal data set separately

Description

Plot each component of a simulated longitudinal data set separately

Usage

```
plot_simdata_by_component(simData, linecolor = "black", nrow = NULL,
    ncol = NULL, plot_point = TRUE, linealpha = 1)
```

Arguments

simData a list returned by simulate_data

linecolor line color

nrow an argument for ggplot2::facet_wrap ncol an argument for ggplot2::facet_wrap

plot_point should points be plotted also

linealpha line alpha

Value

a ggplot object

```
plot_simdata_by_individual
```

Plot a simulated longitudinal data set for each individual separately

Description

Plot a simulated longitudinal data set for each individual separately

Usage

```
plot_simdata_by_individual(simData, linecolor = "gray70", nrow = NULL,
    ncol = NULL, i_test = NULL, color_test = "steelblue2")
```

Arguments

simData a list returned by simulate_data

linecolor line color

nrow an argument for ggplot2::facet_wrap
ncol an argument for ggplot2::facet_wrap

i_test test point indices color_test test point color

Value

a ggplot object

postproc

Finalize the lgpfit object after sampling

Description

Creates the lgpfit slots

- 1. components Inferred components.
- 2. components_corrected Covariate-effect corrected components.
- 3. component_relevances Inferred component relevances.
- 4. covariate_relevances Inferred covariate relevances.
- 5. signal_variance Signal variance.
- 6. residual_variance Residual variance.
- 7. covariate_selection Covariate selection info

all of which are lists that contain the fields samples and average.

60 predict_preproc

Usage

```
postproc(fit, threshold = 0.95, ell_smooth = "ell_shared",
  ell_smooth_multip = 1, sample_idx = NULL,
  average_before_variance = FALSE)
```

Arguments

fit An (incomplete) object of class lgpfit.

threshold Covariate selection threshold.

ell_smooth Defines how to determine smoothing lengthscale for corrected shared age effect

inference. Possible options are

1. "ell_shared" (default) - the sampled lengthscale of the shared age component is used as ell_smooth

2. "none" - no correction will be performed

3. A numeric argument that directly defines ell_smooth

ell_smooth_multip

a multiplier for ell_smooth

average_before_variance

Should the variances be computed using average components?

Value

An updated object of class lgpfit.

predict_preproc

Preprocess some things before computing predictions

Description

This is a helper function for lgp_predict.

Usage

```
predict_preproc(fit, X_test, samples)
```

Arguments

fit An object of class lgpfit.

X_test The test points where the predictions should be computed.

samples The samples argument to lgp_predict

print_prior 61

print_prior

Human-readable description of a specified prior

Description

Print human-readable info about the prior specification that was used or will be used

Usage

```
print_prior(object)
```

Arguments

object

An object of class lgpfit or a valid prior argument for the 'lgp' function.

Value

nothing

prior_default

Create the default prior

Description

Create the default prior

Usage

```
prior_default(sigma_alpha = 1)
```

Arguments

sigma_alpha

Sigma parameter of the student-t distribution for all alpha.

Value

A list defining a valid prior argument for the 1gp function.

prior_stan_to_readable

prior_LonGP

Create a similar default prior as in LonGP (Cheng et. al, 2019)

Description

Not recommended, because a lengthscale close to 0 is possible.

Usage

```
prior_LonGP()
```

Value

A list defining a valid prior argument for the lgp_model function.

```
prior_stan_to_readable
```

Human-readable information about the priors in the Stan data object

Description

Human-readable information about the priors in the Stan data object

Usage

```
prior_stan_to_readable(stan_dat)
```

Arguments

stan_dat

The list that is passed as data to rstan::sampling.

Value

Info as a string.

prior_statement 63

prior_statement	Human-readable	prior statement
-----------------	----------------	-----------------

Description

Human-readable prior statement

Usage

```
prior_statement(parname, TYP, P, dist, row_change = TRUE)
```

Arguments

parname parameter name
TYP two integers

P three real numbers

dist list of distribution names

row_change should a newline be last character?

Value

Sampling statement as a string.

prior_to_stan Get priors as a format that can be input to Stan

Description

Get priors as a format that can be input to Stan

Usage

```
prior_to_stan(D, prior, HMGNS, UNCRT, N_cases, T_observed, T_last)
```

Arguments

D an integer vector of length 6

prior The prior argument supplied to lgp().

HMGNS Is diseaseAge assumed to have a homogenous effect (1) or not (0)?

UNCRT Boolean value, is uncertainty of disease onset modeled?

N_cases number of case individuals
T_observed observed disease onsets

T_last last time point for each diseased individual

rtgeom rtgeom

Value

a list with all things related to priors that Stan needs

repvec

Repeat a vector as a rows of an array

Description

Repeat a vector as a rows of an array

Usage

```
repvec(v, n)
```

Arguments

v a vector of length m

n number of times to repeat

Value

returns an array of size n x m

rtgeom

Sample from the 'truncated geometric' distribution

Description

Sample from the 'truncated geometric' distribution

Usage

```
rtgeom(s, p, n = 1)
```

Arguments

s an integer

p a number between 0 and 1

n number of samples

Value

an integer from the interval 1...n

scaleRelevances 65

scaleRelevances	Scale the effect sizes
-----------------	------------------------

Description

Scale the effect sizes

Usage

```
scaleRelevances(FFF, relevances, force_zero_mean = TRUE, i_dis)
```

Arguments

FFF matrix where one column corresponds to one additive data component

relevances the desired variance of each component (column)

force_zero_mean

should each component be forced to have zero mean?

i_dis index of a component for which the zero-mean forcing is skipped

Value

a new matrix FFF

separate_effects	Separate the covariate effects from an interaction components of a
	categorical covariate and age

Description

Separate the covariate effects from an interaction components of a categorical covariate and age

Usage

```
separate_effects(f_post, t, D, ell, i_edit)
```

Arguments

f_post	a matrix of size n x sum(D)
t	vector of n time points corresponding to f_post
_	

D a vector of length 6 ell kernel lengthscale

i_edit Indices of columns whose effect should be moved to shared age.

Value

```
a corrected f\_post
```

show,lgpfit-method

Show a summary of results of the 1gp function

Description

Show a summary of results of the 1gp function

Usage

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

Arguments

object

an object of class lgpfit

Value

nothing

show,lgpmodel-method Show a summary of an lgpmodel

Description

Show a summary of an lgpmodel

Usage

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

Arguments

object

an object of class lgpmodel

Value

nothing

show_relevances 67

show_relevances

Print info about component and covariate relevances

Description

Print info about component and covariate relevances

Usage

```
show_relevances(fit)
```

Arguments

fit

an object of class lgpfit

Value

nothing

```
simdata_colnames_pretty
```

Simulated data column names in a prettier form

Description

Simulated data column names in a prettier form

Usage

```
simdata_colnames_pretty(cn)
```

Arguments

cn

column names

Value

names of model components

68 simulate_data

simulate_data

Generate an artificial longitudinal data set

Description

Generate an artificial longitudinal data set.

Usage

```
simulate_data(N, 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, 3))
  2 + sum(covariates %in% c(0, 1, 2))), f_var = 1,
  noise_type = "Gaussian", snr = 3, phi = 1,
 N_affected = round(N/2), onset_range = "auto",
  t_observed = "after_0", C_hat = 0, dis_fun = "gp_vm",
  useBinKernel = TRUE, 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)))
```

Arguments

Ν Number of individuals.

t_data

Measurement times.

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

names Covariate names.

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

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

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

age component, respectively.

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_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)).

simulate_data 69

f_var variance of f

noise_type Either "Gaussian", "Poisson" or "NB" (negative binomial).

snr The desired signal-to-noise ratio. This argument is valid only with

noise_type = "Gaussian".

phi The dispersion parameter for negative binomial noise.

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.

onset_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 onset 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).

useBinKernel Should the binary kernel be used for categorical covariates? If this is TRUE, the

effect will exist only for group 1.

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

 $x \leftarrow \sin(a*t + b) + c$, 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 out, where

- out\$data is a data frame containing the actual data and
- out\$components contains more points for smoother visualizations of the generating process.
- out\$onsets contains the real disease effect times
- out\$p_signal proportion of variance explained by signal

70 simulate_kernels

Examples

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

simulate_kernels

Compute all kernel matrices when simulating data

Description

Compute all kernel matrices when simulating data

Usage

```
simulate_kernels(X, types, lengthscales, X_affected, useBinKernel,
 useMaskedVarianceKernel, steepness, vm_params)
```

Arguments

Χ covariates

vector of covariate types, so that types

• 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

useBinKernel whether or not binary (mask) kernel should be used for categorical covariates useMaskedVarianceKernel

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

steepness of the input warping function steepness parameters of the variance mask function vm_params

Value

a 3D array

sim_check_covariates 71

Description

Input check for the covariates-related arguments of simulate_data

Usage

```
sim_check_covariates(covariates, relevances, names, n_cat)
```

Arguments

covariates argument to simulate_data
relevances argument to simulate_data
names argument to simulate_data

n_cat the n_categs argument to simulate_data

Value

the covariate names

sim_data_to_observed Real generated disease ages to observed ones

Description

Real generated disease ages to observed ones

Usage

```
sim_data_to_observed(dat, t_observed)
```

Arguments

data frame

t_observed Determines how the disease onset is observed. See documentation of simulate_data.

Value

a new data frame and observed onsets

72 sim_parse_t_obs

sim_generate_names

Generate names for covariates

Description

Generate names for covariates

Usage

```
sim_generate_names(covariates)
```

Arguments

covariates

vector of covariate types

Value

covariate names

sim_parse_t_obs

Parse the t_observed argument of simulate_data

Description

Parse the $t_observed$ argument of $simulate_data$

Usage

```
sim_parse_t_obs(t_observed)
```

Arguments

t_observed a string

Value

a list with a name and number

split_data 73

split_data

Split data into training and test data according to given row indices

Description

Split data into training and test data according to given row indices

Usage

```
split_data(data, i_test, sort_ids = TRUE)
```

Arguments

data a data frame

i_test test data row indices

sort_ids should the test indices be sorted into increasing order

Value

```
a list(train, test)
```

split_data_by_id

Split data into training and test data according to given individuals

Description

Split data into training and test data according to given individuals

Usage

```
split_data_by_id(data, test_ids, id_variable = "id")
```

Arguments

data a data frame

test_ids test data individual identifiers

id_variable name of id variable

Value

```
a list(train, test)
```

74 split_data_random

```
split_data_by_timepoint
```

Split data into training and test data according to time point indices

Description

Split data into training and test data according to time point indices

Usage

```
split_data_by_timepoint(data, test_idx, id_variable = "id",
   time_variable = "age")
```

Arguments

data a data frame

Value

```
a list(train, test)
```

split_data_random

Split data into training and test data randomly

Description

Split data into training and test data randomly

Usage

```
split_data_random(data, p_test = 0.1, n_test = NULL)
```

Arguments

data a data frame

p_test desired proportion of test data

n_test desired number of test data points (if NULL, p_test is used to compute this)

Value

```
a list(train, test)
```

split_data_random_each 75

```
split_data_random_each
```

Split data into training and test data by selecting randomly k points from each individual

Description

Split data into training and test data by selecting randomly k points from each individual

Usage

```
split_data_random_each(data, n_test = 1, id_variable = "id",
   time_variable = "age")
```

Arguments

data a data frame

n_test desired number of test data points per individual

id_variable name of id variable
time_variable name of time variable

Value

```
a list(train, test)
```

standardize_inputs

Standardize continuous input variables in X

Description

Standardize continuous input variables in X

Usage

```
standardize_inputs(X, D)
```

Arguments

X the design matrix

D the covariate types, a vector of length 6

Value

updated X and info about scaling

76 validate_prior

stan_input_X_and_D

Predictor covariates and types to Stan input

Description

Reorders covariates and takes only those that are needed

Usage

```
stan_input_X_and_D(data, varInfo, types, formula, verbose)
```

Arguments

data a data frame containing the covariates

varInfo original variable type info types types of the covariates

formula model formula

verbose can this print some info?

Value

X and needed types and updated varInfo

validate_prior

Validate prior by sampling the signal and noise from it

Description

Validate prior by sampling the signal and noise from it

Usage

```
validate_prior(model, chains = 4, iter = 1000, parallel = FALSE)
```

Arguments

model An object of class lgpmodel.

chains how many chains are used to sample from the prior

iter for how many iterations are the chains run parallel should the chains be run in parallel?

Value

An object of class lgpfit and random samples of both 'f' and 'y'.

varsel 77

varsel

Covariate selection

Description

Covariate selection

Usage

```
varsel(object, threshold = 0.95, verbose = TRUE)
```

Arguments

object An object of class lgpfit.

threshold A threshold for proportion of explained variance

verbose should this print some output

Value

the selected covariates

warp_input

Warp inputs

Description

Warp inputs

Usage

```
warp_input(t, a, b, c)
```

Arguments

t.	a vector
L	a vector

a steepness of the rise

b location of the effective time window

c maximum range

Value

```
a vector of warped inputs w(t)
```

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