

# R documentation

of ‘cfderiv.Rd’

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cfderiv	<i>Auto-constructing Frechet derivative of D-criterion based on general equivalence theorem</i>
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## Description

Auto-constructs Frechet derivative of D-criterion at  $M(\xi, \beta)$  and in direction  $M(\xi_x, \beta)$  where  $M$  is Fisher information matrix,  $\beta$  is vector of parameters,  $\xi$  is the interested design and  $\xi_x$  is a unique design which only has point  $x$ . The constructed Frechet derivative is an R function with argument  $x$ .

## Usage

```
cfderiv(ymean, yvar, param, points, weights)
```

## Arguments

ymean	a character string, formula of $E(y)$ with specific standard: characters b1, b2, b3, ... symbolize model parameters and x1, x2, x3, ... symbolize explanatory variables. See ‘Examples’.
yvar	a character string, formula of $Var(y)$ with specific standard as ymean. See ‘Details’ and ‘Examples’.
param	a vector of values of parameters which must correspond to b1, b2, b3, ... in ymean.
points	a vector of points which belong to design $\xi$ . See ‘Details’.
weights	a vector of $\xi$ points weights. The sum of weights should be 1; otherwise they will be normalized.

## Details

If response variables have the same constant variance, for example  $\sigma^2$ , then yvar must be 1.

Consider design  $\xi$  with  $n$   $m$ -dimensional points. Then, the vector of  $\xi$  points is

$$(x_1, x_2, \dots, x_i, \dots, x_n),$$

where  $x_i = (x_{i1}, x_{i2}, \dots, x_{im})$ . Hence the length of vector points is  $mn$ .

**Value**

cfderiv a function in which its argument is a vector  $x$ , an  $m$ -dimensional design point, and its output is the value of Frechet derivative at  $M(\xi, \beta)$  and in direction  $M(\xi_x, \beta)$ .

**Note**

A design  $\xi$  is D-optimal if and only if Frechet derivative at  $M(\xi, \beta)$  and in direction  $M(\xi_x, \beta)$  is greater than or equal to 0 on the design space. The equality must be achieved just at  $\xi$  points. Here,  $x$  is an arbitrary point on design space.

This function is applicable for models that can be written as  $E(Y_i) = f(x_i, \beta)$  where  $y_i$  is the  $i$ th response variable,  $x_i$  is the observation vector of the  $i$ th explanatory variables,  $\beta$  is the vector of parameters and  $f$  is a continuous and differentiable function with respect to  $\beta$ . In addition, response variables must be independent with distributions that belong to the Natural exponential family. Logistic, Poisson, Negative Binomial, Exponential, Richards, Weibull, Log-linear, Inverse Quadratic and Michaelis-Menten are examples of these models.

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**References**

- Masoudi, E., Sarmad, M. and Talebi, H. 2012, An Almost General Code in R to Find Optimal Design, In Proceedings of the 1st ISM International Statistical Conference 2012, 292-297.
- Kiefer, J. C. 1974, General equivalence theory for optimum designs (approximate theory), Ann. Statist., 2, 849-879.

**Examples**

```
## Logistic dose response model:
ymean <- "(1/(exp(-b2 * (x1 - b1)) + 1))"
yvar <- "(1/(exp(-b2 * (x1 - b1)) + 1))*(1 - (1/(exp(-b2 * (x1 - b1)) + 1)))"
func <- cfderiv(ymean, yvar, param = c(.9, .8), points = c(-1.029256, 2.829256),
  weights = c(.5, .5))
## plot func on the design interval to verify the optimality of the given design
x <- seq(-5, 5, by = .1)
plot(x, -func(x), type = "l")

## Inverse Quadratic model
ymean <- "x1/(b1 + b2 * x1 + b3 * (x1)^2)"
yvar <- "1"
func <- cfderiv(ymean, yvar, param = c(17, 15, 9), points = c(0.33, 1.37, 5.62),
  weights = rep(.33, 3))
## plot func on the design interval to verify the optimality of the given design
x <- seq(0, 15, by = .1)
plot(x, -func(x), type = "l")

#####
## In the following, ymean and yvar for some famous models are given:

## Inverse Quadratic model (another form):
ymean <- "(b1 * x1)/(b2 + x1 + b3 * (x1)^2)"
yvar <- "1"
```

```

## Logistic dose response model:
ymean <- "(1/(exp(-b2 * (x1 - b1)) + 1))"
yvar <- "(1/(exp(-b2 * (x1 - b1)) + 1)) * (1 - (1/(exp(-b2 * (x1 - b1)) + 1)))"

## Logistic model:
ymean <- "1/(exp(-b1 - b2 * x1) + 1)"
yvar <- "(1/(exp(-b1 - b2 * x1) + 1)) * (1 - (1/(exp(-b1 - b2 * x1) + 1)))"

## Poisson model:
ymean <- yvar <- "exp(b1 + b2 * x1)"

## Poisson dose response model:
ymean <- yvar <- "b1 * exp(-b2 * x1)"

## Weibull model:
ymean <- "b1 - b2 * exp(-b3 * x1^b4)"
yvar <- "1"

## Richards model:
ymean <- "b1/(1 + b2 * exp(-b3 * x1))^b4"
yvar <- "1"

## Michaelis-Menten model:
ymean <- "(b1 * x1)/(1 + b2 * x1)"
yvar <- "1"
#
ymean <- "(b1 * x1)/(b2 + x1)"
yvar <= "1"
#
ymean <- "x1/(b1 + b2 * x1)"
yvar <- "1"

## log-linear model:
ymean <- "b1 + b2 * log(x1 + b3)"
yvar <- "1"

## Exponential model:
ymean <- "b1 + b2 * exp(x1/b3)"
yvar <- "1"

## Emax model:
ymean <- "b1 + (b2 * x1)/(x1 + b3)"
yvar <- "1"

## Negative binomial model  $Y \sim \text{NB}(E(Y), \text{theta})$  where  $E(Y) = b1 \cdot \exp(-b2 \cdot x1)$ :
theta = 5
ymean <- "b1 * exp(-b2 * x1)"
yvar <- paste ("b1 * exp(-b2 * x1) * (1 + (1/", theta, ") * b1 * exp(-b2 * x1))" , sep = "")

## Linear regression model:
ymean <- "b1 + b2 * x1 + b3 * x2 + b4 * x1 * x2"
yvar = "1"

```

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