Package ‘ExaGeoStatCPP’

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Type Package

Title R Package demonstrates the R/C++ Language Interface for Exascale GeoStatistics software (ExaGeoStat)

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Description An R-Interface for the ExaGeoStatCPP software: a parallel high performance unified framework for geostatistics on manycore systems. Its abbreviation stands for Exascale Geostatistics. The framework aims at optimizing the likelihood function for a given spatial data to provide an efficient way to predict missing observations. The framework targets many-core systems: clusters of CPUs and GPUs.

License GPL (>= 3)

Imports assertthat (>= 0.2.1), MASS, methods, Rcpp (>= 1.0.9)

Depends R (>= 3.5.0), assertthat (>= 0.2.1)

RoxygenNote 7.2.3

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NeedsCompilation yes

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URL https://github.com/ecrc/ExaGeoStatCPP

BugReports https://github.com/ecrc/ExaGeoStatCPP/issues

Encoding UTF-8

R topics documented:

`ExaGeoStatData` *ExaGeoStatData Class*

Description

The `ExaGeoStatData` class is designed to facilitate the handling and manipulation of geospatial statistics data within the ExaGeoStat framework. It provides a structured way to store and manage data points based on their dimensions. Instances of this class can hold a specified number of location points, and support different data dimensions including two-dimensional (2D), three-dimensional (3D), and spatiotemporal (ST) configurations.

Value

An object of class `ExaGeoStatData` representing a data component with the specified size and dimension.

Constructor

`ExaGeoStatData` Creates a new instance of the `ExaGeoStatData` class. This is achieved by calling:

```
new(ExaGeoStatData, problem_size, dimension)
```

`size` An integer representing the size of the locations data.

`dimension` A string representing the dimensions of the data. Available dimensions are "2D", "3D", and "ST".

Examples

```
problem_size <- 4
dimension = "3D"
empty_data <- new(Data, problem_size, dimension)
```

`ExaGeoStatHardware` *ExaGeoStatHardware Class*

Description

The ExaGeoStatHardware class represents a hardware component in the ExaGeoStat system. It is initialized with computation mode, and two integers representing number of CPU cores and number of GPU cores.

Value

An object of class `ExaGeoStatHardware` representing a hardware component with the specified component and number of CPU cores and GPU cores.

Constructor

`ExaGeoStatHardware` Creates a new instance of the `ExaGeoStatHardware` class. This is achieved by calling:

```
new(Hardware, computation, ncores, ngpus)
```

`computation` A string specifying the computation method, either "exact" or "dst" or "tlr".

`num_of_cpus` An integer representing number of CPU cores.

`num_of_gpus` An integer representing number of GPU cores.

Methods

finalize_hardware: `finalize_hardware()` Manually finalizes the hardware by resetting the context.

Examples

```
ncores <- 2
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)
hardware$finalize_hardware()
```

fisher *Fisher Function*

Description

This function computes the Fisher information matrix for a given dataset and theta vector, using a specified kernel and distance metric. It also allows for the inclusion of missing values and the specification of data dimensions.

Usage

```
fisher(kernel, distance_matrix = "euclidean", estimated_theta, dts,
lts = 0, dimension = "2D", train_data, test_data)
```

Arguments

`kernel` A string specifying the kernel to use. Available kernels include:
- "BivariateMaternFlexible"
- "BivariateMaternParsimonious"
- "BivariateSpacetimeMaternStationary"
- "TrivariateMaternParsimonious"
- "UnivariateExpNonGaussian"
- "UnivariateMaternDbeta"
- "UnivariateMaternDdbetaBeta"
- "UnivariateMaternDdbetaNu"
- "UnivariateMaternDdnuNu"
- "UnivariateMaternDdsigmaSquare"
- "UnivariateMaternDdsigmaSquareBeta"
- "UnivariateMaternDdsigmaSquareNu"
- "UnivariateMaternDnu"
- "UnivariateMaternDsigmaSquare"
- "UnivariateMaternNonGaussian"
- "UnivariateMaternNuggetsStationary"
- "UnivariateMaternStationary"
- "UnivariatePowExpStationary"
- "UnivariateSpacetimeMaternStationary"

`distance_matrix` A string specifying the distance metric, either "euclidean" or "great_circle". Default is "euclidean".

`estimated_theta` A list of estimated theta parameters.

`dts` A numeric value representing the time step size.

`lts` A numeric value representing the length step size. Default is 0.

dimension	A string specifying the data dimension, either "2D" or "3D". Default is "2D".
train_data	A numeric vector contains the locations and z measurements for training
test_data	A numeric vector contains the locations for testing.

Value

A vector containing the Fisher information matrix elements.

Examples

```
dimension = "2D"
ncores <- 1
ngpus <- 0
dts <- 2
kernel <- "univariate_matern_stationary"
estimated_theta <- c(1,0.1,0.5)
computation <- "exact"

hardware <- new(Hardware, computation, ncores, ngpus)

z_value <- c(-1.272336140360187606, -2.590699695867695773,
             0.512142584178685967, -0.163880452049749520)
locations_x <- c(0.092042420080872822,  0.193041886015106440,
             0.330556191348134576, 0.181612878614480805)
locations_y <- c(0.928648813611047563, 0.103883421072709245,
             0.135790035858701447,  0.434683756771190977)

test_x <- c(0.347951, 0.62768)
test_y <- c(0.806332, 0.105196)

fisher_matrix <- fisher(train_data=list(locations_x, locations_y, z_value),
test_data=list(test_x, test_y), kernel=kernel, dts=dts, estimated_theta=estimated_theta)
```

---

get_locationsX *Get Locations X Function*

Description

Retrieves X coordinates of locations from ExaGeoStatData object.

Usage

```
get_locationsX(data)
```

Arguments

data	A list of ExaGeoStatData that contains the locations.

Value

A numeric vector of X locations.

Examples

```
ncores <- 1
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)

dimension = "2D"
problem_size <- 4
empty_data <- new(Data, problem_size, dimension)

dts <- 2
kernel <- "univariate_matern_stationary"
initial_theta <- c(1,0.1,0.5)
exageostat_data <- simulate_data(kernel=kernel, initial_theta=initial_theta,
problem_size=problem_size, dts=dts, dimension=dimension)
x <- get_locationsX(data=exageostat_data)
```

`get_locationsY` *Get Locations Y Function*

Description

This function retrieves the Y locations from the provided data.

Usage

```
get_locationsY(data)
```

Arguments

`data`	A list of ExaGeoStatData that contains the locations.

Value

A numeric vector of Y locations.

Examples

```
ncores <- 2
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)

dimension = "2D"
problem_size <- 4
```

```
empty_data <- new(Data, problem_size, dimension)

dts <- 2
kernel <- "univariate_matern_stationary"
initial_theta <- c(1,0.1,0.5)
exageostat_data <- simulate_data(kernel=kernel, initial_theta=initial_theta,
problem_size=problem_size, dts=dts, dimension=dimension)
y <- get_locationsY(data=exageostat_data)
```

`get_locationsZ` *Get Locations Z Function*

Description

Retrieves Z coordinates of locations from ExaGeoStatData object.

Usage

```
get_locationsZ(data)
```

Arguments

`data`	A list of ExaGeoStatData that contains the locations.

Value

A numeric vector of Z locations.

Examples

```
ncores <- 2
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)

dimension = "3D"
problem_size <- 4
empty_data <- new(Data, problem_size, dimension)

dts <- 2
kernel <- "univariate_matern_stationary"
initial_theta <- c(1,0.1,0.5)
exageostat_data <- simulate_data(kernel=kernel, initial_theta=initial_theta,
problem_size=problem_size, dts=dts, dimension=dimension)
z <- get_locationsZ(data=exageostat_data)
```

get_Z_measurement_vector

Get descriptive Z values Function

Description

Retrieves descriptive Z values from ExaGeoStat data based on type.

Usage

```
get_Z_measurement_vector(data,type)
```

Arguments

data	A list of ExaGeoStatData that contains the locations.
type	A string specifying the type of descriptor value to retrieve (e.g., "Chameleon", "HiCMA").

Value

A numeric vector of descriptive Z values.

Examples

```
ncores <- 2
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)

dimension = "3D"
problem_size <- 4
empty_data <- new(Data, problem_size, dimension)

dts <- 2
kernel <- "univariate_matern_stationary"
initial_theta <- c(1,0.1,0.5)
exageostat_data <- simulate_data(kernel=kernel, initial_theta=initial_theta,
problem_size=problem_size, dts=dts, dimension=dimension)
Z <- get_Z_measurement_vector(data=exageostat_data, type="chameleon")
```

idw — *IDW Function*

Description

This function performs Inverse Distance Weighting (IDW) interpolation for a given dataset and theta vector.

Usage

```
idw(kernel, distance_matrix = "euclidean", estimated_theta, dts, lts = 0,
dimension = "2D", train_data, test_data, test_measurements)
```

Arguments

`kernel`
: A string specifying the kernel to use. Available kernels include:
  - "BivariateMaternFlexible"
  - "BivariateMaternParsimonious"
  - "BivariateSpacetimeMaternStationary"
  - "TrivariateMaternParsimonious"
  - "UnivariateExpNonGaussian"
  - "UnivariateMaternDbeta"
  - "UnivariateMaternDdbetaBeta"
  - "UnivariateMaternDdbetaNu"
  - "UnivariateMaternDdnuNu"
  - "UnivariateMaternDdsigmaSquare"
  - "UnivariateMaternDdsigmaSquareBeta"
  - "UnivariateMaternDdsigmaSquareNu"
  - "UnivariateMaternDnu"
  - "UnivariateMaternDsigmaSquare"
  - "UnivariateMaternNonGaussian"
  - "UnivariateMaternNuggetsStationary"
  - "UnivariateMaternStationary"
  - "UnivariatePowExpStationary"
  - "UnivariateSpacetimeMaternStationary"

`distance_matrix`
: A string specifying the distance metric, either "euclidean" or "great_circle". Default is "euclidean"

`estimated_theta`
: A list of estimated theta parameters

`dts`
: A numeric value representing the time step size

`lts`
: A numeric value representing the length step size. Default is 0

`dimension`
: A string specifying the data dimension, either "2D" or "3D". Default is "2D"

`train_data` A numeric vector contains the locations and z measurements for training

`test_data` A numeric vector contains the locations for testing.

`test_measurements`
A numeric vector contains the z measurements for testing.

Value

A vector containing the IDW error.

Examples

```
ncores <- 2
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)

problem_size <- 4
dimension = "2D"
dts <- 2
kernel <- "univariate_matern_stationary"
estimated_theta <- c(1,0.1,0.5)

z_value <- c( -1.272336140360187606, -2.590699695867695773, 0.512142584178685967,
             -0.163880452049749520)
locations_x <- c(0.193041886015106440, 0.330556191348134576, 0.181612878614480805,
             0.370473792629892440)
locations_y <- c(0.103883421072709245, 0.135790035858701447, 0.434683756771190977,
             0.400778210116731537)
test_x <- c(0.347951, 0.62768)
test_y <- c(0.806332, 0.105196)
test_measurements = c(-1.05428, -1.47441)

idw_error = idw(kernel=kernel, estimated_theta=estimated_theta, dts=dts,
train_data=list(locations_x, locations_y, z_value),
test_data=list(test_x, test_y), test_measurements=test_measurements)
```

`mloe_mmom` *MLOE MMOM Function*

Description

This function calculates Mean Misspecification of the Mean Square Error (MMOM) and Mean Loss of Efficiency (MLOE).

Usage

```
mloe_mmom(kernel, distance_matrix="euclidean", estimated_theta, true_theta,
dts, lts=0, dimension="2D", train_data, test_data)
```

Arguments

kernel — A string specifying the kernel to use. Available kernels include:

- "BivariateMaternFlexible"
- "BivariateMaternParsimonious"
- "BivariateSpacetimeMaternStationary"
- "TrivariateMaternParsimonious"
- "UnivariateExpNonGaussian"
- "UnivariateMaternDbeta"
- "UnivariateMaternDdbetaBeta"
- "UnivariateMaternDdbetaNu"
- "UnivariateMaternDdnuNu"
- "UnivariateMaternDdsigmaSquare"
- "UnivariateMaternDdsigmaSquareBeta"
- "UnivariateMaternDdsigmaSquareNu"
- "UnivariateMaternDnu"
- "UnivariateMaternDsigmaSquare"
- "UnivariateMaternNonGaussian"
- "UnivariateMaternNuggetsStationary"
- "UnivariateMaternStationary"
- "UnivariatePowExpStationary"
- "UnivariateSpacetimeMaternStationary"

distance_matrix — A string specifying the distance metric, either "euclidean" or "great_circle". Default is "euclidean"

estimated_theta — A list of estimated theta parameters

true_theta — A list of truth theta parameters

dts — A numeric value representing the time step size

lts — A numeric value representing the length step size. Default is 0

dimension — A string specifying the data dimension, either "2D" or "3D". Default is "2D"

train_data — A numeric vector contains the locations and z measurements for training

test_data — A numeric vector contains the locations for testing.

Value

A vector of MLOE/MMOM values

Examples

```
ncores <- 2
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)
```

```
problem_size <- 4
dimension = "2D"
dts <- 2
kernel <- "univariate_matern_stationary"
estimated_theta <- c(1,0.1,0.5)
true_theta <- c(1.1,0.2,0.5)

z_value <- c(-1.272336140360187606, -2.590699695867695773, 0.512142584178685967,
             -0.163880452049749520)
locations_x <- c(0.092042420080872822,  0.193041886015106440,  0.330556191348134576,
             0.181612878614480805)
locations_y <- c(0.928648813611047563, 0.103883421072709245,  0.135790035858701447,
             0.434683756771190977)

test_x <- c(0.347951, 0.62768)
test_y <- c(0.806332, 0.105196)

result_mloe_mmom = mloe_mmom(train_data=list(locations_x, locations_y, z_value),
test_data=list(test_x, test_y), kernel=kernel, dts=dts,
estimated_theta=estimated_theta, true_theta=true_theta)
```

---

model_data *Model Data Function*

Description

This function models data based on the provided computation method, kernel, distance matrix, and other parameters.

Usage

```
model_data(computation = "exact", kernel, distance_matrix = "euclidean", lb,
ub, tol = 4, mle_itr, dts, lts = 0, dimension = "2D", band = 0, max_rank = 500,
data = NULL, matrix = NULL, x = NULL, y = NULL, z = NULL)
```

Arguments

`computation` A string specifying the computation method, either "exact" or "dst" or "tlr". Default is "exact".

`kernel` A string specifying the kernel to use. Available kernels include:

- "BivariateMaternFlexible"
- "BivariateMaternParsimonious"
- "BivariateSpacetimeMaternStationary"
- "TrivariateMaternParsimonious"
- "UnivariateExpNonGaussian"
- "UnivariateMaternDbeta"
- "UnivariateMaternDdbetaBeta"

- "UnivariateMaternDdbetaNu"
- "UnivariateMaternDdnuNu"
- "UnivariateMaternDdsigmaSquare"
- "UnivariateMaternDdsigmaSquareBeta"
- "UnivariateMaternDdsigmaSquareNu"
- "UnivariateMaternDnu"
- "UnivariateMaternDsigmaSquare"
- "UnivariateMaternNonGaussian"
- "UnivariateMaternNuggetsStationary"
- "UnivariateMaternStationary"
- "UnivariatePowExpStationary"
- "UnivariateSpacetimeMaternStationary"

`distance_matrix`
: A string specifying the distance metric, either "euclidean" or "great_circle". Default is "euclidean".

`lb` A numeric value representing the lower bound for the computation.

`ub` A numeric value representing the upper bound for the computation.

`tol` A numeric value specifying the tolerance for the computation. Default is 4.

`mle_itr` A numeric value specifying the maximum number of iterations for the computation.

`dts` A numeric value representing the time step size.

`lts` A numeric value representing the length step size. Default is 0.

`dimension` A string specifying the data dimension, either "2D" or "3D". Default is "2D".

`band` A numeric value Bandwidth for band matrices, applicable in certain computational kernels.. Default is 0.

`max_rank` A numeric value specifying the Maximum rank for low-rank approximations.. Default is 500.

`data` A list of data vectors. Default is ‘R_NilValue‘.

`matrix` A matrix object. Default is ‘R_NilValue‘.

`x` A numeric vector. Default is ‘R_NilValue‘.

`y` A numeric vector. Default is ‘R_NilValue‘.

`z` A numeric vector. Default is ‘R_NilValue‘.

Value

A vector containing the starting theta.

Examples

```
ncores <- 2
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)
```

```
dimension = "2D"
problem_size <- 4
empty_data <- new(Data, problem_size, dimension)

dts <- 2
kernel <- "univariate_matern_stationary"
lower_bound <- c(0.1,0.1,0.1)
upper_bound <- c(5,5,5)

z_value <- c( -1.272336140360187606, -2.590699695867695773, 0.512142584178685967,
              -0.163880452049749520)
locations_x <- c(0.193041886015106440, 0.330556191348134576, 0.181612878614480805,
              0.370473792629892440)
locations_y <- c(0.103883421072709245, 0.135790035858701447, 0.434683756771190977,
              0.400778210116731537)

theta <- model_data(kernel=kernel, lb=lower_bound, ub=upper_bound,
mle_itr=10, dts=dts, matrix=z_value, x=locations_x, y=locations_y)
```

`predict_data` *Predict Data Function*

Description

This function predicts data based on the provided kernel, distance matrix, estimated theta, and other parameters.

Usage

```
predict_data(kernel, distance_matrix = "euclidean", estimated_theta,
dts, lts = 0, dimension = "2D", train_data, test_data)
```

Arguments

`kernel` A string specifying the kernel to use. Available kernels include:

- "BivariateMaternFlexible"
- "BivariateMaternParsimonious"
- "BivariateSpacetimeMaternStationary"
- "TrivariateMaternParsimonious"
- "UnivariateExpNonGaussian"
- "UnivariateMaternDbeta"
- "UnivariateMaternDdbetaBeta"
- "UnivariateMaternDdbetaNu"
- "UnivariateMaternDdnuNu"
- "UnivariateMaternDdsigmaSquare"
- "UnivariateMaternDdsigmaSquareBeta"

- "UnivariateMaternDdsigmaSquareNu"
- "UnivariateMaternDnu"
- "UnivariateMaternDsigmaSquare"
- "UnivariateMaternNonGaussian"
- "UnivariateMaternNuggetsStationary"
- "UnivariateMaternStationary"
- "UnivariatePowExpStationary"
- "UnivariateSpacetimeMaternStationary"

`distance_matrix`
A string specifying the distance metric, either "euclidean" or "great_circle". Default is "euclidean"

`estimated_theta`
A list of estimated theta parameters

`dts` A numeric value representing the time step size

`lts` A numeric value representing the length step size. Default is 0

`dimension` A string specifying the data dimension, either "2D" or "3D". Default is "2D"

`train_data` A numeric vector contains the locations and z measurements for training

`test_data` A numeric vector contains the locations for testing.

Value

A vector of predicted z values

Examples

```
ncores <- 2
ngpus <- 0
problem_size <- 4
dts <- 2
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)
kernel <- "univariate_matern_stationary"
estimated_theta <- c(1,0.1,0.5)

z_value <- c( -1.272336140360187606, -2.590699695867695773, 0.512142584178685967,
              -0.163880452049749520)
locations_x <- c(0.193041886015106440, 0.330556191348134576, 0.181612878614480805,
              0.370473792629892440)
locations_y <- c(0.103883421072709245, 0.135790035858701447, 0.434683756771190977,
              0.400778210116731537)
test_x <- c(0.347951, 0.62768)
test_y <- c(0.806332, 0.105196)

predict_data(train_data=list(locations_x, locations_y, z_value),
test_data=list(test_x, test_y), kernel=kernel, dts=dts,
estimated_theta=estimated_theta)
```

simulate_data *Simulate Data Function*

Description

This function loads data into an ExaGeoStatData object using the provided configuration and computational settings.

Usage

```
simulate_data(kernel, initial_theta, distance_matrix = "euclidean", problem_size,
seed = 0, dts, lts = 0, dimension = "2D", log_path = "", data_path = "",
observations_file = "", recovery_file = "")
```

Arguments

`kernel` A string specifying the kernel to use. Available kernels include:

- "BivariateMaternFlexible"
- "BivariateMaternParsimonious"
- "BivariateSpacetimeMaternStationary"
- "TrivariateMaternParsimonious"
- "UnivariateExpNonGaussian"
- "UnivariateMaternDbeta"
- "UnivariateMaternDdbetaBeta"
- "UnivariateMaternDdbetaNu"
- "UnivariateMaternDdnuNu"
- "UnivariateMaternDdsigmaSquare"
- "UnivariateMaternDdsigmaSquareBeta"
- "UnivariateMaternDdsigmaSquareNu"
- "UnivariateMaternDnu"
- "UnivariateMaternDsigmaSquare"
- "UnivariateMaternNonGaussian"
- "UnivariateMaternNuggetsStationary"
- "UnivariateMaternStationary"
- "UnivariatePowExpStationary"
- "UnivariateSpacetimeMaternStationary"

`initial_theta` A list of initial theta parameters.

`distance_matrix` A string specifying the distance metric, either "euclidean" or "great_circle". Default is "euclidean".

`problem_size` A numeric value representing the size of the problem to simulate.

`seed` A numeric value specifying the seed for random number generation. Default is 0.

dts	A numeric value representing the time step size.
lts	A numeric value representing the length step size. Default is 0.
dimension	A string specifying the data dimension, either "2D" or "3D". Default is "2D".
log_path	A string specifying the path for logging. Default is "".
data_path	A string specifying the path for data storage. Default is "".
observations_file	A string specifying the file name for observations. Default is "".
recovery_file	A string specifying the file name for recovery. Default is "".

Value

A pointer to ExaGeoStatData object that contains the loaded data.

Examples

```
ncores <- 2
ngpus <- 0
computation <- "exact"
hardware <- new(Hardware, computation, ncores, ngpus)

dimension = "2D"
problem_size <- 4
empty_data <- new(Data, problem_size, dimension)

dts <- 2
kernel <- "univariate_matern_stationary"
initial_theta <- c(1,0.1,0.5)

exageostat_data <- simulate_data(kernel=kernel, initial_theta=initial_theta,
problem_size=problem_size, dts=dts, dimension=dimension)
```

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