

# Package ‘Rvolcano’

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**Type** Package

**Title** Robust Volcano Plot: Identification of Influential Metabolites  
in the Presence of Outliers

**Version** 1.0

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**Description** Robust volcano plot (RVP) for detection of influential metabolites in noisy metabolomics data. It is an extension of classical volcano plot. It is achieved by adding a kernel weight function to the calculation of the fold-change and p-values.

**License** GPL (>= 2.10)

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Rvolcano-package	<i>Robust Volcano Plot for Identifying Influential Metabolites in Presence of Outliers.</i>
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## Description

This package implements a kernel weight based robust volcano plot for identifying influential Metabolites from noisy metabolomics dataset. This method is outlier-robust because the kernel weight function produce very smaller weight for outlying cell of the data matrix.

## Details

Package: Rvolcano  
 Type: Package  
 Version: 1.0  
 Date: 2018-01-14  
 License: GPL  
 Depends: R (>=2.10)

Package Rvolcano has the following functions:

weightedMean(): This function calculates the outlier-robust weighted mean using the kernel-weight function.  
 weightedVar(): This function calculates the outlier-robust weighted variance using the kernel-weight function.  
 foldChngCalc(): This function calculates outlier-robust fold change value using the kernel-weight function.  
 p.valcalc(): This function calculates the p-value using the robust version of t-statistic.  
 RobVolPlot(): This function draws a outlier-robust volcano plot using the robust fold change value and robust t-test p-value.

#### Author(s)

Nishith Kumar  
 Maintainer: Nishith Kumar <nk.bru09@gmail.com>

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DummyFullData

*Artificially generated Metabolomic Study on Cancer*

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#### Description

This dataset is a matrix containing measurements of metabolite concentration.

#### Usage

```
data("DummyFullData")
```

#### Format

A datamatrix with 40 rows and 40 columns. Each row is a metabolite. The columns are the concentration measurements of metabolites from different subjects.

#### Details

This is an artificially generated dataset that contain first 5 metabolites('Guanidoacetate', 'O-Acetylcarnitine', '2-Aminobutyrate', 'Formate' and 'Xylose') with lower concentration and next 5 metabolites i.e., no. 6-10 metabolites('Valine', 'Hypoxanthine', 'Fumarate', 'Tyrosine' and 'Pantothenate') with higher concentration for the cancer patient.

**Examples**

```
data(DummyFullData)
## View the artificially generated dataset.
View(DummyFullData)
```

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foldChngCalc

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*Robust Fold Change Calculation for Differential Calculation*


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**Description**

This function calculates the outlier-robust fold change value in presence of outliers. A kernel weight function has been used in this function.

**Usage**

```
foldChngCalc(data, nSampG1, nSampG2)
```

**Arguments**

data	a numerical vector or matrix of metabolomic measurements.
nSampG1	number of subjects in group-1.
nSampG2	number of subjects in group-2.

**Value**

Calculate the fold change values.

**Author(s)**

Nishith Kumar <nk.bru09@gmail.com>

**Examples**

```
data(DummyFullData)
fcval<-foldChngCalc(DummyFullData,nSampG1=20,nSampG2=20)
fcval
```

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p.valcalc

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*p-Value Calculation Using Robust t-Test*


---

**Description**

This function calculates the p-value using the robust version of t-test. A kernel weight function has been used behind the test statistic to robustify the t-test.

**Usage**

```
p.valcalc(x, y)
```

**Arguments**

x	a numerical vector of metabolomic measurements.
y	a numerical vector of metabolomic measurements.

**Value**

p-value of robust t-test.

**Author(s)**

Nishith Kumar <nk.bru09@gmail.com>

**Examples**

```
x<-rnorm(20,3,2)
y<-rnorm(20,6,2)
p.valcalc(x,y)
```

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RobVolPlot

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*Outlier-Robust Volcano Plot for Identifying Influential metabolites*


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**Description**

This function draws a volcano plot using the robust fold change value and the p-value obtained from robust t-test.

**Usage**

```
RobVolPlot(folds, pvals, cexcutoff = 0.7, cexlab = 0.5,
plimit = 0.05, fclimit = 2, xlab = "log2 Robust Fold Change",
tab ylab = "-log10 Robust t-Test P-value", main = "Robust Volcano Plot", ...)
```

**Arguments**

folds	A vector of fold changes with metabolite names.
pvals	A vector of corresponding p-values with metabolite names.
cexcutoff	Font size of the cut-off labels.
cexlab	Font size of the variable labels.
plimit	A numeric indicating the p value cutoff. The default is set to 0.05.
fclimit	A numeric indicating the lower fold cutoff. The default is set to 2.
xlab	x-axis label.
ylab	y-axis label.
main	Plot title.
...	Other graphical parameters.

**Author(s)**

Nishith Kumar <nk.bru09@gmail.com>

**Examples**

```

data(DummyFullData)
##Calculation of fold change values
fcval<-foldChngCalc(DummyFullData,nSampG1=20,nSampG2=20)
##Calculation of p-values
pval<-NULL
for (i in 1:dim(DummyFullData)[1]){
  pval[i]<-p.valcalc(DummyFullData[i,1:20],DummyFullData[i,21:40])
}
##Robust volcano plot
RobVolPlot(fcval,pval , cexcutoff = 0.7, cexlab = 0.8, plimit = .05,fclimit = 2)

```

weightedMean

*Calculation of Outlier-Robust Weighted Mean***Description**

This function calculates the outlier-robust weighted mean in presence of outliers. A kernel weight function has been used in this function.

**Usage**

```
weightedMean(x, b)
```

**Arguments**

x	a numerical vector of metabolomic measurements.
b	value of tuning parameter. Default value is 0.2.

**Value**

Computed the weighted mean.

**Author(s)**

Nishith Kumar <nk.bru09@gmail.com>

**Examples**

```

set.seed(2345)
x<-c(rnorm(200,3,1))
x1<-c(rnorm(180,3,1),rnorm(20,60,3)) #contain 20 outliers#
weightedMean(x)
mean(x)
weightedMean(x1)
mean(x1)

```

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`weightedVar`*Calculation of Outlier-Robust Weighted Variance*

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**Description**

This function calculates the outlier-robust weighted variance in presence of outliers. A kernel weight function has been used behind this function.

**Usage**

```
weightedVar(x, b)
```

**Arguments**

<code>x</code>	a numerical vector of metabolomic measurements.
<code>b</code>	value of tuning parameter. Default value is 0.25.

**Value**

Computed the weighted variance.

**Author(s)**

Nishith Kumar <nk.bru09@gmail.com>

**Examples**

```
set.seed(2345)
x<-c(rnorm(100,0,1))
x1<-c(rnorm(90,0,1),rnorm(10,50,3)) # contain 10 outliers#
weightedVar(x)
var(x)
weightedVar(x1)
var(x1)
```

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