Package 'ppwdeming'

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Title Precision Profile Weighted Deming Regression

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Depends R (>= 3.6.0)

Suggests testthat (>= 3.0.0)

Imports stats

Description Weighted Deming regression, also known as ``errors-in-variable'' regression, is applied with suitable weights. Weights are modeled via a precision profile; functions are provided for implementing it in both known and unknown precision profile situations. The package provides tools for precision profile weighted Deming (PWD) regression.
It covers two settings – one where the precision profiles are known either from external studies or from adequate replication of the X and Y readings, and one in which there is a plausible functional form for the precision profiles but the exact function must be estimated from the (generally singlicate) readings.
The function set includes tools for: estimated standard errors (via jackknifing); standardized-residual analysis function with regression diagnostic tools for normality, linearity and constant variance; and an outlier analysis identifying significant outliers for closer investigation.
Further information on mathematical derivations and applications can be found on arXiv: Hawkins and Kraker (2025) <doi:10.48550/arXiv.2508.02888>.

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Contents

`PWD_get_gh` *Estimate of Variance Profile Functions (proportional)*

Description

This code estimates the variance profiles, assumed proportional, of the Rocke-Lorenzato form; also provides the resulting weighted Deming fit and residuals.

Usage

```
PWD_get_gh(X, Y, lambda=1, epsilon=1.e-8, printem=FALSE)
```

Arguments

`X`	the vector of predicate readings,
`Y`	the vector of test readings,
`lambda`	*optional* (default of 1) - the ratio of the X to the Y precision profile (defaults to 1),
`epsilon`	*optional* (default of 1.e-8) - convergence tolerance limit,
`printem`	*optional* - if TRUE, routine will print out results as a `message`.

Details

This workhorse routine optimizes the likelihood in the **unknown** g, h setting over its n+4 parameters (the two Rocke-Lorenzato precision profile parameters σ and κ, the intercept α and slope β, and the n latent true concentrations μ_i).

That is, the assumed forms are:

- predicate precision profile model: $g_i = var(X_i) = \lambda \left(\sigma^2 + [\kappa \cdot \mu_i]^2 \right)$ and
- test precision profile model: $h_i = var(Y_i) = \sigma^2 + [\kappa \cdot (\alpha + \beta \mu_i)]^2$.

Value

A list containing the following components:

`alpha`	the fitted intercept
`beta`	the fitted slope
`fity`	the vector of predicted Y
`mu`	the vector of estimated latent true values
`resi`	the vector of residuals
`sigma`	the estimate of the Rocke-Lorenzato σ
`kappa`	the estimate of the Rocke-Lorenzato κ
`like`	the -2 log likelihood L

Author(s)

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References

Hawkins DM and Kraker JJ. Precision Profile Weighted Deming Regression for Methods Comparison, on *Arxiv* (2025) doi:10.48550/arXiv.2508.02888

Rocke DM, Lorenzato S (2012). A Two-Component Model for Measurement Error in Analytical Chemistry. *Technometrics*, **37:2**:176-184.

Examples

```
# library
library(ppwdeming)

# parameter specifications
sigma <- 1
kappa <- 0.08
alpha <- 1
beta  <- 1.1
true  <- 8*10^((0:99)/99)
truey <- alpha+beta*true
# simulate single sample - set seed for reproducibility
set.seed(1039)
# specifications for predicate method
X     <- sigma*rnorm(100)+true *(1+kappa*rnorm(100))
# specifications for test method
Y     <- sigma*rnorm(100)+truey*(1+kappa*rnorm(100))

# fit with RL precision profile to estimate parameters
RL_gh_fit  <- PWD_get_gh(X,Y,printem=TRUE)
# RL precision profile estimated parameters
cat("\nsigmahat=", signif(RL_gh_fit$sigma,6),
    "and kappahat=", signif(RL_gh_fit$kappa,6))
```

PWD_inference *Weighted Deming Regression – Inference*

Description

This routine fits the regression, uses the jackknife to get its precision, and optionally prints it out. Currently implements Rocke-Lorenzato as the variance profile model.

Usage

```
PWD_inference(X, Y, lambda=1, MDL=NA, epsilon=1e-8, printem=FALSE)
```

Arguments

X	the vector of predicate readings,
Y	the vector of test readings,
lambda	*optional* (default of 1) - the ratio of the X to the Y precision profile.
MDL	*optional* (default to missing) - medical decision level(s),
epsilon	*optional* (default of 1.e-8) - convergence tolerance limit,
printem	*optional* - if TRUE, routine will print out results as a message.

Details

For the linear model relating the predicate and test readings, the standard errors of the estimators $\hat{\alpha}$, $\hat{\beta}$, and their covariance are estimated by the jackknife. The estimates of the intercept and slope are output, along with their standard errors and covariance.

These estimates are further used to estimate the predictions at the input MDL.

Value

A list containing the following components:

alpha	the fitted intercept
beta	the fitted slope
cor	the Pearson correlation between X and Y
fity	the vector of predicted Y
mu	the vector of estimated latent true values
resi	the vector of residuals
preresi	the vector of leave-one-out predicted residuals
sigma	the estimate of the Rocke-Lorenzato σ
kappa	the estimate of the Rocke-Lorenzato κ
like	the -2 log likelihood L
sealpha	the jackknife standard error of alpha

sebeta	the jackknife standard error of beta
covar	the jackknife covariance between alpha and beta
preMDL	the predictions at the MDL(s)
preMDLl	the lower confidence limit(s) of preMDL
preMDLu	the upper confidence limit(s) of preMDL

Author(s)

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References

Hawkins DM and Kraker JJ. Precision Profile Weighted Deming Regression for Methods Comparison, on *Arxiv* (2025) doi:10.48550/arXiv.2508.02888

Efron, B (1982). The jackknife, the bootstrap and other resampling plans. Society for Industrial and Applied Mathematics.

Examples

```
# library
library(ppwdeming)

# parameter specifications
sigma <- 1
kappa <- 0.08
alpha <- 1
beta  <- 1.1
true  <- 8*10^((0:99)/99)
truey <- alpha+beta*true
# simulate single sample - set seed for reproducibility
set.seed(1039)
# specifications for predicate method
X     <- sigma*rnorm(100)+true *(1+kappa*rnorm(100))
# specifications for test method
Y     <- sigma*rnorm(100)+truey*(1+kappa*rnorm(100))

# fit with RL precision profile to estimate parameters and variability
RL_inf <- PWD_inference(X,Y,MDL=12,printem=TRUE)
```

PWD_known *Weighted Deming Regression – general weights*

Description

This code is used for the setting of known precision profiles implemented in user-provided R functions called gfun and hfun.

Usage

```
PWD_known(X, Y, gfun, hfun, gparms, hparms, epsilon=1e-10,
          MDL=NA, getCI=TRUE, printem=FALSE)
```

Arguments

X	the vector of predicate readings,
Y	the vector of test readings,
gfun	a function with two arguments, a vector of size *n* and a vector of parameters,
hfun	a function with two arguments, a vector of size *n* and a vector of parameters,
gparms	a numeric vector containing any parameters referenced by gfun,
hparms	a numeric vector containing any parameters referenced by hfun,
epsilon	*optional* convergence tolerance limit,
MDL	*optional* medical decision level(s),
getCI	*optional* - allows for jackknifed standard errors on the regression and MDL,
printem	*optional* - if TRUE, routine will print out results as a message.

Details

The functions gfun and hfun are allowed as inputs, to support flexibility in specification of the forms of these variance functions. The known precision profiles specified by the functions gfun and hfun, when provided with estimated vectors of μ and $\alpha + \beta\mu$ respectively and with any required parameters, will produce the vectors g and h. These vectors are then integrated into the iterative estimation of the slope and intercept of the linear relationship between predicate and test readings.

Value

A list containing the following components:

alpha	the fitted intercept
beta	the fitted slope
cor	the Pearson correlation between X and Y
fity	the vector of predicted Y
mu	the vector of estimated latent true values
resi	the vector of residuals
scalr	the vector of scaled residuals using the specified g and h
like	the -2 log likelihood L
sealpha	the jackknife standard error of alpha
sebeta	the jackknife standard error of beta
covar	the jackknife covariance between alpha and beta
preMDL	the predictions at the MDL(s)
preMDLl	the lower confidence limit(s) of preMDL
preMDLu	the upper confidence limit(s) of preMDL

Author(s)

Douglas M. Hawkins, Jessica J. Kraker krakerjj@uwec.edu

Examples

```
# library
library(ppwdeming)

# parameter specifications
alpha <- 1
beta  <- 1.1
true  <- 8*10^((0:99)/99)
truey <- alpha+beta*true
# forms of precision profiles
gfun    <- function(true, gparms) {
  gvals = gparms[1]+gparms[2]*true^gparms[3]
  gvals
}
hfun    <- function(true, hparms) {
  hvals = hparms[1]+hparms[2]*true^hparms[3]
  hvals
}

# Loosely motivated by Vitamin D data set
g     <- 4e-16+0.07*true^1.27
h     <- 6e-2+7e-5*truey^2.2
# simulate single sample - set seed for reproducibility
set.seed(1039)
# specifications for predicate method
X     <- true +sqrt(g)*rnorm(100)
# specifications for test method
Y     <- truey+sqrt(h)*rnorm(100)

# fit with to estimate linear parameters
pwd_known_fit <- PWD_known(X, Y, gfun, hfun,
                           gparms=c(4e-16, 0.07, 1.27),
                           hparms=c(6e-2, 7e-5, 2.2),
                           printem=TRUE)
```

PWD_outlier *Weighted Deming Regression – Outlier scanning*

Description

This function tests for outliers from the fitted regression, and refits on a sanitized data set (with outliers removed).

Usage

```
PWD_outlier(X, Y, K, lambda=1, Pcut=0.01, printem=FALSE)
```

Arguments

X	the vector of predicate readings,
Y	the vector of test readings,
K	the maximum number of outliers to seek,
lambda	*optional* the ratio of the X to the Y precision profile (defaults to 1),
Pcut	*optional*, default 0.01 (1%), cutoff for statistical significance of Bonferroni P,
printem	*optional* - if TRUE, routine will print out results as a message.

Details

The method is modeled on the Rosner sequential ESD outlier procedure and assumes the sample is large enough to assume normality of the predicted residuals.

Value

A list containing the following components:

ndrop	the number of significant outliers
drop	a vector of the indices of the outliers
cor	the Pearson correlation between X and Y
cleancor	the Pearson correlation between cleaned X and Y (after outliers removed)
scalr	the scaled residuals of all cases from the sanitized fit
keep	logical vector identifying which cases retained in sanitized data set
basepar	the sigma, kappa, alpha, beta of the full data set
lastpar	the sigma, kappa, alpha, beta of the sanitized data set

Author(s)

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References

Hawkins DM and Kraker JJ. Precision Profile Weighted Deming Regression for Methods Comparison, on *Arxiv* (2025) doi:10.48550/arXiv.2508.02888

Hawkins DM (2008). *Outliers* in Wiley Encyclopedia of Clinical Trials, eds R. D'Agostino, L. Sullivan, and J. Massaro. Wiley, New York.

Examples

```
# library
library(ppwdeming)

# parameter specifications
sigma <- 1
kappa <- 0.08
alpha <- 1
beta  <- 1.1
true  <- 8*10^((0:99)/99)
truey <- alpha+beta*true
# simulate single sample - set seed for reproducibility
set.seed(1039)
# specifications for predicate method
X     <- sigma*rnorm(100)+true *(1+kappa*rnorm(100))
# specifications for test method
Y     <- sigma*rnorm(100)+truey*(1+kappa*rnorm(100))
# add some outliers
Y[c(1,2,100)] <- Y[c(1,2,100)] + c(7,4,-45)

# check for outliers, re-fit, and store output
outliers_assess <- PWD_outlier(X, Y, K=5, printem=TRUE)
```

PWD_resi *Fit Rocke-Lorenzato profile model to residuals*

Description

This routine fits the Rocke-Lorenzato precision profile model to the **residuals** from the fit (via PWD_inference).

Usage

```
PWD_resi(true, resi, epsilon=1e-5, printem=FALSE)
```

Arguments

true	the vector of values used to predict the precision – commonly X,
resi	the vector of residuals whose variance is thought to be a function of "true",
epsilon	*optional* (default of 1e-5) - convergence tolerance limit,
printem	*optional* - if TRUE, routine will print out results as a message.

Details

The Rocke-Lorenzato precision profile model is

$$SD^2 = \sigma_r^2 + (\kappa_r \cdot true)^2$$

for the *residuals* from a precision-profile model fit.

Under this model, the approach for reviewing residuals is to fit a variance profile model to the residuals r_i themselves. This function includes a check for the special cases of

- constant variance ($\kappa_r = 0$) - in this case, one could switch to the simpler unweighted Deming model;
- and of constant coefficient of variation ($\sigma_r = 0$) - in this case, one could switch to the constant CV weighted Deming model.

using chi-squared tests.

Value

A list containing the following components:

`sigmar`	the estimate of σ_r
`kappar`	the estimate of κ_r
`like`	the likelihood
`scalr`	the scaled residuals
`poolsig`	the maximum likelihood estimate of σ_r if κ_r =0
`poolkap`	the maximum likelihood estimate of κ_r if σ_r =0
`tests`	the chi-squared test statistics for κ_r=0 and for σ_r=0
`Pvals`	the P values for the two chi-squared tests

Author(s)

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References

Hawkins DM and Kraker JJ. Precision Profile Weighted Deming Regression for Methods Comparison, on *Arxiv* (2025) doi:10.48550/arXiv.2508.02888

Hawkins DM (2014). A Model for Assay Precision. *Statistics in Biopharmaceutical Research*, **6**, 263-269. http://dx.doi.org/10.1080/19466315.2014.899511

Examples

```
# library
library(ppwdeming)

# parameter specifications
sigma <- 1
kappa <- 0.08
```

```
alpha <- 1
beta  <- 1.1
true  <- 8*10^((0:99)/99)
truey <- alpha+beta*true
# simulate single sample - set seed for reproducibility
set.seed(1039)
# specifications for predicate method
X     <- sigma*rnorm(100)+true *(1+kappa*rnorm(100))
# specifications for test method
Y     <- sigma*rnorm(100)+truey*(1+kappa*rnorm(100))

# fit the model and store output
RL_gh_fit  <- PWD_get_gh(X,Y,printem=FALSE)
# run the residual analysis from the model output
post  <- PWD_resi(X, RL_gh_fit$resi, printem=TRUE)
```

PWD_RL *Weighted Deming – Rocke-Lorenzato - known sigma, kappa*

Description

This code fits the weighted Deming regression on predicate readings (X) and test readings (Y), with user-supplied Rocke-Lorenzato ("RL") parameters sigma (σ) and kappa (κ).

Usage

```
PWD_RL(X, Y, sigma, kappa, lambda=1, epsilon=1e-6)
```

Arguments

X	the vector of predicate readings,
Y	the vector of test readings,
sigma	the RL sigma parameter,
kappa	the RL kappa parameter,
lambda	*optional* (default of 1) - the ratio of the X to the Y precision profile,
epsilon	*optional* - convergence tolerance limit.

Details

The Rocke-Lorenzato precision profile model assumes the following forms for the variances, with proportionality constant λ:

- predicate precision profile model: $g_i = var(X_i) = \lambda \left(\sigma^2 + [\kappa \cdot \mu_i]^2 \right)$ and
- test precision profile model: $h_i = var(Y_i) = \sigma^2 + [\kappa \cdot (\alpha + \beta \mu_i)]^2$.

The algorithm uses maximum likelihood estimation. Proportionality constant λ is assumed to be known or estimated externally.

Value

A list containing the following components:

`alpha`	the fitted intercept
`beta`	the fitted slope
`fity`	the vector of predicted Y
`mu`	the vector of estimated latent true values
`resi`	the vector of residuals
`like`	the -2 log likelihood L
`innr`	the number of inner refinement loops executed
`error`	an error code if the iteration fails

Author(s)

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References

Hawkins DM and Kraker JJ. Precision Profile Weighted Deming Regression for Methods Comparison, on *Arxiv* (2025) doi:10.48550/arXiv.2508.02888

Hawkins DM (2014). A Model for Assay Precision. *Statistics in Biopharmaceutical Research*, **6**, 263-269. doi:10.1080/19466315.2014.899511

Examples

```
# library
library(ppwdeming)

# parameter specifications
sigma <- 1
kappa <- 0.08
alpha <- 1
beta  <- 1.1
true  <- 8*10^((0:99)/99)
truey <- alpha+beta*true
# simulate single sample - set seed for reproducibility
set.seed(1039)
# specifications for predicate method
X     <- sigma*rnorm(100)+true *(1+kappa*rnorm(100))
# specifications for test method
Y     <- sigma*rnorm(100)+truey*(1+kappa*rnorm(100))

# fit RL with given sigma and kappa
RL_results <- PWD_RL(X,Y,sigma,kappa)
cat("\nWith given sigma and kappa, the estimated intercept is",
    signif(RL_results$alpha,4), "and the estimated slope is",
    signif(RL_results$beta,4), "\n")
```

WD_General *Weighted Deming Regression*

Description

This code fits the weighted Deming regression on predicate readings (X) and test readings (Y).

Usage

```
WD_General(X, Y, g, h, epsilon=1e-10)
```

Arguments

X	the vector of predicate readings,
Y	the vector of test readings,
g	the vector of variances of the X,
h	the vector of variances of the Y,
epsilon	*optional* convergence tolerance limit.

Details

For input vectors g and h containing the variances of predicate readings X and test readings Y, respectively, iteratively fits weighted Deming regression.

Value

A list containing the following components:

alpha	the fitted intercept
beta	the fitted slope
cor	the Pearson correlation between X and Y
fity	the vector of predicted Y
mu	the vector of estimated latent true values
resi	the vector of residuals
like	the -2 log likelihood L
innr	the number of inner refinement loops executed

Author(s)

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References

Ripley BD and Thompson M (1987). Regression techniques for the detection of analytical bias. *Analyst*, **112**, 377-383.

Examples

```
# library
library(ppwdeming)

# parameter specifications
alpha <- 1
beta  <- 1.1
true  <- 8*10^((0:99)/99)
truey <- alpha+beta*true
# Loosely motivated by Vitamin D data set
g     <- 4e-16+0.07*true^1.27
h     <- 6e-2+7e-5*truey^2.2

# simulate single sample - set seed for reproducibility
set.seed(1039)
# specifications for predicate method
X     <- true +sqrt(g)*rnorm(100)
# specifications for test method
Y     <- truey+sqrt(h)*rnorm(100)

# fit with to estimate linear parameters
wd_fit <- WD_General(X,Y,g,h)
cat("\nWith given g and h, the estimated intercept is",
    signif(wd_fit$alpha,4), "and the estimated slope is",
    signif(wd_fit$beta,4), "\n")
```

`WD_Linnet` *Linnet proportional CV weighted Deming*

Description

This routine, provided for convenience, makes Linnet's constant CV fit.

Usage

```
WD_Linnet(X, Y, lambda=1, MDL=NA, getCI=TRUE, epsilon=1e-9, printem=FALSE)
```

Arguments

`X`	the vector of predicate readings,
`Y`	the vector of test readings,
`lambda`	ratio of g function to h function,
`MDL`	optional medical decision limit(s),
`getCI`	if TRUE, generates jackknife standard errors,
`epsilon`	optional tolerance limit,
`printem`	if TRUE, prints out results as a `message`.

Value

A list containing the following components:

alpha	the fitted intercept
beta	the fitted slope
cor	the Pearson correlation between X and Y
sealpha	the jackknife standard error of alpha
sebeta	the jackknife standard error of beta
covar	the jackknife covariance between alpha and beta
preMDL	the predictions at the MDL(s)
preMDLl	the lower confidence limit(s) of preMDL
preMDLu	the upper confidence limit(s) of preMDL

Author(s)

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References

Linnet K (1993). Evaluation of regression procedures for methods comparison studies. *Clinical Chemistry*, **39**, 424-432.

Examples

```
# library
library(ppwdeming)

# parameter specifications
alpha <- 1
beta  <- 1.1
true  <- 8*10^((0:99)/99)
truey <- alpha+beta*true
kappa <- 0.1

# simulate single sample - set seed for reproducibility
set.seed(1039)
# specifications for predicate method
X     <- true *(1+kappa*rnorm(100))
# specifications for test method
Y     <- truey *(1+kappa*rnorm(100))

# fit with to estimate linear parameters
wd_fit <- WD_Linnet(X, Y, MDL=12, printem=TRUE)
cat("\nThe Linnet constant-CV estimated intercept is",
    signif(wd_fit$alpha,4), "and the estimated slope is",
    signif(wd_fit$beta,4), "\n")
```

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