Package 'fdaPDE'

January 8, 2025

Version 1.1-21 **Date** 2025-01-01

Title Physics-Informed Spatial and Functional Data Analysis

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Depends R (>= 3.5.0), stats, grDevices, graphics, rgl, Matrix, plot3D, methods

LinkingTo RcppEigen, Rcpp

Suggests MASS, testthat (>= 3.0.0)

Description An implementation of regression models with partial differential regularizations, making use of the Finite Element Method. The models efficiently handle data distributed over irregularly shaped domains and can comply with various conditions at the boundaries of the domain. A priori information about the spatial structure of the phenomenon under study can be incorporated in the model via the differential regularization. See Sangalli, L. M. (2021) <doi:10.1111/insr.12444> ``Spatial Regression With Partial Differential Equation Regularisation" for an overview. The release 1.1-9 requires R (>= 4.2.0) to be installed on windows machines.

License GPL-3

NeedsCompilation yes

SystemRequirements GNU make

RoxygenNote 7.2.3

Encoding UTF-8

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Repository CRAN

Date/Publication 2025-01-08 18:00:02 UTC

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covs.	test Covariate test function for the horseshoe domain	

Description

Implements a finite area test function the horseshoe domain.

Usage

```
covs.test(x, y)
```

Arguments

x, y Points at which to evaluate the test function.

Value

Returns function evaluations.

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create.FEM.basis

Create a FEM basis

Description

Sets up a Finite Element basis. It requires a mesh. 2D, mesh. 2.5D or mesh. 3D object, as input. The basis' functions are globally continuos functions, that are polynomials once restricted to a triangle in the mesh. The current implementation includes linear finite elements (when order = 1 in the input mesh) and quadratic finite elements (when order = 2 in the input mesh). If saveTree flag is TRUE, it saves the tree mesh information in advance inside mesh object and can be used later on to save mesh construction time.

Usage

```
create.FEM.basis(mesh, saveTree = FALSE)
```

Arguments

mesh A mesh. 2D, mesh. 2.5D or mesh. 3D object representing the domain triangula-

tion. See create.mesh.2D, create.mesh.2.5D, create.mesh.3D.

saveTree a flag to decide to save the tree mesh information in advance (default is FALSE)

Value

A FEMbasis object. This contains the mesh, along with some additional quantities:

order Either "1" or "2" for the 2D and 2.5D case, and "1" for the 3D case. Order of the Finite Element basis.

nbasis Scalar. The number of basis.

See Also

```
create.mesh.2D, create.mesh.2.5D,create.mesh.3D
```

Examples

```
library(fdaPDE)
## Upload the quasicircle2D data
data(quasicircle2D)

## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(quasicircle2D$boundary_nodes,
quasicircle2D$locations), segments = quasicircle2D$boundary_segments)
## Plot it
plot(mesh)
## Create the basis
FEMbasis = create.FEM.basis(mesh)
## Upload the hub2.5D data
```

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```
data(hub2.5D)
hub2.5D.nodes = hub2.5D$hub2.5D.nodes
hub2.5D.triangles = hub2.5D$hub2.5D.triangles
## Create the 2.5D mesh
mesh = create.mesh.2.5D(nodes = hub2.5D.nodes, triangles = hub2.5D.triangles)
## Plot it
plot(mesh)
## Create the basis
FEMbasis = create.FEM.basis(mesh)
```

create.mesh.1.5D

Create a 1.5D linear network mesh

Description

Create a 1.5D linear network mesh

Usage

```
create.mesh.1.5D(nodes, edges = NULL, order = 1, nodesattributes = NULL)
```

Arguments

nodes A #nodes-by

A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.

edges

A #edges-by-2 (when order = 1) or #triangles-by-3 (when order = 2) matrix. This option is used when a triangulation is already available. It specifies the edges giving the row's indices in nodes of the edges' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints are ordered as 1—3—2 In this case the function create.mesh.1.5D is used to

produce a complete mesh.1.5D object.

order

Either '1' or '2'. It specifies wether each mesh should be represented by 2 nodes (the edges vertices) or by 3 nodes (the edges's vertices and midpoint). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements.

Default is order = 1.

nodesattributes

A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. If a node is added during the triangulation process or mesh refinement, its attributes are computed by linear interpolation using the attributes of neighboring nodes. This functionality is for instance used to compute the value of a Dirichlet boundary condition at boundary nodes added during the triangulation process.

Value

An object of the class mesh.1.5D with the following output:

nodes A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.

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nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.

- nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- edges A #edges-by-2 matrix containing all the edges of the triangles in the output triangulation. Each row contains the row's indices in nodes, indicating the nodes where the edge starts from and ends to.
- neighbors A #edges-by-2 matrix of list. Each row contains the indices of the neighbouring edges. An empty entry indicates that one node of the edge is a boundary node.
- order Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements.

create.mesh.2.5D

Create a mesh.2.5D object from the nodes locations and the connectivity matrix

Description

Create a mesh. 2.5D object from the nodes locations and the connectivity matrix

Usage

```
create.mesh.2.5D(
  nodes,
  triangles = NULL,
  order = 1,
  nodesattributes = NULL,
  segments = NULL,
  holes = NULL
```

Arguments

nodes

A #nodes-by-3 matrix containing the x, y, z coordinates of the mesh nodes.

triangles

A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix. It specifies the triangles giving the row's indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints are ordered as described at https://www.cs.cmu.edu/~quake/triangle.highorder.html.

order

Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements. Default is order = 1.

create.mesh.2.5D

nodesattributes

A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. This has been added for consistency with the function create.mesh.2D.

segments

A #segments-by-2 matrix. Each row contains the row's indices in nodes of the vertices where the segment starts from and ends to. Segments are edges that are not splitted during the triangulation process. These are for instance used to define the boundaries of the domain. This has been added for consistency with the function create.mesh.2D.

holes

A #holes-by-3 matrix containing the x, y, z coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes. This has been added for consistency with the function create.mesh.2D.

Value

An object of the class mesh.2.5D with the following output:

nodes A #nodes-by-3 matrix containing the x, y, z coordinates of the mesh nodes.

- nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.
- nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix. It specifies the triangles giving the indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints are ordered as described at
 - https://www.cs.cmu.edu/~quake/triangle.highorder.html.
- segmentsmarkers A vector of length #segments with entries either '1' or '0'. An entry '1' indicates that the corresponding element in segments is a boundary segment; an entry '0' indicates that the corresponding segment is not a boundary segment.
- edges A #edges-by-2 matrix containing all the edges of the triangles in the output triangulation. Each row contains the row's indices in nodes, indicating the nodes where the edge starts from and ends to.
- edgesmarkers A vector of lenght #edges with entries either '1' or '0'. An entry '1' indicates that the corresponding element in edge is a boundary edge; an entry '0' indicates that the corresponding edge is not a boundary edge.
- neighbors A #triangles-by-3 matrix. Each row contains the indices of the three neighbouring triangles. An entry '-1' indicates that one edge of the triangle is a boundary edge.
- holes A #holes-by-3 matrix containing the x, y, z coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes. These are passed unchanged from the input.
- order Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements.

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Examples

```
library(fdaPDE)

## Upload the hub2.5D the data
data(hub2.5D)
hub2.5D.nodes = hub2.5D$hub2.5D.nodes
hub2.5D.triangles = hub2.5D$hub2.5D.triangles

## Create mesh from nodes and connectivity matrix:
mesh = create.mesh.2.5D(nodes = hub2.5D.nodes, triangles = hub2.5D.triangles)
plot(mesh)
```

create.mesh.2D

Create a 2D triangular mesh

Description

This function is a wrapper of the Triangle library (http://www.cs.cmu.edu/~quake/triangle.html). It can be used to create a triangulation of the domain of interest starting from a list of points, to be used as triangles' vertices, and a list of segments, that define the domain boundary. The resulting mesh is a Constrained Delaunay triangulation. This is constructed in a way to preserve segments provided in the input segments without splitting them. This imput can be used to define the boundaries of the domain. If this imput is NULL, it generates a triangulation over the convex hull of the points. It is also possible to create a mesh.2D from the nodes locations and the connectivity matrix.

Usage

Arguments

nodes

A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.

nodesattributes

A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. If a node is added during the triangulation process or mesh refinement, its attributes are computed by linear interpolation using the attributes of neighboring nodes. This functionality is for instance used to compute the value of a Dirichlet boundary condition at boundary nodes added during the triangulation process.

segments

A #segments-by-2 matrix. Each row contains the row's indices in nodes of the vertices where the segment starts from and ends to. Segments are edges that are not splitted during the triangulation process. These are for instance used to define the boundaries of the domain. If this is input is NULL, it generates a triangulation over the convex hull of the points specified in nodes.

create.mesh.2D

holes A #holes-by-2 matrix containing the x and y coordinates of a point internal to

each hole of the mesh. These points are used to carve holes in the triangulation,

when the domain has holes.

triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) ma-

trix. This option is used when a triangulation is already available. It specifies the triangles giving the row's indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and

midpoints are ordered as described at

https://www.cs.cmu.edu/~quake/triangle.highorder.html. In this case the func-

tion create.mesh.2D is used to produce a complete mesh.2D object.

order Either '1' or '2'. It specifies wether each mesh triangle should be represented

by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic

(order = 2) Finite Elements. Default is order = 1.

verbosity This can be '0', '1' or '2'. It indicates the level of verbosity in the triangulation

process. When verbosity = 0 no message is returned during the triangulation. When verbosity = 2 the triangulation process is described step by step by

displayed messages. Default is verbosity = 0.

Value

An object of the class mesh.2D with the following output:

nodes A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.

nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.

nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.

triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix. This option is used when a triangulation is already available. It specifies the triangles giving the indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints are ordered as described at https://www.cs.cmu.edu/~quake/triangle.highorder.html.

- segmentsmarkers A vector of length #segments with entries either '1' or '0'. An entry '1' indicates that the corresponding element in segments is a boundary segment; an entry '0' indicates that the corresponding segment is not a boundary segment.
- edges A #edges-by-2 matrix containing all the edges of the triangles in the output triangulation. Each row contains the row's indices in nodes, indicating the nodes where the edge starts from and ends to.
- edgesmarkers A vector of lenght #edges with entries either '1' or '0'. An entry '1' indicates that the corresponding element in edge is a boundary edge; an entry '0' indicates that the corresponding edge is not a boundary edge.
- neighbors A #triangles-by-3 matrix. Each row contains the indices of the three neighbouring triangles. An entry '-1' indicates that one edge of the triangle is a boundary edge.

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holes A #holes-by-2 matrix containing the x and y coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes.

order Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements.

See Also

```
refine.mesh.2D, create.FEM.basis
```

Examples

```
library(fdaPDE)
## Upload the quasicirle2D data
data(quasicircle2D)
boundary_nodes = quasicircle2D$boundary_nodes
boundary_segments = quasicircle2D$boundary_segments
locations = quasicircle2D$locations
data = quasicircle2D$data
## Create mesh from boundary
## if the domain is convex it is sufficient to call:
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations))
plot(mesh)
## if the domain is not convex, pass in addition the segments the compose the boundary:
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create mesh from data locations (without knowing the boundary)
mesh = create.mesh.2D(nodes = locations)
plot(mesh)
## In this case the domain is the convex hull of the data locations.
## Do this only if you do not have any information about the shape of the domain of interest.
```

create.mesh.3D

Create a mesh. 3D object from the connectivity matrix and nodes locations

Description

Create a mesh. 3D object from the connectivity matrix and nodes locations

Usage

```
create.mesh.3D(
  nodes,
  tetrahedrons,
```

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```
order = 1,
nodesattributes = NULL,
segments = NULL,
holes = NULL
)
```

Arguments

nodes A #nodes-by-3 matrix containing the x, y, z coordinates of the mesh nodes.

tetrahedrons A #tetrahedrons-by-4 (when order = 1) or #tetrahedrons-by-10 (when order

= 2) matrix. It specifies the tetrahedrons giving the row's indices in nodes of the tetrahedrons' vertices and (when nodes = 2) also if the tetrahedrons' edges midpoints. The tetrahedrons' vertices and midpoints are ordered as described in "The Finite Element Method its Basis and Fundamentals" by O. C. Zienkiewicz,

R. L. Taylor and J.Z. Zhu

order Either '1' or '2'. It specifies wether each mesh tetrahedron should be represented

by 4 nodes (the tetrahedron's vertices) or by 10 nodes (the tetrahedron's vertices and edge midpoints). These are respectively used for linear (order = 1) and

quadratic (order = 2) Finite Elements. Default is order = 1.

nodesattributes

A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. This has been added for consistency with the function

create.mesh.2D.

segments A #segments-by-2 matrix. Each row contains the row's indices in nodes of the

vertices where the segment starts from and ends to. Segments are edges that are not splitted during the triangulation process. These are for instance used to define the boundaries of the domain. This has been added for consistency with

the function create.mesh.2D.

holes A #holes-by-3 matrix containing the x, y, z coordinates of a point internal to each

hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes. This has been added for consistency with the function

create.mesh.2D.

Value

An object of the class mesh.3D with the following output:

nodes A #nodes-by-3 matrix containing the x, y, z coordinates of the mesh nodes.

nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.

nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.

tetrahedrons A #tetrahedrons-by-4 (when order = 1) or #tetrahedrons-by-10 (when order = 2) matrix. It specifies the tetrahedrons giving the indices in nodes of the tetrahedrons' vertices and (when nodes = 2) also if the tetrahedrons' edges midpoints.

segmentsmarkers A vector of length #segments with entries either '1' or '0'. An entry '1' indicates that the corresponding element in segments is a boundary segment; an entry '0' indicates that the corresponding segment is not a boundary segment.

- faces A #faces-by-3 matrix containing all the faces of the tetrahedrons in the output triangulation. Each row contains the row's indices in nodes, indicating the nodes where the face starts from and ends to.
- facesmarkers A vector of lenght #faces with entries either '1' or '0'. An entry '1' indicates that the corresponding element in faces is a boundary face; an entry '0' indicates that the corresponding edge is not a boundary face.
- neighbors A #triangles-by-4 matrix. Each row contains the indices of the four neighbouring tetrahedrons An entry '-1' indicates that one face of the tetrahedrons is a boundary face.
- holes A #holes-by-3 matrix containing the x, y, z coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes. These are passed unchanged from the input.
- order Either '1' or '2'. It specifies wether each mesh tetrahedron should be represented by 3 nodes (the tetrahedron's vertices) or by 6 nodes (the tetrahedron's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements.

Examples

library(fdaPDE)

##Load the matrix nodes and tetrahedrons
data(sphere3Ddata)

nodes=sphere3Ddata\$nodes
tetrahedrons=sphere3Ddata\$tetrahedrons

##Create the triangulated mesh from the connectivity matrix and nodes locations
mesh=create.mesh.3D(nodes,tetrahedrons)

DE.FEM

Nonparametric density estimation with differential regularization

Description

This function implements a nonparametric density estimation method with differential regularization (given by the square root of the L2 norm of the laplacian of the density function), when points are located over a planar mesh. The computation relies only on the C++ implementation of the algorithm.

Usage

Arguments

data A matrix of dimensions #observations-by-ndim. Data are locations: each row

corresponds to one point, the first column corresponds to the x-coordinates, the second column corresponds to the y-coordinates and, if ndim=3, the third col-

umn corresponds to the z-coordinates.

FEMbasis A FEMbasis object describing the Finite Element basis, as created by create. FEM. basis.

lambda A scalar or vector of smoothing parameters. If it is a vector, the optimal smooth-

ing parameter is chosen with a k-fold cross-validation procedure based on the

L2 norm.

scaling A positive factor needed to scale the smoothing parameter in the construction of

confidence intervals. If the scaling is not specified, it is automatically set as the

square root of the number of observations.

fvec A vector of length #nodes of the mesh. It corresponds to the node values of the

initial density function. If this is NULL the initial density is estimated thanks to a discretized heat diffusion process that starts from the empirical density of the data. Default is NULL. N.B. This vector cannot be the constant vector of zeros

since the algorithm works with the log(f).

heatStep A real specifying the time step for the discretized heat diffusion process. Default

is 0.1.

heatIter An integer specifying the number of iterations to perform the discretized heat

diffusion process. Default is 500.

stepProposals A scalar or a vector containing the step parameters useful for the descent algo-

rithm. If there is a vector of parameters, the biggest one such that the functional decreases at each iteration is chosen. If it is NULL the following vector c(0.1, 0.01, 0.001, 0.0001, 0.00001, 0.000001, 1e-7, 1e-8, 1e-9) is proposed. Default is NULL. N.B. If the program does not receive a right parameter, it aborts

the R session. Try a smaller parameter.

tol1 A scalar specifying the tolerance to use for the termination criterion based on the

percentage difference between two consecutive iterations of the minimization algorithm of the loss function, the log-likelihood and the penalization. Default

is 1e-5.

tol2 A scalar specifying the tolerance to use for the termination criterion based on

the norm of the gradient of the functional to be minimized (the true minimum is such that this norm is zero). The default does not use this criterion. Default is 0.

print A boolean that is TRUE if the user wants the value of the functional, of the log-

likelihood and of the penalization term printed on console at each iteration of the descent algorithm. Default is FALSE. N.B. We suggest to let it FALSE if

preprocess_method is 'RightCV' or 'SimplifiedCV'.

nfolds An integer specifying the number of folds used in cross validation technique to

find the best lambda parameter. If there is only one lambda it can be 0. Default

is 0.

nsimulations An integer specifying the number of iterations used in the optimization algo-

rithms. Default value is 500.

step_method

String. This parameter specifies which step method use in the descent algorithm. If it is Fixed_Step, the step is constant during all the algorithm and it is chosen according to stepProposals; if it is Backtracking_Method, the step is computed at each iteration according to the backtracking method; finally if it is Wolfe_Method, the step is computed at each iteration according to the Wolfe method. Default is Fixed_Step.

direction_method

String. This parameter specifies which descent direction use in the descent algorithm. If it is Gradient, the direction is the one given by the gradient descent method (the opposite to the gradient of the functional); if instead it is BFGS the direction is the one given by the BFGS method (Broyden Fletcher Goldfarb and Shanno, a Quasi-Newton method). Default is BFGS. Other possible choices: Conjugate Gradient direction with Fletcher-Reeves formula (ConjugateGradientFR), Conjugate Gradient direction with Polak-Ribiére-Polyak formula (ConjugateGradientPRP), Conjugate Gradient direction with Hestenes-Stiefel formula (ConjugateGradientHS), Conjugate Gradient direction with Dai-Yuan formula (ConjugateGradientDY), Conjugate Gradient direction with Conjugate-Descent formula (ConjugateGradientCD), Conjugate Gradient direction with Liu-Storey formula (ConjugateGradientLS), L-BFGS direction with 5 correction vectors (L-BFGS5), L-BFGS direction with 10 correction vectors (L-BFGS10).

preprocess_method

String. This parameter specifies the k fold cross validation technique to use, if there is more than one smoothing parameter lambda (otherwise it should be NULL). If it is RightCV the usual k fold cross validation method is performed. If it is SimplifiedCV a simplified version is performed. In the latter case the number of smoothing parameters lambda must be equal to the number of folds nfolds. Default is NULL.

search

a flag to decide the search algorithm type (tree or naive or walking search algorithm). Default is tree.

inference

A boolean that is TRUE if the user wants to estimate confidence intervals. Default is FALSE.

Value

A list with the following variables:

FEMbasis	Given FEMbasis with tree information.
g	A vector of length #nodes that represents the value of the g-function estimated for each node of the mesh. The density is the exponential of this function.
f_init	A #nodes-by-#lambda parameters matrix. Each column contains the node values of the initial density used for the lambda given by the column.
lambda	A scalar representing the optimal smoothing parameter selected via k fold cross validation, if in the input there is a vector of parameters; the scalar given in input otherwise.
data	A matrix of dimensions #observations-by-ndim containing the data used in the algorithm. They are the same given in input if the domain is 2D pr 3D; they are the original data projected on the mesh if the domain is 2.5D.

CV_err

A vector of length nfolds containing the cross validation errors obtained in each fold, if preprocess_method is either RightCV or SimplifiedCV.

References

- Ferraccioli, F., Arnone, E., Finos, L., Ramsay, J. O., Sangalli, L. M. (2021). Nonparametric density estimation over complicated domains. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 83(2), 346-368.
- Arnone, E., Ferraccioli, F., Pigolotti, C., Sangalli, L.M. (2021), A roughness penalty approach to estimate densities over two-dimensional manifolds, Computational Statistics and Data Analysis, to appear.

Examples

```
library(fdaPDE)
## Create a 2D mesh over a squared domain
Xbound \leftarrow seq(-3, 3, length.out = 10)
Ybound \leftarrow seq(-3, 3, length.out = 10)
grid_XY <- expand.grid(Xbound, Ybound)</pre>
Bounds <- grid_XY[(grid_XY$Var1 %in% c(-3, 3)) | (grid_XY$Var2 %in% c(-3, 3)), ]
mesh <- create.mesh.2D(nodes = Bounds, order = 1)</pre>
mesh <- refine.mesh.2D(mesh, maximum_area = 0.2)</pre>
FEMbasis <- create.FEM.basis(mesh)</pre>
## Generate data
n <- 50
set.seed(10)
data_x <- rnorm(n)</pre>
data_y <- rnorm(n)</pre>
data <- cbind(data_x, data_y)</pre>
plot(mesh)
points(data, col="red", pch=19, cex=0.5)
## Density Estimation
lambda = 0.1
sol <- DE.FEM(data = data, FEMbasis = FEMbasis, lambda = lambda, fvec=NULL, heatStep=0.1,
              heatIter=500, nsimulations=300, step_method = "Fixed_Step", inference = TRUE)
## Visualization
n = 100
X \leftarrow seq(-3, 3, length.out = n)
Y < - seq(-3, 3, length.out = n)
grid <- expand.grid(X, Y)</pre>
evaluation <- eval.FEM(FEM(FEMbasis, coeff = sol$g), locations = grid)
lower_bound_g <- eval.FEM(FEM(FEMbasis, coeff = sol$g_CI_L), locations = grid)</pre>
upper_bound_g <- eval.FEM(FEM(FEMbasis, coeff = sol$g_CI_U), locations = grid)</pre>
evaluation <- exp(evaluation)</pre>
lower_bound_g <- exp(lower_bound_g)</pre>
upper_bound_g <- exp(upper_bound_g)</pre>
```

DE.FEM.time

Nonparametric spatio-temporal density estimation with differential regularization

Description

This function implements a nonparametric spatio-temporal density estimation method with differential regularization (given by the sum of the square of the L2 norm of the laplacian of the density function and the square of the L2 norm of the second- order time-derivative), when points are located over a planar mesh. The computation relies only on the C++ implementation of the algorithm.

Usage

Arguments

data	A matrix of dimensions #observations-by-ndim. Data are locations: each row corresponds to one point, the first column corresponds to the x-coordinates, the second column corresponds to the y-coordinates and, if ndim=3, the third column corresponds to the z-coordinates.
data_time	A vector of length #observations. The i-th datum is the time instant during which the i-th location is observed (according to the order in which locations are provided in data).
FEMbasis	A FEMbasis object describing the Finite Element basis, as created by create.FEM.basis.
mesh_time	A vector containing the b-splines knots for separable smoothing. It is the time mesh of the considered time domain (interval). Its nodes are in increasing order.
lambda	A scalar or vector of smoothing parameters in space. If it is a vector, the optimal smoothing parameter in space is chosen, together with the optimal smoothing parameter in time, with a k-fold cross-validation procedure based on the L2 norm.

lambda_time A scalar or vector of smoothing parameters in time. If it is a vector, the optimal

smoothing parameter in time is chosen, together with the optimal smoothing parameter in space, with a k-fold cross-validation procedure based on the L2

norm.

scaling A positive factor needed to scale the smoothing parameters in the construction

of confidence intervals. If the scaling is not specified, it is automatically set as

the square root of the number of observations.

fvec A vector of length #nodes of the spatial mesh times #B-spline temporal func-

tional basis. It corresponds to the node values of the initial density function. If this is NULL the initial density is estimated thanks to a discretized heat diffusion process that starts from the empirical density of the data. Default is NULL. N.B. This vector cannot be the constant vector of zeros since the algorithm works

with the log(f).

heatStep A real specifying the time step for the discretized heat diffusion process. Default

is 0.1.

heatIter An integer specifying the number of iterations to perform the discretized heat

diffusion process. Default is 10.

stepProposals A scalar or a vector containing the step parameters useful for the descent algo-

rithm. If there is a vector of parameters, the biggest one such that the functional decreases at each iteration is chosen. If it is NULL the following vector c(0.1, 0.01, 0.001, 0.0001, 0.00001, 0.000001, 1e-7, 1e-8, 1e-9) is proposed. Default is NULL. N.B. If the program does not receive a right parameter, it aborts

the R session. Try a smaller parameter.

tol1 A scalar specifying the tolerance to use for the termination criterion based on the

percentage difference between two consecutive iterations of the minimization algorithm of the loss function, the log-likelihood and the penalizations. Default

is 1e-5.

tol2 A scalar specifying the tolerance to use for the termination criterion based on

the norm of the gradient of the functional to be minimized (the true minimum is such that this norm is zero). The default version does not use this criterion.

Default is 0.

print A boolean that is TRUE if the user wants the value of the functional, of the log-

likelihood and of the penalization terms printed on console at each iteration of the descent algorithm (plus some other information/warnings). Default is FALSE. N.B. We suggest to let it FALSE if preprocess_method is 'RightCV' or 'Sim-

plifiedCV'.

nfolds An integer specifying the number of folds used in cross validation technique to

find the best pair of (lambda, lambda_time) smoothing parameters. If there is

only one pair of (lambda, lambda_time) it can be 0. Default is 0.

nsimulations An integer specifying the number of iterations used in the optimization algo-

rithms. Default value is 500.

step_method A string specifying which step method to use in the descent algorithm. If it is

Fixed_Step, the step is constant during the algorithm and it is chosen according to stepProposals; if it is Backtracking_Method, the step is computed at each iteration according to the backtracking method; finally if it is Wolfe_Method,

> the step is computed at each iteration according to the Wolfe method. Default is Fixed_Step.

direction_method

A string specifying which descent direction to use in the descent algorithm. If it is Gradient, the direction is the one given by the gradient descent method (the opposite to the gradient of the functional); if instead it is BFGS the direction is the one given by the BFGS method (Broyden-Fletcher-Goldfarb-Shanno, a Quasi-Newton method). Default is BFGS. Other possible choices: Conjugate Gradient direction with Fletcher-Reeves formula (ConjugateGradientFR), Conjugate Gradient direction with Polak-Ribiére-Polyak formula (ConjugateGradientPRP), Conjugate Gradient direction with Hestenes-Stiefel formula (ConjugateGradientHS), Conjugate Gradient direction with Dai-Yuan formula (ConjugateGradientDY), Conjugate Gradient direction with Conjugate-Descent formula (ConjugateGradientCD), Conjugate Gradient direction with Liu-Storey formula (ConjugateGradientLS), L-BFGS direction with 5 correction vectors (L-BFGS5), L-BFGS direction with 10 correction vectors (L-BFGS10).

preprocess_method

A string specifying the k fold cross validation technique to use, if there is more than one pair of smoothing parameters in space and in time (lambda, lambda_time); otherwise it should be NULL. If it is RightCV the usual k fold cross validation method is performed. If it is SimplifiedCV a simplified version is performed. In the latter case the number of possible pairs of smoothing parameters in space and in time (lambda, lambda_time) must be equal to the number of folds nfolds. Default is NULL.

search

A flag to decide the search algorithm type (tree or naive or walking search algorithm). Default is tree.

isTimeDiscrete A boolean specifying the time data type: TRUE for discrete (with many duplicates) time data; FALSE for continuous time data. Default is FALSE.

flagMass

A boolean specifying whether to consider full mass matrices (TRUE) or identity mass matrices (FALSE) for the computation of space and time penalty matrices. Default is FALSE.

flagLumped

A boolean specifying whether to perform mass lumping. This numerical technique presents computational advantages during the procedure involving a mass matrix inversion for the computation of the space penalty matrix. Default is FALSE. N.B. We suggest to use it as TRUE in case of a large spatial domain or in case of a dense/refined spatial mesh.

inference

A boolean that is TRUE if the user wants to estimate confidence intervals. Default is FALSE.

Value

A list with the following variables:

FEMbasis

Given FEMbasis with tree information.

A vector of length #nodes times #B-splines that represents the value of the g-function estimated for each node of the spatial mesh and at each time instant of the time mesh. The density is the exponential of this function.

f_init A #nodes-by-#lambdax#lambda_time parameters matrix. Each column contains the node values of the initial density used for the pair (lambda, lambda_time)

given by the column.

lambda A scalar representing the optimal smoothing parameter in space selected, to-

gether with lambda_time, via k fold cross validation, if in the input there is a vector of parameters (in space and/or in time); the scalar given in input other-

wise.

lambda_time A scalar representing the optimal smoothing parameter in time selected, together

with lambda, via k fold cross validation, if in the input there is a vector of

parameters (in space and/or in time); the scalar given in input otherwise.

data A matrix of dimensions #observations-by-ndim containing the spatial data used

in the algorithm. They are the same given in input if the domain is 2D pr 3D; they are the original data projected on the mesh if the domain is 2.5D. Data lying

outside the spatial domain, defined through its mesh, are not considered.

data_time A vector of length #observations containing the time data used in the algorithm.

Data lying outside the temporal domain, defined through its mesh, are not con-

sidered.

CV_err A vector of length nfolds containing the cross validation errors obtained in each

fold, if preprocess_method is either RightCV or SimplifiedCV.

Examples

```
library(fdaPDE)
```

```
## Create a 2D mesh over a squared domain
Xbound \leftarrow seq(-3, 3, length.out = 10)
Ybound \leftarrow seq(-3, 3, length.out = 10)
grid_XY <- expand.grid(Xbound, Ybound)</pre>
Bounds <- grid_XY[(grid_XY$Var1 %in% c(-3, 3)) | (grid_XY$Var2 %in% c(-3, 3)), ]
mesh <- create.mesh.2D(nodes = Bounds, order = 1)</pre>
mesh <- refine.mesh.2D(mesh, maximum_area = 0.25, minimum_angle = 20)</pre>
FEMbasis <- create.FEM.basis(mesh)</pre>
## Create a 1D time mesh over a (non-negative) interval
mesh_time <- seq(0, 1, length.out=3)</pre>
## Generate data
n <- 50
set.seed(10)
x <- rnorm(n, 0, 2)
y \leftarrow rnorm(n,0,2)
locations <- cbind(x,y)</pre>
times <- runif(n,0,1)
data <- cbind(locations, times)</pre>
t <- 0.5 \# time instant in which to evaluate the solution
plot(mesh)
sample <- data[abs(data[,3]-t)<0.05,1:2]</pre>
points(sample, col="red", pch=19, cex=1, main=paste('Sample | ', t-0.05,' < t < ', t+0.05))</pre>
```

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```
## Density Estimation
lambda <- 0.1
lambda_time <- 0.001</pre>
sol <- DE.FEM.time(data = locations, data_time = times, FEMbasis = FEMbasis, mesh_time = mesh_time,</pre>
             lambda = lambda, lambda_time = lambda_time, nsimulations=300, inference=TRUE)
## Visualization
n = 100
X \leftarrow seq(-3, 3, length.out = n)
Y \leftarrow seq(-3, 3, length.out = n)
grid <- expand.grid(X, Y)</pre>
FEMfunction = FEM.time(sol$g, mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation <- eval.FEM.time(FEM.time = FEMfunction, locations = grid, time.instants = t)
FEMfunction_L = FEM.time(sol$g_CI_L, mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation_L <- eval.FEM.time(FEM.time = FEMfunction_L, locations = grid, time.instants = t)
FEMfunction_U = FEM.time(sol$g_CI_U, mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation_U <- eval.FEM.time(FEM.time = FEMfunction_U, locations = grid, time.instants = t)
image2D(x = X, y = Y, z = matrix(exp(evaluation_L), n, n), col = heat.colors(100),
        xlab = "x", ylab = "y", contour = list(drawlabels = FALSE),
        main = paste("Estimated CI lower bound at t = ", t), zlim=c(0,0.3), asp = 1)
image2D(x = X, y = Y, z = matrix(exp(evaluation), n, n), col = heat.colors(100),
        xlab = "x", ylab = "y", contour = list(drawlabels = FALSE),
        main = paste("Estimated density at t = ", t), zlim=c(0,0.3), asp = 1)
image2D(x = X, y = Y, z = matrix(exp(evaluation_U), n, n), col = heat.colors(100),
        xlab = "x", ylab = "y", contour = list(drawlabels = FALSE),
        main = paste("Estimated CI upper bound at t = ", t), zlim=c(0,0.3), asp = 1)
```

DE.heat.FEM

Density initialization

Description

This function implements two methods for the density initialization procedure.

Usage

Arguments

data

A matrix of dimensions #observations-by-ndim. Data are locations: each row corresponds to one point, the first column corresponds to the x-coordinates, the second column corresponds to the y-coordinates and, if ndim=3, the third column corresponds to the z-coordinates.

FEMbasis

A FEMbasis object describing the Finite Element basis, as created by create.FEM.basis.

DE.heat.FEM

lambda	A scalar or vector of smoothing parameters. Default is NULL. It is useful only if init='Heat'.
heatStep	Real specifying the time step for the discretized heat diffusionn process.
heatIter	Integer specifying the number of iteriations to perform the discretized heat diffusion process.
init	String. This parameter specifies the initialization procedure. It can be either 'Heat' or 'CV'.
nFolds	An integer specifying the number of folds used in cross validation techinque. It is useful only for the case init = 'CV'.
search	a flag to decide the search algorithm type (tree or naive or walking search algorithm).

Value

If init = 'Heat' it returns a matrix in which each column contains the initial vector for each lambda. If init = 'CV' it returns the initial vector associated to the lambda given.

Examples

```
library(fdaPDE)
## Create a 2D mesh over a squared domain
Xbound <- seq(-3, 3, length.out = 10)
Ybound \leftarrow seq(-3, 3, length.out = 10)
grid_XY <- expand.grid(Xbound, Ybound)</pre>
Bounds <- grid_XY[(grid_XY$Var1 %in% c(-3, 3)) | (grid_XY$Var2 %in% c(-3, 3)), ]
mesh <- create.mesh.2D(nodes = Bounds, order = 1)</pre>
mesh <- refine.mesh.2D(mesh, maximum_area = 0.2)</pre>
FEMbasis <- create.FEM.basis(mesh)</pre>
## Generate data
n <- 50
set.seed(10)
data_x <- rnorm(n)</pre>
data_y <- rnorm(n)</pre>
data <- cbind(data_x, data_y)</pre>
plot(mesh)
points(data, col="red", pch=19, cex=0.5)
## Density initialization
sol = DE.heat.FEM(data, FEMbasis, lambda, heatStep=0.1, heatIter=500, init="Heat")
## Visualization
plot(FEM(coeff=sol$f_init, FEMbasis=FEMbasis))
```

DE.heat.FEM.time

DE.heat.FEM.time	Spatio-temporal density initialization	

Description

This function implements two methods for the density initialization procedure.

Usage

Arguments

٤	,uments	
	data	A matrix of dimensions #observations-by-ndim. Data are locations: each row corresponds to one point, the first column corresponds to the x-coordinates, the second column corresponds to the y-coordinates and, if ndim=3, the third column corresponds to the z-coordinates.
	data_time	A vector of dimensions #observations. The i-th datum is the time instant during which the i-th location is observed (according to the order in which data are provided).
	FEMbasis	$A \ FEMbasis \ object \ describing \ the \ Finite \ Element \ basis, \ as \ created \ by \ create. \\ FEM.basis.$
	mesh_time	A vector containing the b-splines knots for separable smoothing. It is the time mesh of the considered time domain (interval). Its nodes are in increasing order.
	lambda	A scalar or vector of smoothing parameters in space. Default is NULL. It is useful only if init='Heat'.
	lambda_time	A scalar or vector of smoothing parameters in time. Default is NULL. It is useful only if init='Heat'.
	heatStep	A real specifying the time step for the discretized heat diffusion process.
	heatIter	An integer specifying the number of iterations to perform the discretized heat diffusion process.
	init	A string specifying the initialization procedure. It can be either 'Heat' or 'CV'.
	nFolds	An integer specifying the number of folds used in the cross validation technique. It is useful only for the case init = 'CV'.
	search	A flag to decide the search algorithm type (tree or naive or walking search algorithm).
	isTimeDiscrete	A boolean specifying the time data type: TRUE for discrete (with many duplicates) time data; FALSE for continuous time data. Default is FALSE.
	flagMass	A boolean specifying whether to consider full mass matrices (TRUE) or identity mass matrices (FALSE) for the computation of space and time penalty matrices. Default is FALSE.

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flagLumped

A boolean specifying whether to perform mass lumping. This numerical technique presents computational advantages during the procedure involving a mass matrix inversion for the computation of the space penalty matrix. Default is FALSE. N.B. We suggest to put it TRUE in case of a large spatial domain or in case of a dense/refined spatial mesh.

Value

If init = 'Heat' it returns a matrix in which each column contains the initial vector for each possible pair (lambda, lambda_time). If init = 'CV' it returns the initial vector associated to the unique pair (lambda, lambda_time) given.

Examples

```
library(fdaPDE)
## Create a 2D mesh over a squared domain
Xbound \leftarrow seq(-3, 3, length.out = 10)
Ybound \leftarrow seq(-3, 3, length.out = 10)
grid_XY <- expand.grid(Xbound, Ybound)</pre>
Bounds <- grid_XY[(grid_XY$Var1 %in% c(-3, 3)) | (grid_XY$Var2 %in% c(-3, 3)), ]
mesh <- create.mesh.2D(nodes = Bounds, order = 1)</pre>
mesh <- refine.mesh.2D(mesh, maximum_area = 0.25, minimum_angle = 20)</pre>
FEMbasis <- create.FEM.basis(mesh)</pre>
## Create a 1D time mesh over a (non-negative) interval
mesh_time <- seq(0, 1, length.out=3)</pre>
## Generate data
n <- 50
set.seed(10)
x <- rnorm(n,0,2)
y <- rnorm(n,0,2)
locations <- cbind(x,y)</pre>
times <- runif(n,0,1)</pre>
data <- cbind(locations, times)</pre>
t <- 0.5 # time instant in which to evaluate the solution
plot(mesh)
sample <- data[abs(data[,3]-t)<0.05,1:2]</pre>
points(sample, col="red", pch=19, cex=1, main=paste('Sample | ', t-0.05,' < t < ', t+0.05))</pre>
## Density initialization
lambda = 0.1
lambda_time <- 0.001</pre>
sol = DE.heat.FEM.time(data = locations, data_time = times, FEMbasis = FEMbasis,
                        mesh_time = mesh_time, lambda = lambda, lambda_time = lambda_time,
                         heatStep=0.1, heatIter=10, init="Heat")
```

Visualization

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eval.FEM

Evaluate a FEM object at a set of point locations

Description

It evaluates a FEM object at the specified set of locations or areal regions. The locations are used for pointwise evaluations and incidence matrix for areal evaluations. The locations and the incidence matrix cannot be both NULL or both provided.

Usage

Arguments

FEM A FEM object to be evaluated.

locations A 2-columns (in 1.5D or 2D) or 3-columns (in 2.5D and 3D) matrix with the

spatial locations where the FEM object should be evaluated.

incidence_matrix

In case of areal evaluations, the #regions-by-#elements incidence matrix defin-

ing the regions where the FEM object should be evaluated.

search a flag to decide the search algorithm type (tree or naive or walking search algo-

rithm).

bary.locations A list with three vectors: locations, location points which are same as the

given locations options. (checks whether both locations are the same); element ids, a vector of element id of the points from the mesh where they are located;

barycenters, a vector of barycenter of points from the located element.

Value

A vector or a matrix of numeric evaluations of the FEM object. If the FEM object contains multiple finite element functions the output is a matrix, and each row corresponds to the location (or areal region) where the evaluation has been taken, while each column corresponds to the function evaluated.

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References

Sangalli, L. M., Ramsay, J. O., & Ramsay, T. O. (2013). Spatial spline regression models.
 Journal of the Royal Statistical Society: Series B (Statistical Methodology), 75(4), 681-703.

• Azzimonti, L., Sangalli, L. M., Secchi, P., Domanin, M., & Nobile, F. (2015). Blood flow velocity field estimation via spatial regression with PDE penalization. Journal of the American Statistical Association, 110(511), 1057-1071.

Examples

```
library(fdaPDE)
## Upload the horseshoe2D data
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations
## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
## Compute the coeff vector evaluating the desired function at the mesh nodes
## In this case we consider the fs.test() function introduced by Wood et al. 2008
coeff = fs.test(mesh$nodes[,1], mesh$nodes[,2])
## Create the FEM object
FEMfunction = FEM(coeff, FEMbasis)
## Evaluate the finite element function in the location (1,0.5)
eval.FEM(FEMfunction, locations = matrix(c(1, 0.5), ncol = 2))
## Evaluate the mean of the finite element function over the fifth triangle of the mesh
incidence_matrix = matrix(0, ncol = nrow(mesh$triangles))
incidence_matrix[1,5] = 1
eval.FEM(FEMfunction, incidence_matrix = incidence_matrix)
```

eval.FEM.time

Evaluate a FEM.time object at a set of point locations

Description

It evaluates a FEM. time object at the specified set of locations or regions. If space.time.locations is provided locations, incidence_matrix and time.instants must be NULL. Otherwise time.instants and one of locations and incidence_matrix must be given. In this case the evaluation is perform on the tensor grid time.instants-by-locations (or time.instants-by-areal domains).

Usage

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Arguments

FEM. time A FEM. time object to be evaluated.

locations A 2-columns (in case of planar mesh) or 3-columns (in case of 2D manifold in a

3D space or a 3D volume) matrix with the spatial locations where the FEM.time

object should be evaluated.

time.instants A vector with the time instants where the FEM.time object should be evaluated.

space.time.locations

A 3-columns (in case of planar mesh) or 4-columns(in case of 2D manifold in a 3D space or a 3D volume) matrix with the time instants and spatial locations where the FEM.time object should be evaluated. The first column is for the time instants. If given, locations, incidence_matrix and time.instants must be

NULL.

incidence_matrix

In case of areal data, the #regions x #elements incidence matrix defining the

regions.

lambdaS The index of the lambdaS choosen for the evaluation.

lambdaT The index of the lambdaT choosen for the evaluation.

search a flag to decide the search algorithm type (tree or naive or walking search algo-

rithm).

bary.locations A list with three vectors: locations, location points which are same as the

given locations options. (checks whether both locations are the same); element ids, a vector of element id of the points from the mesh where they are located;

barycenters, a vector of barycenter of points from the located element.

Value

A matrix of numeric evaluations of the FEM. time object. Each row indicates the location where the evaluation has been taken, the column indicates the function evaluated.

References

Devillers, O. et al. 2001. Walking in a Triangulation, Proceedings of the Seventeenth Annual Symposium on Computational Geometry

Examples

```
library(fdaPDE)
## Upload the horseshoe2D data
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations

## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
```

fdaPDE-deprecated

Deprecated Functions

Description

Only executed when smooth. FEM. basis is run with the option CPP_CODE = FALSE. It computes the mass matrix. The element (i,j) of this matrix contains the integral over the domain of the product between the ith and kth element of the Finite Element basis. As common practise in Finite Element Analysis, this quantities are computed iterating over all the mesh triangles.

Only executed when smooth.FEM.basis is run with the option $CPP_CODE = FALSE$. It computes the stifness matrix. The element (i,j) of this matrix contains the integral over the domain of the scalar product between the gradient of the ith and kth element of the Finite Element basis. As common practise in Finite Element Analysis, this quantities are computed iterating over all the mesh triangles.

Only executed when the function smooth.FEM.basis is run with the option CPP_CODE = FALSE. It evaluates the Finite Element basis functions and their derivatives up to order 2 at the specified set of locations. This version of the function is implemented using only R code. It is called by R_smooth.FEM.basis.

Only executed when the function smooth.FEM.basis is run with the option CPP_CODE = FALSE. It evaluates a FEM object at the specified set of locations.

This function implements a spatial regression model with differential regularization; isotropic and stationary case. In particular, the regularizing term involves the Laplacian of the spatial field. Spacevarying covariates can be included in the model. The technique accurately handle data distributed over irregularly shaped domains. Moreover, various conditions can be imposed at the domain boundaries.

This function implements a spatial regression model with differential regularization; anysotropic case. In particular, the regularizing term involves a second order elliptic PDE, that models the space-variation of the phenomenon. Space-varying covariates can be included in the model. The technique accurately handle data distributed over irregularly shaped domains. Moreover, various conditions can be imposed at the domain boundaries.

This function implements a spatial regression model with differential regularization; anysotropic and non-stationary case. In particular, the regularizing term involves a second order elliptic PDE with space-varying coefficients, that models the space-variation of the phenomenon. Space-varying covariates can be included in the model. The technique accurately handle data distributed over irregularly shaped domains. Moreover, various conditions can be imposed at the domain boundaries.

This function is a wrapper of the Triangle library (http://www.cs.cmu.edu/~quake/triangle.html). It can be used to create a triangulation of the domain of interest starting from a list of points, to be used as triangles' vertices, and a list of segments, that define the domain boundary. The resulting mesh is a Constrained Delaunay triangulation. This is constructed in a way to preserve segments provided in the input segments without splitting them. This imput can be used to define the boundaries of the domain. If this imput is NULL, it generates a triangulation over the convex hull of the points.

This function refines a Constrained Delaunay triangulation into a Conforming Delaunay triangulation. This is a wrapper of the Triangle library (http://www.cs.cmu.edu/~quake/triangle.html). It can be used to refine a mesh created previously with create.MESH.2D. The algorithm can add Steiner points (points through which the segments are splitted) in order to meet the imposed refinement conditions.

Plot a mesh MESH2D object, generated by create.MESH.2D or refine.MESH.2D. Circles indicate the mesh nodes.

Usage

```
R_mass(FEMbasis)
R_stiff(FEMbasis)
R_smooth.FEM.basis(
  locations,
  observations,
  FEMbasis,
  lambda,
  covariates = NULL,
  GCV
R_{eval.FEM.basis}(FEMbasis, locations, nderivs = matrix(0, 1, 2))
R_eval.FEM(FEM, locations)
smooth.FEM.basis(
  locations = NULL,
  observations,
  FEMbasis,
  lambda,
  covariates = NULL,
  BC = NULL,
  GCV = FALSE,
  CPP\_CODE = TRUE
smooth.FEM.PDE.basis(
  locations = NULL,
  observations,
  FEMbasis,
```

```
lambda,
 PDE_parameters,
  covariates = NULL,
 BC = NULL,
  GCV = FALSE
 CPP\_CODE = TRUE
)
smooth.FEM.PDE.sv.basis(
  locations = NULL,
  observations,
  FEMbasis,
  lambda,
  PDE_parameters,
  covariates = NULL,
  BC = NULL,
  GCV = FALSE,
  CPP_CODE = TRUE
)
create.MESH.2D(nodes, nodesattributes = NA, segments = NA, holes = NA,
                     triangles = NA, order = 1, verbosity = 0)
refine.MESH.2D(mesh, minimum_angle, maximum_area, delaunay, verbosity)
## S3 method for class 'MESH2D'
plot(x, ...)
```

Arguments

FEMbasis A FEMbasis object describing the Finite Element basis, as created by create.FEM.basis.

locations A #observations-by-2 matrix where each row specifies the spatial coordinates

x and y of the corresponding observations in the vector observations. This parameter can be NULL. In this case the spatial coordinates of the corresponding

observations are assigned as specified in observations.

observations A vector of length #observations with the observed data values over the domain.

The locations of the observations can be specified with the locations argument. Otherwise if only the vector of observations is given, these are consider to be located in the corresponding node in the table nodes of the mesh. In this last case, an NA value in the observations vector indicates that there is no observation

associated to the corresponding node.

lambda A scalar or vector of smoothing parameters.

covariates A #observations-by-#covariates matrix where each row represents the covariates

associated with the corresponding observed data value in observations.

Boolean. If TRUE the following quantities are computed: the trace of the smooth-

ing matrix, the estimated error standard deviation, and the Generalized Cross Validation criterion, for each value of the smoothing parameter specified in

lambda.

nderivs A vector of lenght 2 specifying the order of the partial derivatives of the bases

to be evaluated. The vectors' entries can be 0,1 or 2, where 0 indicates that only

the basis functions, and not their derivatives, should be evaluated.

FEM A FEM object to be evaluated

BC A list with two vectors: BC_indices, a vector with the indices in nodes of

boundary nodes where a Dirichlet Boundary Condition should be applied; BC_values, a vector with the values that the spatial field must take at the nodes indicated in

BC_indices.

CPP_CODE Boolean. If TRUE the computation relies on the C++ implementation of the al-

gorithm. This usually ensures a much faster computation.

PDE_parameters A list specifying the space-varying parameters of the elliptic PDE in the regu-

larizing term: K, a function that for each spatial location in the spatial domain (indicated by the vector of the 2 spatial coordinates) returns a 2-by-2 matrix of diffusion coefficients. This induces an anisotropic smoothing with a local preferential direction that corresponds to the first eigenvector of the diffusion matrix K.The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be an array with dimensions 2-by-2-by-#points.b, a function that for each spatial location in the spatial domain returns a vector of length 2 of transport coefficients. This induces a local smoothing only in the direction specified by the vector b. The function must support recycling for efficiency reasons, thus if the input parameter is a #pointby-2 matrix, the output should be a matrix with dimensions 2-by-#points; c, a function that for each spatial location in the spatial domain returns a scalar reaction coefficient. c induces a shrinkage of the surface to zero. The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be a vector with length #points; u, a function that for each spatial location in the spatial domain returns a scalar reaction coefficient. u induces a reaction effect. The function must support recycling for

nodes A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.

should be a vector with length #points.

A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. If a node is added during the triangulation process or mesh refinement, its attributes are computed by linear interpolation using the attributes of neighboring nodes. This functionality is for instance used to compute the value of a Dirichlet boundary condition at boundary nodes added during the triangulation process.

efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output

A #segments-by-2 matrix. Each row contains the row's indices in nodes of the vertices where the segment starts from and ends to. Segments are edges that are not splitted during the triangulation process. These are for instance used to define the boundaries of the domain. If this is input is NULL, it generates a triangulation over the convex hull of the points specified in nodes.

A #holes-by-2 matrix containing the x and y coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes.

nodesattributes

segments

holes

triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) ma-

trix. This option is used when a triangulation is already available. It specifies the triangles giving the row's indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and

midpoints are ordered as described at

https://www.cs.cmu.edu/~quake/triangle.highorder.html. In this case the func-

tion create. MESH. 2D is used to produce a complete MESH2D object.

order Either '1' or '2'. It specifies wether each mesh triangle should be represented

by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic

(order = 2) Finite Elements. Default is order = 1.

verbosity This can be '0', '1' or '2'. It indicates the level of verbosity in the triangulation

process.

mesh A MESH2D object representing the triangular mesh, created by create.MESH.2D.

minimum_angle A scalar specifying a minimum value for the triangles angles.

maximum_area A scalar specifying a maximum value for the triangles areas.

delaunay A boolean parameter indicating whether or not the output mesh should satisfy

the Delaunay condition.

x A MESH2D object defining the triangular mesh, as generated by create. Mesh. 2D

or refine.Mesh.2D.

... Arguments representing graphical options to be passed to par.

Details

These functions are Deprecated in this release of fdaPDE, they will be marked as Defunct and removed in a future version.

Value

A square matrix with the integrals of all the basis' functions pairwise products. The dimension of the matrix is equal to the number of the nodes of the mesh.

A square matrix with the integrals of all the basis functions' gradients pairwise dot products. The dimension of the matrix is equal to the number of the nodes of the mesh.

A list with the following quantities:

fit. FEM A FEM object that represents the fitted spatial field.

PDEmisfit.FEM A FEM object that represents the Laplacian of the estimated spatial field.

beta If covariates is not NULL, a vector of length #covariates with the regression co-

efficients associated with each covariate.

edf If GCV is TRUE, a scalar or vector with the trace of the smoothing matrix for

each value of the smoothing parameter specified in lambda.

stderr If GCV is TRUE, a scalar or vector with the estimate of the standard deviation of

the error for each value of the smoothing parameter specified in lambda.

GCV If GCV is TRUE, a scalar or vector with the value of the GCV criterion for each

value of the smoothing parameter specified in lambda.

A matrix of basis function values. Each row indicates the location where the evaluation has been taken, the column indicates the basis function evaluated

A matrix of numeric evaluations of the FEM object. Each row indicates the location where the evaluation has been taken, the column indicates the function evaluated.

A list with the following variables:

fit.FEM A FEM object that represents the fitted spatial field.

PDEmisfit.FEM A FEM object that represents the Laplacian of the estimated spatial field.

solution A list, note that all terms are matrices or row vectors: the jth column represents the vector of related to lambda[j] if lambda.selection.criterion="grid" and lambda.selection.lossfunction="unus In all the other cases is returned just the column related to the best penalization parameter

- f Matrix, estimate of function f, first half of solution vector
- g Matrix, second half of solution vector
- z_hat Matrix, prediction of the output in the locations

beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. It is the regression coefficients estimate

rmse Estimate of the root mean square error in the locations

estimated_sd Estiimate of the standard deviation of the error

optimization A detailed list of optimization related data:

lambda_solution numerical value of best lambda acording to lambda.selection.lossfunction,

-1 if lambda.selection.lossfunction="unused"

 $lambda_position\ in teger, postion\ in\ lambda_vector\ of\ best\ lambda\ acording\ to\ lambda\ .\ selection\ .\ loss function\ ,$

-1 if lambda.selection.lossfunction="unused" GCV numeric value of GCV in correspondence of the optimum

optimization_details list containing further information about the optimization method used and the nature of its termination, eventual number of iterations

dof numeric vector, value of dof for all the penalizations it has been computed, empty if not computed

lambda_vector numeric value of the penalization factors passed by the user or found in the iterations of the optimization method

GCV_vector numeric vector, value of GCV for all the penalizations it has been computed

time Duration of the entire optimization computation

bary.locations A barycenter information of the given locations if the locations are not mesh nodes.

A list with the following variables:

fit.FEM A FEM object that represents the fitted spatial field.

PDEmisfit.FEM A FEM object that represents the Laplacian of the estimated spatial field.

solution A list, note that all terms are matrices or row vectors: the jth column represents the vector of related to lambda[j] if lambda.selection.criterion="grid" and lambda.selection.lossfunction="unus In all the other cases is returned just the column related to the best penalization parameter

f Matrix, estimate of function f, first half of solution vector

- g Matrix, second half of solution vector
- z_hat Matrix, prediction of the output in the locations

beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. It is the regression coefficients estimate

rmse Estimate of the root mean square error in the locations

estimated_sd Estimate of the standard deviation of the error

optimization A detailed list of optimization related data:

lambda_solution numerical value of best lambda acording to lambda.selection.lossfunction,

-1 if lambda.selection.lossfunction="unused"

lambda_position integer, postion in lambda_vector of best lambda acording to lambda.selection.lossfunction, -1 if lambda.selection.lossfunction="unused"

GCV numeric value of GCV in correspondence of the optimum

optimization_details list containing further information about the optimization method used and the nature of its termination, eventual number of iterations

dof numeric vector, value of dof for all the penalizations it has been computed, empty if not computed

lambda_vector numeric value of the penalization factors passed by the user or found in the iterations of the optimization method

GCV_vector numeric vector, value of GCV for all the penalizations it has been computed

time Duration of the entire optimization computation

bary.locations A barycenter information of the given locations if the locations are not mesh nodes.

A list with the following variables:

fit.FEM A FEM object that represents the fitted spatial field.

PDEmisfit.FEM A FEM object that represents the Laplacian of the estimated spatial field.

solution A list, note that all terms are matrices or row vectors: the jth column represents the vec-

tor of related to lambda[j] if lambda.selection.criterion="grid" and lambda.selection.lossfunction="unus In all the other cases is returned just the column related to the best penalization parameter

- f Matrix, estimate of function f, first half of solution vector
- g Matrix, second half of solution vector
- z_hat Matrix, prediction of the output in the locations

beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. It is the regression coefficients estimate

rmse Estimate of the root mean square error in the locations

estimated_sd Estiimate of the standard deviation of the error

optimization A detailed list of optimization related data:

lambda_solution numerical value of best lambda acording to lambda.selection.lossfunction,

-1 if lambda.selection.lossfunction="unused"

lambda_position integer, postion in lambda_vector of best lambda acording to lambda.selection.lossfunction, -1 if lambda.selection.lossfunction="unused"

GCV numeric value of GCV in correspondence of the optimum

optimization_details list containing further information about the optimization method used and the nature of its termination, eventual number of iterations

dof numeric vector, value of dof for all the penalizations it has been computed, empty if not computed

lambda_vector numeric value of the penalization factors passed by the user or found in the iterations of the optimization method

GCV_vector numeric vector, value of GCV for all the penalizations it has been computed time Duration of the entire optimization computation

bary.locations A barycenter information of the given locations if the locations are not mesh nodes.

An object of the class MESH2D with the following output:

nodes A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.

nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates

that the corresponding node is a boundary node; an entry '0' indicates that the

corresponding node is not a boundary node.

nodesattributes

nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. If a node is added during the triangulation process or mesh refinement, its attributes are computed by linear interpolation using the attributes of neighboring nodes. This functionality is for instance used to compute the value of a Dirichlet boundary condition at boundary nodes added

during the triangulation process.

triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix.

This option is used when a triangulation is already available. It specifies the triangles giving the indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints

are ordered as described at

https://www.cs.cmu.edu/~quake/triangle.highorder.html.

segmentsmarker A vector of length #segments with entries either '1' or '0'. An entry '1' indicates

that the corresponding element in segments is a boundary segment; an entry '0'

indicates that the corresponding segment is not a boundary segment.

edges A #edges-by-2 matrix containing all the edges of the triangles in the output

triangulation. Each row contains the row's indices in nodes, indicating the nodes

where the edge starts from and ends to.

edgesmarkers A vector of lenght #edges with entries either '1' or '0'. An entry '1' indicates

that the corresponding element in edge is a boundary edge; an entry '0' indicates

that the corresponding edge is not a boundary edge.

neighbors A #triangles-by-3 matrix. Each row contains the indices of the three neighbour-

ing triangles. An entry '-1' indicates that one edge of the triangle is a boundary

edge.

holes A #holes-by-2 matrix containing the x and y coordinates of a point internal to

each hole of the mesh. These points are used to carve holes in the triangulation,

when the domain has holes.

order

Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements. Default is order = 1.

A MESH2D object representing the refined triangular mesh, with the following output:

nodes A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.

nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates

that the corresponding node is a boundary node; an entry '0' indicates that the

corresponding node is not a boundary node.

nodesattributes

nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. If a node is added during the triangulation process or mesh refinement, its attributes are computed by linear interpolation using the attributes of neighboring nodes. This functionality is for instance used to compute the value of a Dirichlet boundary condition at boundary nodes added during the triangulation process.

triangles

A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix. This option is used when a triangulation is already available. It specifies the triangles giving the row's indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints are ordered as described at

https://www.cs.cmu.edu/~quake/triangle.highorder.html.

edges

A #edges-by-2 matrix. Each row contains the row's indices of the nodes where the edge starts from and ends to.

edgesmarkers

A vector of lenght #edges with entries either '1' or '0'. An entry '1' indicates that the corresponding element in edge is a boundary edge; an entry '0' indicates that the corresponding edge is not a boundary edge.

neighbors

A #triangles-by-3 matrix. Each row contains the indices of the three neighbouring triangles. An entry '-1' indicates that one edge of the triangle is a boundary edge.

holes

A #holes-by-2 matrix containing the x and y coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes.

order

Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements. Default is order = 1.

See Also

refine.MESH.2D, create.FEM.basis create.MESH.2D, create.FEM.basis

36 FEM

FEM

Define a surface or spatial field by a Finite Element basis expansion

Description

This function defines a FEM object.

Usage

```
FEM(coeff,FEMbasis)
```

Arguments

coeff A vector or a matrix containing the coefficients for the Finite Element basis ex-

pansion. The number of rows (or the vector's length) corresponds to the number of basis in FEMbasis. The number of columns corresponds to the number of

functions.

FEMbasis A FEMbasis object defining the Finite Element basis, created by create.FEM.basis.

Value

An FEM object. This contains a list with components coeff and FEMbasis.

Examples

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FEM.time	Define a spatio-temporal field by a Finite Element basis expansion

Description

This function defines a FEM.time object.

Usage

```
FEM.time(coeff,time_mesh,FEMbasis,FLAG_PARABOLIC=FALSE)
```

Arguments

coeff A vector or a matrix containing the coefficients for the spatio-temporal basis expansion. The number of rows (or the vector's length) corresponds to the number

of basis in FEMbasis times the number of knots in time_mesh.

time_mesh A vector containing the b-splines knots for separable smoothing and the nodes

for finite differences for parabolic smoothing

FEMbasis A FEMbasis object defining the Finite Element basis, created by create.FEM.basis.

FLAG_PARABOLIC Boolean. If TRUE the coefficients are from parabolic smoothing, if FALSE the

separable one.

Value

A FEM.time object. This contains a list with components coeff, mesh_time, FEMbasis and FLAG_PARABOLIC.

```
library(fdaPDE)
## Upload the horseshoe2D data
data(horseshoe2D)
## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(horseshoe2D$boundary_nodes, horseshoe2D$locations),
                      segments = horseshoe2D$boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
## Compute the coeff vector evaluating the desired function at the mesh nodes
## In this case we consider the fs.test() function introduced by Wood et al. 2008
coeff = rep(fs.test(mesh$nodes[,1], mesh$nodes[,2]),5)
time_mesh = seq(0,1,length.out = 5)
## Create the FEM object
FEMfunction = FEM.time(coeff, time_mesh, FEMbasis, FLAG_PARABOLIC = TRUE)
## Plot it at desired time
plot(FEMfunction, 0.7)
```

38 FPCA.FEM

FPCA.	FEM
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Smooth Functional Principal Component Analysis

Description

This function implements a smooth functional principal component analysis over a planar mesh, a smooth manifold or a volume.

Usage

Arguments

locations A #observations-by-2 matrix in the 2D case and #observations-by-3 matrix in

the 2.5D and 3D case, where each row specifies the spatial coordinates x and y (and z in 2.5D and 3D) of the corresponding observation in the datamatrix. If the locations of the observations coincide with (or are a subset of) the nodes of the mesh in the FEMbasis, leave the parameter locations = NULL for a faster

implementation.

datamatrix A matrix of dimensions #samples-by-#locations with the observed data values

over the domain for each sample. The datamatrix needs to have zero mean. If the locations argument is left NULL the datamatrix has to be dimensions #samples-by-#nodes where #nodes is the number of nodes of the mesh in the FEMbasis. In this case, each observation is associated to the corresponding node in the mesh. If the data are observed only on a subset of the mesh nodes, fill with NA the

values of the datamatrix in correspondence of unobserved data.

FEMbasis A FEMbasis object describing the Finite Element basis, as created by create.FEM.basis.

lambda A scalar or vector of smoothing parameters.

nPC An integer specifying the number of Principal Components to compute.

validation A string specifying the type of validation to perform. If lambda is a vector, it has

to be specified as "GCV" or "KFold". This parameter specify which method of cross-validation is used to select the best parameter lambda among those values of the smoothing parameter specified in lambda for each Principal Component.

NFolds This parameter is used only in case validation = "KFold". It is an integer

specifying the number of folds to use if the KFold cross-validation method for

the selection of the best parameter lambda is chosen. Default value is 5.

GCVmethod This parameter is considered only when validation = "GCV". It can be either

"Exact" or "Stochastic". If set to "Exact" the algoritm performs an exact (but possibly slow) computation of the GCV index. If set to "Stochastic" the GCV is

approximated by a stochastic algorithm.

nrealizations The number of realizations to be used in the stochastic algorithm for the estima-

tion of GCV.

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search a flag to decide the search algorithm type (tree or naive or walking search algorithm).

bary.locations A list with three vectors: locations, location points which are same as the

given locations options. (checks whether both locations are the same); element ids, a vector of element id of the points from the mesh where they are located; barycenters, a vector of barycenter of points from the located element.

Value

A list with the following variables:

loadings.FEM A FEM object that represents the L^2-normalized functional loadings for each Principal Component computed.

scores A #samples-by-#PrincipalComponents matrix that represents the unnormalized scores or PC vectors.

lambda A vector of length #PrincipalComponents with the values of the smoothing parameter lambda chosen for that Principal Component.

variance_explained A vector of length #PrincipalComponents where each value represent the variance explained by that component.

cumsum_percentage A vector of length #PrincipalComponents containing the cumulative percentage of the variance explained by the first components.

bary.locations A barycenter information of the given locations if the locations are not mesh nodes.

References

Lila, E., Aston, J.A.D., Sangalli, L.M., 2016a. Smooth Principal Component Analysis over two-dimensional manifolds with an application to neuroimaging. Ann. Appl. Stat., 10(4), pp. 1854-1879.

```
library(fdaPDE)

## Load the hub data
data(hub2.5D)
hub2.5D.nodes = hub2.5D$hub2.5D.nodes
hub2.5D.triangles = hub2.5D$hub2.5D.triangles

mesh = create.mesh.2.5D(nodes = hub2.5D.nodes, triangles = hub2.5D.triangles)

## Create the Finite Element basis
FEMbasis = create.FEM.basis(mesh)

## Create a datamatrix
datamatrix = NULL
for(ii in 1:50){
    a1 = rnorm(1, mean = 1, sd = 1)
    a2 = rnorm(1, mean = 1, sd = 1)
    a3 = rnorm(1, mean = 1, sd = 1)
```

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```
func_evaluation = numeric(nrow(mesh$nodes))
  for (i in 0:(nrow(mesh$nodes)-1)){
    func_evaluation[i+1] = a1* sin(2*pi*mesh$nodes[i+1,1]) +
                           a2* sin(2*pi*mesh$nodes[i+1,2]) +
                           a3*sin(2*pi*mesh$nodes[i+1,3]) + 1
  }
  data = func_evaluation + rnorm(nrow(mesh$nodes), mean = 0, sd = 0.5)
  datamatrix = rbind(datamatrix, data)
## Compute the mean of the datamatrix and subtract it to the data
data_bar = colMeans(datamatrix)
data_demean = matrix(rep(data_bar,50), nrow=50, byrow=TRUE)
datamatrix_demeaned = datamatrix - data_demean
## Set the smoothing parameter lambda
lambda = 0.00375
## Estimate the first 2 Principal Components
FPCA_solution = FPCA.FEM(datamatrix = datamatrix_demeaned,
                      FEMbasis = FEMbasis, lambda = lambda, nPC = 2)
## Plot the functional loadings of the estimated Principal Components
plot(FPCA_solution$loadings.FEM)
```

fs.test

FELSPLINE test function

Description

Implements a finite area test function based on one proposed by Tim Ramsay (2002) proposed by Simon Wood (2008).

Usage

```
fs.test(x, y, r0 = 0.1, r = 0.5, l = 3, b = 1, exclude = FALSE)
```

Arguments

x, y	Points at which to evaluate the test function.
r0	The test domain is a sort of bent sausage. This is the radius of the inner bend.
r	The radius of the curve at the centre of the sausage.
1	The length of an arm of the sausage.
b	The rate at which the function increases per unit increase in distance along the centre line of the sausage.
exclude	Should exterior points be set to NA?

Value

Returns function evaluations, or NAs for points outside the horseshoe domain.

fs.test.3D 41

References

- Ramsay, T. 2002. Spline smoothing over difficult regions. J.R. Statist. Soc. B 64(2):307-319
- Wood, S. N., Bravington, M. V., & Hedley, S. L. (2008). Soap film smoothing. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 70(5), 931-955.

Examples

```
library(fdaPDE)
## Upload the horseshoe2D data
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations
## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
## Compute the coeff vector evaluating the desired function at the mesh nodes
## In this case we consider the fs.test() function introduced by Wood et al. 2008
coeff = fs.test(mesh$nodes[,1], mesh$nodes[,2], exclude = FALSE)
## Create the FEM object
FEMfunction = FEM(coeff, FEMbasis)
## Plot it
plot(FEMfunction)
```

fs.test.3D

FELSPLINE 3D test function

Description

Implements a finite area test function based on one proposed by Tim Ramsay (2002) and by Simon Wood (2008) in 3D.

Usage

```
fs.test.3D(x, y, z, r0 = 0.25, r = 1.25, l = 5, b = 1, exclude = FALSE)
```

Arguments

x, y, z	Points at which to evaluate the test function.
r0	The test domain is a sort of bent sausage. This is the radius of the inner bend.
r	The radius of the curve at the centre of the sausage.
1	The length of an arm of the sausage.
b	The rate at which the function increases per unit increase in distance along the centre line of the sausage.
exclude	Should exterior points be set to NA?

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Value

Returns function evaluations, or NAs for points outside the horseshoe domain.

Examples

```
library(fdaPDE)

data(horseshoe2.5D)
mesh = horseshoe2.5D
FEMbasis=create.FEM.basis(mesh)

# Evaluation at nodes
sol_exact=fs.test.3D(mesh$nodes[,1],mesh$nodes[,3],mesh$nodes[,2])
plot(FEM(sol_exact, FEMbasis))
```

horseshoe2.5D

Horseshoe2.5D domain

Description

A mesh2.5D object with nodes and connectivity matrix of a triangular mesh of the horseshoe 2.5D domain.

horseshoe2D

Horseshoe domain

Description

The boundary and interior nodes and connectivity matrix of a triangular mesh of the horseshoe domain. This dataset can be used to create a mesh. 2D object with the function create.mesh. 2D.

hub2.5D

Hub domain

Description

The nodes and connectivity matrix of a triangular mesh of a manifold representing a hub geometry. This dataset can be used to create a MESH. 2.5D object with the function create. MESH. 2.5D.

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image.FEM

Image Plot of a 2D FEM object

Description

Image plot of a FEM object, generated by the function FEM or returned by smooth. FEM and FPCA. FEM. Only FEM objects defined over a 2D mesh can be plotted with this method.

Usage

```
## S3 method for class 'FEM'
image(x, num_refinements, ...)
```

Arguments

x A 2D-mesh FEM object. num refinements

A natural number specifying how many bisections should by applied to each triangular element for plotting purposes. This functionality is useful where a discretization with 2nd order Finite Element is applied.

... Arguments representing graphical options to be passed to plot3d.

Value

No return value

See Also

FEM plot.FEM

```
library(fdaPDE)
## Upload the horseshoe2D data
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations

## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
## Compute the coeff vector evaluating the desired function at the mesh nodes
## In this case we consider the fs.test() function introduced by Wood et al. 2008
coeff = fs.test(mesh$nodes[,1], mesh$nodes[,2])
## Create the FEM object
FEMfunction = FEM(coeff, FEMbasis)
```

44 image.FEM.time

```
## Plot the FEM function
image(FEMfunction)
```

image.FEM.time

Image plot of a 2D FEM.time object at a given time

Description

Image plot of a FEM. time object, generated by the function FEM. time or returned by smooth. FEM. time. Only FEM objects defined over a 2D mesh can be plotted with this method.

Usage

```
## S3 method for class 'FEM.time'
image(x,t,lambdaS=1,lambdaT=1,num_refinements=NULL,...)
```

Arguments

x A 2D-mesh FEM. time object.
t time at which do the plot

lambdaS index of the space penalization parameter to use for the plot, useful when FEM. time

returned by smooth.FEM.time using GCV

lambdaT index of the time penalization parameter to use for the plot, useful when FEM. time

returned by smooth.FEM.time using GCV

num_refinements

A natural number specifying how many bisections should by applied to each triangular element for plotting purposes. This functionality is useful where a

discretization with 2nd order Finite Element is applied.

... Arguments representing graphical options to be passed to plot3d.

Value

No return value

See Also

```
FEM.time image.FEM.time
```

```
library(fdaPDE)
## Upload the horseshoe2D data
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations
```

```
## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
## Compute the coeff vector evaluating the desired function at the mesh nodes
## In this case we consider the fs.test() function introduced by Wood et al. 2008
time = 1:5
coeff = rep(fs.test(mesh$nodes[,1], mesh$nodes[,2]),5)*time
## Create the FEM.time object
FEM_time_function = FEM.time(coeff=coeff, time_mesh=1:5,FEMbasis=FEMbasis,FLAG_PARABOLIC=TRUE)
## Plot the FEM function
t = c(1.2,1.5,3.6,2.4,4.5)
image(FEM_time_function,t)
```

inferenceDataObject-class

Class for inference data

Description

A class that contains all possible information for inference over linear parameters and/or nonparametric field in spatial regression with differential regularization problem. This object can be used as parameter in smoothing function of the fdaPDE library smooth.FEM.

Details

At least one between test and interval must be nonzero. n_cov, coeff and beta0, if provided, need to be coherent. dim and locations, if provided, need to be coherent. The usage of inferenceDataObjectBuilder is recommended for the construction of an object of this class.

Slots

- test A vector of integers taking value 0, 1 or 2; if 0 no test is performed, if 1 one-at-the-time tests are performed, if 2 a simultaneous test is performed.
- interval A vector of integers taking value 0, 1, 2 or 3; if 0 no confidence interval is computed, if 1 one-at-the-time confidence intervals are computed, if 2 simultaneous confidence intervals are computed, if 3 Bonferroni confidence intervals are computed.
- type A vector of integers taking value 1, 2, 3, 4 or 5 corresponding to Wald, Speckman, Eigen-Sign-Flip, Enhanced-Eigen-Sign-Flip or Sign-Flip inferential approach.
- component A vector of integers taking value 1, 2 or 3, indicating whether the inferential analysis should be carried out respectively for the parametric, nonparametric or both the components.
- exact An integer taking value 1 or 2. If 1 an exact computation of the test statistics will be performed, whereas if 2 an approximated computation will be carried out (not implemented in this version).

- dim Dimension of the problem, it is equal to 2 in the 1.5D and 2D cases and equal to 3 in the 2.5D and 3D cases.
- n_cov Number of covariates taken into account in the linear part of the regression problem.
- locations A matrix of numeric coefficients with columns of dimension dim. When nonparametric inference is requested it represents the set of spatial locations for which the inferential analysis should be performed. The default values is a one-dimensional matrix of value 1 indicating that all the observed location points should be considered. In the sign-flip and eigen-sign-flip implementations only observed points are allowed.
- locations_indices A vector of indices indicating which spatial points have to be considered among the observed ones for nonparametric inference. If a vector of location indices is provided then the slot 'location' is discarded.
- locations_are_nodes An integer taking value 1 or 2; in the first case it indicates that the selected locations to perform inference on f are all coinciding with the nodes; otherwise it takes value 2;
- coeff A matrix of numeric coefficients with columns of dimension n_cov and each row represents a linear combination of the linear parameters to be tested and/or to be estimated via confidence interval.
- beta0 Vector of null hypothesis values for the linear parameters of the model. Used only if test is not 0 and component is not 2.
- f0 Function representing the expression of the nonparametric component f under the null hypothesis. Used only if component is not 1.
- f0_eval Vector of f0 evaluations at the chosen test locations. It will be eventually set later in checkInferenceParameters, if nonparametric inference is required.
- f_var An integer taking value 1 or 2. If 1 local variance estimates for the nonlinear part of the model will be computed, whereas if 2 they will not.
- quantile Vector of quantiles needed for confidence intervals, used only if interval is not 0.
- alpha 1 minus confidence level vector of sign-flipping approaches confidence intervals. Used only if interval is not 0.
- n_flip An integer representing the number of sign-flips in the case of sign-flipping approaches.
- tol_fspai A real number greater than 0 specifying the tolerance for FSPAI algorithm, in case of non-exact inference (not implemented in this version).
- definition An integer taking value 0 or 1. If set to 1, the class will be considered as created by the function inferenceDataObjectBuilder, leading to avoid some of the checks that are performed on inference data within smoothing functions.

Description

A function that build an inferenceDataObject. In the process of construction many checks over the input parameters are carried out so that the output is a well defined object, that can be used as parameter in smooth.FEM or smooth.FEM.time functions. Notice that this constructor ensures well-posedness of the object, but a further check on consistency with the smoothing functions parameters will be carried out.

Usage

```
inferenceDataObjectBuilder(test = NULL,
interval = NULL,
type = 'w',
component = 'parametric',
dim = NULL,
n_cov = NULL,
locations = NULL,
locations_indices = NULL,
locations_by_nodes = FALSE,
coeff = NULL,
beta0 = NULL,
f0 = NULL,
f_var = FALSE,
level = 0.95,
n_flip = 1000)
```

Arguments

test

A string defining the type of test to be performed. Multiple tests can be required. In this case the length of the list needs to be coherent with the ones of type, component and interval. The default is NULL, and can take values:

'oat' : one-at-the-time tests, available only when component is 'parametric'.

'sim': simultaneous tests.

'none' : no test required. interval must be set.

interval

A string defining the type of confidence intervals to be computed. Multiple intervals can be required. In this case the length of the list needs to be coherent with the ones of type, component and test. The default is NULL, and can take values:

'oat' : one-at-the-time intervals.

'sim': simultaneous intervals, available only when component is 'parametric' and no sign-flipping approaches are required.

'bonf': Bonferroni intervals, available only when component is 'parametric'

'none': no interval required. test must be set.

type

A list of strings defining the type of implementation for the inferential analysis. The possible values are:

'w': Wald parametric approach (default).

's' : Speckman parametric approach.

dim

'sf': sign-flip nonparametric approach.

'esf': eigen-sign-flip nonparametric approach.

'enh-esf': enhanced-eigen-sign-flip nonparametric approach.

component A list of strings defining on which model component inference has to be per-

formed. It can take values 'parametric' (default), 'nonparametric' or 'both'.

Dimension of the problem, defaulted to NULL. It can take value 2 or 3 corre-

sponding to 1.5D/2D or 2.5D/3D problems (Must be set by the user)

n_cov Number of the covariates, defaulted to NULL. (Must be set by the user)

locations A matrix of the locations of interest when testing the nonparametric component

f, defaulted to NULL

locations_indices

A vector of indices indicating the locations to be considered among the observed ones for nonparametric inference, defaulted to NULL. If a vector of indices is provided, then the slot 'locations' is discarded.

locations_by_nodes

A logical used to indicate whether the selected locations to perform inference

on f are all coinciding with the nodes;

coeff A matrix, with n_cov number of columns, of numeric coefficients representing

the linear combinations of the parametric components of the model. The default is NULL, corresponding to an identity matrix. If at least one sing-flipping

approach is required in type, needs to be an identity matrix.

beta0 Vector of real numbers (default NULL). It is used only if the test parameter is

set, and component is not 'nonparametric'; its length is the number of rows of matrix coeff if provided. If test is set and beta0 is NULL, will be set to a

vector of zeros.

f0 A function object representing the expression of the nonparametric component

f under the null hypothesis. Taken into account if test is set and component is not parametric. If NULL, the default is the null function, hence a test on the

significance of the nonparametric component is carried out.

f_var A logical used to decide whether to estimate the local variance of the nonlinear

part of the model. The possible values are: FALSE (default) and TRUE.

level A vector containing the level of significance used to compute quantiles for con-

fidence intervals, defaulted to 0.95. It is taken into account only if interval is

set.

n_flip Number of flips performed in sign-flipping approaches, defaulted to 1000.

Value

The output is a well defined inferenceDataObject, that can be used as input parameter in the smooth.FEM function.

```
obj<-inferenceDataObjectBuilder(test = 'oat', dim = 2, beta0 = rep(1,4), n_cov = 4);
obj2<-inferenceDataObjectBuilder(test = 'sim', dim = 3, component = 'nonparametric', n_cov = 3);</pre>
```

inferenceDataObjectTime-class

Class for inference data in ST case

Description

A class that contains all possible information for inference over linear parameters and/or nonparametric field in spatio-temporal regression with differential regularization problem. This object can be used as parameter in smoothing function of the fdaPDE library smooth.FEM.time.

Details

At least one between test and interval must be nonzero. n_cov, coeff and beta0, if provided, need to be coherent. dim and locations, if provided, need to be coherent. The usage of inferenceDataObjectTimeBuilder is recommended for the construction of an object of this class.

Slots

- test A vector of integers taking value 0, 1 or 2; if 0 no test is performed, if 1 one-at-the-time tests are performed, if 2 a simultaneous test is performed.
- interval A vector of integers taking value 0, 1, 2 or 3; if 0 no confidence interval is computed, if 1 one-at-the-time confidence intervals are computed, if 2 simultaneous confidence intervals are computed, if 3 Bonferroni confidence intervals are computed.
- type A vector of integers taking value 1, 2, 3 or 4 corresponding to Wald, Speckman, Eigen-Sign-Flip, Enhanced-Eigen-Sign-Flip inferential approach.
- component A vector of integers taking value 1, 2 or 3, indicating whether the inferential analysis should be carried out respectively for the parametric, nonparametric or both the components.
- exact An integer taking value 1 or 2. If 1 an exact computation of the test statistics will be performed, whereas if 2 an approximated computation will be carried out (not implemented in this version).
- dim Dimension of the problem, it is equal to 2 in the 1.5D and 2D cases and equal to 3 in the 2.5D and 3D cases.
- n_cov Number of covariates taken into account in the linear part of the regression problem.
- locations A matrix of numeric coefficients with columns of dimension dim. When nonparametric inference is requested it represents the set of spatial locations for which the inferential analysis should be performed. The default values is a one-dimensional matrix of value 1 indicating that all the observed location points should be considered. In the sign-flip and eigen-sign-flip implementations only observed points are allowed.
- locations_indices A vector of indices indicating which spatial points have to be considered among the observed ones for nonparametric inference. If a vector of location indices is provided then the slot 'location' is discarded.
- locations_are_nodes An integer taking value 1 or 2; in the first case it indicates that the selected locations to perform inference on f are all coinciding with the nodes; otherwise it takes value 2;

- time_locations A vector of numeric coefficients containing the set of times of interest for inference on the nonparametric component. This parameter can be NULL. In this case the temporal locations are assumed to coincide with the time_locations provided to the smoothing functions. Used only if component is not 1.
- coeff A matrix of numeric coefficients with columns of dimension n_cov and each row represents a linear combination of the linear parameters to be tested and/or to be estimated via confidence interval.
- beta0 Vector of null hypothesis values for the linear parameters of the model. Used only if test is not 0 and component is not 2.
- f0 Function representing the expression of the nonparametric component f under the null hypothesis. Used only if component is not 1.
- f0_eval Matrix of f0 evaluations at the chosen space and time locations. It will be eventually set later in checkInferenceParametersTime, if nonparametric inference is required.
- f_var An integer taking value 1 or 2. If 1 local variance estimates for the nonlinear part of the model will be computed, whereas if 2 they will not.
- quantile Vector of quantiles needed for confidence intervals, used only if interval is not 0.
- alpha 1 minus confidence level vector of sign-flipping approaches confidence intervals. Used only if interval is not 0.
- n_flip An integer representing the number of sign-flips in the case of sign-flipping approaches.
- tol_fspai A real number greater than 0 specifying the tolerance for FSPAI algorithm, in case of non-exact inference (not implemented in this version).
- definition An integer taking value 0 or 1. If set to 1, the class will be considered as created by the function inferenceDataObjectTimeBuilder, leading to avoid some of the checks that are performed on inference data within smoothing functions.

inferenceDataObjectTimeBuilder

Constructor for inferenceDataObjectTime class

Description

A function that build an inferenceDataObjectTime. In the process of construction many checks over the input parameters are carried out so that the output is a well defined object, that can be used as parameter in smooth.FEM or smooth.FEM.time functions. Notice that this constructor ensures well-posedness of the object, but a further check on consistency with the smoothing functions parameters will be carried out.

Usage

```
inferenceDataObjectTimeBuilder(test = NULL,
interval = NULL,
type = 'w',
component = 'parametric',
dim = NULL,
```

```
n_{cov} = NULL
locations = NULL,
locations_indices = NULL,
locations_by_nodes = F,
time_locations = NULL,
coeff = NULL,
beta0 = NULL,
f0 = NULL,
f_{var} = F,
level = 0.95,
n_flip = 1000)
```

Arguments

test

A string defining the type of test to be performed. Multiple tests can be required. In this case the length of the list needs to be coherent with the ones of type, component and interval. The default is NULL, and can take values:

'oat': one-at-the-time tests, available only when component is 'parametric'.

'sim': simultaneous tests.

'none': no test required. interval must be set.

interval

A string defining the type of confidence intervals to be computed. Multiple intervals can be required. In this case the length of the list needs to be coherent with the ones of type, component and test. The default is NULL, and can take values:

'oat': one-at-the-time intervals.

'sim': simultaneous intervals, available only when component is 'parametric' and no sign-flipping approaches are required.

'bonf': Bonferroni intervals, available only when component is 'parametric'

'none': no interval required, test must be set.

type

A list of strings defining the type of implementation for the inferential analysis. The possible values are:

'w': Wald parametric approach (default).

's': Speckman parametric approach, available only when component is 'parametric'.

'esf': eigen-sign-flip nonparametric approach, available only when component is 'parametric'.

'enh-esf': enhanced-eigen-sign-flip nonparametric approach, available only when component is 'parametric'.

component

A list of strings defining on which model component inference has to be performed. It can take values 'parametric' (default), 'nonparametric' or 'both'.

dim

Dimension of the problem, defaulted to NULL. It can take value 2 or 3 corresponding to 1.5D/2D or 2.5D/3D problems (Must be set by the user)

n_cov

Number of the covariates, defaulted to NULL. (Must be set by the user)

locations

A matrix of the locations of interest when testing the nonparametric component f, defaulted to NULL.

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locations_indices

A vector of indices indicating the locations to be considered among the observed ones for nonparametric inference, defaulted to NULL. If a vector of indices is provided, then the slot 'locations' is discarded.

locations_by_nodes

A logical used to indicate whether the selected locations to perform inference on f are all coinciding with the nodes.

time_locations A vector of times of interest when testing the nonparametric component f, defaulted to NULL. If FLAG_parabolic = TRUE, time_locations need to be NULL

or to coincide with the time mesh.

coeff A matrix, with n_cov number of columns, of numeric coefficients representing

the linear combinations of the parametric components of the model. The default is NULL, corresponding to an identity matrix. If at least one sing-flipping

approach is required in type, needs to be an identity matrix.

beta0 Vector of real numbers (default NULL). It is used only if the test parameter is

set, and component is not 'nonparametric'; its length is the number of rows of matrix coeff if provided. If test is set and beta0 is NULL, will be set to a

vector of zeros.

f0 A function object representing the expression of the nonparametric component

f under the null hypothesis. Taken into account if test is set and component is not parametric. If NULL, the default is the null function, hence a test on the

significance of the nonparametric component is carried out.

f_var A logical used to decide whether to estimate the local variance of the nonlinear

part of the model. The possible values are: FALSE (default) and TRUE.

level A vector containing the level of significance used to compute quantiles for con-

fidence intervals, defaulted to 0.95. It is taken into account only if interval is

set.

n_flip Number of flips performed in sign-flipping approaches, defaulted to 1000.

Value

The output is a well defined inferenceDataObjectTime, that can be used as input parameter in the smooth.FEM function.

Examples

```
obj<-inferenceDataObjectTimeBuilder(test = 'oat', dim = 2, beta0 = rep(1,4), n_cov = 4);
obj2<-inferenceDataObjectTimeBuilder(test = 'sim', dim = 3, component = 'nonparametric', n_cov = 3);</pre>
```

plot.FEM Plot a FEM object

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Description

Three-dimensional plot of a FEM object, generated by FEM or returned by smooth. FEM or FPCA. FEM. If the mesh of the FEMbasis component is of class mesh. 2D both the 3rd axis and the color represent the value of the coefficients for the Finite Element basis expansion (coeff component of the FEM object). If the mesh is of class mesh. 3D, the color of each triangle or tetrahedron represent the mean value of the coefficients for the Finite Element basis expansion (coeff).

Usage

```
## S3 method for class 'FEM'
plot(x, colormap = "heat.colors", num_refinements = NULL, ...)
```

Arguments

x A FEM object.

colormap A colormap exploited in the plot. The default value is the heat colormap.

num_refinements

A natural number specifying how many bisections should be applied to each triangular element for plotting purposes. This functionality is useful where a discretization with 2nd order Finite Element is applied. This parameter can be specified only when a FEM object defined over a 2D mesh is plotted.

... Arguments representing graphical options to be passed to plot3d.

Value

No return value

See Also

```
FEM, image.FEM
```

```
library(fdaPDE)
## Upload the horseshoe2D data
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations

## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
## Compute the coeff vector evaluating the desired function at the mesh nodes
## In this case we consider the fs.test() function introduced by Wood et al. 2008
coeff = fs.test(mesh$nodes[,1], mesh$nodes[,2])
## Create the FEM object
FEMfunction = FEM(coeff, FEMbasis)
```

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```
## Plot the FEM function
plot(FEMfunction)
```

plot.FEM.time

Plot a FEM. time object at a given time

Description

Plot of a FEM. time object, generated by FEM. time or returned by smooth. FEM. time. time_locations and locations must not be both provided. If time_locations is provided, the spatial field is plotted for the provided temporal instnts. If locations is provided, the temporal evolution in the provided space locations is plotted. If both time_locations and locations are NULL a default plot is provided. If the mesh of the FEMbasis component is of class mesh. 2D both the 3rd axis and the color represent the value of the coefficients for the Finite Element basis expansion (coeff component of the FEM. time object). If the mesh is of class mesh. 3D, the color of each triangle or tetrahedron represent the mean value of the coefficients for the Finite Element basis expansion (coeff).

Usage

Arguments

x A FEM. time object.

time_locations A vector with the instants in which plot the spatial field

locations A 2-column matrix when x\$FEMbasis\$mesh is of class mesh. 2D or a 3-column

matrix otherwise with the spatial locations for which plot the temporal evolution

lambdaS Index of the space penalization parameter to use for the plot, useful when FEM. time

returned by smooth.FEM.time using GCV

lambdaT Index of the time penalization parameter to use for the plot, useful when FEM. time

returned by smooth.FEM.time using GCV

num_refinements

A natural number specifying how many bisections should be applied to each triangular element for plotting purposes. This functionality is useful where a discretization with 2nd order Finite Element is applied. This parameter can be

specified only when a FEM object defined over a 2D mesh is plotted.

Nt The number of instants to plot when locations is not NULL

add Boolean, used only when locations is not NULL, if TURE it performs the graphic

over the last plot

main The title of the plot when locations is not NULL

col The color of the plot when locations is not NULL. May be a single color or a

vector of colors

... Arguments representing graphical options to be passed to plot3d.

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Value

No return value

See Also

```
FEM.time, image.FEM.time
```

Examples

```
library(fdaPDE)
## Upload the horseshoe2D data
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations
## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
## Compute the coeff vector evaluating the desired function at the mesh nodes
## In this case we consider the fs.test() function introduced by Wood et al. 2008
time = 1:5
coeff = rep(fs.test(mesh$nodes[,1], mesh$nodes[,2]),5)*time
## Create the FEM.time object
FEM_time_function = FEM.time(coeff=coeff, time_mesh=1:5, FEMbasis=FEMbasis, FLAG_PARABOLIC=TRUE)
## Plot the FEM function
plot(FEM_time_function)
## plot spatial field in some instants
t = c(1.2, 1.5, 3.6, 2.4, 4.5)
plot(FEM_time_function, t)
## plot time evolution in some locations
plot(FEM_time_function, locations = locations[1:10,])
```

plot.mesh.1.5D

Plot a mesh.1.5D object

Description

Plot a mesh.1.5D object, generated by create.mesh.1.5D or refine.mesh.1.5D.

Usage

```
## S3 method for class 'mesh.1.5D'
plot(x, ...)
```

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Arguments

x A mesh.1.5D object defining the triangular mesh, as generated by create.mesh.1.5D or refine.mesh.1.5D.

... Arguments representing graphical options to be passed to par.

Value

No return value

plot.mesh.2.5D

Plot a mesh.2.5D object

Description

Plot the triangulation of a mesh. 2.5D object, generated by create.mesh. 2.5D

Usage

```
## S3 method for class 'mesh.2.5D' plot(x, ...)
```

Arguments

x A mesh. 2.5D object generated by create.mesh. 2.5D.

Arguments representing graphical options to be passed to par.

Value

No return value

```
library(fdaPDE)

## Upload the hub2.5D the data
data(hub2.5D)
hub2.5D.nodes = hub2.5D$hub2.5D.nodes
hub2.5D.triangles = hub2.5D$hub2.5D.triangles

## Create mesh
mesh = create.mesh.2.5D(nodes = hub2.5D.nodes, triangles = hub2.5D.triangles)
plot(mesh)
```

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plot.mesh.2D

Plot a mesh.2D object

Description

Plot a mesh.2D object, generated by create.mesh.2D or refine.mesh.2D.

Usage

```
## S3 method for class 'mesh.2D' plot(x, ...)
```

Arguments

x A mesh. 2D object defining the triangular mesh, as generated by create.mesh. 2D or refine.mesh. 2D.

Arguments representing graphical options to be passed to par.

Value

No return value

```
library(fdaPDE)

## Upload the quasicirle2D data
data(quasicircle2D)
boundary_nodes = quasicircle2D$boundary_nodes
boundary_segments = quasicircle2D$boundary_segments
locations = quasicircle2D$locations
data = quasicircle2D$data

## Create mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)

## Plot the mesh
plot(mesh)
```

plot.mesh.3D

Plot a mesh.3D object

Description

Plot a mesh. 3D object, generated by create.mesh. 3D.

Usage

```
## S3 method for class 'mesh.3D' plot(x, ...)
```

Arguments

x A mesh.3D object generated by create.mesh.3D.

... Arguments representing graphical options to be passed to par.

Value

No return value

Examples

```
library(fdaPDE)

##Load the matrix nodes and tetrahedrons
data(sphere3Ddata)

nodes = sphere3Ddata$nodes
tetrahedrons = sphere3Ddata$tetrahedrons

##Create the triangulated mesh from the connectivity matrix and nodes locations
mesh = create.mesh.3D(nodes,tetrahedrons)

##Plot the triangulation of the object
plot(mesh)
```

```
projection.points.1.5D
```

Project 2D points onto 1.5D linear network mesh

Description

This function projects any 2D points onto 1.5D linear network mesh.

Usage

```
projection.points.1.5D(mesh, locations)
```

Arguments

mesh A mesh.1.5D object representing the graph mesh, created by create.mesh.1.5D.

locations 2D points to be projected onto 1.5D mesh.

Value

2D points projected onto 1.5D linear network mesh.

Examples

```
library(fdaPDE)
##Create Mesh

nodes=matrix(c(0.25,0.25,0.5,0.25,0.75,0.5,0.75,0.), nrow = 4, byrow=TRUE)
edges=matrix(c(1,2,2,3,2,4),nrow = 3,byrow = TRUE)
mesh_ = create.mesh.1.5D(nodes,edges,order=1)

## Create 2D points to be projected
locations=matrix(nrow=5,ncol=2)
locations[,1] = runif(5,min=0.25,max=0.75)
locations[,2] = runif(5,min=0.25,max=0.5)

## Project the points on the mesh
loc = projection.points.1.5D(mesh_, locations)
```

projection.points.2.5D

Project 3D points onto 2D 2.5D triangular mesh

Description

This function projects any 3D points onto 2.5D triangular mesh.

Usage

```
projection.points.2.5D(mesh, locations)
```

Arguments

mesh A mesh.2.5D object representing the triangular mesh, created by create.mesh.2.5D.

locations 3D points to be projected onto 2.5D triangular mesh.

Value

3D points projected onto 2.5D triangluar mesh.

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Examples

```
library(fdaPDE)

## Upload the hub2.5D the data
data(hub2.5D)
hub2.5D.nodes = hub2.5D$hub2.5D.nodes
hub2.5D.triangles = hub2.5D$hub2.5D.triangles

## Create mesh
mesh = create.mesh.2.5D(nodes = hub2.5D.nodes, triangles = hub2.5D.triangles)

## Create 3D points to be projected
x <- cos(seq(0,2*pi, length.out = 9))
y <- sin(seq(0,2*pi, length.out = 9))
z <- rep(0.5, 9)
locations = cbind(x,y,z)

## Project the points on the mesh
loc = projection.points.2.5D(mesh, locations)</pre>
```

quasicircle2D

Quasicircle2D domain

Description

The boundary and interior nodes and connectivity matrix of a triangular mesh of a quasicircular domain, together with a non-stationary field observed over the nodes of the mesh. This dataset can be used to create a mesh. 2D object with the function create.mesh. 2D and to test the smooth.FEM function.

quasicircle2Dareal

Quasicircle2Dareal domain

Description

The mesh of a quasicircular domain, together with a non-stationary field observed over seven circular subdomains and the incindence matrix defining the subdomains used by Azzimonti et. al 2015. This dataset can be used to test the smooth.FEM function for areal data.

References

Azzimonti, L., Sangalli, L. M., Secchi, P., Domanin, M., & Nobile, F. (2015). Blood flow velocity field estimation via spatial regression with PDE penalization. Journal of the American Statistical Association, 110(511), 1057-1071.

```
refine.by.splitting.mesh.1.5D
```

Create a mesh. 1.5D object by splitting each edge of a given mesh into two subedges.

Description

Create a mesh. 1.5D object by splitting each edge of a given mesh into two subedges.

Usage

```
refine.by.splitting.mesh.1.5D(mesh = NULL)
```

Arguments

mesh

a mesh. 1.5D object to split

Value

An object of class mesh.1.5D with splitted edges

```
refine.by.splitting.mesh.2.5D
```

Create a mesh.2.5D object by splitting each triangle of a given mesh into four subtriangles.

Description

Create a mesh. 2.5D object by splitting each triangle of a given mesh into four subtriangles.

Usage

```
refine.by.splitting.mesh.2.5D(mesh = NULL)
```

Arguments

mesh

a mesh. 2.5D object to split

Value

An object of class mesh.2.5D with splitted triangles

```
refine.by.splitting.mesh.2D
```

Create a mesh. 2D object by splitting each triangle of a given mesh into four subtriangles.

Description

Create a mesh. 2D object by splitting each triangle of a given mesh into four subtriangles.

Usage

```
refine.by.splitting.mesh.2D(mesh = NULL)
```

Arguments

mesh

a mesh. 2D object to split

Value

An object of class mesh.2D with splitted triangles

```
refine.by.splitting.mesh.3D
```

Create a mesh. 3D object by splitting each tetrahedron of a given mesh into eight subtetrahedrons.

Description

Create a mesh. 3D object by splitting each tetrahedron of a given mesh into eight subtetrahedrons.

Usage

```
refine.by.splitting.mesh.3D(mesh = NULL)
```

Arguments

mesh

a mesh. 3D object to split

Value

An object of class mesh.3D with splitted tetrahedrons

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refine.mesh.1.5D Refine 1.5D mesh

Description

Refine 1.5D mesh

Usage

```
refine.mesh.1.5D(mesh, delta)
```

Arguments

mesh a mesh.1.5D object to refine delta the maximum allowed length

Value

An object of class mesh.1.5D with refined edges

refine.mesh.2D Refine a 2D triangular mesh

Description

This function refines a Constrained Delaunay triangulation into a Conforming Delaunay triangulation. This is a wrapper of the Triangle library (http://www.cs.cmu.edu/~quake/triangle.html). It can be used to refine a mesh previously created with create.mesh.2D. The algorithm can add Steiner points (points through which the segments are splitted) in order to meet the imposed refinement conditions.

Usage

```
refine.mesh.2D(mesh, minimum_angle, maximum_area, delaunay, verbosity)
```

Arguments

mesh	A mesh.2D object representing the triangular mesh, created by create.mesh.2D.
minimum_angle	A scalar specifying a minimun value for the triangles angles.

maximum_area A scalar specifying a maximum value for the triangles areas.

delaunay A boolean parameter indicating whether or not the output mesh should satisfy

the Delaunay condition.

verbosity This can be '0', '1' or '2'. It indicates the level of verbosity in the triangulation

process.

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Value

A mesh.2D object representing the refined triangular mesh, with the following output:

nodes A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.

nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.

nodesattributes nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. If a node is added during the triangulation process or mesh refinement, its attributes are computed by linear interpolation using the attributes of neighboring nodes. This functionality is for instance used to compute the value of a Dirichlet boundary condition at boundary nodes added during the triangulation process.

triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix.

edges A #edges-by-2 matrix. Each row contains the row's indices of the nodes where the edge starts from and ends to.

edgesmarkers A vector of lenght #edges with entries either '1' or '0'. An entry '1' indicates that the corresponding element in edge is a boundary edge; an entry '0' indicates that the corresponding edge is not a boundary edge.

neighbors A #triangles-by-3 matrix. Each row contains the indices of the three neighbouring triangles. An entry '-1' indicates that one edge of the triangle is a boundary edge.

holes A #holes-by-2 matrix containing the x and y coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes.

order Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order = 1) and quadratic (order = 2) Finite Elements.

See Also

```
create.mesh.2D, create.FEM.basis
```

```
library(fdaPDE)

## Upload the quasicircle2D data
data(quasicircle2D)
boundary_nodes = quasicircle2D$boundary_nodes
boundary_segments = quasicircle2D$boundary_segments
locations = quasicircle2D$locations
data = quasicircle2D$data

## Create mesh from boundary:
mesh = create.mesh.2D(nodes = boundary_nodes, segments = boundary_segments)
plot(mesh)
## Refine the mesh with the maximum area criterion:
finemesh = refine.mesh.2D(mesh = mesh, maximum_area = 0.1)
plot(finemesh)
```

```
## Refine the mesh with the minimum angle criterion:
finemesh2 = refine.mesh.2D(mesh = mesh, minimum_angle = 30)
plot(finemesh2)
```

smooth.FEM

Spatial regression with differential regularization

Description

This function implements a spatial regression model with differential regularization. The regularizing term involves a Partial Differential Equation (PDE). In the simplest case the PDE involves only the Laplacian of the spatial field, that induces an isotropic smoothing. When prior information about the anisotropy or non-stationarity is available the PDE involves a general second order linear differential operator with possibly space-varying coefficients. The technique accurately handle data distributed over irregularly shaped domains. Moreover, various conditions can be imposed at the domain boundaries

Usage

```
smooth.FEM(locations = NULL, observations, FEMbasis,
  covariates = NULL, PDE_parameters = NULL, BC = NULL,
  incidence_matrix = NULL, areal.data.avg = TRUE,
  search = "tree", bary.locations = NULL,
  family = "gaussian", mu0 = NULL, scale.param = NULL, threshold.FPIRLS = 0.0002020,
  max.steps.FPIRLS = 15, lambda.selection.criterion = "grid", DOF.evaluation = NULL,
  lambda.selection.lossfunction = NULL, lambda = NULL, DOF.stochastic.realizations = 100,
  DOF.stochastic.seed = 0, DOF.matrix = NULL, GCV.inflation.factor = 1,
  lambda.optimization.tolerance = 0.05,
  inference.data.object=NULL)
```

Arguments

locations

A #observations-by-2 matrix in the 2D case and #observations-by-3 matrix in the 2.5D and 3D case, where each row specifies the spatial coordinates x and y (and z in 2.5D and 3D) of the corresponding observation in the vector observations. If the locations of the observations coincide with (or are a subset of) the nodes of the mesh in the FEMbasis, leave the parameter locations = NULL for a faster implementation.

observations

A vector of length #observations with the observed data values over the domain. If the locations argument is left NULL the vector of the observations have to be of length #nodes of the mesh in the FEMbasis. In this case, each observation is associated to the corresponding node in the mesh. If the observations are observed only on a subset of the mesh nodes, fill with NA the values of the vector observations in correspondence of unobserved data.

FEMbasis A FEMbasis object describing the Finite Element basis, as created by create. FEM. basis.

covariates

A #observations-by-#covariates matrix where each row represents the covariates associated with the corresponding observed data value in observations and each column is a different covariate.

PDE_parameters

A list specifying the parameters of the PDE in the regularizing term. Default is NULL, i.e. regularization is by means of the Laplacian (stationary, isotropic case). If the coefficients of the PDE are constant over the domain PDE_parameters must contain:

- K, a 2-by-2 matrix of diffusion coefficients. This induces an anisotropic smoothing with a preferential direction that corresponds to the first eigenvector of the diffusion matrix K;
- b, a vector of length 2 of advection coefficients. This induces a smoothing only in the direction specified by the vector b;
- c, a scalar reaction coefficient. c induces a shrinkage of the surface to zero.

If the coefficients of the PDE are space-varying PDE_parameters must contain:

- K, a function that for each spatial location in the spatial domain (indicated by the vector of the 2 spatial coordinates) returns a 2-by-2 matrix of diffusion coefficients. The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be an array with dimensions 2-by-2-by-#points.
- b, a function that for each spatial location in the spatial domain returns a vector of length 2 of transport coefficients. The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be a matrix with dimensions 2-by-#points;
- c, a function that for each spatial location in the spatial domain returns a scalar reaction coefficient. The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be a vector with length #points;
- u, a function that for each spatial location in the spatial domain returns a scalar reaction coefficient. u induces a reaction effect. The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be a vector with length #points.

For 2.5D and 3D, only the Laplacian is available (PDE_parameters=NULL).

ВС

A list with two vectors: BC_indices, a vector with the indices in nodes of boundary nodes where a Dirichlet Boundary Condition should be applied; BC_values, a vector with the values that the spatial field must take at the nodes indicated in BC_indices.

incidence_matrix

A #regions-by-#triangles/tetrahedrons matrix where the element (i,j) equals 1 if the j-th triangle/tetrahedron is in the i-th region and 0 otherwise. This is needed only for areal data. In case of pointwise data, this parameter is set to NULL.

areal.data.avg Boolean. It involves the computation of Areal Data. If TRUE the areal data are averaged, otherwise not.

search

a flag to decide the search algorithm type (tree or naive or walking search algorithm).

bary.locations A list with three vectors: locations, location points which are same as the given locations options. (checks whether both locations are the same); element ids, a vector of element id of the points from the mesh where they are located; barycenters, a vector of barycenter of points from the located element.

family

This parameter specify the distibution within exponential family used for GLM model. The following distribution are implemented: "binomial", "exponential", "gamma", "poisson", "gaussian", "invgaussian". The default link function for binomial is logit if you want either probit or clogloc set family = "probit", family = "cloglog".

mu0

This parameter is a vector that set the starting point for FPIRLS algorithm. It represent an initial guess of the location parameter. Default is set to observation for non binary distribution while equal to 0.5(observations + 0.5) for binary data.

scale.param

Dispersion parameter of the chosen distribution. This is only required for "gamma", "gaussian", "invgaussian". User may specify the parameter as a positive real number. If the parameter is not supplied, it is estimated from data according to Wilhelm Sangalli 2016.

threshold.FPIRLS

This parameter is used for arresting algorithm iterations. Algorithm stops when two successive iterations lead to improvement in penalized log-likelihood smaller than threshold.FPIRLS. Default value threshold.FPIRLS = 0.0002020.

max.steps.FPIRLS

This parameter is used to limit the maximum number of iteration. Default value max.steps.FPIRLS=15.

lambda.selection.criterion

This parameter is used to select the optimization method for the smoothing parameter lambda. The following methods are implemented: 'grid', 'newton', 'newton fd'. The former is a pure evaluation method. A test vector of lambda must be provided. The remaining two are optimization methods that automatically select the best penalization according to lambda.selection.lossfunction criterion. They implement respectively a pure Newton method and a finite differences Newton method. Default value lambda.selection.criterion='grid'

DOF. evaluation This parameter is used to identify if and how to perform degrees of freedom computation. The following possibilities are allowed: NULL, 'exact' and 'stochastic' In the former case no degree of freedom is computed, while the other two methods enable computation. Stochastic computation of DOFs may be slightly less accurate than its deterministic counterpart, but it is fairly less time consuming. Stochastic evaluation is highly suggested for meshes with more than 5000 nodes. Default value DOF.evaluation=NULL

lambda.selection.lossfunction

This parameter is used to determine if some loss function has to be evaluated. The following possibilities are allowed: NULL and 'GCV' (generalized cross validation) If NULL is selected, lambda.selection.criterion='grid' is required. 'GCV' is employed for both lambda.selection.criterion='grid' and optimization methods. Default value lambda.selection.lossfunction=NULL

lambda

a vector of spatial smoothing parameters provided if lambda.selection.criterion='grid'. An optional initialization otherwise.

DOF.stochastic.realizations

This positive integer is considered only when DOF.evaluation = 'stochastic'. It is the number of uniform random variables used in stochastic DOF evaluation. Default value DOF.stochastic.realizations=100.

DOF.stochastic.seed

This positive integer is considered only when DOF.evaluation = 'stochastic'. It is a user defined seed employed in stochastic DOF evaluation. Default value DOF.stochastic.seed = 0 means random.

DOF.matrix

Matrix of degrees of freedom. This parameter can be used if the DOF.matrix corresponding to lambda is available from precedent computation. This allows to save time, since the computation of the DOFs is the most time consuming part of GCV evaluation.

GCV.inflation.factor

Tuning parameter used for the estimation of GCV. Default value GCV.inflation.factor = 1.0 or 1.8 in GAM. It is advised to set GCV.inflation.factor larger than 1 to avoid overfitting.

lambda.optimization.tolerance

Tolerance parameter, a double between 0 and 1 that fixes how much precision is required by the optimization method: the smaller the parameter, the higher the accuracy. Used only if lambda.selection.criterion='newton' or

lambda.selection.criterion='newton_fd'. Default value lambda.optimization.tolerance=0.05

inference.data.object

An inferenceDataObject that stores all the information regarding inference over the linear and nonlinear parameters of the model. This parameter needs to be consistent with covariates, otherwise will be discarded. If set and well defined, the function will have in output the inference results. It is suggested to create this object via inferenceDataObjectBuilder function, so that the object is guaranteed to be well defined.

Value

A list with the following variables:

fit.FEM A FEM object that represents the fitted spatial field.

PDEmisfit.FEM A FEM object that represents the Laplacian of the estimated spatial field.

solution A list, note that all terms are matrices or row vectors: the jth column represents the vector related to lambda[j] if lambda.selection.criterion="grid" and lambda.selection.lossfunction=NULL. In all the other cases, only the column related to the best smoothing parameter is returned.

- f Matrix, estimate of function f, first half of solution vector.
- g Matrix, second half of solution vector.
- z_hat Matrix, prediction of the output in the locations.

beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. It is the regression coefficients estimate.

rmse Estimate of the root mean square error in the locations.

estimated_sd Estimate of the standard deviation of the error.

optimization A detailed list of optimization related data:

- lambda_solution numerical value of best lambda according to lambda.selection.lossfunction, -1 if lambda.selection.lossfunction=NULL.
- lambda_position integer, position in lambda_vector of best lambda according to lambda.selection.lossfunctio -1 if lambda.selection.lossfunction=NULL.
- GCV numeric value of GCV in correspondence of the optimum.
- optimization_details list containing further information about the optimization method used and the nature of its termination, eventual number of iterations.
- dof vector of positive numbers, DOFs for all the lambdas in lambda_vector, empty or invalid if not computed.
- lambda_vector vector of positive numbers: penalizations either passed by the user or found in the iterations of the optimization method.
- GCV_vector vector of positive numbers, GCV values for all the lambdas in lambda_vector
- time Duration of the entire optimization computation.
- bary.locations Barycenter information of the given locations, if the locations are not mesh nodes.
- GAM_output A list of GAM related data:
 - fn_hat A matrix with number of rows equal to number of locations and number of columns equal to length of lambda. Each column contains the evaluation of the spatial field in the location points.
 - J_minima A vector of the same length of lambda, containing the reached minima for each value of the smoothing parameter.
 - variance.est A vector which returns the variance estimates for the Generative Additive Models.
- inference A list set only if a well defined inferenceDataObject is passed as parameter to the function; contains all inference outputs required:
 - p_values list of lists set only if at least one p-value is required; contains the p-values divided by implementation:
 - wald list containing all the Wald p-values required, in the same order of the type list in inference.data.object. If one-at-the-time tests are required, the corresponding item is a vector of p values ordered as the rows of coeff matrix in inference.data.object.
 - speckman list containing all the Speckman p-values required, in the same order of the type list in inference.data.object. If one-at-the-time tests are required, the corresponding item is a vector of p values ordered as the rows of coeff matrix in inference.data.object.
 - eigen_sign_flip list containing all the Eigen-Sign-Flip p-values required, in the same order of the type list in inference.data.object. If one-at-the-time tests are required, the corresponding item is a vector of p values ordered as the rows of coeff matrix in inference.data.object.
 - CI list of lists set only if at least one confidence interval is required; contains the confidence intervals divided by implementation:
 - wald list containing all the Wald confidence intervals required, in the same order of the type list in inference.data.object. Each item is a matrix with 3 columns and p rows, p being the number of rows of coeff matrix in inference.data.object; each row is the CI for the corresponding row of coeff matrix.

speckman list containing all the Speckman confidence intervals required, in the same order of the type list in inference.data.object. Each item is a matrix with 3 columns and prows, p being the number of rows of coeff matrix in inference.data.object; each row is the CI for the corresponding row of coeff matrix.

References

- Sangalli, L. M., Ramsay, J. O., Ramsay, T. O. (2013). Spatial spline regression models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 75(4), 681-703.
- Azzimonti, L., Sangalli, L. M., Secchi, P., Domanin, M., Nobile, F. (2015). Blood flow velocity field estimation via spatial regression with PDE penalization. Journal of the American Statistical Association, 110(511), 1057-1071.
- Matthieu Wilhelm & Laura M. Sangalli (2016). Generalized spatial regression with differential regularization. Journal of Statistical Computation and Simulation, 86:13, 2497-2518.
- Federico Ferraccioli, Laura M. Sangalli & Livio Finos (2022). Some first inferential tools for spatial regression with differential regularization. Journal of Multivariate Analysis, 189, 104866.

```
library(fdaPDE)
#### No prior information about anysotropy/non-stationarity (laplacian smoothing) ####
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
FEMbasis = create.FEM.basis(mesh)
lambda = 10^{-1}
# no covariate
data = fs.test(mesh$nodes[,1], mesh$nodes[,2]) + rnorm(nrow(mesh$nodes), sd = 0.5)
solution = smooth.FEM(observations = data, FEMbasis = FEMbasis, lambda = lambda)
plot(solution$fit.FEM)
# with covariates
covariate = covs.test(mesh$nodes[,1], mesh$nodes[,2])
data = fs.test(mesh$nodes[,1], mesh$nodes[,2]) + 2*covariate + rnorm(nrow(mesh$nodes), sd = 0.5)
#Inferential tests and confidence intervals
inference.data.object = inferenceDataObjectBuilder(test = 'oat', type = 'w', dim = 2, n_cov = 1)
solution = smooth.FEM(observations = data, covariates = covariate,
                      FEMbasis = FEMbasis, lambda = lambda,
                      inference.data.object=inference.data.object)
# beta estimate:
solution$solution$beta
# tests over beta estimates p-values:
```

```
solution$inference$beta$p_values
# confidence intervals for beta estimates:
solution$inference$beta$CI
# non-parametric estimate:
plot(solution$fit.FEM)
# Choose lambda with GCV - stochastic grid evaluation:
lambda = 10^{(-2:0)}
solution = smooth.FEM(observations = data,
                            covariates = covariate,
                            FEMbasis = FEMbasis,
                            lambda = lambda, DOF.evaluation = 'stochastic',
                            lambda.selection.lossfunction = 'GCV')
bestLambda = solution$optimization$lambda_solution
# Choose lambda with GCV - Newton finite differences stochastic evaluation -:
solution = smooth.FEM(observations = data,
                            covariates = covariate,
                            FEMbasis = FEMbasis,
                    DOF.evaluation = 'stochastic', lambda.selection.lossfunction = 'GCV')
bestLambda = solution$optimization$lambda_solution
#### Smoothing with prior information about anysotropy/non-stationarity and boundary conditions ####
# See Azzimonti et al. for reference to the current example
data(quasicircle2D)
boundary_nodes = quasicircle2D$boundary_nodes
boundary_segments = quasicircle2D$boundary_segments
locations = quasicircle2D$locations
data = quasicircle2D$data
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
FEMbasis = create.FEM.basis(mesh)
lambda = 10^-2
# Set the PDE parameters
R = 2.8
K1 = 0.1
K2 = 0.2
beta = 0.5
K_func<-function(points)</pre>
  output = array(0, c(2, 2, nrow(points)))
  for (i in 1:nrow(points))
  output[,,i]=10*rbind(c(points[i,2]^2+K1*points[i,1]^2+K2*(R^2-points[i,1]^2-points[i,2]^2),
                            (K1-1)*points[i,1]*points[i,2]),
                         c((K1-1)*points[i,1]*points[i,2],
                   points[i,1]^2+K1*points[i,2]^2+K2*(R^2-points[i,1]^2-points[i,2]^2)))
  output
}
b_func<-function(points)</pre>
  output = array(0, c(2, nrow(points)))
```

```
for (i in 1:nrow(points))
   output[,i] = 10*beta*c(points[i,1],points[i,2])
  output
}
c_func<-function(points)</pre>
  rep(c(0), nrow(points))
}
u_func<-function(points)</pre>
  rep(c(0), nrow(points))
PDE_parameters = list(K = K_func, b = b_func, c = c_func, u = u_func)
# Set the boundary conditions
BC = NULL
BC$BC_indices = which(mesh$nodesmarkers == 1) # b.c. on the complete boundary
BC$BC_values = rep(0,length(BC$BC_indices)) # homogeneus b.c.
# Since the data locations are a subset of the mesh nodes for a faster solution use:
dataNA = rep(NA, FEMbasis$nbasis)
dataNA[mesh$nodesmarkers == 0] = data
#grid evaluation
solution = smooth.FEM(observations = dataNA,
                            FEMbasis = FEMbasis,
                            lambda = lambda,
                            PDE_parameters = PDE_parameters,
                            BC = BC)
plot(solution$fit.FEM)
image(solution$fit.FEM)
# Newton's method
solution = smooth.FEM(observations = dataNA,
                            FEMbasis = FEMbasis,
                            PDE_parameters = PDE_parameters,
                            BC = BC)
plot(solution$fit.FEM)
image(solution$fit.FEM)
#### Smoothing with areal data ####
# See Azzimonti et al. for reference to the current exemple
data(quasicircle2Dareal)
incidence_matrix = quasicircle2Dareal$incidence_matrix
data = quasicircle2Dareal$data
mesh = quasicircle2Dareal$mesh
FEMbasis = create.FEM.basis(mesh)
lambda = 10^-4
# Set the PDE parameters
R = 2.8
K1 = 0.1
```

```
K2 = 0.2
beta = 0.5
K_func<-function(points)</pre>
  output = array(0, c(2, 2, nrow(points)))
  for (i in 1:nrow(points))
  output[,,i]=10*rbind(c(points[i,2]^2+K1*points[i,1]^2+K2*(R^2-points[i,1]^2-points[i,2]^2),
                            (K1-1)*points[i,1]*points[i,2]),
                          c((K1-1)*points[i,1]*points[i,2],
                   points[i,1]^2+K1*points[i,2]^2+K2*(R^2-points[i,1]^2-points[i,2]^2)))
  output
}
b_func<-function(points)</pre>
{
  output = array(0, c(2, nrow(points)))
  for (i in 1:nrow(points))
    output[,i] = 10*beta*c(points[i,1],points[i,2])
  output
}
c_func<-function(points)</pre>
  rep(c(0), nrow(points))
u_func<-function(points)</pre>
  rep(c(0), nrow(points))
PDE_parameters = list(K = K_func, b = b_func, c = c_func, u = u_func)
# Set the boundary conditions
BC = NULL
BC$BC_indices = which(mesh$nodesmarkers == 1) # b.c. on the complete boundary
BC\BC_values = rep(0, length(BC\BC_indices)) \# homogeneus b.c.
#grid evaluation
solution = smooth.FEM(observations = data,
                             incidence_matrix = incidence_matrix,
                             FEMbasis = FEMbasis,
                             lambda = lambda,
                             PDE_parameters = PDE_parameters,
                             BC = BC)
plot(solution$fit.FEM)
image(solution$fit.FEM)
#Newton's method
solution = smooth.FEM(observations = data,
                             incidence_matrix = incidence_matrix,
                             FEMbasis = FEMbasis,
                             PDE_parameters = PDE_parameters,
                             BC = BC)
plot(solution$fit.FEM)
image(solution$fit.FEM)
```

smooth.FEM.time

Space-time regression with differential regularization

Description

Space-time regression with differential regularization. Space-varying covariates can be included in the model. The technique accurately handle data distributed over irregularly shaped domains. Moreover, various conditions can be imposed at the domain boundaries.

Usage

```
smooth.FEM.time(locations = NULL, time_locations = NULL, observations, FEMbasis,
time_mesh=NULL, covariates = NULL, PDE_parameters = NULL, BC = NULL,
incidence_matrix = NULL, areal.data.avg = TRUE,
FLAG_MASS = FALSE, FLAG_PARABOLIC = FALSE, FLAG_ITERATIVE = FALSE,
threshold = 10^(-4), max.steps = 50, IC = NULL,
search = "tree", bary.locations = NULL,
family = "gaussian", mu0 = NULL, scale.param = NULL,
threshold.FPIRLS = 0.0002020, max.steps.FPIRLS = 15,
lambda.selection.criterion = "grid", DOF.evaluation = NULL,
lambda.selection.lossfunction = NULL, lambdaS = NULL, lambdaT = NULL,
DOF.stochastic.realizations = 100, DOF.stochastic.seed = 0,
DOF.matrix = NULL, GCV.inflation.factor = 1, lambda.optimization.tolerance = 0.05,
inference.data.object.time=NULL)
```

Arguments

locations	A matrix where each row specifies the spatial coordinates x and y (and z if ndim=3) of the corresponding observations in the vector observations. This parameter can be NULL. In this case, if also the incidence matrix is NULL the spatial coordinates are assumed to coincide with the nodes of the mesh.
time_locations	A vector containing the times of the corresponding observations in the vector observations. This parameter can be NULL. In this case the temporal locations are assumed to coincide with the nodes of the time_mesh.
observations	A matrix of #locations x #time_locations with the observed data values over the spatio-temporal domain. The spatial locations of the observations can be specified with the locations argument.
FEMbasis	$A \ FEMbasis \ object \ describing \ the \ Finite \ Element \ basis, as \ created \ by \ create. \ FEM.basis.$
time_mesh	A vector specifying the time mesh.
covariates	A #observations-by-#covariates matrix where each row represents the covariates associated with the corresponding observed data value in observations.

PDE_parameters A list specifying the parameters of the PDE in the regularizing term. Default is NULL, i.e. regularization is by means of the Laplacian (stationary, isotropic case). If the PDE is elliptic it must contain: K, a 2-by-2 matrix of diffusion coefficients. This induces an anisotropic smoothing with a preferential direction that corresponds to the first eigenvector of the diffusion matrix K; b, a vector of length 2 of advection coefficients. This induces a smoothing only in the direction specified by the vector b; c, a scalar reaction coefficient. c induces a shrinkage of the surface to zero If the PDE is space-varying it must contain: K, a function that for each spatial location in the spatial domain (indicated by the vector of the 2 spatial coordinates) returns a 2-by-2 matrix of diffusion coefficients. This induces an anisotropic smoothing with a local preferential direction that corresponds to the first eigenvector of the diffusion matrix K.The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be an array with dimensions 2-by-2-by-#points.b, a function that for each spatial location in the spatial domain returns a vector of length 2 of transport coefficients. This induces a local smoothing only in the direction specified by the vector b. The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be a matrix with dimensions 2-by-#points; c, a function that for each spatial location in the spatial domain returns a scalar reaction coefficient. c induces a shrinkage of the surface to zero. The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be a vector with length #points; u, a function that for each spatial location in the spatial domain returns a scalar reaction coefficient. u induces a reaction effect. The function must support recycling for efficiency reasons, thus if the input parameter is a #point-by-2 matrix, the output should be a vector with length #points. For 2.5D and 3D only the Laplacian is available (PDE_parameters=NULL)

BC

A list with two vectors: BC_indices, a vector with the indices in nodes of boundary nodes where a Dirichlet Boundary Condition should be applied; BC_values, a vector with the values that the spatial field must take at the nodes indicated in BC_indices.

incidence_matrix

A #regions-by-#triangles/tetrahedrons matrix where the element (i,j) equals 1 if the j-th triangle/tetrahedron is in the i-th region and 0 otherwise. This is only for areal data. In case of pointwise data, this parameter is set to NULL.

areal.data.avg Boolean. It involves the computation of Areal Data. If TRUE the areal data are averaged, otherwise not.

Boolean. This parameter is considered only for separable problems i.e. when FLAG_MASS FLAG_PARABOLIC==FALSE. If TRUE the mass matrix in space and in time are used, if FALSE they are substituted with proper identity matrices.

FLAG_PARABOLIC Boolean. If TRUE the parabolic problem problem is selected, if FALSE the separable one.

FLAG_ITERATIVE Boolean. If TRUE the iterative method is selected, if FALSE the monolithic one. threshold

This parameter is used for arresting algorithm iterations. Algorithm stops when two successive iterations lead to improvement in penalized log-likelihood smaller than threshold. Default value threshold = 10^{-4} .

This parameter is used to limit the maximum number of iteration. Default value max.steps

max.steps=50.

IC Initial condition needed in case of parabolic problem i.e. when FLAG_PARABOLIC==TRUE.

> If FLAG_PARABOLIC==FALSE this parameter is ignored. If FLAG_PARABOLIC=TRUE and IC=NULL it is necessary to provide also data at the initial time. IC will be

estimated from them.

a flag to decide the search algorithm type (tree or naive or walking search algo-

rithm).

bary.locations A list with three vectors: locations, location points which are same as the

given locations options. (checks whether both locations are the same); element ids, a vector of element id of the points from the mesh where they are located;

barycenters, a vector of barycenter of points from the located element.

family This parameter specify the distribution within exponential family used for GLM

> model. The following distribution are implemented: "binomial", "exponential", "gamma", "poisson", "gaussian", "invgaussian". The default link function for binomial is logit if you want either probit or clogloc set family = "probit",

family = "cloglog".

mu0 This parameter is a vector that set the starting point for FPIRLS algorithm. It represent an initial guess of the location parameter. Default is set to observation

for non binary distribution while equal to 0.5(observations + 0.5) for binary

scale.param Dispersion parameter of the chosen distribution. This is only required for "gamma",

"gaussian", "invgaussian". User may specify the parameter as a positive real number. If the parameter is not supplied, it is estimated from data according to

Wilhelm Sangalli 2016.

threshold.FPIRLS

This parameter is used for arresting algorithm iterations. Algorithm stops when two successive iterations lead to improvement in penalized log-likelihood smaller

than threshold.FPIRLS. Default value threshold.FPIRLS = 0.0002020.

max.steps.FPIRLS

This parameter is used to limit the maximum number of iteration. Default value

max.steps.FPIRLS=15.

This parameter is used to select the optimization method related to smoothing parameter lambda. The following methods are implemented: 'grid', further optimization methods are yet to come. The 'grid' is a pure evaluation method,

therefore a vector of lambda testing penalizations must be provided. Default value lambda.selection.criterion='grid'

DOF. evaluation This parameter is used to identify if and how degrees of freedom computation

has to be performed. The following possibilities are allowed: NULL, 'exact' and 'stochastic' In the former case no degree of freedom is computed, while the other two methods enable computation. Stochastic computation of DOFs may be slightly less accurate than its deterministic counterpart, but is highly suggested for meshes of more than 5000 nodes, being fairly less time consuming. Default

value DOF.evaluation=NULL

search

lambda.selection.criterion

lambda.selection.lossfunction

This parameter is used to understand if some loss function has to be evaluated. The following possibilities are allowed: NULL and 'GCV' (generalized cross validation) The former case is that of lambda.selection.criterion='grid' pure evaluation, while the second can be employed for optimization methods. Default value lambda.selection.lossfunction=NULL

lambdaS A scalar or vector of spatial smoothing parameters.

lambdaT A scalar or vector of temporal smoothing parameters.

DOF.stochastic.realizations

This parameter is considered only when DOF.evaluation = 'stochastic'. It is a positive integer that represents the number of uniform random variables used in stochastic GCV computation. Default value DOF.stochastic.realizations=100.

DOF.stochastic.seed

This parameter is considered only when DOF.evaluation = 'stochastic'. It is a positive integer that represents user defined seed employed in stochastic GCV computation. Default value DOF.stochastic.seed=0.

DOF.matrix Matrix of degrees of freedom. This parameter can be used if the DOF.matrix corresponding to lambdaS and lambdaT is available from precedent computation. This allows to save time since the computation of the DOFs is the most expensive part of GCV.

GCV.inflation.factor

Tuning parameter used for the estimation of GCV. Default value GCV. inflation. factor = 1.0. It is advised to set it grather than 1 to avoid overfitting.

lambda.optimization.tolerance

Tolerance parameter, a double between 0 and 1 that fixes how much precision is required by the optimization method: the smaller the parameter, the higher the accuracy. Used only if lambda.selection.criterion='newton' or lambda.selection.criterion='newton_fd', thus ot implemented yet. Default value lambda.optimization.tolerance=0.05.

inference.data.object.time

An inferenceDataObjectTime that stores all the information regarding inference over the linear and nonlinear parameters of the model. This parameter needs to be consistent with covariates and mesh dimension number, otherwise will be discarded. If set and well defined, the function will have in output the inference results. It is suggested to create this object via inferenceDataObjectTimeBuilder function, so that the object is guaranteed to be well defined.

Value

A list with the following variables:

fit.FEM.time A FEM.time object that represents the fitted spatio-temporal field.

PDEmisfit.FEM.time A FEM.time object that represents the misfit of the penalized PDE.

beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. The jth column represents the vector of regression coefficients when the smoothing parameter is equal to lambda[j].

edf If GCV is TRUE, a scalar or matrix with the trace of the smoothing matrix for each combination of the smoothing parameters specified in lambdaS and lambdaT.

- stderr If GCV is TRUE, a scalar or matrix with the estimate of the standard deviation of the error for each combination of the smoothing parameters specified in lambdaS and lambdaT.
- GCV If GCV is TRUE, a scalar or matrix with the value of the GCV criterion for each combination of the smoothing parameters specified in lambdaS and lambdaT.
- ICestimated If FLAG_PARABOLIC is TRUE and IC is NULL, a list containing a FEM object with the initial conditions, the value of the smoothing parameter lambda returning the lowest GCV and, in presence of covariates, the estimated beta coefficients
- bary.locations A barycenter information of the given locations if the locations are not mesh nodes.
- inference A list set only if a well defined inferenceDataObjectTime is passed as parameter to the function; contains all inference outputs required:
 - p_values list of lists set only if at least one p-value is required; contains the p-values divided by implementation:
 - wald list containing all the Wald p-values required, in the same order of the type list in inference.data.object.time. If one-at-the-time tests are required, the corresponding item is a vector of p values ordered as the rows of coeff matrix in inference.data.object.time.
 - speckman list containing all the Speckman p-values required, in the same order of the type list in inference.data.object.time. If one-at-the-time tests are required, the corresponding item is a vector of p values ordered as the rows of coeff matrix in inference.data.object.time.
 - eigen_sign_flip list containing all the Eigen-Sign-Flip p-values required, in the same
 order of the type list in inference.data.object.time. If one-at-the-time tests are
 required, the corresponding item is a vector of p values ordered as the rows of coeff
 matrix in inference.data.object.time.
 - CI list of lists set only if at least one confidence interval is required; contains the confidence intervals divided by implementation:
 - wald list containing all the Wald confidence intervals required, in the same order of the type list in inference.data.object.time. Each item is a matrix with 3 columns and prows, p being the number of rows of coeff matrix in inference.data.object.time; each row is the CI for the corresponding row of coeff matrix.
 - speckman list containing all the Speckman confidence intervals required, in the same order of the type list in inference.data.object.time. Each item is a matrix with 3 columns and prows, p being the number of rows of coeff matrix in inference.data.object.time; each row is the CI for the corresponding row of coeff matrix.

References

#' @references Arnone, E., Azzimonti, L., Nobile, F., & Sangalli, L. M. (2019). Modeling spatially dependent functional data via regression with differential regularization. Journal of Multivariate Analysis, 170, 275-295. Bernardi, M. S., Sangalli, L. M., Mazza, G., & Ramsay, J. O. (2017). A penalized regression model for spatial functional data with application to the analysis of the

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production of waste in Venice province. Stochastic Environmental Research and Risk Assessment, 31(1), 23-38. Federico Ferraccioli, Laura M. Sangalli & Livio Finos (2022). Some first inferential tools for spatial regression with differential regularization. Journal of Multivariate Analysis, 189, 104866.

Examples

```
library(fdaPDE)
 data(horseshoe2D)
 boundary_nodes = horseshoe2D$boundary_nodes
 boundary_segments = horseshoe2D$boundary_segments
 locations = horseshoe2D$locations
 time_locations = seq(0,1,length.out = 5)
 mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
 space_time_locations = cbind(rep(time_locations,each=nrow(mesh$nodes)),
                               rep(mesh$nodes[,1],5),rep(mesh$nodes[,2],5))
 FEMbasis = create.FEM.basis(mesh)
 lambdaS = 10^{-1}
 lambdaT = 10^-1
 data = fs.test(space_time_locations[,2],
                space_time_locations[,3])*cos(pi*space_time_locations[,1]) +
        rnorm(nrow(space_time_locations), sd = 0.5)
 data = matrix(data, nrow = nrow(mesh$nodes), ncol = length(time_locations), byrow = TRUE)
 solution = smooth.FEM.time(observations = data, time_locations = time_locations,
                             FEMbasis = FEMbasis, lambdaS = lambdaS, lambdaT = lambdaT)
 plot(solution$fit.FEM)
sphere3Ddata
                         Sphere3Ddata
```

Description

A dataset with information about the connectivity matrix and the nodes locations of a sphere geometry. It containes:

- nodes. A #nodes-by-3 matrix specifying the locations of each node.
- tetrahedrons. A #tetrahedrons-by-4 matrix specifying the indices of the nodes in each tetrahedron

This dataset can be used to create a MESH. 3D object with the function create. MESH. 3D

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