# Package: GPTreeO (via r-universe)

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Type Package

Title Dividing Local Gaussian Processes for Online Learning Regression

Version 1.0.1

**Description** We implement and extend the Dividing Local Gaussian Process algorithm by Lederer et al. (2020)

<doi:10.48550/arXiv.2006.09446>. Its main use case is in online learning where it is used to train a network of local GPs (referred to as tree) by cleverly partitioning the input space. In contrast to a single GP, 'GPTreeO' is able to deal with larger amounts of data. The package includes methods to create the tree and set its parameter, incorporating data points from a data stream as well as making joint predictions based on all relevant local GPs.

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2 CreateWrappedGP

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# Description

Factory function called by GPNode to create the wrapper for a specified GP package

# Usage

```
CreateWrappedGP(
  wrapper,
  X,
  y,
  y_var,
  gp_control,
  init_covpars,
  retrain_buffer_length,
  add_buffer_in_prediction
)
```

# Arguments

wrapper	A string specifying what GP implementation is used
X	Input data matrix with x_dim columns and at maximum Nbar rows. Is used to create the first iteration of the local GP.
У	Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored
y_var	Variance of the target variable; has to be a one-dimensional matrix or vector
gp_control	A list of GP implementation-specific options, passed directly to the wrapped GP implementation
init_covpars	Initial covariance parameters of the local GP
retrain_buffer_	length
	Only retrain when the number of buffer points or collected points exceeds this value

add\_buffer\_in\_prediction

If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated.

#### **Details**

A detailed list of expected functions from GPTree and GPNode can be found in the comments of this file. Currently, GPs from the DiceKriging package (WrappedDiceKrigingGP) and mlegp package (WrappedmlegpGP) are implemented. The user can create their own wrapper using WrappedGP.

# Value

The wrapper of the chosen GP package, containing the respective GP and information on the shared points and those stored in the buffer.

**GPNode** 

R6 Class for the nodes / leaves in the GPTree tree

# Description

The nodes contain the local GP if they are leaves (at the end of a branch). Nodes that are just nodes contain information on how the input space was split. They are responsible for computing and updating the splitting probabilities. Also, the tree interacts with the local GPs through the nodes.

Currently, GPs from the DiceKriging package (WrappedDiceKrigingGP) and mlegp package (WrappedmlegpGP) are implemented. The user can create their own wrapper using WrappedGP.

## Public fields

key A string like "0110100" to identify the node in the binary tree

x\_dim Dimensionality of input points. It is set once the first point is received through the GPTree method update. It needs to be specified if min\_ranges should be different from default.

theta Overlap ratio between two leafs in the split direction. The default value is 0.

split\_direction\_criterion A string that indicates which spitting criterion to use. The options are:

- "max\_spread": Split along the direction which has the largest data spread.
- "min\_lengthscale": split along the direction with the smallest length-scale hyperparameter from the local GP.
- "max\_spread\_per\_lengthscale": Split along the direction with the largest data spread relative to the corresponding GP length-scale hyperparameter.
- "max\_corr": Split along the direction where the input data is most strongly correlated with the target variable.
- "principal\_component": Split along the first principal component.

The default value is "max\_spread\_per\_lengthscale".

split\_position\_criterion A string indicating how the split position along the split direction should be set. Possible values are ("mean" and "median"). The default is "mean".

shape\_decay A string specifying how the probability function for a point to be assigned to the left leaf should fall off in the overlap region. The available options are a linear shape ("linear"), an exponential shape ("exponential") or a Gaussian shape ("gaussian"). Another option is to select no overlap region. This can be achieved by selecting "deterministic" or to set theta to 0. The default is "linear".

prob\_min\_theta Minimum probability after which the overlap shape gets truncated (either towards 0 or 1). The default value is 0.01.

Nbar Maximum number of data points for each GP in a leaf before it is split. The default value is 1000.

min\_ranges Smallest allowed input data spread (per dimension) before node splitting stops. It is set to its default min\_ranges = rep(0.0, x\_dim) once the first point is received through the update method. x\_dim needs to be specified by the user if it should be different from the default.

is\_leaf If TRUE, this node a leaf, i.e the last node on its branch

wrapped\_gp An instance of the WrappedGP type

can\_split If TRUE for a given dimension, the leaf can be split along that dimension

rotation\_matrix A rotation matrix, used for transforming the data

shift A shift, used for transforming the data

use\_pc\_transform TRUE if principal components transformation is used for node splitting

x\_spread Vector of data spread for each dimension

split\_index Index for the split dimension

position\_split Position of the split along dimension split\_index

width\_overlap Width of overlap region along dimension split\_index

point\_ids IDs of the points assigned to this node

residuals Vector of residuals

pred\_errs Vector of prediction uncertainties

error\_scaler Scaling factor for the prediction error to ensure desired coverage

use\_n\_residuals Number of past residuals to use in calibrating the error\_scaler

#### Methods

#### **Public methods:**

- GPNode\$new()
- GPNode\$transform()
- GPNode\$update\_prob\_pars()
- GPNode\$get\_prob\_child\_1()
- GPNode\$register\_residual()
- GPNode\$update\_empirical\_error\_pars()
- GPNode\$delete\_gp()

#### • GPNode\$clone()

```
Method new(): Create a new node object
 Usage:
 GPNode$new(
   key,
   x_dim,
   theta,
   split_direction_criterion,
   split_position_criterion,
   shape_decay,
   prob_min_theta,
   Nbar,
   wrapper,
   gp_control,
   retrain_buffer_length,
   add_buffer_in_prediction,
   min_ranges = NULL,
   is_leaf = TRUE
 )
```

Arguments:

key A string like "0110100" to identify the node in the binary tree

x\_dim Dimensionality of input points. It is set once the first point is received through the GPTree method update. It needs to be specified if min\_ranges should be different from default.

theta Overlap ratio between two leafs in the split direction. The default value is 0.

split\_direction\_criterion A string that indicates which spitting criterion to use. The options are:

- "max\_spread": Split along the direction which has the largest data spread.
- "min\_lengthscale": split along the direction with the smallest length-scale hyperparameter from the local GP.
- "max\_spread\_per\_lengthscale": Split along the direction with the largest data spread relative to the corresponding GP length-scale hyperparameter.
- "max\_corr": Split along the direction where the input data is most strongly correlated with the target variable.
- "principal\_component": Split along the first principal component.

The default value is "max\_spread\_per\_lengthscale".

split\_position\_criterion A string indicating how the split position along the split direction should be set. Possible values are ("mean" and "median"). The default is "mean".

shape\_decay A string specifying how the probability function for a point to be assigned to the left leaf should fall off in the overlap region. The available options are a linear shape ("linear"), an exponential shape ("exponential") or a Gaussian shape ("gaussian"). Another option is to select no overlap region. This can be achieved by selecting "deterministic" or to set theta to 0. The default is "linear".

prob\_min\_theta Minimum probability after which the overlap shape gets truncated (either towards 0 or 1). The default value is 0.01.

Nbar Maximum number of data points for each GP in a leaf before it is split. The default value is 1000.

- wrapper A string that indicates which GP implementation should be used. The current version includes wrappers for the packages "DiceKriging" and "mlegp". The default setting is "DiceKriging".
- gp\_control A list of control parameter that is forwarded to the wrapper. Here, the covariance function is specified. DiceKriging allows for the following kernels, passed as string:
   "gauss", "matern5\_2", "matern3\_2", "exp", "powexp" where "matern3\_2" is set as default.
- retrain\_buffer\_length Size of the retrain buffer. The buffer for a each node collects data points and holds them until the buffer length is reached. Then the GP in the node is updated with the data in the buffer. For a fixed Nbar, higher values for retrain\_buffer\_length lead to faster run time (less frequent retraining), but the trade-off is a temporary reduced prediction accuracy. We advise that the choice for retrain\_buffer\_length should depend on the chosen Nbar. By default retrain\_buffer\_length is set equal to Nbar.
- add\_buffer\_in\_prediction If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated. The default is FALSE.
- min\_ranges Smallest allowed input data spread (per dimension) before node splitting stops. It is set to its default min\_ranges = rep(0.0, x\_dim) once the first point is received through the GPTree method update. x\_dim needs to be specified by the user if it should be different from the default.

is\_leaf If TRUE, this node a leaf, i.e the last node on its branch.

n\_points\_train\_limit Number of points at which a GP is created in the leaf

*Returns:* A new GPNode object. Contains the local GP in the field wrapped\_gp, and information used for and related to splitting the node. If the node has been split, the local GP is removed.

**Method** transform(): Method to transform input data through a shift and a rotation. IS EXPECTED TO NOT BE CALLED BY THE USER

Usage:

GPNode\$transform(X)

Arguments:

X Matrix with x points

Returns: The transformed X matrix

**Method** update\_prob\_pars(): Method to update the probability parameters (x\_spread, can\_split, split\_index, position\_split, width\_overlap). IS EXPECTED TO NOT BE CALLED BY THE USER

Usage:

GPNode\$update\_prob\_pars()

**Method** get\_prob\_child\_1(): Method to compute the probability that a point x should go to child 1. IS EXPECTED TO NOT BE CALLED BY THE USER

Usage:

```
GPNode$get_prob_child_1(x)
 Arguments:
 x Single data point for which probability is computed; has to be a vector with length equal to
     x_dim
 Returns: The probability that a point x should go to child 1
Method register_residual(): Method to register prediction performance
 Usage:
 GPNode$register_residual(x, y)
 Arguments:
 x Most recent single input data point from the data stream; has to be a vector with length equal
     to x_dim
 y Target variable which has to be a one-dimensional matrix or a vector; any further columns
     will be ignored
Method update_empirical_error_pars(): Method for updating the empirical error parame-
ters
 Usage:
 GPNode$update_empirical_error_pars()
Method delete_gp(): Method to delete the GP. IS EXPECTED TO NOT BE CALLED BY
THE USER
 Usage:
 GPNode$delete_gp()
Method clone(): The objects of this class are cloneable with this method.
 Usage:
 GPNode$clone(deep = FALSE)
 Arguments:
 deep Whether to make a deep clone.
```

# See Also

GPTree() for the main methods

**GPTree** 

*Tree structure storing all nodes containing local GPs* 

#### **Description**

The base class which contains and where all parameters are set. Here, all information on how and when the splitting is carried out is stored. wrapper and gp\_control specify the Gaussian process (GP) implementation and its parameters. Moreover, minimum errors and calibration of the predictions are specified here, too.

#### **Essential methods**

The following three methods are essential for the package. The remaining ones are mostly not expected to be called by the user.

- GPTree\$new(): Creates a new tree with specified parameters
- GPTree\$update(): Adds the information from the input point to the tree and updates local GPs
- GPTree\$joint\_prediction(): Computes the joint prediction for a given input point

#### Brief package functionality overview

The tree collects the information from all GPNodes which in turn contain the local GP. Currently, GPs from the DiceKriging package (WrappedDiceKrigingGP) and mlegp package (WrappedmlegpGP) are implemented. The user can create their own wrapper using WrappedGP.

# **Public fields**

Nbar Maximum number of data points for each GP in a leaf before it is split. The default value is

retrain\_buffer\_length Size of the retrain buffer. The buffer for a each node collects data points and holds them until the buffer length is reached. Then the GP in the node is updated with the data in the buffer. For a fixed Nbar, higher values for retrain\_buffer\_length lead to faster run time (less frequent retraining), but the trade-off is a temporary reduced prediction accuracy. We advise that the choice for retrain\_buffer\_length should depend on the chosen Nbar. By default retrain\_buffer\_length is set equal to Nbar.

gradual\_split If TRUE, gradual splitting is used for splitting. The default value is TRUE.

theta Overlap ratio between two leafs in the split direction. The default value is 0.

- wrapper A string that indicates which GP implementation should be used. The current version includes wrappers for the packages "DiceKriging" and "mlegp". The default setting is "DiceKriging".
- gp\_control A list of control parameter that is forwarded to the wrapper. Here, the covariance function is specified. DiceKriging allows for the following kernels, passed as string:
   "gauss", "matern5\_2", "matern3\_2", "exp", "powexp" where "matern3\_2" is set as default.
- split\_direction\_criterion A string that indicates which spitting criterion to use. The options are:

- "max\_spread": Split along the direction which has the largest data spread.
- "min\_lengthscale": split along the direction with the smallest length-scale hyperparameter from the local GP.
- "max\_spread\_per\_lengthscale": Split along the direction with the largest data spread relative to the corresponding GP length-scale hyperparameter.
- "max\_corr": Split along the direction where the input data is most strongly correlated with the target variable.
- "principal\_component": Split along the first principal component.

The default value is "max\_spread\_per\_lengthscale".

- split\_position\_criterion A string indicating how the split position along the split direction should be set. Possible values are ("median" and "mean"). The default is "median".
- shape\_decay A string specifying how the probability function for a point to be assigned to the left leaf should fall off in the overlap region. The available options are a linear shape ("linear"), an exponential shape ("exponential") or a Gaussian shape ("gaussian"). Another option is to select no overlap region. This can be achieved by selecting "deterministic" or to set theta to 0. The default is "linear".
- use\_empirical\_error If TRUE, the uncertainty is calibrated using recent data points. The default value is TRUE.
  - The most recent 25 observations are used to ensure that the prediction uncertainty yields approximately 68 % coverage. This coverage is only achieved if theta = 0 (also together with gradual\_split = TRUE) is used. Nevertheless, the coverage will be closer to 68 % than it would be without calibration. The prediction uncertainties at the beginning are conservative and become less conservative with increasing number of input points.
- use\_reference\_gp If TRUE, the covariance parameters determined for the GP in node 0 will be used for all subsequent GPs. The default is FALSE.
- min\_abs\_y\_err Minimum absolute error assumed for y data. The default value is 0.
- min\_rel\_y\_err Minimum relative error assumed for y data. The default value is 100 \* .Machine\$double.eps.
- min\_abs\_node\_pred\_err Minimum absolute error on the prediction from a single node. The default value is 0.
- min\_rel\_node\_pred\_err Minimum relative error on the prediction from a single node. The default value is 100 \* .Machine\$double.eps.
- prob\_min\_theta Minimum probability after which the overlap shape gets truncated (either towards 0 or 1). The default value is 0.01.
- add\_buffer\_in\_prediction If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated. The default is FALSE.
- x\_dim Dimensionality of input points. It is set once the first point is received through the update()
   or joint\_prediction() method. It needs to be specified if min\_ranges should be different
   from default.
- min\_ranges Smallest allowed input data spread (per dimension) before node splitting stops. It is set to its default min\_ranges = rep(0.0, x\_dim) once the first point is received through the update() method. x\_dim needs to be specified by the user if it should be different from the default.

max\_cond\_num Add additional noise if the covariance matrix condition number exceeds this value. The default is NULL.

max\_points The maximum number of points the tree is allowed to store. The default value is Inf. End of the user-defined input fields.

nodes A hash to hold the GP tree, using string keys to identify nodes and their position in the tree ("0", "00", "01", "000", "011", "010", "011", etc.)

leaf\_keys Stores the keys ("0", "00", "01", "000", "001", "010", "011", etc.) for the leaves  $n_points$  Number of points in the tree

n\_fed Number of points fed to the tree

#### Methods

#### **Public methods:**

```
• GPTree$new()
```

- GPTree\$add\_node()
- GPTree\$get\_marginal\_point\_prob()
- GPTree\$update()
- GPTree\$get\_data\_split\_table()
- GPTree\$joint\_prediction()
- GPTree\$clone()

# Method new():

```
Usage:
GPTree$new(
  Nbar = 1000,
  retrain_buffer_length = Nbar,
  gradual_split = TRUE,
  theta = 0,
  wrapper = "DiceKriging",
  gp_control = list(covtype = "matern3_2"),
  split_direction_criterion = "max_spread_per_lengthscale",
  split_position_criterion = "median",
  shape_decay = "linear",
  use_empirical_error = TRUE,
  use_reference_gp = FALSE,
 min_abs_y_err = 0,
 min_rel_y_err = 100 * .Machine$double.eps,
 min_abs_node_pred_err = 0,
 min_rel_node_pred_err = 100 * .Machine$double.eps,
  prob_min_theta = 0.01,
  add_buffer_in_prediction = FALSE,
  x_dim = 0,
 min_ranges = NULL,
 max_cond_num = NULL,
 max_points = Inf
)
```

Arguments:

Nbar Maximum number of data points for each GP in a leaf before it is split. The default value is 1000.

retrain\_buffer\_length Size of the retrain buffer. The buffer for a each node collects data points and holds them until the buffer length is reached. Then the GP in the node is updated with the data in the buffer. For a fixed Nbar, higher values for retrain\_buffer\_length lead to faster run time (less frequent retraining), but the trade-off is a temporary reduced prediction accuracy. We advise that the choice for retrain\_buffer\_length should depend on the chosen Nbar. By default retrain\_buffer\_length is set equal to Nbar.

 ${\tt gradual\_split}\ \ {\tt If}\ TRUE,\ {\tt gradual}\ {\tt splitting}\ {\tt is}\ {\tt used}\ {\tt for}\ {\tt splitting}.\ {\tt The}\ {\tt default}\ {\tt value}\ {\tt is}\ {\tt TRUE}.$ 

theta Overlap ratio between two leafs in the split direction. The default value is 0.

- wrapper A string that indicates which GP implementation should be used. The current version includes wrappers for the packages "DiceKriging" and "mlegp". The default setting is "DiceKriging".
- gp\_control A list of control parameter that is forwarded to the wrapper. Here, the covariance function is specified. DiceKriging allows for the following kernels, passed as string:
   "gauss", "matern5\_2", "matern3\_2", "exp", "powexp" where "matern3\_2" is set as default.
- split\_direction\_criterion A string that indicates which spitting criterion to use. The options are:
  - "max\_spread": Split along the direction which has the largest data spread.
  - "min\_lengthscale": split along the direction with the smallest length-scale hyperparameter from the local GP.
  - "max\_spread\_per\_lengthscale": Split along the direction with the largest data spread relative to the corresponding GP length-scale hyperparameter.
  - "max\_corr": Split along the direction where the input data is most strongly correlated with the target variable.
  - "principal\_component": Split along the first principal component.

The default value is "max\_spread\_per\_lengthscale".

- split\_position\_criterion A string indicating how the split position along the split direction should be set. Possible values are ("median" and "mean"). The default is "median".
- shape\_decay A string specifying how the probability function for a point to be assigned to the left leaf should fall off in the overlap region. The available options are a linear shape ("linear"), an exponential shape ("exponential") or a Gaussian shape ("gaussian"). Another option is to select no overlap region. This can be achieved by selecting "deterministic" or to set theta to 0. The default is "linear".
- use\_empirical\_error If TRUE, the uncertainty is calibrated using recent data points. The default value is TRUE.
  - The most recent 25 observations are used to ensure that the prediction uncertainty yields approximately 68 % coverage. This coverage is only achieved if theta = 0 (also together with gradual\_split = TRUE) is used. Nevertheless, the coverage will be closer to 68 % than it would be without calibration. The prediction uncertainties at the beginning are conservative and become less conservative with increasing number of input points.
- use\_reference\_gp If TRUE, the covariance parameters determined for the GP in node 0 will be used for all subsequent GPs. The default is FALSE.
- min\_abs\_y\_err Minimum absolute error assumed for y data. The default value is 0.

min\_rel\_y\_err Minimum relative error assumed for y data. The default value is 100 \* .Machine\$double.eps. min\_abs\_node\_pred\_err Minimum absolute error on the prediction from a single node. The default value is 0.

- min\_rel\_node\_pred\_err Minimum relative error on the prediction from a single node. The default value is 100 \* .Machine\$double.eps.
- prob\_min\_theta Minimum probability after which the overlap shape gets truncated (either towards 0 or 1). The default value is 0.01.
- add\_buffer\_in\_prediction If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated. The default is FALSE.
- x\_dim Dimensionality of input points. It is set once the first point is received through the update method. It needs to be specified if min\_ranges should be different from default.
- min\_ranges Smallest allowed input data spread (per dimension) before node splitting stops. It is set to its default min\_ranges = rep(0.0, x\_dim) once the first point is received through the update method. x\_dim needs to be specified by the user if it should be different from the default.
- max\_cond\_num Add additional noise if the covariance matrix condition number exceeds this value. The default is NULL.
- max\_points The maximum number of points the tree is allowed to store. The default value is Inf.

*Returns:* A new GPTree object. Tree-specific parameters are listed in this object. The field nodes contains a hash with all GPNodes and information related to nodes. The nodes in turn contain the local GPs. Nodes that have been split no longer contain a GP.

## Examples:

```
set.seed(42)
## Use the 1d toy data set from Higdon (2002)
X <- as.matrix(sample(seq(0, 10, length.out = 31)))</pre>
y \leftarrow \sin(2 * pi * X / 10) + 0.2 * \sin(2 * pi * X / 2.5)
y_{variance} < - rep(0.1**2, 31)
## Initialize a tree with Nbar = 15, retrain_buffer_length = 15, use_empirical_error = FALSE,
## and default parameters otherwise
gptree <- GPTree$new(Nbar = 15, retrain_buffer_length = 15, use_empirical_error = FALSE)</pre>
## For the purpose of this example, we simulate the data stream through a simple for loop.
## In actual applications, the input stream comes from e.g. a differential evolutionary scanner.
## We follow the procedure in the associated paper, thus letting the tree make a prediction
## first before we update the tree with the point.
for (i in 1:nrow(X)) {
y_pred_with_err = gptree$joint_prediction(X[i,], return_std = TRUE)
## Update the tree with the true (X,y) pair
gptree$update(X[i,], y[i], y_variance[i])
## In the following, we go over different initializations of the tree
## 1. The same tree as before, but using the package mlegp:
```

```
## Note: since the default for gp_control is gp_control = list(covtype = "matern3_2"),
 ## we set gp_control to an empty list when using mlegp.
 gptree <- GPTree$new(Nbar = 15, retrain_buffer_length = 15, use_empirical_error = FALSE,</pre>
 wrapper = "mlegp", gp_control = list())
 ## 2. Minimum working example:
 gptree <- GPTree$new()</pre>
 ## 3. Fully specified example corresponding to the default settings
 ## Here, we choose to specify x_dim and min_ranges so that they correspond to the default values.
 ## If we do not specifiy them here, they will be automatically specified once
 ## the update or predict method is called.
 gptree <- GPTree$new(Nbar = 1000, retrain_buffer_length = 1000,</pre>
 gradual_split = TRUE, theta = 0, wrapper = "DiceKriging",
 gp_control = list(covtype = "matern3_2"),
 split_direction_criterion = "max_spread_per_lengthscale", split_position_criterion = "mean",
 shape_decay = "linear", use_empirical_error = TRUE,
 use_reference_gp = FALSE, min_abs_y_err = 0, min_rel_y_err = 100 * .Machine$double.eps,
 min_abs_node_pred_err = 0, min_rel_node_pred_err = 100 * .Machine$double.eps,
 prob_min_theta = 0.01, add_buffer_in_prediction = FALSE, x_dim = ncol(X),
 min_ranges = rep(0.0, ncol(X)), max_cond_num = NULL, max_points = Inf)
Method add_node(): Add a new GPNode to the tree. IS EXPECTED TO NOT BE CALLED
BY THE USER
 Usage:
 GPTree$add_node(key)
 Arguments:
 key Key of the new leaf
Method get_marginal_point_prob(): Marginal probability for point x to belong to node with
given key. IS EXPECTED TO NOT BE CALLED BY THE USER
 Usage:
 GPTree$get_marginal_point_prob(x, key)
 x Single input data point from the data stream; has to be a vector with length equal to x_dim
 key Key of the node
 Returns: Returns the marginal probability for point x to belong to node with given key
Method update(): Assigns the given input point x with target variable y and associated variance
y_var to a node and updates the tree accordingly
 Usage:
 GPTree$update(x, y, y_var = 0, retrain_node = TRUE)
```

x Most recent single input data point from the data stream; has to be a vector with length equal to x\_dim

Arguments:

y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored

y\_var Variance of the target variable; has to be a one-dimensional matrix or vector retrain\_node If TRUE, the GP node will be retrained after the point is added.

*Details:* The methods takes care of both updating an existing node and splitting the parent node into two child nodes. It ensures that the each child node has at least n\_points\_train\_limit in each GP. Further handling of duplicate points is also done here.

**Method** get\_data\_split\_table(): Generates a table used to distribute data points from a node to two child nodes

```
Usage:
GPTree$get_data_split_table(current_node)
Arguments:
current_node The GPNode whose data should be distributed
Returns: A matrix object
```

**Method** joint\_prediction(): Compute the joint prediction from all relevant leaves for an input point x

```
Usage:
GPTree$joint_prediction(x, return_std = TRUE)
Arguments:
```

x Single data point for which the predicted joint mean (and standard deviation) is computed; has to be a vector with length equal to x\_dim

return\_std If TRUE, the standard error of the prediction is returned

```
Details: We follow Eqs. (5) and (6) in this paper
```

Returns: The prediction (and its standard error) for input point x from this tree

**Method** clone(): The objects of this class are cloneable with this method.

```
Usage:
GPTree$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

### **Examples**

```
## -----
## Method `GPTree$new`
## ------
set.seed(42)
## Use the 1d toy data set from Higdon (2002)
X <- as.matrix(sample(seq(0, 10, length.out = 31)))
y <- sin(2 * pi * X / 10) + 0.2 * sin(2 * pi * X / 2.5)
y_variance <- rep(0.1**2, 31)</pre>
```

```
## Initialize a tree with Nbar = 15, retrain_buffer_length = 15, use_empirical_error = FALSE,
## and default parameters otherwise
gptree <- GPTree$new(Nbar = 15, retrain_buffer_length = 15, use_empirical_error = FALSE)</pre>
## For the purpose of this example, we simulate the data stream through a simple for loop.
## In actual applications, the input stream comes from e.g. a differential evolutionary scanner.
## We follow the procedure in the associated paper, thus letting the tree make a prediction
## first before we update the tree with the point.
for (i in 1:nrow(X)) {
y_pred_with_err = gptree$joint_prediction(X[i,], return_std = TRUE)
## Update the tree with the true (X,y) pair
gptree$update(X[i,], y[i], y_variance[i])
}
## In the following, we go over different initializations of the tree
## 1. The same tree as before, but using the package mlegp:
## Note: since the default for gp_control is gp_control = list(covtype = "matern3_2"),
## we set gp_control to an empty list when using mlegp.
gptree <- GPTree$new(Nbar = 15, retrain_buffer_length = 15, use_empirical_error = FALSE,</pre>
wrapper = "mlegp", gp_control = list())
## 2. Minimum working example:
gptree <- GPTree$new()</pre>
## 3. Fully specified example corresponding to the default settings
## Here, we choose to specify x_dim and min_ranges so that they correspond to the default values.
## If we do not specifiy them here, they will be automatically specified once
## the update or predict method is called.
gptree <- GPTree$new(Nbar = 1000, retrain_buffer_length = 1000,</pre>
gradual_split = TRUE, theta = 0, wrapper = "DiceKriging",
gp_control = list(covtype = "matern3_2"),
split_direction_criterion = "max_spread_per_lengthscale", split_position_criterion = "mean",
shape_decay = "linear", use_empirical_error = TRUE,
use_reference_gp = FALSE, min_abs_y_err = 0, min_rel_y_err = 100 * .Machine$double.eps,
min_abs_node_pred_err = 0, min_rel_node_pred_err = 100 * .Machine$double.eps,
prob_min_theta = 0.01, add_buffer_in_prediction = FALSE, x_dim = ncol(X),
min_ranges = rep(0.0, ncol(X)), max_cond_num = NULL, max_points = Inf)
```

WrappedDiceKrigingGP R6 class WrappedDiceKrigingGP

#### **Description**

Contains the GP created by DiceKriging::km from the DiceKriging package

#### Public fields

```
gp The DiceKriging GP object (DiceKriging::km in the DiceKriging manual)

X_buffer Buffer matrix to collect x points until first GP can be trained
```

y\_buffer Buffer vector to collect y points until first GP can be trained

y\_var\_buffer Buffer vector to collect variance of y points until first GP can be trained

add\_y\_var Small additional variance used to keep the covariance matrix condition number under control

n\_points\_train\_limit Number of points needed before we can create the GP

n\_points The number of collected points belonging to this GP

x\_dim Dimensionality of input points

gp\_control A list of GP implementation-specific options, passed directly to the wrapped GP implementation

init\_covpars The initial covariance parameters when training the DiceKriging GP object in self@gp estimate\_covpars If TRUE, the parameters are estimated by the package. Otherwise, the parameters from init\_covpars are taken

retrain\_buffer\_length Only retrain after this many new points have been added to the buffer retrain\_buffer\_counter Counter for the number of new points added since last retraining add\_buffer\_in\_prediction If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated.

X\_shared Matrix with x points that this GP shares with the GP in the sibling node y\_shared Vector of y points that this GP shares with the GP in the sibling node y\_var\_shared Vector of y\_var points that this GP shares with the GP in the sibling node n\_shared\_points The number of own points shared with the GP in the sibling node

## Methods

# **Public methods:**

- WrappedDiceKrigingGP\$new()
- WrappedDiceKrigingGP\$update\_init\_covpars()
- WrappedDiceKrigingGP\$get\_lengthscales()
- WrappedDiceKrigingGP\$get\_X\_data()
- WrappedDiceKrigingGP\$get\_y\_data()
- WrappedDiceKrigingGP\$get\_y\_var\_data()
- WrappedDiceKrigingGP\$get\_cov\_mat()
- WrappedDiceKrigingGP\$update\_add\_y\_var()
- WrappedDiceKrigingGP\$store\_point()
- WrappedDiceKrigingGP\$delete\_buffers()
- WrappedDiceKrigingGP\$train()
- WrappedDiceKrigingGP\$predict()
- WrappedDiceKrigingGP\$delete\_gp()
- WrappedDiceKrigingGP\$create\_DiceKriging\_gp()
- WrappedDiceKrigingGP\$call\_DiceKriging\_predict()
- WrappedDiceKrigingGP\$clone()

# Method new(): Create a new WrappedDiceKrigingGP object

```
WrappedDiceKrigingGP$new(
    X,
    y,
    y_var,
    gp_control,
    init_covpars,
    retrain_buffer_length,
    add_buffer_in_prediction,
    estimate_covpars = TRUE,
    X_shared = NULL,
    y_shared = NULL,
    y_var_shared = NULL
)
```

### Arguments:

- X Input data matrix with x\_dim columns and at maximum Nbar rows. Is used to create the first iteration of the local GP.
- y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored
- y\_var Variance of the target variable; has to be a one-dimensional matrix or vector
- gp\_control A list of GP implementation-specific options, passed directly to the wrapped GP implementation
- init\_covpars Initial covariance parameters of the local GP
- retrain\_buffer\_length Only retrain when the number of buffer points or collected points exceeds this value
- add\_buffer\_in\_prediction If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated.
- estimate\_covpars If TRUE, the parameters are estimated by the package. Otherwise, the parameters from init\_covpars are taken
- X\_shared Matrix with x points that this GP shares with the GP in the sibling node
- y\_shared Vector of y points that this GP shares with the GP in the sibling node
- y\_var\_shared Vector of y\_var points that this GP shares with the GP in the sibling node

*Returns:* A new WrappedDiceKrigingGP object. Besides the local GP, information on the shared points and those stored in the buffer are collected. For more information on the GP, consult the method DiceKriging::km in the DiceKriging package.

**Method** update\_init\_covpars(): Stores the initial covariance parameters (length-scales, standard deviation and trend coefficients) of the GP in the field init\_covpars

```
Usage:
```

```
WrappedDiceKrigingGP$update_init_covpars()
```

**Method** get\_lengthscales(): Retrieves the length-scales of the kernel of the local GP *Usage*:

```
WrappedDiceKrigingGP$get_lengthscales()
Method get_X_data(): Retrieves the design matrix X
 Usage:
 WrappedDiceKrigingGP$get_X_data(include_shared = FALSE)
 Arguments:
 include_shared If TRUE, shared points between this GP and its sibling GP are included
Method get_y_data(): Retrieves the response
 Usage:
 WrappedDiceKrigingGP$get_y_data(include_shared = FALSE)
 Arguments:
 include_shared If TRUE, shared points between this GP and its sibling GP are included
Method get_y_var_data(): Retrieves the individual variances from the response
 Usage:
 WrappedDiceKrigingGP$get_y_var_data(include_shared = FALSE)
 Arguments:
 include_shared If TRUE, shared points between this GP and its sibling GP are included
Method get_cov_mat(): Retrieves the covariance matrix
 Usage:
 WrappedDiceKrigingGP$get_cov_mat()
 Returns: the covariance matrix
Method update_add_y_var(): Method for updating add_y_var based on a bound for the co-
variance matrix condition number, based on this paper, Section 5.4
 Usage:
 WrappedDiceKrigingGP$update_add_y_var(max_cond_num)
 Arguments:
 max_cond_num Max allowed condition number
Method store_point(): Stores a new point into the respective buffer method
 Usage:
 WrappedDiceKrigingGP$store_point(
   Х,
   у,
   y_var,
   shared = FALSE,
    remove_shared = TRUE
 )
 Arguments:
 x Single input data point from the data stream; has to be a vector or row matrix with length
     equal to x_dim
```

y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored

y\_var Variance of the target variable; has to be a one-dimensional matrix or vector shared If TRUE, this point is shared between this GP and its sibling GP remove\_shared If TRUE, the last of the shared points is removed

**Method** delete\_buffers(): Method for clearing the buffers

Usage:

WrappedDiceKrigingGP\$delete\_buffers()

**Method** train(): Method for (re)creating / (re)training the GP

Usage:

WrappedDiceKrigingGP\$train(do\_buffer\_check = TRUE)

Arguments:

do\_buffer\_check If TRUE, only train the GP if the number of stored points is larger than retrain\_buffer\_length

Returns: TRUE if training was performed, otherwise FALSE

Method predict(): Method for prediction

Usage:

WrappedDiceKrigingGP\$predict(x, return\_std = TRUE)

Arguments:

x Single data point for which the predicted mean (and standard deviation) is computed; has to be a vector or row matrix with length equal to x\_dim

return\_std If TRUE, the standard error is returned in addition to the prediction

Returns: Prediction for input point x

Method delete\_gp(): Method to delete the GP object in self\$gp

Usage:

WrappedDiceKrigingGP\$delete\_gp()

**Method** create\_DiceKriging\_gp(): Method for calling the 'km' function in DiceKriging to create a GP object, stored in self\$gp

Usage:

WrappedDiceKrigingGP\$create\_DiceKriging\_gp(X, y, y\_var)

Arguments:

- X Input data matrix with x\_dim columns and at maximum Nbar rows for the local GP.
- y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored

y\_var Variance of the target variable; has to be a one-dimensional matrix or vector

Returns: TRUE

**Method** call\_DiceKriging\_predict(): Method for calling the 'predict' function in DiceKriging

Usage:

WrappedDiceKrigingGP\$call\_DiceKriging\_predict(x, use\_gp = NULL)

Arguments:

x Single data point for which the predicted mean (and standard deviation) is computed; has to be a vector with length equal to x\_dim

use\_gp optional user-defined GP which is evaluated instead of the local GP

Returns: The predictions for x from the specified GP, by default the local GP

**Method** clone(): The objects of this class are cloneable with this method.

Usage:

WrappedDiceKrigingGP\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

WrappedGP

R6 class WrappedGP

## Description

Contains the GP created by a user-defined GP package

#### **Details**

This is effectively a dummy wrapper based on the wrapper for the mlegp package (see WrappedmlegpGP). It contains a basic implementation of the wrapper. The vignette offers a tutorial on how to change this wrapper for the new GP package.

# **Public fields**

gp The mlegp GP object (mlegp::mlegp in the mlegp manual)

X\_buffer Buffer matrix to collect x points until first GP can be trained

y\_buffer Buffer vector to collect y points until first GP can be trained

y\_var\_buffer Buffer vector to collect variance of y points until first GP can be trained

add\_y\_var Small additional variance used to keep the covariance matrix condition number under control

n\_points\_train\_limit Number of points needed before we can create the GP

n\_points The number of collected points belonging to this GP

x\_dim Dimensionality of input points

gp\_control A list of GP implementation-specific options, passed directly to the wrapped GP implementation

init\_covpars The initial covariance parameters when training the mlegp GP object in self@gp

estimate\_covpars If TRUE, the parameters are estimated by the package. Otherwise, the parameters from init\_covpars are taken

retrain\_buffer\_length Only retrain after this many new points have been added to the buffer retrain\_buffer\_counter Counter for the number of new points added since last retraining add\_buffer\_in\_prediction If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated.

X\_shared Matrix with x points that this GP shares with the GP in the sibling node y\_shared Vector of y points that this GP shares with the GP in the sibling node y\_var\_shared Vector of y\_var points that this GP shares with the GP in the sibling node n\_shared\_points The number of own points shared with the GP in the sibling node

# Methods

#### **Public methods:**

```
WrappedGP$new()
WrappedGP$update_init_covpars()
WrappedGP$get_lengthscales()
WrappedGP$get_X_data()
WrappedGP$get_y_data()
WrappedGP$get_y_var_data()
WrappedGP$get_cov_mat()
WrappedGP$update_add_y_var()
WrappedGP$store_point()
WrappedGP$delete_buffers()
WrappedGP$call_create_gp()
WrappedGP$call_predict()
WrappedGP$train()
WrappedGP$predict()
```

# Method new(): Create a new WrappedmlegpGP object

```
Usage:
WrappedGP$new(
    X,
    y,
    y_var,
    gp_control,
    init_covpars,
    retrain_buffer_length,
    add_buffer_in_prediction,
    estimate_covpars = TRUE,
    X_shared = NULL,
```

• WrappedGP\$clone()

```
y_shared = NULL,
   y_var_shared = NULL
 Arguments:
 X Input data matrix with x dim columns and at maximum Nbar rows. Is used to create the first
     iteration of the local GP.
 y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any
     further columns will be ignored
 y_var Variance of the target variable; has to be a one-dimensional matrix or vector
 gp_control A list of GP implementation-specific options, passed directly to the wrapped GP
     implementation
 init_covpars Initial covariance parameters of the local GP
 retrain_buffer_length Only retrain when the number of buffer points or collected points
     exceeds this value
 add_buffer_in_prediction If TRUE, points in the data buffers are added to the GP before
     prediction. They are added into a temporarily created GP which contains the not yet in-
     cluded points. The GP in the node is not yet updated.
 estimate_covpars If TRUE, the parameters are estimated by the package. Otherwise, the
     parameters from init covpars are taken
 X_shared Matrix with x points that this GP shares with the GP in the sibling node
 y_shared Vector of y points that this GP shares with the GP in the sibling node
 y_var_shared Vector of y_var points that this GP shares with the GP in the sibling node
 Returns: A new WrappedGP object. Besides the local GP, information on the shared points and
 those stored in the buffer are collected. For more information on the GP, consult the respective
 met in the GP package.
Method update_init_covpars(): Stores the initial covariance parameters (length-scales, stan-
dard deviation and trend coefficients) of the GP in the field init_covpars
 Usage:
 WrappedGP$update_init_covpars()
Method get_lengthscales(): Retrieves the length-scales of the kernel of the local GP
 Usage:
 WrappedGP$get_lengthscales()
Method get_X_data(): Retrieves the design matrix X
 Usage:
 WrappedGP$get_X_data(include_shared = FALSE)
 Arguments:
 include_shared If TRUE, shared points between this GP and its sibling GP are included
```

**Method** get\_y\_data(): Retrieves the response

WrappedGP\$get\_y\_data(include\_shared = FALSE)

Usage:

Usage:

Arguments: include\_shared If TRUE, shared points between this GP and its sibling GP are included **Method** get\_y\_var\_data(): Retrieves the individual variances from the response Usage: WrappedGP\$get\_y\_var\_data(include\_shared = FALSE) Arguments: include\_shared If TRUE, shared points between this GP and its sibling GP are included **Method** get\_cov\_mat(): Retrieves the covariance matrix Usage: WrappedGP\$get\_cov\_mat() Returns: the covariance matrix Method update\_add\_y\_var(): Method for updating add\_y\_var based on a bound for the covariance matrix condition number, based on this paper, Section 5.4 WrappedGP\$update\_add\_y\_var(max\_cond\_num) Arguments: max\_cond\_num Max allowed condition number **Method** store\_point(): Stores a new point into the respective buffer method Usage: WrappedGP\$store\_point(x, y, y\_var, shared = FALSE, remove\_shared = TRUE) Arguments: x Single input data point from the data stream; has to be a vector or row matrix with length equal to x dim y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored y\_var Variance of the target variable; has to be a one-dimensional matrix or vector shared If TRUE, this point is shared between this GP and its sibling GP remove\_shared If TRUE, the last of the shared points is removed **Method** delete\_buffers(): Method for clearing the buffers Usage: WrappedGP\$delete\_buffers() **Method** delete\_gp(): Method to delete the GP object in self\$gp Usage: WrappedGP\$delete\_gp() **Method** call\_create\_gp(): Method for calling the 'mlegp' function in mlegp to create a GP object, stored in self\$gp

```
WrappedGP$call_create_gp(X, y, y_var)
```

Arguments:

X Input data matrix with x\_dim columns and at maximum Nbar rows for the local GP.

y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored

y\_var Variance of the target variable; has to be a one-dimensional matrix or vector

Returns: TRUE

**Method** call\_predict(): Method for calling the 'predict' function in mlegp

Usage:

```
WrappedGP$call_predict(x, use_gp = NULL)
```

Arguments:

x Single data point for which the predicted mean (and standard deviation) is computed; has to be a vector with length equal to x\_dim

use\_gp Optional user-defined GP which is evaluated instead of the local GP

*Returns:* The predictions for x from the specified GP, by default the local GP. The output needs to be a list with fields mean and sd for the prediction and prediction error, respectively.

**Method** train(): Method for (re)creating / (re)training the GP

Usage.

```
WrappedGP$train(do_buffer_check = TRUE)
```

Arguments:

do\_buffer\_check If TRUE, only train the GP if the number of stored points is larger than retrain\_buffer\_length

Returns: TRUE if training was performed, otherwise FALSE

**Method** predict(): Method for prediction

Usage:

```
WrappedGP$predict(x, return_std = TRUE)
```

Arguments:

x Single data point for which the predicted mean (and standard deviation) is computed; has to be a vector or row matrix with length equal to x\_dim

return\_std If TRUE, the standard error is returned in addition to the prediction

Returns: Prediction for input point x

**Method** clone(): The objects of this class are cloneable with this method.

Usage:

```
WrappedGP$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

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	WrappedmlegpGP	R6 class WrappedmlegpGP	
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# **Description**

Contains the GP created by mlegp::mlegp from the mlegp package

#### **Details**

This package is by default not able to include individual uncertainties for input points. For this reason, all fields related to y\_var are not used when updating the GP. No covariance kernel can be specified either. This implementation also assumes a vector for y (and not a matrix with multiple columns). Moreover, since no parameters can be specified for the GP, we will only update the GP parameters due to internal dependencies, but not use init\_covpars.

#### **Public fields**

gp The mlegp GP object (mlegp::mlegp in the mlegp manual)

X\_buffer Buffer matrix to collect x points until first GP can be trained

y\_buffer Buffer vector to collect y points until first GP can be trained

y\_var\_buffer Buffer vector to collect variance of y points until first GP can be trained

add\_y\_var Small additional variance used to keep the covariance matrix condition number under control

n\_points\_train\_limit Number of points needed before we can create the GP

n\_points The number of collected points belonging to this GP

x\_dim Dimensionality of input points

gp\_control A list of GP implementation-specific options, passed directly to the wrapped GP implementation

init\_covpars The initial covariance parameters when training the mlegp GP object in self@gp

estimate\_covpars If TRUE, the parameters are estimated by the package. Otherwise, the parameters from init\_covpars are taken

retrain\_buffer\_length Only retrain after this many new points have been added to the buffer

retrain\_buffer\_counter Counter for the number of new points added since last retraining

add\_buffer\_in\_prediction If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated.

X\_shared Matrix with x points that this GP shares with the GP in the sibling node

y\_shared Vector of y points that this GP shares with the GP in the sibling node

y\_var\_shared Vector of y\_var points that this GP shares with the GP in the sibling node

n\_shared\_points The number of own points shared with the GP in the sibling node

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#### Methods

#### **Public methods:**

```
WrappedmlegpGP$new()
WrappedmlegpGP$update_init_covpars()
WrappedmlegpGP$get_lengthscales()
WrappedmlegpGP$get_X_data()
WrappedmlegpGP$get_y_data()
WrappedmlegpGP$get_y_var_data()
WrappedmlegpGP$get_cov_mat()
WrappedmlegpGP$get_cov_mat()
WrappedmlegpGP$update_add_y_var()
WrappedmlegpGP$store_point()
WrappedmlegpGP$delete_buffers()
WrappedmlegpGP$train()
WrappedmlegpGP$predict()
WrappedmlegpGP$create_mlegp_gp()
WrappedmlegpGP$create_mlegp_predict()
```

#### **Method** new(): Create a new WrappedmlegpGP object

```
Usage:
WrappedmlegpGP$new(
    X,
    y,
    y_var,
    gp_control,
    init_covpars,
    retrain_buffer_length,
    add_buffer_in_prediction,
    estimate_covpars = TRUE,
    X_shared = NULL,
    y_var_shared = NULL
)
```

• WrappedmlegpGP\$clone()

Arguments:

- X Input data matrix with x\_dim columns and at maximum Nbar rows. Is used to create the first iteration of the local GP.
- y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored
- y\_var Variance of the target variable; has to be a one-dimensional matrix or vector
- gp\_control A list of GP implementation-specific options, passed directly to the wrapped GP implementation

init\_covpars Initial covariance parameters of the local GP

retrain\_buffer\_length Only retrain when the number of buffer points or collected points exceeds this value

add\_buffer\_in\_prediction If TRUE, points in the data buffers are added to the GP before prediction. They are added into a temporarily created GP which contains the not yet included points. The GP in the node is not yet updated.

estimate\_covpars If TRUE, the parameters are estimated by the package. Otherwise, the parameters from init\_covpars are taken

X\_shared Matrix with x points that this GP shares with the GP in the sibling node

y\_shared Vector of y points that this GP shares with the GP in the sibling node

y\_var\_shared Vector of y\_var points that this GP shares with the GP in the sibling node

*Returns:* A new WrappedmlegpGP object. Besides the local GP, information on the shared points and those stored in the buffer are collected. For more information on the GP, consult the method mlegp::mlegp in the mlegp package.

**Method** update\_init\_covpars(): Stores the initial covariance parameters (length-scales, standard deviation and trend coefficients) of the GP in the field init\_covpars

Usage:

WrappedmlegpGP\$update\_init\_covpars()

Method get\_lengthscales(): Retrieves the length-scales of the kernel of the local GP

Usage:

WrappedmlegpGP\$get\_lengthscales()

**Method** get\_X\_data(): Retrieves the design matrix X

Usage:

WrappedmlegpGP\$get\_X\_data(include\_shared = FALSE)

Arguments:

include\_shared If TRUE, shared points between this GP and its sibling GP are included

**Method** get\_y\_data(): Retrieves the response

Usage:

WrappedmlegpGP\$get\_y\_data(include\_shared = FALSE)

Arguments:

include\_shared If TRUE, shared points between this GP and its sibling GP are included

**Method** get\_y\_var\_data(): Retrieves the individual variances from the response

Usage:

WrappedmlegpGP\$get\_y\_var\_data(include\_shared = FALSE)

Arguments:

include\_shared If TRUE, shared points between this GP and its sibling GP are included

Method get\_cov\_mat(): Retrieves the covariance matrix

Usage:

WrappedmlegpGP\$get\_cov\_mat()

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Returns: the covariance matrix

**Method** update\_add\_y\_var(): Method for updating add\_y\_var based on a bound for the covariance matrix condition number, based on this paper, Section 5.4

Usage:

WrappedmlegpGP\$update\_add\_y\_var(max\_cond\_num)

Arguments:

max\_cond\_num Max allowed condition number

**Method** store\_point(): Stores a new point into the respective buffer method

Usage:

WrappedmlegpGP\$store\_point(x, y, y\_var, shared = FALSE, remove\_shared = TRUE)

Arguments:

- x Single input data point from the data stream; has to be a vector or row matrix with length equal to  $x_dim$
- y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored

y\_var Variance of the target variable; has to be a one-dimensional matrix or vector shared If TRUE, this point is shared between this GP and its sibling GP remove\_shared If TRUE, the last of the shared points is removed

**Method** delete\_buffers(): Method for clearing the buffers

Usage:

WrappedmlegpGP\$delete\_buffers()

**Method** train(): Method for (re)creating / (re)training the GP

Usage:

WrappedmlegpGP\$train(do\_buffer\_check = TRUE)

Arguments:

do\_buffer\_check If TRUE, only train the GP if the number of stored points is larger than retrain\_buffer\_length

Returns: TRUE if training was performed, otherwise FALSE

**Method** predict(): Method for prediction

Usage:

WrappedmlegpGP\$predict(x, return\_std = TRUE)

Arguments:

x Single data point for which the predicted mean (and standard deviation) is computed; has to be a vector or row matrix with length equal to x\_dim

return\_std If TRUE, the standard error is returned in addition to the prediction

Returns: Prediction for input point x

**Method** delete\_gp(): Method to delete the GP object in self\$gp

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```
Usage:
```

WrappedmlegpGP\$delete\_gp()

**Method** create\_mlegp\_gp(): Method for calling the 'mlegp' function in mlegp to create a GP object, stored in self\$gp

Usage:

WrappedmlegpGP\$create\_mlegp\_gp(X, y, y\_var)

Arguments:

- X Input data matrix with x\_dim columns and at maximum Nbar rows for the local GP.
- y Value of target variable at input point x; has to be a one-dimensional matrix or a vector; any further columns will be ignored

y\_var Variance of the target variable; has to be a one-dimensional matrix or vector

Returns: TRUE

Method call\_mlegp\_predict(): Method for calling the 'predict' function in mlegp

Usage.

WrappedmlegpGP\$call\_mlegp\_predict(x, use\_gp = NULL)

Arguments:

x Single data point for which the predicted mean (and standard deviation) is computed; has to be a vector with length equal to x\_dim

use\_gp Optional user-defined GP which is evaluated instead of the local GP

*Returns:* The predictions for x from the specified GP, by default the local GP. The output needs to be a list with fields mean and sd for the prediction and prediction error, respectively.

**Method** clone(): The objects of this class are cloneable with this method.

Usage:

WrappedmlegpGP\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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