

Package ‘fdaPDE’

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Title Physics-Informed Spatial and Functional Data Analysis

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

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Suggests MASS, testthat

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](https://doi.org/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

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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.

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 continuous 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 triangulation. 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:

- orderEither "1" or "2" for the 2D and 2.5D case, and "1" for the 3D case. Order of the Finite Element basis.
- nbasisScalar. 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
```

```

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-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 whether 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:

- nodesA #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.
- **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 whether each mesh triangle should be represented by 3 nodes (the triangle's 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.

<code>create.mesh.2.5D</code>	<i>Create a mesh.2.5D object from the nodes locations and the connectivity matrix</i>
-------------------------------	---

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

<code>nodes</code>	A <code>#nodes-by-3</code> matrix containing the x, y, z coordinates of the mesh nodes.
<code>triangles</code>	A <code>#triangles-by-3</code> (when order = 1) or <code>#triangles-by-6</code> (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 .
<code>order</code>	Either '1' or '2'. It specifies whether each mesh triangle should be represented by 3 nodes (the triangle's 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.

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:

- nodesA #nodes-by-3 matrix containing the x, y, z coordinates of the mesh nodes.
- nodesmarkersA 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.
- nodesattributesA matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- trianglesA #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>.
- segmentsmarkerA 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.
- edgesA #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.
- edgesmarkersA vector of length #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.
- neighborsA #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.
- holesA #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.
- orderEither '1' or '2'. It specifies whether each mesh triangle should be represented by 3 nodes (the triangle's 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.

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 input can be used to define the boundaries of the domain. If this input 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

```
create.mesh.2D(nodes, nodesattributes = NA, segments = NA, holes = NA,
               triangles = NA, order = 1, verbosity = 0)
```

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 input is NULL, it generates a triangulation over the convex hull of the points specified in nodes.

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) 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 . In this case the function create.mesh.2D is used to produce a complete mesh.2D object.
order	Either '1' or '2'. It specifies whether each mesh triangle should be represented by 3 nodes (the triangle's 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:

- nodesA #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.
- nodesmarkersA 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.
- nodesattributesA matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- trianglesA #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>.
- segmentsmarkerA 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.
- edgesA #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.
- edgesmarkersA vector of length #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.
- neighborsA #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.

- holesA #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.
- orderEither '1' or '2'. It specifies whether each mesh triangle should be represented by 3 nodes (the triangle's 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 quasicircle2D 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 that 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	<i>Create a mesh.3D object from the connectivity matrix and nodes locations</i>
----------------	---

Description

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

Usage

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

```

    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 whether 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:

- nodesA #nodes-by-3 matrix containing the x, y, z coordinates of the mesh nodes.
- nodesmarkersA 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.
- nodesattributesA matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- tetrahedronsA #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.

- `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.
- `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 length `#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 whether 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

```
DE.FEM(data, FEMbasis, lambda, fvec=NULL, heatStep=0.1, heatIter=500,
        stepProposals=NULL, tol1=1e-4, tol2=0, print=FALSE, nfolds=NULL,
        nsimulations=500, step_method="Fixed_Step", direction_method="BFGS",
        preprocess_method="NoCrossValidation", search = "tree")
```

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 <code>create.FEM.basis</code> .
lambda	A scalar or vector of smoothing parameters. If it is a vector, the optimal smoothing parameter is chosen with a k-fold cross-validation procedure based on the L2 norm.
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.
heatIter	An integer specifying the number of iterations to perform the discretized heat diffusion process.
stepProposals	A scalar or a vector containing the step parameters useful for the descent algorithm. 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 <code>preprocess_method</code> 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 NULL. Default is NULL.
nsimulations	An integer specifying the number of iterations used in the optimization algorithms. Default value is 500.
step_method	String. This parameter specifies which step method use in the descent algorithm. If it is <code>Fixed_Step</code> , the step is constant during all the algorithm and it is chosen according to <code>stepProposals</code> ; if it is <code>Backtracking_Method</code> , the step is computed at each iteration according to the backtracking method; finally if it is <code>Wolfe_Method</code> , the step is computed at each iteration according to the Wolfe method. Default is <code>Fixed_Step</code> .

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-Ribière-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 n folds. Default is NULL.
search	a flag to decide the search algorithm type (tree or naive or walking search algorithm).

Value

A list with the following variables:

FEMBasis	Given FEMBasis with tree informations.
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 n folds 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 <- seq(-3, 3, length.out = 10)
Ybound <- seq(-3, 3, length.out = 10)
grid_XY <- expand.grid(Xbound, Ybound)
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)
mesh <- refine.mesh.2D(mesh, maximum_area = 0.2)
FEMbasis <- create.FEM.basis(mesh)

## Generate data
n <- 50
set.seed(10)
data_x <- rnorm(n)
data_y <- rnorm(n)
data <- cbind(data_x, data_y)

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, stepProposals=NULL, tol1=1e-4, tol2=0, print=FALSE,
              nolds=NULL, nsimulations=300, step_method = "Fixed_Step",
              direction_method = "BFGS", preprocess_method="NoCrossValidation")

## Visualization
n = 100
X <- seq(-3, 3, length.out = n)
Y <- seq(-3, 3, length.out = n)
grid <- expand.grid(X, Y)

evaluation <- eval.FEM(FEM(FEMbasis, coeff = sol$g), locations = grid)
evaluation <- exp(evaluation)
eval <- matrix(evaluation, n, n)

image2D(x = X, y = Y, z = eval, col = heat.colors(100), xlab = "x", ylab = "y",
        contour = list(drawlabels = FALSE), main = "Estimated density")

```

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

```
DE.FEM.time(data, data_time, FEMbasis, mesh_time, lambda, lambda_time, fvec=NULL,
            heatStep=0.1, heatIter=10, stepProposals=NULL, tol1=1e-4, tol2=0,
            print=FALSE, nolds=NULL, nsimulations=500, step_method="Fixed_Step",
            direction_method="BFGS", preprocess_method="NoCrossValidation",
            search="tree", isTimeDiscrete=FALSE, flagMass=FALSE, flagLumped=FALSE)
```

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.
fvec	A vector of length #nodes of the spatial mesh times #B-spline temporal functional 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.
heatIter	An integer specifying the number of iterations to perform the discretized heat diffusion process.
stepProposals	A scalar or a vector containing the step parameters useful for the descent algorithm. 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 'SimplifiedCV'.
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 NULL. Default is NULL.
nsimulations	An integer specifying the number of iterations used in the optimization algorithms. 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-Ribière-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 (<code>lambda</code> , <code>lambda_time</code>) must be equal to the number of folds <code>nfolds</code> . Default is NULL.
<code>search</code>	A flag to decide the search algorithm type (tree or naive or walking search algorithm).
<code>isTimeDiscrete</code>	A boolean specifying the time data type: TRUE for discrete (with many duplicates) time data; FALSE for continuous time data. Default is FALSE.
<code>flagMass</code>	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.
<code>flagLumped</code>	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

A list with the following variables:

<code>FEMbasis</code>	Given FEMbasis with tree information.
<code>g</code>	A vector of length <code>#nodes</code> times <code>#B-splines</code> that represents the value of the <code>g</code> -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.
<code>f_init</code>	A <code>#nodes-by-#lambda</code> x <code>#lambda_time</code> parameters matrix. Each column contains the node values of the initial density used for the pair (<code>lambda</code> , <code>lambda_time</code>) given by the column.
<code>lambda</code>	A scalar representing the optimal smoothing parameter in space selected, together with <code>lambda_time</code> , via <code>k</code> 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.
<code>lambda_time</code>	A scalar representing the optimal smoothing parameter in time selected, together with <code>lambda</code> , via <code>k</code> 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.
<code>data</code>	A matrix of dimensions <code>#observations-by-ndim</code> 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.
<code>data_time</code>	A vector of length <code>#observations</code> containing the time data used in the algorithm. Data lying outside the temporal domain, defined through its mesh, are not considered.
<code>CV_err</code>	A vector of length <code>nfolds</code> containing the cross validation errors obtained in each fold, if <code>preprocess_method</code> is either <code>RightCV</code> or <code>SimplifiedCV</code> .

Examples

```

library(fdaPDE)

## Create a 2D mesh over a squared domain
Xbound <- seq(-3, 3, length.out = 10)
Ybound <- seq(-3, 3, length.out = 10)
grid_XY <- expand.grid(Xbound, Ybound)
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)
mesh <- refine.mesh.2D(mesh, maximum_area = 0.25, minimum_angle = 20)
FEMbasis <- create.FEM.basis(mesh)

## Create a 1D time mesh over a (non-negative) interval
mesh_time <- seq(0, 1, length.out=3)

## Generate data
n <- 50
set.seed(10)
x <- rnorm(n,0,2)
y <- rnorm(n,0,2)
locations <- cbind(x,y)
times <- runif(n,0,1)
data <- cbind(locations, times)

t <- 0.5 # time instant in which to evaluate the solution

plot(mesh)
sample <- data[abs(data[,3]-t)<0.05,1:2]
points(sample, col="red", pch=19, cex=1, main=paste('Sample | ', t-0.05, ' < t < ', t+0.05))

## Density Estimation
lambda <- 0.1
lambda_time <- 0.001
sol <- DE.FEM.time(data = locations, data_time = times, FEMbasis = FEMbasis,
  mesh_time = mesh_time, lambda = lambda, lambda_time = lambda_time,
  fvec=NULL, heatStep=0.1, heatIter=10, stepProposals=NULL, tol1=1e-4, tol2=0,
  print=FALSE, nfolds=NULL, nsimulations=300, step_method="Fixed_Step",
  direction_method="BFGS", preprocess_method="NoCrossValidation",
  search="tree", isTimeDiscrete=0, flagMass=0, flagLumped=0)

## Visualization
n = 100
X <- seq(-3, 3, length.out = n)
Y <- seq(-3, 3, length.out = n)
grid <- expand.grid(X, Y)

FEMfunction = FEM.time(sol$g, mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation <- eval.FEM.time(FEM.time = FEMfunction, locations = grid, time.instants = t)
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(0,0.2), asp = 1)

```

DE.heat.FEM

*Density initialization***Description**

This function implements two methods for the density initialization procedure.

Usage

```
DE.heat.FEM(data, FEMbasis, lambda=NULL, heatStep=0.1, heatIter=500,
            init="Heat", nFolds=5, search = "tree")
```

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 .
lambda	A scalar or vector of smoothing parameters. Default is NULL. It is useful only if <code>init='Heat'</code> .
heatStep	Real specifying the time step for the discretized heat diffusion process.
heatIter	Integer specifying the number of iterations 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 technique. It is useful only for the case <code>init = 'CV'</code> .
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 <- seq(-3, 3, length.out = 10)
grid_XY <- expand.grid(Xbound, Ybound)
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)
```

```

mesh <- refine.mesh.2D(mesh, maximum_area = 0.2)
FEMbasis <- create.FEM.basis(mesh)

## Generate data
n <- 50
set.seed(10)
data_x <- rnorm(n)
data_y <- rnorm(n)
data <- cbind(data_x, data_y)

plot(mesh)
points(data, col="red", pch=19, cex=0.5)

## Density initialization
lambda = 0.1
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 *Spatio-temporal density initialization*

Description

This function implements two methods for the density initialization procedure.

Usage

```

DE.heat.FEM.time(data, data_time, FEMbasis, mesh_time, lambda=NULL,
                 lambda_time=NULL, heatStep=0.1, heatIter=10,
                 init="Heat", nFolds=5, search="tree",
                 isTimeDiscrete=FALSE, flagMass=FALSE, flagLumped=FALSE)

```

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 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'.

<code>lambda_time</code>	A scalar or vector of smoothing parameters in time. Default is NULL. It is useful only if <code>init='Heat'</code> .
<code>heatStep</code>	A real specifying the time step for the discretized heat diffusion process.
<code>heatIter</code>	An integer specifying the number of iterations to perform the discretized heat diffusion process.
<code>init</code>	A string specifying the initialization procedure. It can be either 'Heat' or 'CV'.
<code>nFolds</code>	An integer specifying the number of folds used in the cross validation technique. It is useful only for the case <code>init = 'CV'</code> .
<code>search</code>	A flag to decide the search algorithm type (tree or naive or walking search algorithm).
<code>isTimeDiscrete</code>	A boolean specifying the time data type: TRUE for discrete (with many duplicates) time data; FALSE for continuous time data. Default is FALSE.
<code>flagMass</code>	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.
<code>flagLumped</code>	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 <- seq(-3, 3, length.out = 10)
Ybound <- seq(-3, 3, length.out = 10)
grid_XY <- expand.grid(Xbound, Ybound)
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)
mesh <- refine.mesh.2D(mesh, maximum_area = 0.25, minimum_angle = 20)
FEMbasis <- create.FEM.basis(mesh)

## Create a 1D time mesh over a (non-negative) interval
mesh_time <- seq(0, 1, length.out=3)

## Generate data
n <- 50
set.seed(10)
x <- rnorm(n,0,2)
y <- rnorm(n,0,2)
```

```

locations <- cbind(x,y)
times <- runif(n,0,1)
data <- cbind(locations, times)

t <- 0.5 # time instant in which to evaluate the solution

plot(mesh)
sample <- data[abs(data[,3]-t)<0.05,1:2]
points(sample, col="red", pch=19, cex=1, main=paste('Sample | ', t-0.05, ' < t < ', t+0.05))

## Density initialization
lambda = 0.1
lambda_time <- 0.001
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

n = 100
X <- seq(-3, 3, length.out = n)
Y <- seq(-3, 3, length.out = n)
grid <- expand.grid(X, Y)

FEMfunction = FEM.time(sol$f_init[,1,1], mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation <- eval.FEM.time(FEM.time = FEMfunction, locations = grid, time.instants = t)
image2D(x = X, y = Y, z = matrix(evaluation, n, n), col = heat.colors(100),
      xlab = "", ylab = "", contour = list(drawlabels = FALSE),
      main = paste("Initial guess at t = ", t), zlim=c(0,0.2), asp = 1)

```

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

```
eval.FEM(FEM, locations = NULL, incidence_matrix = NULL, search = "tree",
        bary.locations = NULL)
```

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.

<code>incidence_matrix</code>	In case of areal evaluations, the <code>#regions-by-#elements</code> incidence matrix defining the regions where the FEM object should be evaluated.
<code>search</code>	a flag to decide the search algorithm type (tree or naive or walking search algorithm).
<code>bary.locations</code>	A list with three vectors: <code>locations</code> , location points which are same as the given <code>locations</code> options. (checks whether both locations are the same); <code>element ids</code> , a vector of element id of the points from the mesh where they are located; <code>barycenters</code> , 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.

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	<i>Evaluate a FEM.time object at a set of point locations</i>
---------------	---

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 performed on the tensor grid time.instants-by-locations (or time.instants-by-areal domains).

Usage

```
eval.FEM.time(FEM.time, locations = NULL, time.instants = NULL,
             space.time.locations = NULL, incidence_matrix = NULL, lambdaS = 1,
             lambdaT = 1, search = "tree", bary.locations = NULL)
```

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 chosen for the evaluation.
lambdaT	The index of the lambdaT chosen for the evaluation.
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 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)
## 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)

evaluations = eval.FEM.time(FEM_time_function, locations = matrix(c(-0.92,0), ncol=2),
                           time.instants = time)
```

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 stiffness 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. 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; anisotropic 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; anisotropic 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 input can be used to define the boundaries of the domain. If this input 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 considered 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.
GCV	Boolean. If TRUE the following quantities are computed: the trace of the smoothing 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 length 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 algorithm. This usually ensures a much faster computation.
PDE_parameters	A list specifying the space-varying parameters of the elliptic PDE in the regularizing 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 #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.

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.
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) 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 . In this case the function <code>create.MESH.2D</code> is used to produce a complete MESH2D object.
order	Either '1' or '2'. It specifies whether each mesh triangle should be represented by 3 nodes (the triangle's 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 <code>create.Mesh.2D</code> or <code>refine.Mesh.2D</code> .
...	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:

<code>fit.FEM</code>	A FEM object that represents the fitted spatial field.
<code>PDEmisfit.FEM</code>	A FEM object that represents the Laplacian of the estimated spatial field.
<code>beta</code>	If <code>covariates</code> is not <code>NULL</code> , a vector of length <code>#covariates</code> with the regression coefficients associated with each covariate.
<code>edf</code>	If <code>GCV</code> is <code>TRUE</code> , a scalar or vector with the trace of the smoothing matrix for each value of the smoothing parameter specified in <code>lambda</code> .
<code>stderr</code>	If <code>GCV</code> is <code>TRUE</code> , a scalar or vector with the estimate of the standard deviation of the error for each value of the smoothing parameter specified in <code>lambda</code> .
<code>GCV</code>	If <code>GCV</code> is <code>TRUE</code> , a scalar or vector with the value of the GCV criterion for each value of the smoothing parameter specified in <code>lambda</code> .

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` FEM object that represents the fitted spatial field.
- `PDEmisfit.FEM` FEM object that represents the Laplacian of the estimated spatial field.
- `solution` A list, note that all terms are matrices or row vectors: the `j`th column represents the vector of related to `lambda[j]` if `lambda.selection.criterion="grid"` and `lambda.selection.lossfunction="u"`. In all the other cases is returned just the column related to the best penalization parameter `fMatrix`, estimate of function `f`, first half of solution vector `gMatrix`, second half of solution vector `z_hatMatrix`, 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="unused"` `lambda_position` integer, position in `lambda_vector` of best `lambda` according 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` FEM object that represents the fitted spatial field.
- `PDEmisfit.FEM` FEM object that represents the Laplacian of the estimated spatial field.
- `solution` A list, note that all terms are matrices or row vectors: the `j`th column represents the vector of related to `lambda[j]` if `lambda.selection.criterion="grid"` and `lambda.selection.lossfunction="u"`. In all the other cases is returned just the column related to the best penalization parameter `fMatrix`, estimate of function `f`, first half of solution vector `gMatrix`, second half of solution vector `z_hatMatrix`, 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 `rmseEstimate` of the root mean square error in the locations `estimated_sdEstimate` 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="unused"` `lambda_position` integer, position in `lambda_vector` of best `lambda` according 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
- `timeDuration` 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` FEM object that represents the fitted spatial field.
- `PDEmisfit.FEM` FEM object that represents the Laplacian of the estimated spatial field.
- `solution` A list, note that all terms are matrices or row vectors: the `j`th column represents the vector of related to `lambda[j]` if `lambda.selection.criterion="grid"` and `lambda.selection.lossfunction="u"`. In all the other cases is returned just the column related to the best penalization parameter `fMatrix`, estimate of function `f`, first half of solution vector `gMatrix`, second half of solution vector `z_hatMatrix`, 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 `rmseEstimate` of the root mean square error in the locations `estimated_sdEstimate` 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="unused"` `lambda_position` integer, position in `lambda_vector` of best `lambda` according 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

- `timeDuration` 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:

<code>nodes</code>	A <code>#nodes-by-2</code> matrix containing the x and y coordinates of the mesh nodes.
<code>nodesmarkers</code>	A vector of length <code>#nodes</code> , 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.
<code>nodesattributes</code>	<code>nodesattributes</code> A matrix with <code>#nodes</code> 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.
<code>triangles</code>	A <code>#triangles-by-3</code> (when <code>order = 1</code>) or <code>#triangles-by-6</code> (when <code>order = 2</code>) 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 <code>nodes = 2</code>) 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 .
<code>segmentsmarker</code>	A vector of length <code>#segments</code> with entries either '1' or '0'. An entry '1' indicates that the corresponding element in <code>segments</code> is a boundary segment; an entry '0' indicates that the corresponding segment is not a boundary segment.
<code>edges</code>	A <code>#edges-by-2</code> 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.
<code>edgesmarkers</code>	A vector of length <code>#edges</code> with entries either '1' or '0'. An entry '1' indicates that the corresponding element in <code>edges</code> is a boundary edge; an entry '0' indicates that the corresponding edge is not a boundary edge.
<code>neighbors</code>	A <code>#triangles-by-3</code> 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.
<code>holes</code>	A <code>#holes-by-2</code> 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.
<code>order</code>	Either '1' or '2'. It specifies whether each mesh triangle should be represented by 3 nodes (the triangle's vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (<code>order = 1</code>) and quadratic (<code>order = 2</code>) Finite Elements. Default is <code>order = 1</code> .

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 length #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](#)

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 expansion. 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

```
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 = fs.test(mesh$nodes[,1], mesh$nodes[,2])
## Create the FEM object
FEMfunction = FEM(coeff, FEMbasis)
## Plot it
plot(FEMfunction)
```

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.

Examples

```
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)
```

FPCA.FEM

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

```
FPCA.FEM(locations = NULL, datamatrix, FEMbasis, lambda, nPC = 1, validation = NULL,
          NFolds = 5, GCVmethod = "Stochastic", nrealizations = 100, search = "tree",
          bary.locations = 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 <code>datamatrix</code> . If the locations of the observations coincide with (or are a subset of) the nodes of the mesh in the <code>FEMbasis</code> , leave the parameter <code>locations = NULL</code> for a faster implementation.
datamatrix	A matrix of dimensions #samples-by-#locations with the observed data values over the domain for each sample. The <code>datamatrix</code> needs to have zero mean. If the <code>locations</code> argument is left <code>NULL</code> the <code>datamatrix</code> has to be dimensions #samples-by-#nodes where #nodes is the number of nodes of the mesh in the <code>FEMbasis</code> . 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 <code>NA</code> the values of the <code>datamatrix</code> in correspondence of unobserved data.
FEMbasis	A <code>FEMbasis</code> object describing the Finite Element basis, as created by <code>create.FEM.basis</code> .
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 <code>lambda</code> 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 <code>lambda</code> among those values of the smoothing parameter specified in <code>lambda</code> for each Principal Component.
NFolds	This parameter is used only in case <code>validation = "KFold"</code> . It is an integer specifying the number of folds to use if the <code>KFold</code> cross-validation method for the selection of the best parameter <code>lambda</code> is chosen. Default value is 5.
GCVmethod	This parameter is considered only when <code>validation = "GCV"</code> . It can be either "Exact" or "Stochastic". If set to "Exact" the algorithm 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 estimation of GCV.
search	a flag to decide the search algorithm type (tree or naive or walking search algorithm).
bary.locations	A list with three vectors: <code>locations</code> , location points which are same as the given <code>locations</code> options. (checks whether both <code>locations</code> are the same); <code>element ids</code> , a vector of element id of the points from the mesh where they are located; <code>barycenters</code> , a vector of barycenter of points from the located element.

Value

A list with the following variables:

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

Examples

```
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)

  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.
l	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.

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.
l	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.

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	<i>Horseshoe2.5D domain</i>
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Description

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

horseshoe2D	<i>Horseshoe domain</i>
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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	<i>Hub domain</i>
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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.

image.FEM	<i>Image Plot of a 2D FEM object</i>
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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 be 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

[FEMplot.FEM](#)

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)

## 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 be 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](#)

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
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.

`inferenceDataObjectBuilder`

Constructor for inferenceDataObject class

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	<p>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:</p> <ul style="list-style-type: none"> • 'oat': one-at-the-time tests, available only when component is 'parametric'. • 'sim': simultaneous tests. • 'none': no test required. interval must be set.
interval	<p>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:</p> <ul style="list-style-type: none"> • '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	<p>A list of strings defining the type of implementation for the inferential analysis. The possible values are:</p> <ul style="list-style-type: none"> • 'w': Wald parametric approach (default). • 's': Speckman parametric approach. • 'sf': sign-flip nonparametric approach. • 'esf': eigen-sign-flip nonparametric approach. • 'enh-esf': enhanced-eigen-sign-flip nonparametric approach.
component	<p>A list of strings defining on which model component inference has to be performed. It can take values 'parametric' (default), 'nonparametric' or 'both'.</p>
dim	<p>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)</p>
n_cov	<p>Number of the covariates, defaulted to NULL. (Must be set by the user)</p>
locations	<p>A matrix of the locations of interest when testing the nonparametric component f, defaulted to NULL</p>
locations_indices	<p>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.</p>

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 <code>n_cov</code> number of columns, of numeric coefficients representing the linear combinations of the parametric components of the model. The default is <code>NULL</code> , corresponding to an identity matrix. If at least one sign-flipping approach is required in <code>type</code> , needs to be an identity matrix.
beta0	Vector of real numbers (default <code>NULL</code>). It is used only if the <code>test</code> parameter is set, and <code>component</code> is not 'nonparametric'; its length is the number of rows of matrix <code>coeff</code> if provided. If <code>test</code> is set and <code>beta0</code> is <code>NULL</code> , 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 <code>test</code> is set and <code>component</code> is not parametric. If <code>NULL</code> , 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: <code>FALSE</code> (default) and <code>TRUE</code> .
level	A vector containing the level of significance used to compute quantiles for confidence intervals, defaulted to 0.95. It is taken into account only if <code>interval</code> 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.

Examples

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

plot.FEM

Plot a FEM object

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](#)

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)

## Plot the FEM function
plot(FEMfunction)

```


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 instants. 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

```
## S3 method for class 'FEM.time'
plot(x, time_locations = NULL, locations = NULL,
      lambdaS = NULL, lambdaT = NULL, num_refinements = NULL, Nt = 100,
      add = FALSE, main = NULL, col = "red", ...)
```

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 TRUE 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 .

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, ...)

```

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	<i>Plot a mesh.2.5D object</i>
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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

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)  
plot(mesh)
```

plot.mesh.2D	<i>Plot a mesh.2D object</i>
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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

Examples

```
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  
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)  
  
## Plot the mesh  
plot(mesh)
```

plot.mesh.3D	<i>Plot a mesh.3D object</i>
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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	<i>Project 2D points onto 1.5D linear network mesh</i>
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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 triangular mesh.

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)

```

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 incidence 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

refine.mesh.1.5D	<i>Refine 1.5D mesh</i>
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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	<i>Refine a 2D triangular mesh</i>
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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 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.
verbosity	This can be '0', '1' or '2'. It indicates the level of verbosity in the triangulation process.

Value

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

- nodesA #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.
- nodesmarkersA 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.
- nodesattributesnodesattributes 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.
- trianglesA #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix.
- edgesA #edges-by-2 matrix. Each row contains the row's indices of the nodes where the edge starts from and ends to.
- edgesmarkersA vector of length #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.
- neighborsA #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.
- holesA #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.
- orderEither '1' or '2'. It specifies whether each mesh triangle should be represented by 3 nodes (the triangle's 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](#)

Examples

```
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	<p>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:</p> <ul style="list-style-type: none"> • 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. <p>If the coefficients of the PDE are space-varying PDE_parameters must contain:</p> <ul style="list-style-type: none"> • 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. <p>For 2.5D and 3D, only the Laplacian is available (PDE_parameters=NULL).</p>
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 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 $0.5(\text{observations} + 0.5)$ 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.

<code>DOF.stochastic.realizations</code>	This positive integer is considered only when <code>DOF.evaluation = 'stochastic'</code> . It is the number of uniform random variables used in stochastic DOF evaluation. Default value <code>DOF.stochastic.realizations=100</code> .
<code>DOF.stochastic.seed</code>	This positive integer is considered only when <code>DOF.evaluation = 'stochastic'</code> . It is a user defined seed employed in stochastic DOF evaluation. Default value <code>DOF.stochastic.seed = 0</code> means random.
<code>DOF.matrix</code>	Matrix of degrees of freedom. This parameter can be used if the <code>DOF.matrix</code> corresponding to <code>lambda</code> 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.
<code>GCV.inflation.factor</code>	Tuning parameter used for the estimation of GCV. Default value <code>GCV.inflation.factor = 1.0</code> or <code>1.8</code> in GAM. It is advised to set <code>GCV.inflation.factor</code> larger than 1 to avoid overfitting.
<code>lambda.optimization.tolerance</code>	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 <code>lambda.selection.criterion='newton'</code> or <code>lambda.selection.criterion='newton_fd'</code> . Default value <code>lambda.optimization.tolerance=0.05</code> .
<code>inference.data.object</code>	An inferenceDataObject that stores all the information regarding inference over the linear parameters of the model. This parameter needs to be consistent with <code>covariates</code> , 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` FEM object that represents the fitted spatial field.
- `PDEmisfit.FEM` FEM object that represents the Laplacian of the estimated spatial field.
- `solutionA` list, note that all terms are matrices or row vectors: the `j`th 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. `fMatrix`, estimate of function `f`, first half of solution vector. `gMatrix`, second half of solution vector. `z_hatMatrix`, prediction of the output in the locations. `betaIf` 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. `rmseEstimate` of the root mean square error in the locations. `estimated_sdEstimate` of the standard deviation of the error.
- `optimizationA` 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.lossfunction` -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`

- `timeDuration` 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 `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.

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 (2021). Some first inferential tools for spatial regression with differential regularization. *Journal of Multivariate Analysis*, to appear

Examples

```

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 anisotropy/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)
{
  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)
{
  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)
{
  rep(c(0), nrow(points))
}

u_func<-function(points)
{
  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)) # homogeneous 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)
{
  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)
{
  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)
  {
    rep(c(0), nrow(points))
  }

  u_func<-function(points)
  {
    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)) # homogeneous 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=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.
FLAG_MASS	Boolean. This parameter is considered only for separable problems i.e. when 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 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} .
max.steps	This parameter is used to limit the maximum number of iteration. Default value 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.
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 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 cloglog set family = "probit", family = "cloglog".

<code>mu0</code>	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 $0.5(\text{observations} + 0.5)$ for binary data.
<code>scale.param</code>	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.
<code>threshold.FPIRLS</code>	This parameter is used for arresting algorithm iterations. Algorithm stops when two successive iterations lead to improvement in penalized log-likelihood smaller than <code>threshold.FPIRLS</code> . Default value <code>threshold.FPIRLS = 0.0002020</code> .
<code>max.steps.FPIRLS</code>	This parameter is used to limit the maximum number of iteration. Default value <code>max.steps.FPIRLS=15</code> .
<code>lambda.selection.criterion</code>	This parameter is used to select the optimization method related to smoothing parameter <code>lambda</code> . 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 <code>lambda.selection.criterion='grid'</code>
<code>DOF.evaluation</code>	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 <code>DOF.evaluation=NULL</code>
<code>lambda.selection.lossfunction</code>	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 <code>lambda.selection.criterion='grid'</code> pure evaluation, while the second can be employed for optimization methods. Default value <code>lambda.selection.lossfunction=NULL</code>
<code>lambdaS</code>	A scalar or vector of spatial smoothing parameters.
<code>lambdaT</code>	A scalar or vector of temporal smoothing parameters.
<code>DOF.stochastic.realizations</code>	This parameter is considered only when <code>DOF.evaluation = 'stochastic'</code> . It is a positive integer that represents the number of uniform random variables used in stochastic GCV computation. Default value <code>DOF.stochastic.realizations=100</code> .
<code>DOF.stochastic.seed</code>	This parameter is considered only when <code>DOF.evaluation = 'stochastic'</code> . It is a positive integer that represents user defined seed employed in stochastic GCV computation. Default value <code>DOF.stochastic.seed=0</code> .
<code>DOF.matrix</code>	Matrix of degrees of freedom. This parameter can be used if the <code>DOF.matrix</code> corresponding to <code>lambdaS</code> and <code>lambdaT</code> 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

An [inferenceDataObject](#) that stores all the information regarding inference over the linear 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.timeA FEM.time object that represents the fitted spatio-temporal field.
- PDEmisfit.FEM.timeA FEM.time object that represents the misfit of the penalized PDE.
- betaIf 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].
- edfIf 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.
- stderrIf 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.
- GCVIf 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.
- best.lambdaIf GCV is TRUE, a 2-elements vector with the indices of smoothing parameters returnig the lowest GCV
- ICestimatedIf 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.locationsA barycenter information of the given locations if the locations are not mesh nodes.
- inferenceA list set only if a well defined [inferenceDataObject] is passed as parameter to the function; contains all inference outputs required: p_valueslist of lists set only if at least one p-value is required; contains the p-values divided by implementation: waldlist 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. speckmanlist 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_fliplist 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.

CIlist of lists set only if at least one confidence interval is required; contains the confidence intervals divided by implementation: waldlist 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. speckmanlist 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 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.

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 production of waste in Venice province. *Stochastic Environmental Research and Risk Assessment*, 31(1), 23-38. Federico Ferraccioli, Laura M. Sangalli & Livio Finos (2021). Some first inferential tools for spatial regression with differential regularization. *Journal of Multivariate Analysis*, to appear

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 contains:

- 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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