

Package ‘polyreg’

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Title Polynomial Regression

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Description Automate formation and evaluation of polynomial regression models. The motivation for this package is described in 'Polynomial Regression As an Alternative to Neural Nets' by Xi Cheng, Bohdan Khomtchouk, Norman Matloff, and Pete Mohanty (<[arXiv:1806.06850](https://arxiv.org/abs/1806.06850)>).

License GPL (>= 2)

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Depends R (>= 3.5)

URL <https://github.com/matloff/polyreg>

BugReports <https://github.com/matloff/polyreg/issues>

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FSR

*FSR***Description**

FSR

Usage

```
FSR(Xy, max_poly_degree = 3, max_interaction_degree = 2,
     outcome = NULL, linear_estimation = FALSE,
     threshold_include = 0.01, threshold_estimate = 0.001,
     min_models = NULL, max_fails = 2, standardize = FALSE,
     pTraining = 0.8, file_name = NULL, store_fit = "none",
     max_block = 250, noisy = TRUE, seed = NULL)
## S3 method for class 'FSR'
summary(object, estimation_overview = TRUE,
         results_overview = TRUE, model_number = NULL, ...)
## S3 method for class 'FSR'
print(x, ...)
```

Arguments

Xy matrix or data.frame; outcome must be in final column. Categorical variables (> 2 levels) should be passed as factors, not dummy variables or integers, to ensure the polynomial matrix is constructed properly.

max_poly_degree highest power to raise continuous features; default 3 (cubic).

max_interaction_degree highest interaction order; default 2 (allow $x_i * x_j$). Also interacts each level of factors with continuous features.

outcome Treat y as either 'continuous', 'binary', 'multinomial', or NULL (auto-detect based on response).

linear_estimation Logical: model outcome as linear and estimate with ordinary least squares? Recommended for speed on large datasets even if outcome is categorical. (For multinomial outcome, this means treated response as vector.) If FALSE, estimator chosen based on 'outcome' (i.e., OLS for continuous outcomes, glm() to estimate logistic regression models for 'binary' outcomes, and nnet::multinom() for 'multinomial').

<code>threshold_include</code>	minimum improvement to include a recently added term in the model (change in fit originally on 0 to 1 scale). -1.001 means 'include all'. Default: 0.01. (Adjust R^2 for linear models, Pseudo R^2 for logistic regression, out-of-sample accuracy for multinomial models. In latter two cases, the same adjustment for number of predictors is applied as pseudo- R^2 .)
<code>threshold_estimate</code>	minimum improvement to keep estimating (pseudo R^2 so scale 0 to 1). -1.001 means 'estimate all'. Default: 0.001.
<code>min_models</code>	minimum number of models to estimate. Defaults to the number of features (unless $P > N$).
<code>max_fails</code>	maximum number of models to FSR() can fail on computationally before exiting. Default == 2.
<code>standardize</code>	if TRUE (not default), standardizes continuous variables.
<code>pTraining</code>	portion of data for training
<code>file_name</code>	If a file name (and path) is provided, saves output after each model is estimated as an .RData file. ex: <code>file_name = "results.RData"</code> . See also <code>store_fit</code> for options as to how much to store in the outputted object.
<code>store_fit</code>	If <code>file_name</code> is provided, FSR() will return coefficients, measures of fit, and call details. Save entire fit objects? Options include "none" (default, just save those other items), "accepted_only" (only models that meet the threshold), and "all".
<code>max_block</code>	Most of the linear algebra is done recursively in blocks to ease memory management. Default 250. Changing up or down may slow things...
<code>noisy</code>	display measures of fit, progress, etc. Recommended.
<code>seed</code>	Automatically set but can also be passed as parameter.
<code>estimation_overview</code>	logical: describe how many models were planned, sample size, etc.?
<code>results_overview</code>	logical: give overview of best fit model, etc?
<code>model_number</code>	If non-null, an integer indicating which model to display a summary of.
<code>object</code>	an FSR object, can be used with <code>predict()</code> .
<code>x</code>	an FSR object, can be used with <code>print()</code> .
<code>...</code>	ignore.

Value

list with slope coefficients, model and estimation details, and measures of fit (object of class 'FSR').

Examples

```
out <- FSR(mtcars)
```

 getPoly

Get polynomial terms

Description

Generate polynomial terms of predictor variables for a data frame or data matrix.

Usage

```
getPoly(xdata = NULL, deg = 1, maxInteractDeg = deg,
        Xy = NULL, standardize = FALSE,
        noisy = TRUE, intercept = FALSE, returnDF = TRUE,
        modelFormula = NULL, retainedNames = NULL, ...)
```

Arguments

xdata	Data matrix or data frame without response variable. Categorical variables (> 2 levels) should be passed as factors, not dummy variables or integers, to ensure the polynomial matrix is constructed properly.
deg	The max degree of power terms. Default 1 so just returns model matrix by default.
maxInteractDeg	The max degree of nondummy interaction terms. $x_1 * x_2$ is degree 2. $x_1^3 * x_2^2$ is degree 5. Implicitly constrained by deg. For example, if deg = 3 and maxInteractDegree = 2, $x_1^1 * x_2^2$ (i.e., degree 3) will be included but $x_1^2 * x_2^2$ (i.e., degree 4) will not.
Xy	The dataframe with the response in the final column (provide xdata or Xy but not both). Categorical variables (> 2 levels) should be passed as factors, not dummy variables or integers, to ensure the polynomial matrix is constructed properly.
standardize	Standardize all continuous variables? (Default: FALSE.)
noisy	Output progress updates? (Default: TRUE.)
intercept	Include intercept? (Default: FALSE.)
returnDF	Return a data.frame (as opposed to model.matrix)? (Default: TRUE.)
modelFormula	Internal use. Formula used to generate the training model matrix. Note: anticipates that polynomial terms are generated using internal functions of library(polyreg). Also, providing modelFormula bypasses deg and maxInteractDeg.
retainedNames	Internal use. colnames of polyMatrix object\$xdata. Requires modelFormula be inputted as well.
...	Additional arguments to be passed to model.matrix() via polyreg:::model_matrix(). Note na.action = "na.omit".

Details

The `getPoly` function takes in a data frame or data matrix and generates polynomial terms of predictor variables.

Note the subtleties involving dummy variables. The square, cubic and so on terms are the same as the original variable, and the various duplicates must be eliminated.

Similarly, after dummy variable are created from a categorical variable having more than two levels, the resulting columns will be orthogonal to each other. In almost all cases, this argument should be set to `TRUE` at the training stage, and then in predictions one should use the vector of names in the component in the return value; `predict.polyFit` does the latter automatically.

Note: If a column that is an R factor has levels with spaces in the names, this will interfere with the parsing, and must be avoided.

Value

The return value of `getPoly` is a `polyMatrix` object. This is an S3 class containing a `model.matrix` `xdata` of the generated polynomial terms. The predictor variables have column names `V1`, `V2`, etc. The object also contains `modelFormula`, the formula used to construct the model matrix, and `XtestFormula`, the formula which should be used out-of-sample (when `y_test` is not available).

Examples

```
N <- 125
rawdata <- data.frame(x1 = rnorm(N),
                     x2 = rnorm(N),
                     group = sample(letters[1:5], N, replace=TRUE),
                     z = sample(c("treatment", "control"), N, replace=TRUE),
                     result = sample(c("win", "lose", "tie"), N, replace=TRUE))

head(rawdata)

P <- length(levels(rawdata$group)) - 1 +
      length(levels(rawdata$z)) - 1 +
      length(levels(rawdata$result)) - 1 +
      sum(unlist(lapply(rawdata, is.numeric)))

# quadratic polynomial, includes interactions
# since maxInteractDeg defaults to deg
X <- getPoly(rawdata, 2)$xdata
ncol(X) # 40

# cubic polynomial, no interactions
X <- getPoly(rawdata, 3, 1)$xdata
ncol(X) # 13

# cubic polynomial, interactions
X <- getPoly(rawdata, 3, 2)$xdata
ncol(X) # 58

# cubic polynomial, interactions
X <- getPoly(rawdata, 3)$xdata
ncol(X) # 101
```

```

# making final column the response variable, y
# results in TRUE (fewer columns)
ncol(getPoly(Xy=rawdata, deg=2)$xdata) < ncol(getPoly(rawdata, 2)$xdata)

# preparing polynomial matrices for crossvalidation
# getPoly() returns a polyMatrix() object containing XtestFormula
# which should be used to ensure factors are handled correctly out-of-sample
Xtrain <- getPoly(rawdata[1:100,],2)
Xtest <- getPoly(rawdata[101:125,], 2, modelFormula = Xtrain$XtestFormula)

```

misc

Miscellaneous

Description

Utilities

Usage

```
toFactors(df, cols)
```

Arguments

df	A data frame.
cols	A vector of column numbers.

Details

The toFactors function converts each df column in cols to a factor, returns new version of df. Should be used on categorical variables stored as integer codes before calling the library's main functions, including getPoly, FSR, or polyFit.

polyFit

Polynomial Fit

Description

Fit polynomial regression using a linear or logistic model; predict new data.

Usage

```

polyFit(xy, deg, maxInteractDeg=deg, use = "lm", pcaMethod=NULL,
        pcaLocation='front', pcaPortion=0.9, glmMethod="one",
        return_xy=FALSE, returnPoly=FALSE, noisy=TRUE)
## S3 method for class 'polyFit'
predict(object, newdata, ...)

```

Arguments

xy	Data frame with response variable in the last column. In the classification case, response is class ID, stored in a vector, not as a factor. Categorical variables (> 2 levels) should be passed as factors, not dummy variables or integers, to ensure the polynomial matrix is constructed properly.
deg	The max degree for polynomial terms.
maxInteractDeg	The max degree of interaction terms.
use	Set to 'lm' for linear regression, 'glm' for logistic regression, or 'mvrlm' for multivariate-response lm.
pcaMethod	NULL for no PCA. For PCA, can be either 'prcomp' (use the prcomp function) or 'RSpectra' (use the eigs function in the RSpectra package).
pcaLocation	In case PCA is applied, specify 'front' to have PCA calculated before forming polynomials, otherwise 'back'.
pcaPortion	If less than 1.0, use as many principal components so as to achieve this portion of total variance. Otherwise, use this many components. In the 'RSpectra' case, this value must be an integer of 1 or more.
glmMethod	Defaults to "one."
newdata	Data frame, one row for each "X" to be predicted. Must have the same column names as in xy (without "Y").
object	An item of class 'polyFit' containing output. Can be used with predict().
return_xy	return data? Default: FALSE
returnPoly	return polyMatrix object? Defaults to FALSE since may be quite large.
noisy	Logical: display messages?
...	Additional arguments for getPoly().

Details

The `polyFit` function calls `getPoly` to generate polynomial terms from predictor variables, then fits the generated data to a linear or logistic regression model. (Powers of dummy variables will not be generated, other than degree 1, but interaction terms will be calculated.)

If `pcaMethod` is not NULL, a principal component analysis is performed before or after generating the polynomials.

When logistic regression for classification is indicated, with more than two classes, All-vs-All or One-vs-All methods, coded 'all' and 'one', can be applied to deal with multiclass problem. Multinomial logit ('multilog') is also available.

Under the 'mvrlm' option in a classification problem, `lm` is called with multivariate response, using `cbind` and dummy variables for class membership as the response. Since predictors are used to form polynomials, this should be a reasonable model, and is much faster than 'glm'.

Value

The return value of `polyFit()` is a `polyFit` object. The original arguments are retained, along with the fitted models and so on.

The prediction function `predict.polyFit` returns the predicted value(s) for newdata. It also contains probability for each class as an attribute named `prob`. In the classification case, these will be the predicted class labels, 1,2,3,...

Examples

```
N <- 125
xyTrain <- data.frame(x1 = rnorm(N),
                     x2 = rnorm(N),
                     group = sample(letters[1:5], N, replace=TRUE),
                     score = sample(100, N, replace = TRUE) # final column is y
                     )

pfOut <- polyFit(xyTrain, 2)

# 4 new test points
xTest <- data.frame(x1 = rnorm(4),
                  x2 = rnorm(4),
                  group = sample(letters[1:5], 4, replace=TRUE))

predict(pfOut, xTest) # returns vector of 4 predictions

# spot checks
stopifnot(length(predict(pfOut, xTest)) == nrow(xTest))
```

`predict.FSR`

predict.FSR

Description

`predict.FSR`

Usage

```
## S3 method for class 'FSR'
predict(object, newdata, model_to_use = NULL,
        standardize = NULL, noisy = TRUE, ...)
```

Arguments

<code>object</code>	FSR output. Predictions will be made based on <code>object\$best_formula</code> unless <code>model_to_use</code> is provided (as an integer).
<code>newdata</code>	New Xdata.
<code>model_to_use</code>	Integer optionally indicating a model to use if <code>object\$best_formula</code> is not selected. Example: <code>model_to_use = 3</code> will use <code>object\$models\$formula[3]</code> .

<code>standardize</code>	Logical—standardize numeric variables? (If NULL, the default, bypasses and decides based on <code>object\$standardize</code> .)
<code>noisy</code>	Display output?
<code>...</code>	ignore

Value

`y_hat` (predictions using chosen model estimates).

Examples

```
out <- FSR(mtcars[1:30,])
forecast <- predict(out, mtcars[31:nrow(mtcars),])
```

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