

# Package ‘mcprofile’

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**Title** Testing Generalized Linear Hypotheses for Generalized Linear Model Parameters by Profile Deviance

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## 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** R (>= 3.1.0), ggplot2

**Imports** quadprog, mvtnorm, splines

**LazyLoad** yes

**LazyData** yes

**License** GPL (>= 2)

**VignetteBuilder** knitr

**Suggests** knitr, markdown, multcomp, MASS

**RoxxygenNote** 6.0.1

**NeedsCompilation** no

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aphidlight	<i>Aphid attraction at different light intensities</i>
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## Description

The light intensity (mumol/m<sup>2</sup>s) 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

`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

Akyazi, G (2009): Zum Einfluss auf Lichtintensitaet und Lichtqualitaet (Hochleistungs-LEDs) auf das Verhalten von *Aphis fabae*. IPP MSc 19.

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confint.mcprofile	<i>Simultaneous Confidence Intervals for Multiple Contrast Profiles</i>
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## Description

Calculates simultaneous confidence intervals based on signed root deviance profiles from function [mcprofile](#).

**Usage**

```
## 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 utilising 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

**See Also**

[confint.glm](#), [mcprofile](#), [confint.glht](#)

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**cta***Cell transformation assay dataset*

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**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**

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

`exp.mcpCI`

*exp transformation of Confidence Intervals*

## Description

Exponential transformation of confidence interval estimates in mcpCI objects.

## Usage

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

## Arguments

`x` An object of class mcpCI

## Value

An object of class mcpCI with transformed estimates.

## See Also

[exp, confint.mcprofile](#)

Other confidence interval transformations: [expit.mcpCI](#)

`expit.mcpCI`

*Inverse logit transformation of Confidence Intervals*

## Description

Inverse logit transformation of confidence interval estimates in mcpCI objects.

## Usage

```
expit.mcpCI(x)
```

## Arguments

`x` An object of class mcpCI

## Value

An object of class mcpCI with transformed estimates.

**See Also**

[exp](#), [confint.mcprofile](#)

Other confidence interval transformations: [exp.mcpCI](#)

hoa

*Higher order asymptotics using the modified likelihood root*

**Description**

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

**Usage**

```
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.

**See Also**

[mcprofile](#)

**Examples**

```
#####
## 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
hp <- hoa(dmcp)

plot(hp)

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

```

**mcprofile***Construction of Multiple Contrast Profiles***Description**

Calculates signed root deviance profiles given a [glm](#) or [lm](#) object. The profiled parameters of interest are defined by providing a contrast matrix.

**Usage**

```

mcprofile(object, CM, control = mcprofileControl(), grid = NULL)

## S3 method for class 'glm'
mcprofile(object, CM, control = mcprofileControl(),
          grid = NULL)

## S3 method for class 'lm'
mcprofile(object, CM, control = mcprofileControl(),
          grid = NULL)

```

**Arguments**

<b>object</b>	An object of class <a href="#">glm</a> or <a href="#">lm</a>
<b>CM</b>	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.
<b>control</b>	A list with control arguments. See <a href="#">mcprofileControl</a> .
<b>grid</b>	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 <a href="#">profile.glm</a> .

## Details

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

## Value

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

## See Also

`profile.glm`, `glht`, `contrMat`, `confint.mcprofile`, `summary.mcprofile`, `solve.QP`

## Examples

```
#####
## 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))
# 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)
del	Suggested change on the scale of the profile t-statistics. Default value chosen to allow profiling at about 10 parameter values.

**See Also**

[mcprofile](#)

**orglm.fit**

*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

<code>x</code>	is a design matrix of dimension $n * p$
<code>y</code>	is a vector of observations of length $n$
<code>weights</code>	an optional vector of ‘prior weights’ to be used in the fitting process. Should be <code>NULL</code> or a numeric vector.
<code>start</code>	starting values for the parameters in the linear predictor.
<code>etastart</code>	starting values for the linear predictor.
<code>mustart</code>	starting values for the vector of means.
<code>offset</code>	this can be used to specify an <i>a priori</i> known component to be included in the linear predictor during fitting. This should be <code>NULL</code> or a numeric vector of length equal to the number of cases. One or more <code>offset</code> terms can be included in the formula instead or as well, and if more than one is specified their sum is used. See <code>model.offset</code> .
<code>family</code>	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 <code>family</code> for details of family functions.)
<code>control</code>	a list of parameters for controlling the fitting process. For <code>orglm.fit</code> this is passed to <code>glm.control</code> .
<code>intercept</code>	logical. Should an intercept be included in the <i>null</i> model?
<code>constr</code>	a matrix with linear constraints. The columns of this matrix should correspond to the columns of the design matrix.
<code>rhs</code>	right hand side of the linear constraint formulation. A numeric vector with a length corresponding to the rows of <code>constr</code> .
<code>nec</code>	Number of equality constraints. The first <code>nec</code> constraints defined in <code>constr</code> 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.
- prior.weights** the weights initially supplied, a vector of 1s if none were.
- df.residual** the residual degrees of freedom of the unconstrained model.
- df.null** the residual degrees of freedom for the null model.
- y** if requested (the default) the y vector used. (It is a vector even for a binomial model.)
- converged** logical. Was the IWLS algorithm judged to have converged?
- boundary** logical. Is the fitted value on the boundary of the attainable values?

### 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

- Dobson, A. J. (1990) *An Introduction to Generalized Linear Models*. London: Chapman and Hall.
- Hastie, T. J. and Pregibon, D. (1992) *Generalized linear models*. Chapter 6 of *Statistical Models in S* eds J. M. Chambers and T. J. Hastie, Wadsworth & Brooks/Cole.
- McCullagh P. and Nelder, J. A. (1989) *Generalized Linear Models*. London: Chapman and Hall.
- Venables, W. N. and Ripley, B. D. (2002) *Modern Applied Statistics with S*. New York: Springer.

### See Also

[glm](#), [solve.QP](#)

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<code>summary.mcprofile</code>	<i>Multiple Testing of General Hypotheses</i>
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## Description

Multiple contrast testing based on signed root deviance profiles.

## Usage

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

## Arguments

<code>object</code>	an object of class <code>mcprofile</code>
<code>margin</code>	test margin, specifying the right hand side of the hypotheses.
<code>adjust</code>	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 <code>p.adjust</code> .
<code>alternative</code>	a character string specifying the alternative hypothesis.
...	...

## Value

An object of class `mcpSummary`

## See Also

[mcprofile](#), [summary.glht](#)

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<code>toxinLD</code>	<i>Identifying the lethal dose of a crop protection product.</i>
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## 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

`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

```
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
mcgrid <- matrix(seq(-11,8,length=15), nrow=15, ncol=nrow(CM))
mc <- mcprofile(fm, CM, grid=mcgrid)

#####
## 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$upper)
wpdat$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)

#####
# estimating the lethal dose LD(25) #
#####

ld <- 0.25
pspf <- splinefun(ppdat$upper, pdose)
pll <- pspf(ld)
wspf <- splinefun(wpdat$upper, pdose)
wll <- wspf(ld)
hspf <- splinefun(hpdat$upper, pdose)
hll <- hspf(ld)

ldest <- data.frame(limit=c(pll, wll, hll), method=c("profile", "wald", "hoa"))

#####
# plot of intervals and LD(25) #
#####

ggplot(toxinLD, aes(x=logdose, y=dead/(dead+alive))) +
  geom_ribbon(data=pdat, aes(y=estimate, ymin=lower, ymax=upper,
                             fill=method, colour=method, linetype=method),
              alpha=0.1, size=0.95) +
  geom_line(data=pdat, aes(y=estimate, linetype=method), size=0.95) +
  geom_point(size=3) +
  geom_hline(yintercept=ld, linetype=2) +
  geom_segment(data=ldest, aes(x=limit, xend=limit, y=0.25, yend=-0.05,
                                linetype=method), size=0.6, colour="grey2") +
  ylab("Mortality rate")

```

**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.

**See Also**

[mcprofile](#)

**Examples**

```
#####
## 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)
```

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