# <span id="page-0-0"></span>Package: fdaPDE (via r-universe)

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Title Physics-Informed Spatial and Functional Data Analysis

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**Suggests** MASS, test that  $(>= 3.0.0)$ 

Description An implementation of regression models with partial differential regularizations, making use of the Finite Element Method. The models efficiently handle data distributed over irregularly shaped domains and can comply with various conditions at the boundaries of the domain. A priori information about the spatial structure of the phenomenon under study can be incorporated in the model via the differential regularization. See Sangalli, L. M. (2021) [<doi:10.1111/insr.12444>](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

NeedsCompilation yes

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#### Config/testthat/edition 3

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# Contents



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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.

<span id="page-3-1"></span><span id="page-3-0"></span>create.FEM.basis *Create a FEM basis*

#### **Description**

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

#### Usage

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



#### Value

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

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

nbasis Scalar. The number of basis.

### See Also

[create.mesh.2D](#page-7-1), [create.mesh.2.5D](#page-5-1),[create.mesh.3D](#page-9-1)

#### 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
```
### <span id="page-4-0"></span>create.mesh.1.5D 5

```
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



#### Value

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

triangulation process.

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

- <span id="page-5-0"></span>nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.
- nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- edges A #edges-by-2 matrix containing all the edges of the triangles in the output triangulation. Each row contains the row's indices in nodes, indicating the nodes where the edge starts from and ends to.
- neighbors A #edges-by-2 matrix of list. Each row contains the indices of the neighbouring edges. An empty entry indicates that one node of the edge is a boundary node.
- order Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order  $= 1$ ) and quadratic (order  $= 2$ ) Finite Elements.

<span id="page-5-1"></span>create.mesh.2.5D *Create a* mesh.2.5D *object from the nodes locations and the connectivity matrix*

#### Description

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

#### Usage

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





### Value

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

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

- nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.
- nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix. It specifies the triangles giving the indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints are ordered as described at

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

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

### 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)
```
<span id="page-7-1"></span>create.mesh.2D *Create a 2D triangular mesh*

#### Description

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

### Usage

```
create.mesh.2D(nodes, nodesattributes = NA, segments = NA, holes = NA,
                      triangles = NA, order = 1, verbosity = \theta)
```
### Arguments

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

#### nodesattributes

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

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

<span id="page-7-0"></span>



### Value

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

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

- nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.
- nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix. This option is used when a triangulation is already available. It specifies the triangles giving the indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints are ordered as described at https://www.cs.cmu.edu/~quake/triangle.highorder.html.
- segmentsmarker A vector of length #segments with entries either '1' or '0'. An entry '1' indicates that the corresponding element in segments is a boundary segment; an entry '0' indicates that the corresponding segment is not a boundary segment.
- edges A #edges-by-2 matrix containing all the edges of the triangles in the output triangulation. Each row contains the row's indices in nodes, indicating the nodes where the edge starts from and ends to.
- edgesmarkers A vector of lenght #edges with entries either '1' or '0'. An entry '1' indicates that the corresponding element in edge is a boundary edge; an entry '0' indicates that the corresponding edge is not a boundary edge.
- neighbors A #triangles-by-3 matrix. Each row contains the indices of the three neighbouring triangles. An entry '-1' indicates that one edge of the triangle is a boundary edge.
- <span id="page-9-0"></span>holes A #holes-by-2 matrix containing the x and y coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes.
- order Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order  $= 1$ ) and quadratic (order  $= 2$ ) Finite Elements.

### See Also

[refine.mesh.2D](#page-62-1), [create.FEM.basis](#page-3-1)

#### Examples

library(fdaPDE)

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

```
## Create mesh from boundary
## if the domain is convex it is sufficient to call:
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations))
plot(mesh)
```

```
## if the domain is not convex, pass in addition the segments the compose the boundary:
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
```

```
## Create mesh from data locations (without knowing the boundary)
mesh = create.mesh.2D(nodes = locations)
plot(mesh)
## In this case the domain is the convex hull of the data locations.
## Do this only if you do not have any information about the shape of the domain of interest.
```
<span id="page-9-1"></span>

#### 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



### Value

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

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

- nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.
- nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged from the input.
- tetrahedrons A #tetrahedrons-by-4 (when  $order = 1$ ) or #tetrahedrons-by-10 (when  $order = 2$ ) matrix. It specifies the tetrahedrons giving the indices in nodes of the tetrahedrons' vertices and (when nodes = 2) also if the tetrahedrons' edges midpoints.
- <span id="page-11-0"></span>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 lenght #faces with entries either '1' or '0'. An entry '1' indicates that the corresponding element in faces is a boundary face; an entry '0' indicates that the corresponding edge is not a boundary face.
- neighbors A #triangles-by-4 matrix. Each row contains the indices of the four neighbouring tetrahedrons An entry '-1' indicates that one face of the tetrahedrons is a boundary face.
- holes A #holes-by-3 matrix containing the x, y, z coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes. These are passed unchanged from the input.
- order Either '1' or '2'. It specifies wether each mesh tetrahedron should be represented by 3 nodes (the tetrahedron's vertices) or by 6 nodes (the tetrahedron's vertices and midpoints). These are respectively used for linear (order  $= 1$ ) and quadratic (order  $= 2$ ) Finite Elements.

#### Examples

library(fdaPDE)

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

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

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

DE.FEM *Nonparametric density estimation with differential regularization*

### Description

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

### Usage

```
DE.FEM(data, FEMbasis, lambda, scaling=NULL, 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", inference = FALSE)
```
#### $DE.FEM$  13

### Arguments





### Value

A list with the following variables:



#### $DE.FEM$  15



### 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 \leq seq(-3, 3, length.out = 10)
Ybound \leq 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 \leq refine.mesh. 2D(mesh, maximum_area = 0.2)
FEMbasis <- create.FEM.basis(mesh)
## Generate data
n < -50set.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 = 0.1sol <- DE.FEM(data = data, FEMbasis = FEMbasis, lambda = lambda, fvec=NULL, heatStep=0.1,
             heatIter=500, nsimulations=300,step_method = "Fixed_Step", inference = TRUE)
## Visualization
n = 100X \leftarrow seq(-3, 3, length.out = n)Y<-seq(-3, 3, length.out = n)grid \leftarrow expand.grid(X, Y)evaluation <- eval.FEM(FEM(FEMbasis, coeff = sol$g), locations = grid)
lower_bound_g <- eval.FEM(FEM(FEMbasis, coeff = sol$g_CI_L), locations = grid)
upper_bound_g <- eval.FEM(FEM(FEMbasis, coeff = sol$g_CI_U), locations = grid)
evaluation <- exp(evaluation)
lower_bound_g <- exp(lower_bound_g)
upper_bound_g <- exp(upper_bound_g)
```

```
eval <- matrix(evaluation, n, n)
eval_L <- matrix(lower_bound_g, n, n)
eval_U <- matrix(upper_bound_g, n, n)
image2D(x = X, y = Y, z = eval_L, col = heat-colors(100), xlab = "x", ylab = "y",contour = list(drawlabels = FALSE), main = "Estimated CI lower bound")
image2D(x = X, y = Y, z = eval, col = heatcolor(100), xlab = "x", ylab = "y",contour = list(drawlabels = FALSE), main = "Estimated density")
image2D(x = X, y = Y, z = eval_U, col = heat.close(100), xlab = "x", ylab = "y",contour = list(drawlabels = FALSE), main = "Estimated CI upper bound")
```
DE.FEM.time *Nonparametric spatio-temporal density estimation with differential regularization*

#### Description

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

#### Usage

```
DE.FEM.time(data, data_time, FEMbasis, mesh_time, lambda, lambda_time, scaling=NULL,
            fvec=NULL, heatStep=0.1, heatIter=10, 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",
                   isTimeDiscrete=FALSE, flagMass=FALSE, flagLumped=FALSE,
                   inference = FALSE)
```
#### Arguments



- lambda\_time A scalar or vector of smoothing parameters in time. If it is a vector, the optimal
	- smoothing parameter in time is chosen, together with the optimal smoothing parameter in space, with a k-fold cross-validation procedure based on the L2 norm.
- scaling A positive factor needed to scale the smoothing parameters in the construction of confidence intervals. If the scaling is not specified, it is automatically set as the square root of the number of observations.
- fvec A vector of length #nodes of the spatial mesh times #B-spline temporal 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  $log(f)$ .
- heat Step A real specifying the time step for the discretized heat diffusion process. Default  $is 0.1$
- heatIter An integer specifying the number of iterations to perform the discretized heat diffusion process. Default is 10.
- stepProposals A scalar or a vector containing the step parameters useful for the descent 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  $c(0.1, 1)$ 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 loglikelihood 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-Ribiére-Polyak formula (ConjugateGradientPRP), Conjugate Gradient direction with Hestenes-Stiefel formula (ConjugateGradientHS), Conjugate Gradient direction with Dai-Yuan formula (ConjugateGradientDY), Conjugate Gradient direction with Conjugate-Descent formula (ConjugateGradientCD), Conjugate Gradient direction with Liu-Storey formula (ConjugateGradientLS), L-BFGS direction with 5 correction vectors (L-BFGS5), L-BFGS direction with 10 correction vectors (L-BFGS10).

preprocess\_method



#### Value

A list with the following variables:



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



### Examples

library(fdaPDE)

```
## Create a 2D mesh over a squared domain
Xbound \leq seq(-3, 3, length.out = 10)
Ybound \leq 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 \leq create.mesh.2D(nodes = Bounds, order = 1)
mesh \le- 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  $\leq$  seq(0, 1, length.out=3)

```
## Generate data
n < -50set.seed(10)
x \leq -rnorm(n, \emptyset, 2)y \leftarrow \text{norm}(n, \emptyset, 2)locations \leq cbind(x,y)times \le 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 < -0.1lambda_time <- 0.001
sol <- DE.FEM.time(data = locations, data_time = times, FEMbasis = FEMbasis, mesh_time = mesh_time,
             lambda = lambda, lambda_time = lambda_time, nsimulations=300, inference=TRUE)
## Visualization
n = 100X \leftarrow seq(-3, 3, length.out = n)Y \leftarrow seq(-3, 3, length.out = n)grid <- expand.grid(X, Y)
FEMfunction = FEM.time(sol$g, mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation <- eval.FEM.time(FEM.time = FEMfunction, locations = grid, time.instants = t)
FEMfunction_L = FEM.time(sol$g_CI_L, mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation_L <- eval.FEM.time(FEM.time = FEMfunction_L, locations = grid, time.instants = t)
FEMfunction_U = FEM.time(sol$g_CI_U, mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation_U <- eval.FEM.time(FEM.time = FEMfunction_U, locations = grid, time.instants = t)
image2D(x = X, y = Y, z = matrix(exp(evaluation_L), n, n), col = heat-colors(100),xlab = "x", ylab = "y", contour = list(drawlabels = FALSE),
        main = paste("Estimated CI lower bound at t = ", t), zlim=c(0,0.3), asp = 1)
image2D(x = X, y = Y, z = matrix(exp(evaluation), n, n), col = heat-colors(100),xlab = "x", ylab = "y", contour = list(drawlabels = FALSE),
        main = paste("Estimated density at t = ", t), zlim=c(0,0.3), asp = 1)
image2D(x = X, y = Y, z = matrix(exp(evaluation_U), n, n), col = heat-colors(100),xlab = "x", ylab = "y", contour = list(drawlabels = FALSE),
        main = paste("Estimated CI upper bound at t = ", t), zlim=c(0,0.3), asp = 1)
```
DE.heat.FEM *Density initialization*

#### Description

This function implements two methods for the density initialization procedure.

#### Usage

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



### DE.heat.FEM 21



### 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 \leq seq(-3, 3, length.out = 10)
Ybound \leq 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 \leq create.mesh. 2D(nodes = Bounds, order = 1)
mesh \leq refine.mesh.2D(mesh, maximum_area = 0.2)
FEMbasis <- create.FEM.basis(mesh)
## Generate data
n < -50set.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 = 0.1sol = DE.heat.FEM(data, FEMbasis, lambda, heatStep=0.1, heatIter=500, init="Heat")
## Visualization
plot(FEM(coeff=sol$f_init, FEMbasis=FEMbasis))
```
<span id="page-21-0"></span>

### 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



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

### Value

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

#### Examples

library(fdaPDE)

```
## Create a 2D mesh over a squared domain
Xbound \leq seq(-3, 3, length.out = 10)
Ybound \leq 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 \leq 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 \leq seq(0, 1, length.out=3)
## Generate data
n < -50set.seed(10)
x \leq -rnorm(n, \emptyset, 2)y \leq -rnorm(n, \emptyset, 2)locations \leq cbind(x,y)
times \le 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 = 0.1lambda_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 = 100X \leftarrow seq(-3, 3, length.out = n)Y \leftarrow seq(-3, 3, length.out = n)grid \leftarrow expand.grid(X, Y)FEMfunction = FEM.time(sol$f_init[,1,1], mesh_time, FEMbasis, FLAG_PARABOLIC = FALSE)
evaluation \leq 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



#### 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.

<span id="page-23-0"></span>

### <span id="page-24-0"></span>eval.FEM.time 25

#### 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$nodes[,2])
## Create the FEM object
FEMfunction = FEM(coeff, FEMbasis)
## Evaluate the finite element function in the location (1,0.5)
eval.FEM(FEMfunction, locations = matrix(c(1, 0.5), ncol = 2))
## Evaluate the mean of the finite element function over the fifth triangle of the mesh
incidence_matrix = matrix(0, ncol = nrow(mesh$triangle)incidence_matrix[1,5] = 1
eval.FEM(FEMfunction, incidence_matrix = incidence_matrix)
```
eval.FEM.time *Evaluate a FEM.time object at a set of point locations*

#### Description

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

#### Usage

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



### 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

FEMbasis = create.FEM.basis(mesh)

```
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
```
#### <span id="page-26-0"></span>fdaPDE-deprecated 27

```
## 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 = 1:5coeff = 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*

### <span id="page-26-1"></span>**Description**

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

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

Only executed when the function smooth.FEM.basis is run with the option CPP\_CODE = FALSE. It evaluates the Finite Element basis functions and their derivatives up to order 2 at the specified set of locations. This version of the function is implemented using only R code. It is called by [R\\_smooth.FEM.basis.](#page-26-1)

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

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

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

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

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

This function refines a Constrained Delaunay triangulation into a Conforming Delaunay triangulation. This is a wrapper of the Triangle library (http://www.cs.cmu.edu/~quake/triangle.html). It can be used to refine a mesh created previously with [create.MESH.2D.](#page-26-1) 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
\mathcal{L}smooth.FEM.PDE.sv.basis(
  locations = NULL,
 observations,
 FEMbasis,
 lambda,
 PDE_parameters,
 covariates = NULL,
 BC = NULL,GCV = FALSE,CPP_CODE = TRUE
\lambdacreate.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, \ldots)
```
### Arguments







### 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:



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

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

A list with the following variables:

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

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

- solution A list, note that all terms are matrices or row vectors: the jth column represents the vector of related to lambda[j] if lambda.selection.criterion="grid" and lambda.selection.lossfunction="unus In all the other cases is returned just the column related to the best penalization parameter
	- f Matrix, estimate of function f, first half of solution vector
	- g Matrix, second half of solution vector
	- z\_hat Matrix, prediction of the output in the locations
	- beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. It is the regression coefficients estimate
	- rmse Estimate of the root mean square error in the locations
	- estimated\_sd Estiimate of the standard deviation of the error
- optimization A detailed list of optimization related data:
	- lambda\_solution numerical value of best lambda acording to lambda.selection.lossfunction, -1 if lambda.selection.lossfunction="unused"
	- lambda\_position integer, postion in lambda\_vector of best lambda acording to lambda.selection.lossfunction, -1 if lambda.selection.lossfunction="unused"
	- GCV numeric value of GCV in correspondence of the optimum
	- optimization\_details list containing further information about the optimization method used and the nature of its termination, eventual number of iterations
	- dof numeric vector, value of dof for all the penalizations it has been computed, empty if not computed
	- lambda\_vector numeric value of the penalization factors passed by the user or found in the iterations of the optimization method

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

- time Duration of the entire optimization computation
- bary.locations A barycenter information of the given locations if the locations are not mesh nodes.

A list with the following variables:

- fit.FEM A FEM object that represents the fitted spatial field.
- PDEmisfit.FEM A FEM object that represents the Laplacian of the estimated spatial field.
- solution A list, note that all terms are matrices or row vectors: the jth column represents the vector of related to lambda[j] if lambda.selection.criterion="grid" and lambda.selection.lossfunction="unus In all the other cases is returned just the column related to the best penalization parameter
	- f Matrix, estimate of function f, first half of solution vector
- g Matrix, second half of solution vector
- z\_hat Matrix, prediction of the output in the locations
- beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. It is the regression coefficients estimate
- rmse Estimate of the root mean square error in the locations
- estimated\_sd Estiimate of the standard deviation of the error
- optimization A detailed list of optimization related data:
	- lambda\_solution numerical value of best lambda acording to lambda.selection.lossfunction, -1 if lambda.selection.lossfunction="unused"
	- lambda\_position integer, postion in lambda\_vector of best lambda acording to lambda.selection.lossfunction, -1 if lambda.selection.lossfunction="unused"
	- GCV numeric value of GCV in correspondence of the optimum
	- optimization\_details list containing further information about the optimization method used and the nature of its termination, eventual number of iterations
	- dof numeric vector, value of dof for all the penalizations it has been computed, empty if not computed
	- lambda\_vector numeric value of the penalization factors passed by the user or found in the iterations of the optimization method
	- GCV\_vector numeric vector, value of GCV for all the penalizations it has been computed
- time Duration of the entire optimization computation
- bary.locations A barycenter information of the given locations if the locations are not mesh nodes.
- A list with the following variables:
- fit.FEM A FEM object that represents the fitted spatial field.
- PDEmisfit.FEM A FEM object that represents the Laplacian of the estimated spatial field.
- solution A list, note that all terms are matrices or row vectors: the jth column represents the vector of related to lambda[j] if lambda.selection.criterion="grid" and lambda.selection.lossfunction="unus In all the other cases is returned just the column related to the best penalization parameter
	- f Matrix, estimate of function f, first half of solution vector
	- g Matrix, second half of solution vector
	- z\_hat Matrix, prediction of the output in the locations
	- beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. It is the regression coefficients estimate
	- rmse Estimate of the root mean square error in the locations
	- estimated\_sd Estiimate of the standard deviation of the error
- optimization A detailed list of optimization related data:

lambda\_solution numerical value of best lambda acording to lambda.selection.lossfunction,

- -1 if lambda.selection.lossfunction="unused"
- lambda\_position integer, postion in lambda\_vector of best lambda acording to lambda.selection.lossfunction,
	- -1 if lambda.selection.lossfunction="unused"
- GCV numeric value of GCV in correspondence of the optimum
- optimization\_details list containing further information about the optimization method used and the nature of its termination, eventual number of iterations
- dof numeric vector, value of dof for all the penalizations it has been computed, empty if not computed
- lambda\_vector numeric value of the penalization factors passed by the user or found in the iterations of the optimization method
- GCV\_vector numeric vector, value of GCV for all the penalizations it has been computed

time Duration of the entire optimization computation

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

An object of the class MESH2D with the following output:





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

- nodes A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.
- nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.

nodesattributes

- nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. If a node is added during the triangulation process or mesh refinement, its attributes are computed by linear interpolation using the attributes of neighboring nodes. This functionality is for instance used to compute the value of a Dirichlet boundary condition at boundary nodes added during the triangulation process.
- triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix. This option is used when a triangulation is already available. It specifies the triangles giving the row's indices in nodes of the triangles' vertices and (when nodes = 2) also if the triangles' edges midpoints. The triangles' vertices and midpoints are ordered as described at

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

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

#### See Also

[refine.MESH.2D](#page-26-1), [create.FEM.basis](#page-3-1) [create.MESH.2D](#page-26-1), [create.FEM.basis](#page-3-1)

<span id="page-35-0"></span>

### **Description**

This function defines a FEM object.

### Usage

FEM(coeff,FEMbasis)

### Arguments



### 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)
```
<span id="page-36-0"></span>

### Description

This function defines a FEM.time object.

# Usage

FEM.time(coeff,time\_mesh,FEMbasis,FLAG\_PARABOLIC=FALSE)

### Arguments



# 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)
```
# 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)
```


- search a flag to decide the search algorithm type (tree or naive or walking search algorithm).
- bary.locations A list with three vectors: locations, location points which are same as the given locations options. (checks whether both locations are the same); element ids, a vector of element id of the points from the mesh where they are located; barycenters, a vector of barycenter of points from the located element.

#### Value

A list with the following variables:

- loadings.FEM A FEM object that represents the L^2-normalized functional loadings for each Principal Component computed.
- scores A #samples-by-#PrincipalComponents matrix that represents the unnormalized scores or PC vectors.
- lambda A vector of length #PrincipalComponents with the values of the smoothing parameter lambda chosen for that Principal Component.
- variance\_explained A vector of length #PrincipalComponents where each value represent the variance explained by that component.
- cumsum\_percentage A vector of length #PrincipalComponents containing the cumulative percentage of the variance explained by the first components.
- bary.locations A barycenter information of the given locations if the locations are not mesh nodes.

#### References

Lila, E., Aston, J.A.D., Sangalli, L.M., 2016a. Smooth Principal Component Analysis over twodimensional 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



#### Value

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

#### $f_{\rm s. test.3D}$  41

# References

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

### Examples

library(fdaPDE)

```
## Upload the horseshoe2D data
data(horseshoe2D)
boundary_nodes = horseshoe2D$boundary_nodes
boundary_segments = horseshoe2D$boundary_segments
locations = horseshoe2D$locations
## Create the 2D mesh
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
## Create the FEM basis
FEMbasis = create.FEM.basis(mesh)
## Compute the coeff vector evaluating the desired function at the mesh nodes
## In this case we consider the fs.test() function introduced by Wood et al. 2008
coeff = fs.test(mesh$nodes[,1], mesh$nodes[,2], exclude = FALSE)
## Create the FEM object
FEMfunction = FEM(coeff, FEMbasis)
## Plot it
plot(FEMfunction)
```
#### fs.test.3D *FELSPLINE 3D test function*

#### Description

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

#### Usage

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


### Value

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

# Examples

```
library(fdaPDE)
```

```
data(horseshoe2.5D)
mesh = horseshoe2.5D
FEMbasis=create.FEM.basis(mesh)
# Evaluation at nodes
sol_exact=fs.test.3D(mesh$nodes[,1],mesh$nodes[,3],mesh$nodes[,2])
plot(FEM(sol_exact, FEMbasis))
```
horseshoe2.5D *Horseshoe2.5D domain*

### Description

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

horseshoe2D *Horseshoe domain*

# Description

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

hub2.5D *Hub domain*

# Description

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

<span id="page-42-0"></span>

#### Description

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

#### Usage

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

x A 2D-mesh FEM object. num\_refinements A natural number specifying how many bisections should by applied to each triangular element for plotting purposes. This functionality is useful where a discretization with 2nd order Finite Element is applied. ... Arguments representing graphical options to be passed to [plot3d.](#page-0-0)

# Value

No return value

### See Also

[FEM](#page-35-0) [plot.FEM](#page-51-0)

### 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)

<span id="page-43-0"></span>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



### Value

No return value

#### See Also

[FEM.time](#page-36-0) [image.FEM.time](#page-43-0)

### 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 = 1:5coeff = 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*

#### <span id="page-44-0"></span>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](#page-64-0).

#### 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](#page-45-0) 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](#page-45-0), leading to avoid some of the checks that are performed on inference data within smoothing functions.

<span id="page-45-0"></span>inferenceDataObjectBuilder

*Constructor for inferenceDataObject class*

# Description

A function that build an [inferenceDataObject](#page-44-0). 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](#page-64-0) or [smooth.FEM.time](#page-73-0) functions. Notice that this constructor ensures wellposedness 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_{\text{cov}} = NULL,
locations = NULL,
locations_indices = NULL,
locations_by_nodes = FALSE,
coeff = NULL,beta = NULL,f0 = NULL,f_{var} = FALSE,level = 0.95,n_flip = 1000)
```




# Value

The output is a well defined [inferenceDataObject](#page-44-0), that can be used as input parameter in the [smooth.FEM](#page-64-0) 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);
```
inferenceDataObjectTime-class *Class for inference data in ST case*

### <span id="page-48-0"></span>**Description**

A class that contains all possible information for inference over linear parameters and/or nonparametric field in spatio-temporal regression with differential regularization problem. This object can be used as parameter in smoothing function of the fdaPDE library [smooth.FEM.time](#page-73-0).

#### Details

At least one between test and interval must be nonzero. n\_cov, coeff and beta0, if provided, need to be coherent. dim and locations, if provided, need to be coherent. The usage of [inferenceDataObjectTimeBuilder](#page-49-0) is recommended for the construction of an object of this class.

### **Slots**

- test A vector of integers taking value 0, 1 or 2; if 0 no test is performed, if 1 one-at-the-time tests are performed, if 2 a simultaneous test is performed.
- interval A vector of integers taking value 0, 1, 2 or 3; if 0 no confidence interval is computed, if 1 one-at-the-time confidence intervals are computed, if 2 simultaneous confidence intervals are computed, if 3 Bonferroni confidence intervals are computed.
- type A vector of integers taking value 1, 2, 3 or 4 corresponding to Wald, Speckman, Eigen-Sign-Flip, Enhanced-Eigen-Sign-Flip inferential approach.
- component A vector of integers taking value 1, 2 or 3, indicating whether the inferential analysis should be carried out respectively for the parametric, nonparametric or both the components.
- exact An integer taking value 1 or 2. If 1 an exact computation of the test statistics will be performed, whereas if 2 an approximated computation will be carried out (not implemented in this version).
- dim Dimension of the problem, it is equal to 2 in the 1.5D and 2D cases and equal to 3 in the 2.5D and 3D cases.
- n\_cov Number of covariates taken into account in the linear part of the regression problem.
- locations A matrix of numeric coefficients with columns of dimension dim. When nonparametric inference is requested it represents the set of spatial locations for which the inferential analysis should be performed. The default values is a one-dimensional matrix of value 1 indicating that all the observed location points should be considered. In the sign-flip and eigen-sign-flip implementations only observed points are allowed.
- locations\_indices A vector of indices indicating which spatial points have to be considered among the observed ones for nonparametric inference. If a vector of location indices is provided then the slot 'location' is discarded.
- locations\_are\_nodes An integer taking value 1 or 2; in the first case it indicates that the selected locations to perform inference on f are all coinciding with the nodes; otherwise it takes value 2;
- time\_locations A vector of numeric coefficients containing the set of times of interest for inference on the nonparametric component. This parameter can be NULL. In this case the temporal locations are assumed to coincide with the time\_locations provided to the smoothing functions. Used only if component is not 1.
- coeff A matrix of numeric coefficients with columns of dimension n\_cov and each row represents a linear combination of the linear parameters to be tested and/or to be estimated via confidence interval.
- beta0 Vector of null hypothesis values for the linear parameters of the model. Used only if test is not 0 and component is not 2.
- f0 Function representing the expression of the nonparametric component f under the null hypothesis. Used only if component is not 1.
- f0\_eval Matrix of f0 evaluations at the chosen space and time locations. It will be eventually set later in checkInferenceParametersTime, if nonparametric inference is required.
- f\_var An integer taking value 1 or 2. If 1 local variance estimates for the nonlinear part of the model will be computed, whereas if 2 they will not.
- quantile Vector of quantiles needed for confidence intervals, used only if interval is not 0.
- alpha 1 minus confidence level vector of sign-flipping approaches confidence intervals. Used only if interval is not 0.
- n\_flip An integer representing the number of sign-flips in the case of sign-flipping approaches.
- tol\_fspai A real number greater than 0 specifying the tolerance for FSPAI algorithm, in case of non-exact inference (not implemented in this version).
- definition An integer taking value  $0$  or 1. If set to 1, the class will be considered as created by the function [inferenceDataObjectTimeBuilder](#page-49-0), leading to avoid some of the checks that are performed on inference data within smoothing functions.

<span id="page-49-0"></span>inferenceDataObjectTimeBuilder

*Constructor for inferenceDataObjectTime class*

# **Description**

A function that build an [inferenceDataObjectTime](#page-48-0). In the process of construction many checks over the input parameters are carried out so that the output is a well defined object, that can be used as parameter in smooth. FEM or smooth. FEM. time functions. Notice that this constructor ensures well-posedness of the object, but a further check on consistency with the smoothing functions parameters will be carried out.

### Usage

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

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




# Value

The output is a well defined [inferenceDataObjectTime](#page-48-0), that can be used as input parameter in the [smooth.FEM](#page-64-0) function.

# Examples

obj<-inferenceDataObjectTimeBuilder(test = 'oat', dim = 2, beta0 =  $rep(1,4)$ , n\_cov = 4); obj2<-inferenceDataObjectTimeBuilder(test = 'sim', dim = 3, component = 'nonparametric', n\_cov = 3);

<span id="page-51-0"></span>plot.FEM *Plot a* FEM *object*

#### plot.FEM 53

#### **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-color", num_refinements = NULL, ...)
```
### **Arguments**



#### Value

No return value

### See Also

[FEM](#page-35-0), [image.FEM](#page-42-0)

#### 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)

plot.FEM.time *Plot a* FEM.time *object at a given time*

### Description

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

#### Usage

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


plot.mesh.1.5D 55

### Value

No return value

### See Also

[FEM.time](#page-36-0), [image.FEM.time](#page-43-0)

### 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 = 1:5coeff = 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, \ldots)
```
### Arguments



# Value

No return value



# 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



# 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 *Plot a mesh.2D object*

### Description

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

### Usage

## S3 method for class 'mesh.2D'  $plot(x, \ldots)$ 

# Arguments



### Value

No return value

# Examples

library(fdaPDE)

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

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

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

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

#### Usage

## S3 method for class 'mesh.3D'  $plot(x, \ldots)$ 

### Arguments



### Value

No return value

### Examples

library(fdaPDE)

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

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

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

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

projection.points.1.5D

*Project 2D points onto 1.5D linear network mesh*

# Description

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

# projection.points.2.5D 59

# Usage

projection.points.1.5D(mesh, locations)

### Arguments



# 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, by row = TRUE)mesh_ = create.mesh.1.5D(nodes,edges,order=1)
## Create 2D points to be projected
locations=matrix(nrow=5,ncol=2)
localions[, 1] = runif(5, min=0.25, max=0.75)localions[, 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



# Value

3D points projected onto 2.5D triangluar 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 \leq \cos(\sec(\theta, 2\pi)x), length.out = 9))
y \le -\sin(\sec(\theta, 2\pi\pi), \text{ length.out} = 9)z \leq -rep(0.5, 9)locations = child(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 incindence matrix defining the subdomains used by Azzimonti et. al 2015. This dataset can be used to test the smooth.FEM function for areal data.

# References

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

refine.by.splitting.mesh.1.5D

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

# Description

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

#### Usage

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

mesh a mesh.1.5D object to split

# Value

An object of class mesh.1.5D with splitted edges

refine.by.splitting.mesh.2.5D

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

# Description

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

# Usage

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

mesh a mesh. 2.5D object to split

#### Value

An object of class mesh.2.5D with splitted triangles

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

# Description

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

#### Usage

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

mesh a mesh.2D object to split

# Value

An object of class mesh.2D with splitted triangles

refine.by.splitting.mesh.3D

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

# Description

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

# Usage

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

mesh a mesh.3D object to split

#### Value

An object of class mesh.3D with splitted tetrahedrons

refine.mesh.1.5D *Refine 1.5D mesh*

# Description

Refine 1.5D mesh

#### Usage

refine.mesh.1.5D(mesh, delta)

# Arguments



### Value

An object of class mesh.1.5D with refined edges

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

### Description

This function refines a Constrained Delaunay triangulation into a Conforming Delaunay triangulation. This is a wrapper of the Triangle library (http://www.cs.cmu.edu/~quake/triangle.html). It can be used to refine a mesh previously created with [create.mesh.2D.](#page-7-0) 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)
```


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

- nodes A #nodes-by-2 matrix containing the x and y coordinates of the mesh nodes.
- nodesmarkers A vector of length #nodes, with entries either '1' or '0'. An entry '1' indicates that the corresponding node is a boundary node; an entry '0' indicates that the corresponding node is not a boundary node.
- nodesattributes nodesattributes A matrix with #nodes rows containing nodes' attributes. These are passed unchanged to the output. If a node is added during the triangulation process or mesh refinement, its attributes are computed by linear interpolation using the attributes of neighboring nodes. This functionality is for instance used to compute the value of a Dirichlet boundary condition at boundary nodes added during the triangulation process.
- triangles A #triangles-by-3 (when order = 1) or #triangles-by-6 (when order = 2) matrix.
- edges A #edges-by-2 matrix. Each row contains the row's indices of the nodes where the edge starts from and ends to.
- edgesmarkers A vector of lenght #edges with entries either '1' or '0'. An entry '1' indicates that the corresponding element in edge is a boundary edge; an entry '0' indicates that the corresponding edge is not a boundary edge.
- neighbors A #triangles-by-3 matrix. Each row contains the indices of the three neighbouring triangles. An entry '-1' indicates that one edge of the triangle is a boundary edge.
- holes A #holes-by-2 matrix containing the x and y coordinates of a point internal to each hole of the mesh. These points are used to carve holes in the triangulation, when the domain has holes.
- order Either '1' or '2'. It specifies wether each mesh triangle should be represented by 3 nodes (the triangle' vertices) or by 6 nodes (the triangle's vertices and midpoints). These are respectively used for linear (order  $= 1$ ) and quadratic (order  $= 2$ ) Finite Elements.

### See Also

[create.mesh.2D](#page-7-0), [create.FEM.basis](#page-3-0)

#### 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)
```
#### $smooth.FEM$  65

```
## Refine the mesh with the minimum angle criterion:
finemesh2 = refine.mesh.2D(mesh = mesh, minimum_angle = 30)
plot(finemesh2)
```
<span id="page-64-0"></span>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, area1.data.argv = 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)
```




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

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

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

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

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

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.





- family This parameter specify the distibution within exponential family used for GLM model. The following distribution are implemented: "binomial", "exponential", "gamma", "poisson", "gaussian", "invgaussian". The default link function for binomial is logit if you want either probit or clogloc set family = "probit", family = "cloglog".
- mu0 This parameter is a vector that set the starting point for FPIRLS algorithm. It represent an initial guess of the location parameter. Default is set to observation for non binary distribution while equal to  $0.5$  (observations  $+0.5$ ) for binary data.
- scale.param Dispersion parameter of the chosen distribution. This is only required for "gamma", "gaussian", "invgaussian". User may specify the parameter as a positive real number. If the parameter is not supplied, it is estimated from data according to Wilhelm Sangalli 2016.

threshold.FPIRLS

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

#### max.steps.FPIRLS

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

lambda.selection.criterion

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

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

lambda.selection.lossfunction

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

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

#### DOF.stochastic.realizations

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

#### DOF.stochastic.seed

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

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

#### GCV.inflation.factor

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

#### lambda.optimization.tolerance

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

### inference.data.object

An [inferenceDataObject](#page-44-0) that stores all the information regarding inference over the linear and nonlinear parameters of the model. This parameter needs to be consistent with covariates, otherwise will be discarded. If set and well defined, the function will have in output the inference results. It is suggested to create this object via [inferenceDataObjectBuilder](#page-45-0) function, so that the object is guaranteed to be well defined.

### Value

A list with the following variables:

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

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

- solution A list, note that all terms are matrices or row vectors: the jth column represents the vector related to lambda[j] if lambda.selection.criterion="grid" and lambda.selection.lossfunction=NULL. In all the other cases, only the column related to the best smoothing parameter is returned.
- f Matrix, estimate of function f, first half of solution vector.
- g Matrix, second half of solution vector.
- z\_hat Matrix, prediction of the output in the locations.
- beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. It is the regression coefficients estimate.
- rmse Estimate of the root mean square error in the locations.
- estimated\_sd Estimate of the standard deviation of the error.
- optimization A detailed list of optimization related data:
- lambda\_solution numerical value of best lambda according to lambda.selection.lossfunction, -1 if lambda.selection.lossfunction=NULL.
- lambda\_position integer, position in lambda\_vector of best lambda according to lambda.selection.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

- time Duration of the entire optimization computation.
- bary.locations Barycenter information of the given locations, if the locations are not mesh nodes.
- GAM\_output A list of GAM related data:
	- fn\_hat A matrix with number of rows equal to number of locations and number of columns equal to length of lambda. Each column contains the evaluaton 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](#page-44-0) 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 (2022). Some first inferential tools for spatial regression with differential regularization. Journal of Multivariate Analysis, 189, 104866.

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

```
solution$inference$beta$p_values
# confidence intervals for beta estimates:
solution$inference$beta$CI
# non-parametric estimate:
plot(solution$fit.FEM)
# Choose lambda with GCV - stochastic grid evaluation:
lambda = 10^(-2:0)solution = smooth.FEM(observations = data,
                            covariates = covariate,
                            FEMbasis = FEMbasis,
                            lambda = lambda, DOF.evaluation = 'stochastic',
                            lambda.selection.lossfunction = 'GCV')
bestLambda = solution$optimization$lambda_solution
# Choose lambda with GCV - Newton finite differences stochastic evaluation -:
solution = smooth.FEM(observations = data,
                            covariates = covariate,
                            FEMbasis = FEMbasis,
                    DOF.evaluation = 'stochastic', lambda.selection.lossfunction = 'GCV')
bestLambda = solution$optimization$lambda_solution
#### Smoothing with prior information about anysotropy/non-stationarity and boundary conditions ####
# See Azzimonti et al. for reference to the current example
data(quasicircle2D)
boundary_nodes = quasicircle2D$boundary_nodes
boundary_segments = quasicircle2D$boundary_segments
locations = quasicircle2D$locations
data = quasicircle2D$data
mesh = create.mesh.2D(nodes = rbind(boundary_nodes, locations), segments = boundary_segments)
FEMbasis = create.FEM.basis(mesh)
lambda = 10^{\circ} - 2# Set the PDE parameters
R = 2.8K1 = 0.1K2 = 0.2beta = 0.5K_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 = NULLBC$BC_indices = which(mesh$nodesmarkers == 1) # b.c. on the complete boundary
BC$BC_values = rep(0,length(BC$BC_indices)) # homogeneus b.c.
# Since the data locations are a subset of the mesh nodes for a faster solution use:
dataNA = rep(NA, FEMbasis$nbasis)
dataNA[mesh$nodesmarkers == 0] = data
#grid evaluation
solution = smooth.FEM(observations = dataNA,
                            FEMbasis = FEMbasis,
                            lambda = lambda,
                            PDE_parameters = PDE_parameters,
                            BC = BCplot(solution$fit.FEM)
image(solution$fit.FEM)
# Newton's method
solution = smooth.FEM(observations = dataNA,
                            FEMbasis = FEMbasis,
                            PDE_parameters = PDE_parameters,
                            BC = BCplot(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^{\circ} - 4# Set the PDE parameters
R = 2.8K1 = 0.1
```
$smooth.FEM$  73

```
K2 = 0.2beta = 0.5K_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 = NULLBC$BC_indices = which(mesh$nodesmarkers == 1) # b.c. on the complete boundary
BC$BC_values = rep(0,length(BC$BC_indices)) # homogeneus b.c.
#grid evaluation
solution = smooth.FEM(observations = data,
                            incidence_matrix = incidence_matrix,
                            FEMbasis = FEMbasis,
                            lambda = lambda,
                            PDE_parameters = PDE_parameters,
                            BC = BCplot(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 = BCplot(solution$fit.FEM)
image(solution$fit.FEM)
```
## <span id="page-73-0"></span>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, area1.data.avg = TRUE,FLAG_MASS = FALSE, FLAG_PARABOLIC = FALSE, FLAG_ITERATIVE = FALSE,
threshold = 10^*(-4), max.steps = 50, IC = NULL,
search = "tree", bary.locations = NULL,
family = "gaussian", mu0 = NULL, scale.param = NULL,
threshold.FPIRLS = 0.0002020, max.steps.FPIRLS = 15,
lambda.selection.criterion = "grid", DOF.evaluation = NULL,
lambda.selection.lossfunction = NULL, lambdaS = NULL, lambdaT = NULL,
DOF.stochastic.realizations = 100, DOF.stochastic.seed = 0,
DOF.matrix = NULL, GCV.inflation.factor = 1, lambda.optimization.tolerance = 0.05,
inference.data.object.time=NULL)
```
## Arguments







<span id="page-76-0"></span>lambda.selection.lossfunction

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

lambdaS A scalar or vector of spatial smoothing parameters.

lambdaT A scalar or vector of temporal smoothing parameters.

DOF.stochastic.realizations

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

#### DOF.stochastic.seed

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

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

### GCV.inflation.factor

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

#### lambda.optimization.tolerance

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

#### inference.data.object.time

An [inferenceDataObjectTime](#page-48-0) that stores all the information regarding inference over the linear and nonlinear parameters of the model. This parameter needs to be consistent with covariates and mesh dimension number, otherwise will be discarded. If set and well defined, the function will have in output the inference results. It is suggested to create this object via [inferenceDataObjectTimeBuilder](#page-49-0) function, so that the object is guaranteed to be well defined.

## Value

A list with the following variables:

- fit.FEM.time A FEM.time object that represents the fitted spatio-temporal field.
- PDEmisfit.FEM.time A FEM.time object that represents the misfit of the penalized PDE.
- beta If covariates is not NULL, a matrix with number of rows equal to the number of covariates and number of columns equal to length of lambda. The jth column represents the vector of regression coefficients when the smoothing parameter is equal to lambda[j].
- <span id="page-77-0"></span>edf If GCV is TRUE, a scalar or matrix with the trace of the smoothing matrix for each combination of the smoothing parameters specified in lambdaS and lambdaT.
- stderr If GCV is TRUE, a scalar or matrix with the estimate of the standard deviation of the error for each combination of the smoothing parameters specified in lambdaS and lambdaT.
- GCV If GCV is TRUE, a scalar or matrix with the value of the GCV criterion for each combination of the smoothing parameters specified in lambdaS and lambdaT.
- bestlambda If GCV is TRUE, a 2-elements vector with the indices of smoothing parameters returning the lowest GCV
- ICestimated If FLAG\_PARABOLIC is TRUE and IC is NULL, a list containing a FEM object with the initial conditions, the value of the smoothing parameter lambda returning the lowest GCV and, in presence of covariates, the estimated beta coefficients
- bary.locations A barycenter information of the given locations if the locations are not mesh nodes.
- inference A list set only if a well defined [inferenceDataObjectTime](#page-48-0) is passed as parameter to the function; contains all inference outputs required:
	- p\_values list of lists set only if at least one p-value is required; contains the p-values divided by implementation:
		- wald list containing all the Wald p-values required, in the same order of the type list in inference.data.object.time. If one-at-the-time tests are required, the corresponding item is a vector of p values ordered as the rows of coeff matrix in inference.data.object.time.
		- speckman list containing all the Speckman p-values required, in the same order of the type list in inference.data.object.time. If one-at-the-time tests are required, the corresponding item is a vector of p values ordered as the rows of coeff matrix in inference.data.object.time.
		- eigen\_sign\_flip list containing all the Eigen-Sign-Flip p-values required, in the same order of the type list in inference.data.object.time. If one-at-the-time tests are required, the corresponding item is a vector of p values ordered as the rows of coeff matrix in inference.data.object.time.
	- CI list of lists set only if at least one confidence interval is required; contains the confidence intervals divided by implementation:
		- wald list containing all the Wald confidence intervals required, in the same order of the type list in inference.data.object.time. Each item is a matrix with 3 columns and p rows, p being the number of rows of coeff matrix in inference.data.object.time; each row is the CI for the corresponding row of coeff matrix.
		- speckman list containing all the Speckman confidence intervals required, in the same order of the type list in inference.data.object.time. Each item is a matrix with 3 columns and p rows, p being the number of rows of coeff matrix in inference.data.object.time; each row is the CI for the corresponding row of coeff matrix.

## References

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

## <span id="page-78-0"></span>sphere3Ddata 79

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

### Examples

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

#### Description

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

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

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

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