

Package ‘prinsurf’

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Type Package

Title Principal Surface Contour Biplots

Version 2.0

Description Fits principal surfaces, the two-dimensional generalisation of the principal curves of Hastie and Stuetzle (1989) [doi:10.1080/01621459.1989.10478797](https://doi.org/10.1080/01621459.1989.10478797), and displays them as biplots in which each variable is read off the contour lines of its fitted surface coordinate function. Sample predictivity, the proportion of a sample's squared length that is reconstructed by the fitted surface, is reported as a per-sample diagnostic of how well the surface represents the data.

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URL <https://raeesaganey91.github.io/prinsurf/>,
<https://github.com/RaeesaGaney91/prinsurf>

BugReports <https://github.com/RaeesaGaney91/prinsurf/issues>

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Depends R (>= 4.1.0)

Imports stats, graphics, grDevices

Suggests testthat (>= 3.0.0), knitr, rmarkdown, biplotEZ

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contour_predictive_error
<i>Contour reading error</i>

Description

For each variable, the root-mean-square difference between the value read from the variable’s contour lines at each sample’s biplot position (as [predict.prinsurf](#) does) and the sample’s actual value. This measures how accurately a variable can be recovered by reading its contours, combining the surface’s lack of fit for that variable with the small loss from interpolating between contour lines; lower is better, in the units of the working data. Samples that fall outside the supported part of the contour grid cannot be read and are excluded; their number is returned as the attribute “n.unread”.

Usage

```
contour_predictive_error(object)
```

Arguments

object A “prinsurf” object.

Value

A named numeric vector of per-variable RMS contour-reading errors, with the mean over all variables as the attribute “overall” and the number of unreadable samples as the attribute “n.unread”.

See Also

[predictivity](#) for whole-sample reconstruction.

fitted.prinsurf	<i>Fitted (reconstructed) values from a principal surface</i>
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Description

Returns the fitted surface values $\hat{f}_j(\lambda_i)$ for every sample and variable: the point on the surface at which sample i sits, written back in the coordinates of the original variables. Row i is the surface's reconstruction of sample i – what the fit says the sample would be if it lay exactly on the surface – and the residual $x_i - \hat{f}(\lambda_i)$ is the part of the sample the surface does not capture, which is what [predictivity](#) summarises.

Usage

```
## S3 method for class 'prinsurf'
fitted(object, ...)
```

Arguments

object	A "prinsurf" object.
...	Ignored.

Details

Values are in the working units used for fitting: centred, and divided by each variable's standard deviation if the surface was fitted with `scale = TRUE`. This is the scale on which residuals and [predictivity](#) are computed. [predict.prinsurf](#) differs in two ways: it reads values off the plotted contour grid rather than evaluating the coordinate functions exactly, and it returns them on the variables' original scales.

Value

An $n \times p$ matrix of fitted values, in working (centred, optionally scaled) units.

See Also

[predictivity](#) for the per-sample quality of this reconstruction, and [predict.prinsurf](#) for the values a reader obtains from the contours.

plot.prinsurf	<i>Plot a principal-surface biplot</i>
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Description

Draws the sample coordinates. If `vars` is given, draws one panel per named variable, each showing the sample coordinates together with that variable's contour lines - the surface's analogue of a biplot axis, read by interpolating between contour lines rather than by projection onto a single calibrated axis. With no `vars`, a single panel of sample coordinates is drawn with no contours.

Usage

```
## S3 method for class 'prinsurf'
plot(
  x,
  vars = NULL,
  group = NULL,
  col_contour = "grey40",
  nlevels = 6,
  pch = 16,
  cex = 0.7,
  asp = 1,
  main = NULL,
  outer_main = NULL,
  ...
)
```

Arguments

<code>x</code>	A "prinsurf" object.
<code>vars</code>	Variables to contour, one panel each (default: none – a bare scatter of sample coordinates).
<code>group</code>	Optional factor to colour the sample points.
<code>col_contour</code>	Colour for the contour lines.
<code>nlevels</code>	Number of contour levels per panel.
<code>pch, cex</code>	Point symbol and size for samples.
<code>asp</code>	Aspect ratio of each panel; the default 1 keeps the two surface coordinates on a common scale, so distances in the biplot are comparable in every direction.
<code>main</code>	Panel title(s), replacing the default (the variable's name, or no title when <code>vars</code> is not given). A single string titles every panel; a vector titles the panels in the order of <code>vars</code> and is recycled to that length. Use "" for no panel titles.
<code>outer_main</code>	A single title for the figure as a whole, drawn in the outer margin above the panels. Can be combined with <code>main</code> , which titles the individual panels.
<code>...</code>	Passed to each panel's initial plot.

Value

Invisibly, vars.

Examples

```
set.seed(1)
s <- runif(120, -1, 1); t <- runif(120, -1, 1)
X <- cbind(x = s, y = t, z = 0.7 * s + 0.9 * t^2) +
  matrix(rnorm(360, 0, 0.03), 120, 3)
fit <- prinsurf(X, max.iter = 6)

## default: each panel is titled with its variable's name
plot(fit, vars = c("x", "z"))

## your own panel titles, and a title for the figure as a whole
plot(fit, vars = c("x", "z"),
     main = c("First coordinate", "Third coordinate"),
     outer_main = "Principal-surface biplot")

## a title on a single, contour-free panel
plot(fit, main = "Sample coordinates")
```

predict.prinsurf	<i>Predict all variables from the biplot contours</i>
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Description

Reads every variable's value for every sample off that variable's contour lines at the sample's biplot position λ_i – the same interpolation used to draw the contours in [plot.prinsurf](#). Values come from the contour grid alone: a sample whose position is not covered by the supported part of the grid has no contours to read, and is returned as NA for every variable.

Usage

```
## S3 method for class 'prinsurf'
predict(object, ...)
```

Arguments

object	A "prinsurf" object.
...	Ignored.

Value

An $n \times p$ matrix of values read from the contours, on the variables' original scales, with NA rows where the biplot cannot be read.

See Also

`contour_predictive_error` to measure this reading against the variables' actual values, and `fitted.prinsurf` for the surface's own reconstruction of the data.

predictivity	<i>Sample predictivity of a principal-surface biplot</i>
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Description

For each sample, the proportion of its squared length reconstructed by the fitted surface, $1 - \|x_i - \hat{f}(\lambda_i)\|^2 / \|x_i\|^2$. This is the principal-surface analogue of biplot sample predictivity and is read from the sample's position on the surface.

Usage

```
predictivity(object)
```

Arguments

object A "prinsurf" object.

Value

A numeric vector of per-sample predictivities (with the overall mean as the attribute "overall").

prinsurf	<i>Fit a principal surface</i>
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Description

Fits a two-dimensional principal surface to a numeric data matrix using the iterative expectation / projection algorithm of Hastie and Stuetzle (1989), with the coordinate functions estimated by local regression (loess).

Usage

```
prinsurf(X, max.iter = 10, span = 0.6, scale = FALSE, verbose = FALSE)
```

Arguments

X	A numeric matrix or data frame, $n \times p$. Column names are used as variable names; if absent, V1, V2, ... are assigned.
max.iter	Maximum number of expectation/projection iterations.
span	The loess span (α) used for the coordinate functions.
scale	Logical; if TRUE each variable is standardised to unit standard deviation before fitting (recommended when variables are on very different scales). Variables are always centred.
verbose	Logical; print the relative change and residual sum of squares at each iteration.

Value

An object of class "prinsurf": a list with elements `lambda` (the $n \times 2$ surface coordinates of the samples), `fj.mat` (the fitted surface coordinates of the samples in the working units), `models` (the per-variable loess coordinate functions), `varnames`, `center`, `scale`, `span` and `iterations`.

References

Hastie, T. and Stuetzle, W. (1989) Principal curves. *Journal of the American Statistical Association* **84**, 502–516.

Examples

```
set.seed(1)
s <- runif(120, -1, 1); t <- runif(120, -1, 1)
X <- cbind(x = s, y = t, z = 0.7 * s + 0.9 * t^2) +
  matrix(rnorm(360, 0, 0.03), 120, 3)
fit <- prinsurf(X, max.iter = 6)
fit
```

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