

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: $\frac{n}{(n-1)(n-2)} \sum \left\{ \frac{(x[i] - \text{Xmean})}{\text{STDDEV}} \right\}^3$

StandardDeviation: $\text{SQRT} \left(\frac{\sum (x[i] - \text{Mean})^2}{(n-1)} \right)$

StandardDeviationN: $\text{SQRT} \left(\frac{\sum (x[i] - \text{Mean})^2}{n} \right)$

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

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

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

Variance: $\frac{\sum (x[i] - \text{Xmean})^2}{(n-1)}$

VarianceN: $\frac{\sum (x[i] - \text{Xmean})^2}{n}$

-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) 2024 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.