Package 'smof'

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Description Starting from a given object representing a fitted model (within a certain set of model classes) whose linear predictor includes some ordered factor(s) among the explanatory variables, a new model is constructed and fitted where each named factor is replaced by a single numeric score, suitably chosen so that the new variable produces a fit comparable with the standard methodology based on a set of polynomial contrasts. Two variants of the present approach have been developed, one in each of the next references: Azzalini (2023) <doi:10.1002 sta4.624="">, (2024) <doi:10.48550 arxiv.2406.15933="">.</doi:10.48550></doi:10.1002>
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smof-package

Description

Starting from a given object representing a fitted model (within a certain set of model classes) whose linear predictor includes some ordered factor(s) among the explanatory variables, a new model is constructed and fitted where each named factor is replaced by a single numeric score, suitably chosen so that the new variable produces a fit comparable with the standard methodology based on a set of polynomial contrasts.

Details

The DESCRIPTION file:

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	improved optimization

Author(s)

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References

Azzalini, A. (2023). On the use of ordered factors as explanatory variables. *Stat* **12**, e624. doi:10.1002/ sta4.624

Examples

```
library(datasets)
data(esoph)
contrasts(esoph$agegp, 2) <- contr.poly(6) # optional
contrasts(esoph$tobgp, 1) <- contr.poly(4) # optional
obj1 <- glm(cbind(ncases, ncontrols) ~ agegp + tobgp + alcgp, family=binomial(), data=esoph)
out0 <- smof(obj1, esoph, "alcgp")
print(summary(out0$object))</pre>
```

```
smof
```

Scoring Methodology for Ordered Factors

Description

Starting from an object representing a fitted model whose linear predictor includes some ordered factor(s) among the explanatory variables, a new model is constructed where each named factor is replaced by a single numeric score, suitably chosen so that the new variable produces a data fit comparable with the standard methodology based on a set of polynomial contrasts.

Usage

Arguments

object	an object produced by a fitting function; see 'Details' below for specification of the admissible classes of objects.
data	the data frame used for producing object.
factors	a character vector with the names of the ordered factors of data which must be converted to numeric scores.
scoring	a list which selects the type of scoring technques and related ingredients. Its key component is the character string scoring\$type with possible values "distr" and "spline"; the other components of the list depend on this value, and are de- scribed in the 'Details'. If scoring is missing, the default value list(type="distr", family="gh") is used.
fast.fit	a logical value (default value: FALSE) indicating whether a fast-fitting procedure must be used. This option is available only under certain circumstances specified in the 'Details' below.
original	a logical value (default value: FALSE) indicating whether the original object must be included in the returned object.

opt.control	a list passed to optim as its control argument. It must not be used to turn the minimization problem into a maximization one.
trace	a logical value (default value: FALSE) indicating whether details of the iterative procedure for parameter estimation must be printed at each iteration.

Details

In its original formulation, function smof implements the methodology proposed by Azzalini (2023), briefly summarized in the 'Background' section. It is recommended to read at least that section in case the referenced paper is not examined. The published paper has open access. Later on, in version 1.2.0 of **smof**, a variant methodology has been included, based on the use of splines instead of quantile functions, presented in Azzalini (2024).

Start from an object obtained as the outcome from some fitting procedure, whose linear predictor includes one or more ordered factor(s) among the explanatory variables. For each ordered factor whose name is included in vector factors, a suitable vector of numeric scores is constructed. The selection process examines the quantiles of the members of a specified parametric class of distributions and selects the member with optimizes (i.e. minimizes) a suitable target criterion. To avoid trivialities, each factor in vector factors must have at least three levels.

There are two quite different options to build the numeric scores assigned to an ordered factor. The selection of one of these options is made via the component type of the list scoring, which can be either "distr" or "spline". The other components of scoring depends on the chosen type and are described below.

If scoring\$type="distr", the numeric scores are obtained as quantiles of a probability distribution belonging to a certain parametric family; this route corresponds to the original construction of smof, following Azzalini (2023). The admissible parametric families are all obtained by monotonic transformations of a standard normal variate. Specifically, the admissible families and corresponding strings to be specified in scoring\$family are as follows:

Johnson's S_U	"SU"
Tukey's g-and-h	"gh", "g-and-h"
Jones and Pewsey's sinh-arcsinh	"sinh-arcsinh","SAS"

where either string name can be used when two of them are indicated. All these families involve two parameters for shape regulation; location and scale parameters are not considered, because irrelevant for our purposes. Of the two shape parameters, the first one regulates asymmetry and can take any value, while the second one regulates tail thickness and must be positive. In each case, the adopted parameterization is the 'standard' one, but explicit specifications are provided in the reference below. The same family is employed for all the components of factors.

If scoring\$type="spline", the numeric scores are obtained via a monotonic spline function. Specifically, the scores are generated using splinefun with method="monoH.FC". Since currently this is the only admissible form of spline, it does not need to be specified. What must be specified is scoring\$in.knots, the number of internal knots between the fixed extremal knots 1 and K, if K denotes the number of levels of any given factor. Hence scoring\$in.knots should be an integer vector with as many components as factors; if a shorter vector is supplied, its values will be recycled. Since each internal knot involves the selection of two numeric values, the total number of fitted parameters will equal the sum of twice the in.knots values, summed over the components of factors.

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Estimation of the transformation parameters is performed by minimization, performed by the optimizer optim, of a suitable target criterion, which depends on class(object). The admissible classes for object are currently as follows, listed along the corresponding target criteria:

class	fitting function (package)	target criterion
lm	lm (stats)	sum of squared residuals
mlm	lm (stats)	[see below]
glm	glm (stats)	deviance
survreg	survreg (survival)	-loglikelihood
coxph	coxph (survival)	-loglikelihood
coxph.penal	coxph (survival)	-loglikelihood

For an object of class mlm, the target function is formed by summing terms where the contribution from the *j*-th response variable is $(1 - R_j^2)$, where R_j^2 is the r-squared statistic for that component of the fitted model. Note that, in the case of a single response variable, its $(1 - R^2)$ value is equivalent, up to an algebraic transformation, to the sum of squared residuals used for lm objects; hence the chosen target criterion for mlm models is a direct extension of the one for lm's. The above list of classes may be expanded in the future, depending on feedback.

In certain cases, models involving a large number of parameters for regulation of the scores transformation(s) can lead to difficulties at the optimization step, which is performed by optim. This situation may be flagged by the message

Non-zero error code returned by optim:...

In these circumstances, one direction for improvement is to make use of the argument opt.control for better tuning the working of optim. In more problematic cases, the axiliary function smof_refit is provided to improve upon an initial fitting.

The rest of this section is slightly of more technical nature, and it may be not of interest to the casual user, especially if the option fast.fit=TRUE is not selected. Operationally, estimation of the scoring\$family parameters is performed via optimization of the pertaining target criterion, as indicated by the table above. For each candidate set of parameters, each factor included in factors is replaced by values determined by the quantiles of scoring\$family and the current parameters. The name of the new constructed variable is formed by adding .score to the original name. For instance, an ordered factor called ordfac is replaced by the numeric variable ordfac.score both in the linear predictor of object and in the data frame. A call to update using the modified linear predictor and data delivers a new fitting, with attached a value of the target criterion. An interative optimization process the target criterion leads to the estimated parameters of scoring\$family with a corresponding fitted model.

There are in fact two variants of the procedure. What has been just described refers to the more 'general' variant form. However, in the prominent cases of an object of class lm or glm, the procedure can be speeded-up by setting fast.fit=TRUE, provided the fitted model is of a basic form, that is, a model specification via a formula, and a family in the glm case, without non-basic arguments such as offset, subset and alike. If these non-basic arguments are included in the object call, they are ignored for estimation of the scoring\$family parameter. However, they are included for producing the final object returned by the function. With this option, the sequence of calls to lm and glm involved by the iterative search procedure is replaced by faster calls to lm.fit

and glm.fit. Correspondingly, the internal target function (target.fit) is slightly different from the one used on the more general case (target.gen). Since the selection of the parameters involves an iterative process with dimensionality equal to twice the length of factors and each iteration involves a new data fitting process, the saving in execution time can be substantial in some cases.

Value

A list with the following components:

call	the calling statement
new.object	an updated version of the original object, with the components of factors in the model replaced by new variables; this object is itself a list, whose structure depends on its class.
new.data	a new data frame where the ordered factors are replaced by numeric variables representing scores.
scoring	a list similar to the input argument with the addition of the estimates of the parameters.
factor.scores	a list of numeric vectors with the scores assigned to the levels of each factor.
original.factor	S
	a list with the names and the levels of the original factors.
target.criterio	n
	the final value of the target criterion used for fitting.
opt	the list returned by optim.

Background

The methodology proposed in the reference below deals with the presence of ordered factors used as explanatory variables, hence included in the linear predictor of some model under consideration. For any given ordered factor with K levels, say, a set of K numeric scores is introduced, with a certain value assigned to each factor level. In the end, the original factor is effectively replaced by a numeric variable. This scheme represents a refinement of the elementary scoring system based on the basic sequence 1, ..., K, which constitutes a simple time-honoured option to deal with ordered factors, but it is not always appropriate.

There are two variants of the methodology, selected with the value of the component type of the list scoring. Here we summarize the working of the original formulation, selected by setting type="distr". The actual construction of numeric scores proceeds by selecting K quantiles of a distribution belonging to some parametric family. The adoption of a sufficiently flexible parametric family helps to find a scoring system best suited for the data under consideration, hence improving upon the basic sequence I, ..., K. A concomitant product of this scheme is the identification of numeric values which indicate how the K levels are "really" spaced. Combining these two features, the key feature of the proposal is interpretability of the construction.

The proposed method represents an alternative to the use of polynomial contrasts, which is the default action taken by R for ordered factors; see the documentation of contr.poly.

In the proposed logic, the constructed scores are intended to be used, and interpreted, without further manipulation. Hence, for instance, building a polynomial form using one such variable would diverge somewhat from the proposed logic, although still conceivable. With a single numeric

smof

variable to represent a given factor, one cannot expect to achieve the same numerical fit to the data as obtained the polynomial contrasts built for the original factor, when these constrasts involve high degrees polynomials, and correspondingly several parameters. However, a range of numerical explorations has indicated that in many cases the resulting fit is equal or similar to the one achieved via polynomial constrasts, with non-negligible simplification in the model specification, and easier interpretation,

In a nutshell, the aim of the approach is to achieve a satisfactory data fit while improving an model parsimony, with simple interpretability of the score system.

The alternative variant of the methodology is selected by setting scoring\$type="spline". The underlying principle is similar to the one just described, but it makes use of splines instead of quantile functions. Its operational working is described in the 'Details'.

For a more comprehensive exposition and discussion, see the references below.

Note

For subsequent computations on the object returned by smof, difficulties may arise if the call to the fitting function does not set model=TRUE. This is not a problem with lm and glm, if their default setting model=TRUE has not been modified. The default setting of coxph is instead model=FALSE. This implies, for instance, that issuing the survival command survfit(smof4\$new.object), right after running the code of Example 4 below, would cause an error. The main route to avoid this issue is to set model=TRUE in the call to the fitting function, that is, coxph or whaterever function is used. Alternatively, if one does not want to refit an already existing object, there exist various ways to overcome this snag; the simplest one is to write

new.data <- smof4\$new.data
s <- survfit(smof4\$new.object)</pre>

This indication is temporary and it may be superseded by a different design in future versions of the package.

Author(s)

Adelchi Azzalini

References

Azzalini, A. (2023). On the use of ordered factors as explanatory variables. *Stat* **12**, e624. doi:10.1002/ sta4.624

Azzalini, A. (2024). On the use of splines for representing ordered factors. *arXiv:2406.15933*, doi:10.48550/arXiv.2406.15933

See Also

smof_refit, optim, contr.poly, update, splinefun, plogis, lm, lm.fit, glm, glm.fit

Examples

```
# Example 1, reconstructs Tables 1 and 2 (second part) of the reference
message("--- Example 1: esoph data ---")
library(datasets)
data(esoph)
contrasts(esoph$agegp, 2) <- contr.poly(6)</pre>
contrasts(esoph$tobgp, 1) <- contr.poly(4)</pre>
fit1 <- glm(cbind(ncases, ncontrols) ~ agegp + tobgp + alcgp, family=binomial(), data=esoph)</pre>
message("original fit:")
print(summary(fit1))
smof1 <- smof(fit1, esoph, "alcgp")</pre>
# to select the Johnson's S_U family of distributions, write instead:
# smof1 <- smof(fit1, esoph, "alcgp", scoring=list(type="distr", family="SU"))</pre>
print(smof1, type="b", pch=20, col=4)
print(summary(smof1))
plot(smof1)
#
# Example 2 , reconstructs Tables 3 and 4 (first part) of the reference
if(require(ggplot2, quietly=TRUE)) {
message("--- Example 2: diamonds data ---")
data(diamonds, package="ggplot2")
dmd <- data.frame(diamonds[seq(1, 53940, by=100),]) # use a subset of the data
dmd <- dmd[-c(518, 519, 523),] # remove three outliers</pre>
contrasts(dmd$clarity, 3) <- contr.poly(8)</pre>
contrasts(dmd$color, 4) <- contr.poly(7)</pre>
contrasts(dmd$cut, 1) <- contr.poly(5)</pre>
fit2 <- lm(sqrt(price) ~ carat + clarity + color + cut, data=dmd)</pre>
smof2 <- smof(fit2, dmd, c("color", "clarity"))</pre>
message("smof fit:")
print(smof2)
print(summary(smof2))
plot(smof2, which="clarity")
} # end diamonds example
#
# Example 3
if(require(survival, quietly=TRUE)) {
message("--- Example 3: lung data ---")
lung0 <- lung
lung0$ph.karno <- ordered(lung0$ph.karno)</pre>
contrasts(lung0$ph.karno, 3) <- contr.poly(6)</pre>
fit3 <- survreg(Surv(time, status) ~ ph.karno, data=lung0)</pre>
smof3 <- smof(fit3, lung0, "ph.karno")</pre>
print(summary(smof3))
plot(smof3) # Karnofsky scores do not seem to be linearly spaced
#
message("--- Example 4: PBC data ---")
data(pbc, package="survival")
pbc$stage <- ordered(pbc$stage)</pre>
fit4 <- coxph(Surv(time) ~ strata(status) + stage, data=pbc)</pre>
smof4 <- smof(fit4, data=pbc, factors="stage")</pre>
print(summary(smof4))
plot(smof4)
```

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smof-methods

} # end of survival examples

smof-methods *Methods for* smof *objects*

Description

The list of methods that apply to smof objects

Usage

```
## S3 method for class 'smof'
print(x, ...)
## S3 method for class 'smof'
plot(x, which, ...)
## S3 method for class 'smof'
summary(object, ...)
## S3 method for class 'summary.smof'
print(x, ...)
## S3 method for class 'smof'
predict(object, newdata, ...)
```

Arguments

object	an object returned by smof.
x	an object returned by smof, except for print.summary.smof where x is the outcome of summary.smof.
which	either a vector or a two-elements list; see 'Details' for full specification.
newdata	a data frame which includes ordered factors with the same names and levels as those in the data frame used to produce object; see 'Details' for additional information.
	arguments passsed through to other methods.

Details

There are two main parts in the outcome of summary.smof. One is the outcome of the selection of the factor(s) transformation(s); the other part, denoted Final fitting call, represents the newly fitted model with the original ordered factors replaced by numeric scores. The corresponding data.frame, denoted new.data, is one of the components of the object returned by smof.

If which is a character vector, its components are interpreted as names of the factors in the calling statement of the object to be plotted, producing a set of graphs where the numeric scores of each named factor are plotted versus the equally spaced ticks associated to the original level names. The same effect is obtained when which is a numeric vector of integers, which then select the corresponding components of the factors sequence.

If which is a list, its first element is assumed to be a vector having the meaning just described. After the pertaining set of graphs has been completed, the second element of the list is passed to the plotting method for the object produced by the model fitting procedure. Currently this option operates only for objects which inherits from class lm; specifically, it works for objects originated by a call to lm or to glm.

With predict.smof, the outcome of a smof fit is applied to new data frame which includes ordered factors analogous to those used to compute the smof transformation. Only the factors of newdata with the same name as those processed by smof to produce object are examined. The levels of these factors must coincide with or be a subset of those of the original data frame.

Note the difference between the role played by predict.smof and the one of predict methods for most other classes. Usually the returned values pertain to the response variable, or to some related entity, while here the outcome refers to explanatory variables.

Value

For summary.smof, a list of class summary.smof. For predict.smof, a data frame. For plot.smof, NULL with graphical side effects.

Author(s)

Adelchi Azzalini

See Also

smof, lm, glm

Examples

```
library(datasets)
data(esoph)
contrasts(esoph$agegp, 2) <- contr.poly(6)
contrasts(esoph$tobgp, 1) <- contr.poly(4)
fit1 <- glm(cbind(ncases, ncontrols) ~ agegp + tobgp + alcgp, family=binomial(), data=esoph)
smof1 <- smof(fit1, esoph, "alcgp")
print(smof1)
print(summary(smof1))
plot(smof1, type="b", pch=19, col="blue")
plot(smof1, which=list(1, 1:4))
predict(smof1, newdata=esoph[seq(1, 88, by=8), ])</pre>
```

smof_refit

Re-fitting an existing smof model for improved optimization

Description

Given a model fitted by smof, this function helps to improve the achieved fitting level by launching new numerical optimizations of the underlying target function. The search process is initiated with parameters randomly chosen in the vicinity of those of the object provided.

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smof_refit

Usage

```
smof_refit(object, searches = 10, sd = 1, opt.control=list(), verbose = 1)
```

Arguments

object	an object returned by a call to smof; that call must include the argument original=TRUE.
searches	a positive integer representing the number of attempted searches.
sd	the standard deviation of the zero-mean normal variates used for earch search to generate the initial set of parameters from which to initiate a numerical opti- mization.
opt.control	a list passed to optim as its control argument. It must not be used to turn the minimization problem into a maximization one.
verbose	an integer regulating the amount of messages displayed; it can be 0 (no messages), 1 (default value) or larger than 1 for a very verbose outcome.

Details

The fitting step of a smof call, performed with the aid of optim, can run into problems with complex optimizations, typically when many parameters regulating the numeric scores are involved. This situation may be flagged by the message

Notice. Non-zero error code returned by optim:...

It is expected that the main usage of this function is to improve the fitting of models produced with scoring\$type="spline", since this option generates model with more parameters than an equivalent model with scoring\$type="distr".

Since the initial values of each optimization step are randomly generated, one may want to make a preliminary call to set.seed. if replicability of the results is required.

Value

an object of class smof

See Also

smof, optim, set.seed

Examples

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