Package 'kpcaIG'

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Title Variables Interpretability with Kernel PCA

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Description

The kernelized version of principal component analysis (KPCA) has proven to be a valid nonlinear alternative for tackling the nonlinearity of biological sample spaces. However, it poses new challenges in terms of the interpretability of the original variables. 'kpcaIG' aims to provide a tool to select the most relevant variables based on the kernel PCA representation of the data as in Briscik et al. (2023) <doi:10.1186/s12859-023-05404-y>. It also includes functions for 2D and 3D visualization of the original variables (as arrows) into the kernel principal components axes, highlighting the contribution of the most important ones.

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Imports grDevices, rgl, kernlab, ggplot2, stats, progress, viridis, WallomicsData, utils

NeedsCompilation no

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kernelpca *Kernel Principal Components Analysis*

Description

Kernel Principal Components Analysis, a nonlinear version of principal component analysis obtrained through the so-called kernel trick.

Usage

```
kernelpca(data, kernel = "vanilladot", kpar = list(), features = 0)
```

Arguments

data	The data matrix organized by rows. Users should scale the data appropriately before applying this function, if relevant.
kernel	The kernel function used for the analysis. It can be chosen from the following strings: • 'rbfdot': Radial Basis kernel function "Gaussian" • 'polydot': Polynomial kernel function • 'vanilladot': Linear kernel function • 'tanhdot': Hyperbolic tangent kernel function
kpar	The list of hyper-parameters (kernel parameters) used with the kernel function. The valid parameters for each kernel type are as follows: • sigma: inverse kernel width for the Radial Basis kernel function "rbfdot". • degree, scale, offset for the Polynomial kernel function "polydot". • scale, offset for the Hyperbolic tangent kernel function "tanhdot".
features	The number of features (kernel principal components) to use for the analysis. Default: 0 , (all)

Value

kernelpca returns an S4 object of formal class kpca as in library(kernlab) containing the principal component vectors along with the corresponding eigenvalues.

pcv	pcv a matrix containing the principal component vectors (column wise)
eig	The corresponding eigenvalues
rotated	The original data projected (rotated) on the principal components
xmatrix	The original data matrix

References

Scholkopf B., Smola A. and Muller K.R. (1998) Nonlinear component analysis as a kernel eigenvalue problem. Neural Computation, 10, 1299-1319.

Examples

```
# Example
library(WallomicsData)
library(kpcaIG)
library(ggplot2)
library(kernlab)
Transcriptomics_Stems_s <- scale(Transcriptomics_Stems)

kpca_tan <-  kernelpca(as.matrix(Transcriptomics_Stems_s),
                          kernel = "tanhdot",
                          kpar = list(scale = 0.0001, offset = 0.01))


ggplot(data = data.frame(rotated(kpca_tan), Genetic_Cluster),
       aes(x = X1, y = X2, shape = Genetic_Cluster)) +
  geom_point(size = 2, aes(color = Genetic_Cluster)) +
  xlab("1st kernel PC") +
  ylab("2nd kernel PC") +
  labs(color = "Genetic_Cluster", shape = "Genetic_Cluster") +
  theme_minimal()


ggplot(data = data.frame(rotated(kpca_tan), Ecotype),
       aes(x = X1, y = X2, shape =  Ecotype)) +
  geom_point(size = 2, aes(color =  Ecotype)) +
  xlab("1st kernel PC") +
  ylab("2nd kernel PC") +
  labs(color = " Ecotype", shape = " Ecotype") +
  theme_minimal()


#Equivalently with function plot_kpca2D

plot_kpca2D(kpca_tan, groups = Genetic_Cluster)
plot_kpca2D(kpca_tan, groups = Ecotype)
```

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kpca_igrad *KPCA-IG: Variables Interpretability in Kernel PCA*

Description

KPCA-IG, kernel pca interpetable gradient. It is the fuction that gives the feature ranking, from the most to the least relevant variable. The ranking is obtained through the kernel's partial derivatives computation. A score, which corresponds to the score mean among the sample points, is assigned to each input feature.

Usage

```
kpca_igrad(kpca_result, dim, mean_type = "arithmetic", trim_ratio = 0.1)
```

Arguments

kpca_result	The result of the previously obtained kernel PCA analysis.
dim	Number of kernel principal component to use for the computation of the scores. It should be less or equal to the number of component of the kPCA.
mean_type	Type of mean. Possible values are "arithmetic", "geometric", "harmonic", "median", or "trimmed". Default = "arithmetic"
trim_ratio	For mean_type == "trimmed", it is the fraction (0 to 0.5) of scores to be trimmed from each end before the mean is computed for a more robust to outliers arithmetic mean computation.

Value

A data frame containing the sorted variables and their scores sorted in decreasing order.

References

Briscik, M., Dillies, MA. & Déjean, S. Improvement of variables interpretability in kernel PCA. BMC Bioinformatics 24, 282 (2023). DOI: doi:10.1186/s1285902305404y

Examples

```
library(WallomicsData)
library(kpcaIG)

Transcriptomics_Stems_s <- scale(Transcriptomics_Stems)

kpca_tan <-  kernelpca(as.matrix(Transcriptomics_Stems_s),
                          kernel = "tanhdot",
                          kpar = list(scale = 0.0001, offset = 0.01))

#Compute the most relevant genes based on the first two components of kpca_tan

kpca_ig_tan <- kpca_igrad(kpca_tan, dim = c(1,2))
head(kpca_ig_tan)
```

---

plot_kpca2D *2D Kernel PCA Plot with Variables Representation*

Description

plot_kpca2D allows to visualize an original variable of interest in the specified principal components. The variable is displayed as an arrow, showing its relevance in the relative position of each sample point in the kernel component space.

Usage

```
plot_kpca2D(kpca_result, target_variable = NULL, groups = NULL, scale = 100,
  components = c(1, 2), arrow_col = "#D3D3D3",
  main_title = "Kernel principal component analysis",
  point_size = 2, arrow_thickness = 0.5, text_size = 16,
  legend_text_size = 11, axis_text_size = 12)
```

Arguments

kpca_result	The result of the previously obtained kernel PCA analysis
target_variable	A string indicating the name of the variable of interest to visualize as arrows on the kernel PCA plot. Default: NULL
groups	A vector indicating the grouping of data points, if applicable. Default: NULL
scale	Coefficient to adjust the lengths of the arrows. Default: 100
components	A numeric vector of length 2 specifying the indices of the components to plot. Default: c(1, 2)
arrow_col	Colour of the arrows. Default: '#D3D3D3'
main_title	Graph title. Default: "Kernel principal component analysis"
point_size	Sample points size. Default: 2
arrow_thickness	Arrows size. Default: 0.5
text_size	Text size. Default: 16
legend_text_size	Legend text size. Default: 11
axis_text_size	Axes text size. Default: 12

Value

Provides a 2D plot of class ggplot that displays the sample points projected onto the specified kernel principal component axes, with the variables of interest represented as arrows.

References

Briscik, M., Dillies, MA. & Déjean, S. Improvement of variables interpretability in kernel PCA. BMC Bioinformatics 24, 282 (2023). DOI: doi:10.1186/s1285902305404y. Variables representation as in Reverter, F., Vegas, E. & Oller, J.M. Kernel-PCA data integration with enhanced interpretability. BMC Syst Biol 8 (Suppl 2), S6 (2014). DOI: doi:10.1186/1752-0509-8-S2-S6

Examples

```
library(WallomicsData)
library(kpcaIG)

Transcriptomics_Stems_s <- scale(Transcriptomics_Stems)
```

```
kpca_tan <-  kernelpca(as.matrix(Transcriptomics_Stems_s),
                          kernel = "tanhdot",
                          kpar = list(scale = 0.0001, offset = 0.01))

# Compute the most relevant genes based on the first two components of kpca_tan

kpca_ig_tan <- kpca_igrad(kpca_tan, dim = c(1,2))
head(kpca_ig_tan)

# Visualize the kpca plot.
plot_kpca2D(kpca_tan, groups = Ecotype)

# Visualize the most relevant variable (gene) according to kpca_igrad, "AT4G12060".

plot_kpca2D(kpca_tan, "AT4G12060", groups = Ecotype, scale = 1000, components = c(1, 2))

# Visualize using the second and third component

plot_kpca2D(kpca_tan, "AT4G12060", groups = Ecotype, scale = 1000, components = c(2, 3))

#The selected gene shows upper expression in the samples with genotype type Col.
```

`plot_kpca3D` *3D Kernel PCA Plot with Variables Representation*

Description

`plot_kpca3D` allows to visualize an original variable of interest in the first three principal components. The variable is displayed as an arrow, showing its relevance in the relative position of each sample point in the kernel component space.

Usage

```
plot_kpca3D(kpca_result, target_variable = NULL, groups, scale=1,
type = "s", size = 3/4, arrow_col = "#999999",
angles = 12, main = NULL)
```

Arguments

`kpca_result`	The result of the previously obtained kernel PCA analysis.
`target_variable`	A string indicating the name of the variable to visualize as arrows on the kernel PCA plot. Default: NULL
`groups`	A vector indicating the grouping of data points, if applicable. Default: NULL
`scale`	Coefficient to adjust the lengths of the arrows. Default 1
`type`	A character indicating the type of point for the observations. Supported types are: 'p' for points, 's' for spheres. Default: 's'

size	The size of the plotted points. Default: 3/4
arrow_col	Colour of the arrows. Default: '#999999
angles	Number of barbs of the arrows. Default: 12
main	Graph title. Default: NULL

Value

Provides an interactive 3D plot that displays the sample points projected onto the first three kernel principal component axes, with the variables of interest represented as arrows.

References

Briscik, M., Dillies, MA. & Déjean, S. Improvement of variables interpretability in kernel PCA. BMC Bioinformatics 24, 282 (2023). DOI: doi:10.1186/s1285902305404y. Variables representation as in Reverter, F., Vegas, E. & Oller, J.M. Kernel-PCA data integration with enhanced interpretability. BMC Syst Biol 8 (Suppl 2), S6 (2014). DOI: doi:10.1186/1752-0509-8-S2-S6

Examples

```
library(WallomicsData)
library(kpcaIG)

Transcriptomics_Stems_s <- scale(Transcriptomics_Stems)

kpca_tan <-  kernelpca(as.matrix(Transcriptomics_Stems_s),
                          kernel = "tanhdot",
                          kpar = list(scale = 0.0001, offset = 0.01))

#Compute the most relevant genes based on the first two components of kpca_tan

kpca_ig_tan <- kpca_igrad(kpca_tan, dim = c(1,2))
head(kpca_ig_tan)


# Visualize the kpca plot.

plot_kpca3D(kpca_tan, groups = Ecotype)

#Visualize the most relevant variable (gene) according to kpca_igrad, "AT4G12060".

plot_kpca3D(kpca_tan, "AT4G12060", groups = Ecotype, scale = 1000)

#The selected gene shows upper expression in the samples with genotype type Col.
```

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