

## NAME

AnalyzeTextFilesData.pl - Analyze numerical column data in TextFile(s)

## SYNOPSIS

AnalyzeTextFilesData.pl TextFile(s)...

```
AnalyzeTextFilesData.pl [-c, --colmode colnum | collabel] [--columns "colnum,[colnum,...]" |
"collabel,[collabel,...]" | All] [--columnpairs "colnum,colnum,[colnum,colnum]..." |
"collabel,collabel,[collabel,collabel]..." | AllPairs] [-d, --detail infolevel] [-f, --fast] [--frequencybins number |
"number,number,[number,...]"] [-h, --help] [--indelim comma | semicolon] [--klargest number] [--ksmallest
number] [-m, --mode DescriptiveStatisticsBasic | DescriptiveStatisticsAll | All | "function1, [function2,...]"] [-o,
--overwrite] [--outdelim comma | tab | semicolon] [-p, --precision number] [-q, --quote yes | no] [-r, --root
rootname] [--trimfraction number] [-w, --workingdir dirname] TextFiles(s)...
```

## DESCRIPTION

Analyze numerical column data in *TextFile(s)* using a combination of various statistical functions; Non-numerical values are simply ignored. For *Correlation, RSquare, and Covariance* analysis, the count of valid values in specified column pair must be same; otherwise, column pair is ignored. The file names are separated by space. The valid file extensions are *.csv* and *.tsv* for comma/semicolon and tab delimited text files respectively. All other file names are ignored. All the text files in a current directory can be specified by *\*.csv*, *\*.tsv*, or the current directory name. The *--indelim* option determines the format of *TextFile(s)*. Any file which doesn't correspond to the format indicated by *--indelim* option is ignored.

## OPTIONS

*-c, --colmode colnum | collabel*

Specify how columns are identified in TextFile(s): using column number or column label. Possible values: *colnum* or *collabel*. Default value: *colnum*.

*--columns "colnum,[colnum,...]" | "collabel,[collabel]..." | All*

This value is mode specific. It's a list of comma delimited columns to use for data analysis. Default value: *First column*.

This value is ignored during *Correlation/Pearson Correlation* and *Covariance* data analysis; *-columnpairs* option is used instead.

For *colnum* value of *-c, --colmode* option, input values format is: *colnum,colnum,....* Example:

```
1,3,5
```

For *collabel* value of *-c, --colmode* option, input values format is: *collabel,collabel,...* Example:

```
ALogP,MolWeight,EC50
```

*--columnpairs "colnum,colnum,[colnum,colnum,...]" | "collabel,collabel,[collabel,collabel,...]" | AllPairs*

This value is mode specific and is only used for *Correlation, PearsonCorrelation, or Covariance* value of *-m, --mode* option. It is a comma delimited list of column pairs to use for data analysis during *Correlation* and *Covariance* calculations. Default value: *First column, Second column*.

For *colnum* value of *-c, --colmode* option, input values format is: *colnum,colnum,[colnum,colnum]...* Example:

```
1,3,5,6,1,6
```

For *collabel* value of *-c, --colmode* option, input values format is: *collabel,collabel,[collabel,collabel]...* Example:

```
MolWeight,EC50,NumN+O,PSA
```

For *AllPairs* value of *--columnpairs* option, all column pairs are used for *Correlation* and *Covariance* calculations.

*-d, --detail infolevel*

Level of information to print about column values being ignored. Default: 1. Possible values: 1, 2, 3, or 4.

*-f, --fast*

In this mode, all the columns specified for analysis are assumed to contain numerical data and no checking is performed before analysis. By default, only numerical data is used for analysis; other types of column

data is ignored.

--frequencybins *number* | "*number,number,[number,...]*"

Specify number of bins or bin range to use for frequency analysis. Default value: 10

Number of bins value along with the smallest and largest value for a column is used to group the column values into different groups.

The bin range list is used to group values for a column into different groups; It must contain values in ascending order. Examples:

```
10,20,30
0.1,0.2,0.3,0.4,0.5
```

The frequency value calculated for a specific bin corresponds to all the column values which are greater than the previous bin value and less than or equal to the current bin value.

-h, --help

Print this help message.

--indelim *comma* | *semicolon*

Input delimiter for CSV *TextFile(s)*. Possible values: *comma* or *semicolon*. Default value: *comma*. For TSV files, this option is ignored and *tab* is used as a delimiter.

--klargest *number*

Kth largest value to find by *KLargest* function. Default value: 2 Valid values: positive integers.

--ksmallest *number*

Kth smallest value to find by *KSmallest* function. Default value: 2. Valid values: positive integers.

-m, --mode *DescriptiveStatisticsBasic* | *DescriptiveStatisticsAll* | *All* | "*function1*, [*function2*,...]"

Specify how to analyze data in *TextFile(s)*: calculate basic or all descriptive statistics; or use a comma delimited list of supported statistical functions. Possible values: *DescriptiveStatisticsBasic* | *DescriptiveStatisticsAll* | "*function1,[function2]...*". Default value: *DescriptiveStatisticsBasic*

*DescriptiveStatisticsBasic* includes these functions: *Count*, *Maximum*, *Minimum*, *Mean*, *Median*, *Sum*, *StandardDeviation*, *StandardError*, *Variance*.

*DescriptiveStatisticsAll*, in addition to *DescriptiveStatisticsBasic* functions, includes: *GeometricMean*, *Frequency*, *HarmonicMean*, *KLargest*, *KSmallest*, *Kurtosis*, *Mode*, *RSquare*, *Skewness*, *TrimMean*.

*All* uses complete list of supported functions: *Average*, *AverageDeviation*, *Correlation*, *Count*, *Covariance*, *GeometricMean*, *Frequency*, *HarmonicMean*, *KLargest*, *KSmallest*, *Kurtosis*, *Maximum*, *Minimum*, *Mean*, *Median*, *Mode*, *RSquare*, *Skewness*, *Sum*, *SumOfSquares*, *StandardDeviation*, *StandardDeviationN*, *StandardError*, *StandardScores*, *StandardScoresN*, *TrimMean*, *Variance*, *VarianceN*. The function names ending with N calculate corresponding values assuming an entire population instead of a population sample.

Here are the formulas for these functions:

Average: See Mean

AverageDeviation:  $\text{SUM}(\text{ABS}(x[i] - X_{\text{mean}})) / n$

Correlation: See Pearson Correlation

Covariance:  $\text{SUM}((x[i] - X_{\text{mean}})(y[i] - Y_{\text{mean}})) / n$

GeometricMean:  $\text{NthROOT}(\text{PRODUCT}(x[i]))$

HarmonicMean:  $1 / (\text{SUM}(1/x[i]) / n)$

Mean:  $\text{SUM}(x[i]) / n$

Median:  $X_{\text{sorted}}[(n - 1)/2 + 1]$  for even values of n;  $(X_{\text{sorted}}[n/2] + X_{\text{sorted}}[n/2 + 1])/2$  for odd values of n.

Kurtosis:  $[\{n(n + 1)/(n - 1)(n - 2)(n - 3)\} \text{SUM}\{((x[i] - X_{\text{mean}})/\text{STDDEV})^4\}] - \{3((n - 1)^2)\}/\{(n - 2)(n - 3)\}$

PearsonCorrelation:  $\text{SUM}((x[i] - X_{\text{mean}})(y[i] - Y_{\text{mean}})) / \text{SQRT}(\text{SUM}(x[i] - X_{\text{mean}})^2) (\text{SUM}(y[i] - Y_{\text{mean}})^2))$

RSquare:  $\text{PearsonCorrelation}^2$

Skewness:  $\{n/(n-1)(n-2)\} \text{SUM}\{((x[i] - X_{\text{mean}})/\text{STDDEV})^3\}$

StandardDeviation:  $\text{SQRT}(\text{SUM}(x[i] - \text{Mean})^2 / (n-1))$

StandardDeviationN:  $\text{SQRT}(\text{SUM}(x[i] - \text{Mean})^2 / n)$

StandardError:  $\text{StandardDeviation} / \text{SQRT}(n)$

StandardScore:  $(x[i] - \text{Mean}) / (n-1)$

StandardScoreN:  $(x[i] - \text{Mean}) / n$

Variance:  $\text{SUM}(x[i] - X_{\text{mean}})^2 / (n-1)$

VarianceN:  $\text{SUM}(x[i] - X_{\text{mean}})^2 / n$

-o, --overwrite

Overwrite existing files.

--outdelim *comma | tab | semicolon*

Output text file delimiter. Possible values: *comma, tab, or semicolon* Default value: *comma*.

-p, --precision *number*

Precision of calculated values in the output file. Default: up to 2 decimal places. Valid values: positive integers.

-q, --quote *yes | no*

Put quotes around column values in output text file. Possible values: *yes or no*. Default value: *yes*.

-r, --root *rootname*

New text file name is generated using the root: *<Root>.<Ext>*. Default new file name: *<InitialTextFileName><Mode>.<Ext>*. Based on the specified analysis, *<Mode>* corresponds to one of these values: *DescriptiveStatisticsBasic, DescriptiveStatisticsAll, AllStatistics, SpecifiedStatistics, Covariance, Correlation, Frequency, or StandardScores*. The *csv*, and *tsv* *<Ext>* values are used for *comma/semicolon, and tab delimited text files* respectively. This option is ignored for multiple input files.

--trimfraction *number*

Fraction of data to exclude from the top and bottom of the data set during *TrimMean* calculation. Default value: *0.1*. Valid values: *> 0 and < 1*.

-w --workingdir *text*

Location of working directory. Default: current directory.

## EXAMPLES

To calculate basic statistics for data in first column and generate a *NewSample1DescriptiveStatisticsBasic.csv* file, type:

```
% AnalyzeTextFilesData.pl -o -r NewSample1 Sample1.csv
```

To calculate basic statistics for data in third column and generate a *NewSample1DescriptiveStatisticsBasic.csv* file, type:

```
% AnalyzeTextFilesData.pl --columns 3 -o -r NewSample1 Sample1.csv
```

To calculate basic statistics for data in *MolWeight* column and generate a *NewSample1DescriptiveStatisticsBasic.csv* file, type:

```
% AnalyzeTextFilesData.pl -colmode collabel --columns MolWeight -o
-r NewSample1 Sample1.csv
```

To calculate all available statistics for data in third column and all column pairs, and generate *NewSample1DescriptiveStatisticsAll.csv, NewSample1CorrelationMatrix.csv, NewSample1CorrelationMatrix.csv, and NewSample1MolWeightFrequencyAnalysis.csv* files, type:

```
% AnalyzeTextFilesData.pl -m DescriptiveStatisticsAll --columns 3 -o
--columnpairs AllPairs -r NewSample1 Sample1.csv
```

To compute frequency distribution of data in third column into five bins and generate NewSample1MolWeightFrequencyAnalysis.csv, type:

```
% AnalyzeTextFilesData.pl -m Frequency --frequencybins 5 --columns 3
-o -r NewSample1 Sample1.csv
```

To compute frequency distribution of data in third column into specified bin range values, and generate NewSample1MolWeightFrequencyAnalysis.csv, type:

```
% AnalyzeTextFilesData.pl -m Frequency --frequencybins "100,200,400"
--columns 3 -o -r NewSample1 Sample1.csv
```

To calculate all available statistics for data in all columns and column pairs, type:

```
% AnalyzeTextFilesData.pl -m All --columns All --columnpairs
AllPairs -o -r NewSample1 Sample1.csv
```

#### AUTHOR

Manish Sud <msud@san.rr.com>

#### SEE ALSO

JoinTextFiles.pl, MergeTextFilesWithSD.pl, ModifyTextFilesFormat.pl, SplitTextFiles.pl, TextFilesToHTML.pl

#### COPYRIGHT

Copyright (C) 2004-2012 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.