Package ‘mcprofile’

February 20, 2015

Title Multiple Contrast Profiles
Date 2014-11-17
Version 0.2-1
Author Daniel Gerhard
Maintainer Daniel Gerhard <dgerhard@gmail.com>
Description Calculation of signed root deviance profiles for linear combinations of parameters in a generalized linear model. Multiple tests and simultaneous confidence intervals are provided.
Depends ggplot2
Imports quadprog, mvtnorm, splines
LazyLoad yes
LazyData yes
License GPL (>= 2)
VignetteBuilder knitr
Suggests knitr, multcomp, MASS
NeedsCompilation no
Repository CRAN
Date/Publication 2014-11-17 00:47:56

R topics documented:

aphidlight .................................................. 2
CItrans ...................................................... 2
confint.mcprofile ......................................... 3
tta ............................................................. 4
hoa ............................................................. 4
mcprofile ..................................................... 5
mcprofileControl .......................................... 7
orglm.fit ..................................................... 8
summary.mcprofile ......................................... 10
toxinLD ...................................................... 11
wald .......................................................... 13
Index

aphidlight  Aphid attraction at different light intensities

Description

The light intensity (mumol/m^2s) of green LED light should be found, which attracts Aphis fabae best. At each of 4 replicates 20 aphids were put in a lightproof box with only one green LED at one end. All aphids that fly to the green light are caught and counted after a period of 5h. This procedure was replicated for 9 increasing light intensities.

Usage

data(aphidlight)

Format

A data frame with 36 observations on the following 3 variables.

  light  a numeric vector denoting the concentration levels  
  black  a numeric vector with the number of aphids remaining in the box.  
  green  a numeric vector with the number of attracted aphids

References


CItrans  Transformation of Confidence Intervals

Description

Transformation of confidence interval estimates in mcpCI objects.

Usage

## S3 method for class 'mcpCI'
exp(x)
## S3 method for class 'mcpCI'
expit(x)

Arguments

x  An object of class mcpCI
Value
An object of class mcpCI with transformed estimates.

Author(s)
Daniel Gerhard

See Also
exp.confint.mcprofile

Description
Calculates simultaneous confidence intervals based on signed root deviance profiles from function mcpcalc.

Usage
```r
## S3 method for class 'mcprofile'
confint(object, parm, level = 0.95,
  adjust = c("single-step", "none", "bonferroni"),
  alternative = c("two.sided", "less", "greater"), ...)
```

Arguments
- `object`: An object of class mcprofile
- `parm`: Just ignore this...
- `level`: Simultaneous confidence level (1-alpha), default at 0.95
- `adjust`: a character string specifying the adjustment for multiplicity. "single-step" controlling the FWER utilizing a multivariate normal- or t-distribution; "none" for comparison-wise error rate; "bonferroni" applying a Bonferroni correction.
- `alternative`: a character string specifying if two- or one-sided confidence intervals should be computed

Value
An object of class mcpCI

Author(s)
Daniel Gerhard
**See Also**

`confint.glm`, `mcprofile`, `confint.glht`

---

**cta**  
*Cell transformation assay dataset*

**Description**

Balb/c 3T3 cells are treated with different concentrations of a carcinogen. Cells treated with a carcinogen do not stop proliferation. Number of foci (cell accumulations) are counted for 10 replicates per concentration level.

**Usage**

```r
data(cta)
```

**Format**

A data frame with 80 observations on the following 2 variables.

- **conc**: a numeric vector denoting the concentration levels
- **foci**: a numeric vector with the number of foci

**References**

Thomas C (2008): ECVAM data

---

**hoa**  
*Higher order asymptotics using the modified likelihood root*

**Description**

Transforms a signed root deviance profile to a modified likelihood root profile.

**Usage**

```r
hoa(object, maxstat=10)
```

**Arguments**

- **object**: An object of class `mcprofile`
- **maxstat**: Limits the statistic to a maximum absolute value (default=10)

**Value**

An object of class `mcprofile` with a hoa profile in the srdp slot.
mcprofile

Author(s)
Daniel Gerhard

See Also
mcprofile

Examples

```
# cell transformation assay example
#
str(cta)
## change class of cta$conc into factor
cta$conc <- factor(cta$conc, levels=unique(cta$conc))
ggplot(cta, aes(y=foci, x=conc)) +
  geom_boxplot() +
  geom_dotplot(binaxis = "y", stackdir = "center", binwidth = 0.2) +
  xlab("concentration")

# glm fit assuming a Poisson distribution for foci counts
# parameter estimation on the log link
# removing the intercept
fm <- glm(foci ~ conc-1, data=cta, family=poisson(link="log"))

### Comparing each dose to the control by Dunnett-type comparisons
# Constructing contrast matrix
library(multcomp)
CM <- contrMat(table(cta$conc), type="Dunnett")

# calculating signed root deviance profiles
(dmcp <- mcprofile(fm, CM))

# computing profiles for the modified likelihood root
hp <- hoa(dmcp)

plot(hp)

# comparing confidence intervals
confint(hp)
confint(dmcp)
```
Description

Calculates signed root deviance profiles given a \texttt{glm} or \texttt{lm} object. The profiled parameters of interest are defined by providing a contrast matrix.

Usage

\[
\text{mcprofile}(\text{object, CM, control} = \text{mcprofileControl}(), \text{grid}=\text{NULL})
\]

## S3 method for class 'lm'
\[
\text{mcprofile}(\text{object, CM, control}=\text{mcprofileControl}(), \text{grid}=\text{NULL})
\]

## S3 method for class 'glm'
\[
\text{mcprofile}(\text{object, CM, control}=\text{mcprofileControl}(), \text{grid}=\text{NULL})
\]

Arguments

- **object**: An object of class \texttt{glm} or \texttt{lm}
- **CM**: A contrast matrix for the definition of parameter linear combinations (CM \%\% coefficients(object)). The number of columns should be equal to the number of estimated parameters. Providing row names is recommendable.
- **control**: A list with control arguments. See \texttt{mcprofileControl}.
- **grid**: A matrix or list with profile support coordinates. Each column of the matrix or slot in a list corresponds to a row in the contrast matrix, each row of the grid matrix or element of a numeric vector in each list slot corresponds to a candidate of the contrast parameter. If NULL (default), a grid is found automatically similar to function \texttt{profile.glm}.

Details

The profiles are calculated separately for each row of the contrast matrix. The profiles are calculated by constrained IRWLS optimization, implemented in function \texttt{orglm}, using the quadratic programming algorithm of package \texttt{quadprog}.

Value

An object of class \texttt{mcprofile}. The slot \texttt{srdp} contains the profiled signed root deviance statistics. The \texttt{optpar} slot contains a matrix with profiled parameter estimates.

Author(s)

Daniel Gerhard

See Also

\texttt{profile.glm}, \texttt{glht.contrMat}, \texttt{confint.mcprofile}, \texttt{summary.mcprofile}, \texttt{solve.QP}
Examples

# cell transformation assay example
str(cta)
str(ccta)
str(cpga)
str(cggplt)
str(cgmp)
str(cmcp)

# ggplot(cta, aes(x=foci, y=conc)) +
# geom_boxplot() +
# geom_dotplot(binaxis = "y", stackdir = "center", binwidth = 0.2) +
# xlab("concentration")

# glm fit assuming a Poisson distribution for foci counts
# parameter estimation on the log link
# removing the intercept
fm <- glm(foci ~ conc-1, data=cta, family=poisson(link="log"))

### Comparing each dose to the control by Dunnett-type comparisons
### Constructing contrast matrix
library(multcomp)
CM <- contrMat(table(cpga$conc), type="Dunnett")

# calculating signed root deviance profiles
(dmcp <- mcprofile(fm, CM))
# plot profiles
plot(dmcp)
# confidence intervals
(ci <- confint(dmcp))
plot(ci)

mcprofileControl

mcprofile Control Arguments

Description

Control arguments for the mcprofile function

Usage

mcprofileControl(maxsteps=10, alpha=0.01, del=function(zmax) zmax/5)

Arguments

maxsteps Maximum number of points to be used for profiling each parameter.
alpha Highest significance level allowed for the profile t-statistics (Bonferroni adjusted)
Suggested change on the scale of the profile t-statistics. Default value chosen to allow profiling at about 10 parameter values.

Author(s)
Daniel Gerhard

See Also
mcprofile

Fitting Order-Restricted Generalized Linear Models

Description
orglm.fit is used to fit generalized linear models with restrictions on the parameters, specified by giving a description of the linear predictor, a description of the error distribution, and a description of a matrix with linear constraints. The quadprog package is used to apply linear constraints on the parameter vector.

Usage
orglm.fit(x, y, weights = rep(1, nobs),
           start = NULL, etastart = NULL, mustart = NULL,
           offset = rep(0, nobs), family = gaussian(),
           control = list(), intercept = TRUE, constr, rhs, nec)

Arguments
- **x, y**  
  x is a design matrix of dimension n * p, and y is a vector of observations of length n.
- **family**  
  a description of the error distribution and link function to be used in the model. This can be a character string naming a family function, a family function or the result of a call to a family function. (See family for details of family functions.)
- **weights**  
  an optional vector of ‘prior weights’ to be used in the fitting process. Should be NULL or a numeric vector.
- **start**  
  starting values for the parameters in the linear predictor.
- **etastart**  
  starting values for the linear predictor.
- **mustart**  
  starting values for the vector of means.
- **offset**  
  this can be used to specify an a priori known component to be included in the linear predictor during fitting. This should be NULL or a numeric vector of length equal to the number of cases. One or more offset terms can be included in the formula instead or as well, and if more than one is specified their sum is used. See model.offset.
control  a list of parameters for controlling the fitting process. For `orglm.fit` this is passed to `glm.control`.

intercept  logical. Should an intercept be included in the null model?

constr  a matrix with linear constraints. The columns of this matrix should correspond to the columns of the design matrix.

rhs  right hand side of the linear constraint formulation. A numeric vector with a length corresponding to the rows of constr.

nec  Number of equality constraints. The first nec constraints defined in constr are treated as equality constraints; the remaining ones are inequality constraints.

Details

Non-NULL weights can be used to indicate that different observations have different dispersions (with the values in weights being inversely proportional to the dispersions); or equivalently, when the elements of weights are positive integers $w_i$, that each response $y_i$ is the mean of $w_i$ unit-weight observations. For a binomial GLM prior weights are used to give the number of trials when the response is the proportion of successes: they would rarely be used for a Poisson GLM.

If more than one of `etastart`, `start` and `mustart` is specified, the first in the list will be used. It is often advisable to supply starting values for a quasi family, and also for families with unusual links such as `gaussian("log")`.

For the background to warning messages about ‘fitted probabilities numerically 0 or 1 occurred’ for binomial GLMs, see Venables & Ripley (2002, pp. 197–8).

Value

An object of class "glm" is a list containing at least the following components:

coefficients  a named vector of coefficients

residuals  the working residuals, that is the residuals in the final iteration of the IWLS fit. Since cases with zero weights are omitted, their working residuals are NA.

fitted.values  the fitted mean values, obtained by transforming the linear predictors by the inverse of the link function.

rank  the numeric rank of the fitted linear model.

family  the family object used.

linear.predictors  the linear fit on link scale.

deviance  up to a constant, minus twice the maximized log-likelihood. Where sensible, the constant is chosen so that a saturated model has deviance zero.

null.deviance  The deviance for the null model, comparable with deviance. The null model will include the offset, and an intercept if there is one in the model. Note that this will be incorrect if the link function depends on the data other than through the fitted mean: specify a zero offset to force a correct calculation.

iter  the number of iterations of IWLS used.

weights  the working weights, that is the weights in the final iteration of the IWLS fit.
description of glm.fit

Author(s)

Modification of the original glm.fit by Daniel Gerhard.

The original R implementation of glm was written by Simon Davies working for Ross Ihaka at the University of Auckland, but has since been extensively re-written by members of the R Core team.

The design was inspired by the S function of the same name described in Hastie & Pregibon (1992).

References


See Also

glm, solve.QP

summary.mcprofile Multiple Testing of General Hypotheses

**Description**

Multiple contrast testing based on signed root deviance profiles.

**Usage**

```r
## S3 method for class 'mcprofile'
summary(object, margin = 0, adjust = "single-step",
        alternative = c("two.sided", "less", "greater"), ...)
```
**toxinLD**

**Arguments**

- **object**: an object of class mcpProfile
- **margin**: test margin, specifying the right hand side of the hypotheses.
- **adjust**: a character string specifying the adjustment for multiplicity. "single-step" controlling the FWER utilizing a multivariate normal- or t-distribution; "none" for comparison-wise error rate, or any other method provided by `p.adjust`
- **alternative**: a character string specifying the alternative hypothesis.
- ...  

**Value**

An object of class mcpSummary

**Author(s)**

Daniel Gerhard

**See Also**

`mcpProfile`, `summary.glht`

---

**Description**

Increasing dose levels of a toxin, used as a pesticide for crop protection, is applied to non-target species. The lethal dose should be identified in this experiment. The dataset represents simulated data based on a real experiment.

**Usage**

`data(toxinLD)`

**Format**

A data frame with 6 observations on the following 3 variables.

- **dose**: a numeric vector denoting the toxin concentration levels
- **dead**: a numeric vector with the number of dead insects.
- **alive**: a numeric vector with the number of surviving insects.
Examples

```r
str(toxinLD)

# logistic regression on the logarithmic dose

toxinLD$logdose <- log(toxinLD$dose)
fm <- glm(cbind(dead, alive) ~ logdose, data=toxinLD, family=binomial(link="logit"))

# profiling

# contrast matrix
pdose <- seq(-1,2.3, length=7)
CM <- model.matrix(~ pdose)

# user defined grid to construct profiles
mcpgrid <- matrix(seq(-11.8, length=15), nrow=15, ncol=nrow(CM))
mc <- mcprofile(fm, CM, grid=mcpgrid)

# confidence interval calculation

# srdp profile
ci <- confint(mc)
ppdat <- data.frame(logdose=pdose)
ppdat$estimate <- fm$family$linkinv(ci$estimate$Estimate)
ppdat$lower <- fm$family$linkinv(ci$confint$lower)
ppdat$upper <- fm$family$linkinv(ci$confint$upper)
ppdat$method <- "profile"

# wald profile
wci <- confint(wald(mc))
wpdat <- ppdat
wpdat$estimate <- fm$family$linkinv(wci$estimate$Estimate)
wpdat$lower <- fm$family$linkinv(wci$confint$lower)
wpdat$upper <- fm$family$linkinv(wci$confint$upper)
wdat$method <- "wald"

# higher order approximation
hci <- confint(hoa(mc))
hpdat <- ppdat
hpdat$estimate <- fm$family$linkinv(hci$estimate$Estimate)
hpdat$lower <- fm$family$linkinv(hci$confint$lower)
hpdat$upper <- fm$family$linkinv(hci$confint$upper)
hpdat$method <- "hoa"

# combine results
pdat <- rbind(ppdat, wpdat, hpdat)
```
wald

Calculate Wald-Profiles

Description

Transforms a signed root deviance profile of a mcprofile object into a profile of Wald-type statistics

Usage

wald(object)

Arguments

object An object of class mcprofile

Value

An object of class mcprofile with a wald profile in the srdp slot.
Author(s)
Daniel Gerhard

See Also
mcprofile

Examples

```r
### cell transformation assay example ###
str(cta)
## change class of cta$conc into factor
cta$concf <- factor(cta$conc, levels=unique(cta$conc))

ggplot(cta, aes(y=foci, x=concf)) +
  geom_boxplot() +
  geom_dotplot(binaxis = "y", stackdir = "center", binwidth = 0.2) +
  xlab("concentration")

# glm fit assuming a Poisson distribution for foci counts
# parameter estimation on the log link
# removing the intercept
fm <- glm(foci ~ concf-1, data=cta, family=poisson(link="log"))

### Comparing each dose to the control by Dunnett-type comparisons
# Constructing contrast matrix
library(multcomp)
CM <- contrMat(table(cta$concf), type="Dunnett")

# calculating signed root deviance profiles
(dmcp <- mcprofile(fm, CM))
# computing profiles for the modified likelihood root
wp <- wald(dmcp)

plot(wp)

# comparing confidence intervals
confint(wp)
confint(dmcp)
```
Index

*Topic datasets
  aphidlight, 2
cia, 4
toxinLD, 11
*Topic htest
  confint.mcprofile, 3
  summary.mcprofile, 10
*Topic misc
  CItrans, 2
  hoa, 4
  mcprofile, 5
  mcprofileControl, 7
  wald, 13
*Topic models
  orglm.fit, 8
  aphidlight, 2
  CItrans, 2
  confint.glht, 4
  confint.glm, 4
  confint.mcprofile, 3, 3, 6
  contrMat, 6
  cia, 4
  exp, 3
  exp.mcpCI(CItrans), 2
  expit.mcpCI(CItrans), 2
  family, 8, 9
  glht, 6
  glm, 6, 10
  glm.control, 9
  hoa, 4
  lm, 6
  mcprofile, 4, 5, 5, 8, 11, 14
  mcprofileControl, 6, 7
  model.offset, 8
  offset, 8
  orglm.fit, 8
  p.adjust, 11
  profile.glm, 6
  quasi, 9
  solve.QP, 6, 10
  summary.glht, 11
  summary.mcprofile, 6, 10
  toxinLD, 11
  wald, 13

15