

Package ‘ppwdeming’

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Title Precision Profile Weighted Deming Regression

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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; thus the methods implemented here are referred to as precision profile weighted Deming (PWD) regression. The package 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 (unknown) 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. The following reference provides further information on mathematical derivations and applications.

Hawkins, D.M., and J.J. Kraker. 'Precision Profile Weighted Deming Regression for Methods Comparison', (in press) <[doi:10.1093/jalm/jfaf183](https://doi.org/10.1093/jalm/jfaf183)>.

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PWD_get_gh	<i>Estimate of Variance Profile Functions (proportional)</i>
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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, rho=NA, alpha=NA, beta=NA, mu=NA,
           epsilon = 1e-8, printem=FALSE)
```

Arguments

X	the vector of predicate readings.
Y	the vector of test readings.
lambda	<i>optional</i> (default of 1) - the ratio of the X to the Y precision profile.
rho	<i>optional</i> (default of NA) - numeric, single value or vector, initial estimate(s) of $\rho = \frac{\sigma}{\kappa}$.
alpha	<i>optional</i> (default of NA) - numeric, single value, initial estimate of α .
beta	<i>optional</i> (default of NA) - numeric, single value, initial estimate of β .
mu	<i>optional</i> (default of NA) - numeric, vector of length of X, initial estimate of μ .
epsilon	<i>optional</i> (default of 1.e-8) - convergence tolerance limit.
printem	<i>optional</i> (default of FALSE) - 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: $g_i = \text{var}(X_i) = \lambda \left(\sigma^2 + [\kappa \cdot \mu_i]^2 \right)$ and
- test precision profile model: $h_i = \text{var}(Y_i) = \sigma^2 + [\kappa \cdot (\alpha + \beta \mu_i)]^2$.

The search algorithm implements an efficient approach via reparameterization to the ratio $\rho = \frac{\sigma}{\kappa}$.

If initial estimates are not provided, the parameters are initialized as:

- alpha and beta are initially intercept and slope from simple linear regression;
- rho is initialized as the vector c(0.01, 1, 100); and
- mu is initialized as the values of X.

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
L	the -2 log likelihood L

Author(s)

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References

Hawkins DM and Kraker JJ (in press). Precision Profile Weighted Deming Regression for Methods Comparison. *The Journal of Applied Laboratory Medicine*. doi:10.1093/jalm/jfaf183

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), "\n")
# with estimated linear coefficients
cat("\nalphahat=", signif(RL_gh_fit$alpha,6),
    "and betahat=", signif(RL_gh_fit$beta,6), "\n")

```

PWD_inference

Weighted Deming Regression – Inference

Description

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

Usage

```

PWD_inference(X, Y, lambda=1, rho=NA, alpha=NA, beta=NA, mu=NA, MDL=NA,
  epsilon=1e-8, printem=FALSE)

```

Arguments

X	the vector of predicate readings.
Y	the vector of test readings.
lambda	<i>optional</i> (default of 1) - the ratio of the X to the Y precision profile.
rho	<i>optional</i> (default of NA) - numeric, single value or vector, initial estimate(s) of $\rho = \frac{\sigma}{\kappa}$.
alpha	<i>optional</i> (default of NA) - numeric, single value, initial estimate of α .
beta	<i>optional</i> (default of NA) - numeric, single value, initial estimate of β .
mu	<i>optional</i> (default of NA) - numeric, vector of length of X, initial estimate of μ .
MDL	<i>optional</i> (default to missing) - medical decision level(s).
epsilon	<i>optional</i> (default of 1.e-8) - convergence tolerance limit.
printem	<i>optional</i> (default of FALSE) - 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 point 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
L	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

References

- Hawkins DM and Kraker JJ (in press). Precision Profile Weighted Deming Regression for Methods Comparison. *The Journal of Applied Laboratory Medicine*. doi:10.1093/jalm/jfaf183
- 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-8,
          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	<i>optional</i> (default of 1.e-8) - convergence tolerance limit.
MDL	<i>optional</i> (default of NA) - medical decision level(s).
getCI	<i>optional</i> (default of TRUE) - allows for jackknifed standard errors on the regression and MDL.
printem	<i>optional</i> (default of FALSE) - 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:

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

Author(s)

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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), MDL=12,
                          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, rho=NA, alpha=NA, beta=NA, mu=NA,
            printem=FALSE)
```

Arguments

X	the vector of predicate readings.
Y	the vector of test readings.
K	the maximum number of outliers to seek.
lambda	<i>optional</i> (default of 1) - the ratio of the X to the Y precision profile.
Pcut	<i>optional</i> , default 0.01 (1%), cutoff for statistical significance of Bonferroni P.
rho	<i>optional</i> (default of NA) - numeric, single value or vector, initial estimate(s) of $\rho = \frac{\sigma}{\kappa}$.
alpha	<i>optional</i> (default of NA) - numeric, single value, initial estimate of α .
beta	<i>optional</i> (default of NA) - numeric, single value, initial estimate of β .
mu	<i>optional</i> (default of NA) - numeric, vector of length of X, initial estimate of μ .
printem	<i>optional</i> (default of FALSE) - 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 ignore the effect of random variability in the parameter estimates on the distribution of the 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 and whose normal tail areas provide the basis for the outlier P values
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 (in press). Precision Profile Weighted Deming Regression for Methods Comparison. *The Journal of Applied Laboratory Medicine*. doi:10.1093/jalm/jfaf183

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.

Usage

```
PWD_resi(true, resi, epsilon=1e-8, 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	<i>optional</i> (default of 1e-8) - convergence tolerance limit.
printem	<i>optional</i> (default of FALSE) - 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. The output of this function includes a maximum-likelihood estimate of the remaining parameter in the special cases of:

- constant variance ($\kappa_r = 0$); and
- constant coefficient of variation ($\sigma_r = 0$).

Value

A list containing the following components:

sigmar	the estimate of σ_r
kappar	the estimate of κ_r
L	the -2 log likelihood
scalr	the scaled residuals
poolsig	the maximum likelihood estimate of σ_r if $\kappa_r = 0$
poolkap	the maximum likelihood estimate of κ_r if $\sigma_r = 0$

Author(s)

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References

Hawkins DM and Kraker JJ (in press). Precision Profile Weighted Deming Regression for Methods Comparison. *The Journal of Applied Laboratory Medicine*. doi:10.1093/jalm/jfaf183

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)
# 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, alpha=NA, beta=NA, mu=NA, epsilon=1e-8)
```

Arguments

X	the vector of predicate readings.
Y	the vector of test readings.
sigma	the RL σ parameter.
kappa	the RL κ parameter.
lambda	<i>optional</i> (default of 1) - the ratio of the X to the Y precision profile.
alpha	<i>optional</i> (default of NA) - numeric, single value, initial estimate of α .
beta	<i>optional</i> (default of NA) - numeric, single value, initial estimate of β .
mu	<i>optional</i> (default of NA) - numeric, vector of length of X, initial estimate of μ .
epsilon	<i>optional</i> (default of 1e-8) - 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: $g_i = \text{var}(X_i) = \lambda \left(\sigma^2 + [\kappa \cdot \mu_i]^2 \right)$ and
- test precision profile model: $h_i = \text{var}(Y_i) = \sigma^2 + [\kappa \cdot (\alpha + \beta \mu_i)]^2$.

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
L	the -2 log likelihood L
innr	the number of inner refinement loops executed
error	an error code if the iteration fails

Author(s)

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

References

- Hawkins DM and Kraker JJ (in press). Precision Profile Weighted Deming Regression for Methods Comparison. *The Journal of Applied Laboratory Medicine*. doi:10.1093/jalm/jfaf183
- 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-8)
```

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	<i>optional</i> (default of 1e-8) - convergence tolerance limit.

Details

This function is used when the variances of X and Y are already known, as can be the case from an adequate number of replicate X and Y readings of each sample. 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
L	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-10, printem=FALSE)
```

Arguments

X	the vector of predicate readings.
Y	the vector of test readings.
lambda	ratio of g function to h function.
MDL	<i>optional</i> (default of NA) - medical decision limit(s).
getCI	<i>optional</i> (default of TRUE) - if TRUE, generates jackknife standard errors.
epsilon	<i>optional</i> (default of 1e-10) - tolerance limit.
printem	<i>optional</i> (default of FALSE) - if TRUE, prints out results as a message.

Details

Note that in cases where sigma happens to come out zero, Linnet's constant CV fit differs from the precision-profile fit since the underlying precision profile models are not the same.

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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