

Package ‘DivMelt’

July 2, 2014

Type Package

Title HRM Diversity Assay Analysis Tool

Version 1.0.3

Author David A. Swan <dswan@fhcrc.org> with contributions from Craig A
Magaret <cmagaret@fhcrc.org> and Matthew M Cousins <matthew.m.cousins@gmail.com>

Maintainer David A. Swan <dswan@fhcrc.org>

Description This package has tools for analyzing DNA melting data to
generate HRM scores, the DNA diversity measure output of the
HRM Diversity Assay. For additional documentation visit <http://code.google.com/p/divmelt/>.

License GPL (>= 2)

Depends R(>= 2.12.0),tcltk,glmnet

Imports

biocViews

URL

Repository CRAN

Date/Publication 2013-01-29 07:31:17

NeedsCompilation no

R topics documented:

DivMelt_gui	2
model	2
modelDivMelt	3
plotPDF	4
plotPNG	6
processDivMelt	7
statDivMelt	9
training	11

Index**12**

DivMelt_gui

User Interface for the Diversity Assay Analysis Tool

Description

DivMelt_gui uses tcl/tk to allow the user to set various input, output, plotting and analysis parameters for performing an analysis on the data from an HRM Diversity Melting Assay. The data consists of fluorescence measures, the analysis identifies candidate melting temperatures, peak changes in fluorescence and other statistics as they relate to the data. A complete user manual for the HRM Diversity Assay Analysis Tool can be found in the "doc" sub directory of the DivMelt package installation directory.

Usage

```
DivMelt_gui()
```

Author(s)

David Swan <dswan@fhcrc.org>

Examples

```
##  
library (DivMelt)  
DivMelt_gui()
```

model*Linear regression model for acceptance of Fluorescence data*

Description

This data set is the output of the glmnet R package when presented with a sample training set of acceptable and unacceptable input samples. The samples are characterized in terms of average, minimum and maximum fluorescence and dfluorescence as well as other measures using the stat-DivMelt function in the DivMelt package.

Format

An R formatted version of the glmnet model output.

modelDivMelt	<i>Routine to generate LASSO model for the Diversity Assay Analysis Tool</i>
--------------	--

Description

modelDivMelt uses the provided training set data to generate and save a LASSO model for linear regression analysis on future samples. The training set must be a comma separated file with the following columns:

Sample,min,max,mean,stddev,sigma,dmin,dmax,dmean,dstddev,positive

where:

Sample = sample name

min,max,mean and stddev - those measures w.r.t. fluorescence

sigma - sigma from linear model of fluorescence

dmin,dmax,dmean and dstddev - those measures w.r.t. delta fluorescence

positive - 0 if rejected (negative control), 1 if accepted

The output file is written as an R object. The default filename is model.rda.

Usage

```
modelDivMelt( trngFile, datFile)
```

Arguments

trngFile CSV file representing training set samples (required)

datFile name of output model file (model.rda by default)

Author(s)

David Swan <dswan@fhcrc.org>

Examples

```
library (DivMelt)
pkgDir<-system.file(package="DivMelt")
modelDivMelt(trngFile=paste(pkgDir,"/sample_data/training.csv",sep=''),datFile="new_model.rda")
```

Description

plotPDF uses various passed input, output and analysis parameters for performing an analysis on the data from an HIV Diversity Assay. The data consists of fluorescence measures, the analysis identifies candidate melting temperatures, peak changes in fluorescence and other statistics as they relate to the data. A PDF showing the fluorescence and dFluorescence curves together with the identified points for T1, T2 and Tm is generated for each sample. Parameters are listed below (default values are in parenthesis).

Usage

```
plotPDF(dir,  
singleFile,  
selectList,  
sampleMask,  
theta1=50,  
theta2=30,  
excludeEarly,  
earlyCutoff,  
excludeLate,  
lateCutoff,  
includeShoulders,  
shoulderCutoff,  
t1Cutoff,  
t2Cutoff,  
t1SlopeWindow,  
t2SlopeWindow,  
scoreFile,  
showFlorSmooth,  
showDFlorSmooth,  
useLasso,  
modelFile,  
xrangeOverride,  
xrangemin,  
xrangemax,  
rejectsFile,  
statsFile,  
progressFunc)
```

Arguments

dir	directory containing desired ABT/FLO files (required)
singleFile	a single file in that directory (for just one file)

selectList	a list of samples to plot (searched for in the file or files above), the default is to do all
sampleMask	a full or partial sample name or regular expression used to select individual samples
theta1	T1 cutoff angle (50 deg)
theta2	T2 cutoff angle as absolute value (30 deg)
excludeEarly	exclude peaks before main peak (T)
earlyCutoff	spacing required for exclusion (3 deg C)
excludeLate	exclude peaks after main peak (F)
lateCutoff	spacing required for exclusion (3 deg C)
includeShoulders	include premature shoulders in rising curve (T)
shoulderCutoff	fractional height at which to start inclusion (0.1)
showFlorSmooth	flag to enable drawing of smoothing curve for Florescence plot (F)
showDFlorSmooth	flag to enable drawing of smoothing curve for dFlorescence plot (T)
useLasso	flag to indicate whether to use regression model to filter bad data files (T)
t1Cutoff	delta temp that Theta 1 must be exceeded for T1 candidates (1 deg C)
t2Cutoff	delta temp that Theta 2 must be exceeded for T2 candidates (1 deg C)
t1SlopeWindow	Interval used to approximate slope at T1 (1 deg C)
t2SlopeWindow	Interval used to approximate slope at T2 (1 deg C)
scoreFile	DivMelt score file to compare against
modelFile	Alternate Lasso model file saved as an R object
rejectsFile	File to which to write names of Lasso rejected samples ("rejected.csv")
statsFile	File to which to write statistics like mean, max, etc. - used to help make a Lasso model training set
xrangeOverride	Option to override x-axis range (FALSE)
xrangemin	Value to use as override to x-axis min (75)
xrangemax	Value to use as override to x-axis min (100)
progressFunc	Optional function to call during processing passing it the fraction complete as a real

Author(s)

David Swan <dswan@fhcrc.org>

plotPNG

Routine to generate PNG plots using the Diversity Assay Analysis Tool

Description

plotPNG uses various passed input, output and analysis parameters for performing an analysis on the data from an HIV Diversity Assay. The data consists of fluorescence measures, the analysis identifies candidate melting temperatures, peak changes in fluorescence and other statistics as they relate to the data. A PNG showing the fluorescence and dFluorescence curves together with the identified points for T1, T2 and Tm is generated for each sample. Parameters are listed below (default values are in parenthesis).

Usage

```
plotPNG(dir,  
singleFile,  
selectList,  
sampleMask,  
theta1=50,  
theta2=30,  
excludeEarly,  
earlyCutoff,  
excludeLate,  
lateCutoff,  
includeShoulders,  
showFlorSmooth,  
showDFlorSmooth,  
shoulderCutoff,  
t1Cutoff,  
t2Cutoff,  
t1SlopeWindow,  
t2SlopeWindow,  
xrangeOverride,  
xrangemin,  
xrangemax,  
progressFunc)
```

Arguments

dir	directory containing desired ABT/FLO files (required)
singleFile	a single file in that directory (for just one file)
selectList	a list of samples to plot (searched for in the file or files above), the default is to do all
sampleMask	a full or partial sample name or regular expression used to select individual samples

theta1	T1 cutoff angle (50 deg)
theta2	T2 cutoff angle as absolute value (30 deg)
excludeEarly	exclude peaks before main peak (T)
earlyCutoff	spacing required for exclusion (3 deg C)
excludeLate	exclude peaks after main peak (F)
lateCutoff	spacing required for exclusion (3 deg C)
includeShoulders	include premature shoulders in rising curve (T)
shoulderCutoff	fractional height at which to start inclusion (0.1)
showFlorSmooth	flag to enable drawing of smoothing curve for Florescence plot (F)
showDFlorSmooth	flag to enable drawing of smoothing curve for dFlorescence plot (T)
t1Cutoff	delta temp that Theta 1 must be exceeded for T1 candidates (1 deg C)
t2Cutoff	delta temp that Theta 2 must be exceeded for T2 candidates (1 deg C)
t1SlopeWindow	Interval used to approximate slope at T1 (1 deg C)
t2SlopeWindow	Interval used to approximate slope at T2 (1 deg C)
xrangeOverride	Option to override x-axis range (FALSE)
xrangemin	Value to use as override to x-axis min (75)
xrangemax	Value to use as override to x-axis min (100)
progressFunc	Optional function to call during processing passing it the fraction complete as a real

Author(s)

David Swan <dswan@fhcrc.org>

processDivMelt

Main Routine of the Diversity Assay Analysis Tool

Description

processDivMelt uses various passed input, output and analysis parameters for performing an analysis on the data from an HIV Diversity Assay. The data consists of fluorescence measures, the analysis identifies candidate melting temperatures, peak changes in fluorescence and other statistics as they relate to the data. Parameters are listed below (default values are in parenthesis).

Usage

```

processDivMelt(dir,
singleFile,
selectList,
sampleMask,
theta1=50,
theta2=30,
format,
showStats,
excludeEarly,
earlyCutoff,
excludeLate,
lateCutoff,
includeShoulders,
shoulderCutoff,
showFlorSmooth,
showDFlorSmooth,
useLasso,
t1Cutoff,
t2Cutoff,
t1SlopeWindow,
t2SlopeWindow,
scoreFile,
dataFile,
modelFile,
rejectsFile,
statsFile,
xrangeOverride,
xrangemin,
xrangemax,
progressFunc)

```

Arguments

<code>dir</code>	directory containing desired ABT/FLO files (required)
<code>singleFile</code>	a single file in that directory (for just one file)
<code>selectList</code>	a list of samples to plot (searched for in the file or files above), the default is to do all
<code>sampleMask</code>	a full or partial sample name or regular expression used to select individual samples
<code>theta1</code>	T1 cutoff angle (50 deg)
<code>theta2</code>	T2 cutoff angle as absolute value (30 deg)
<code>format</code>	format for output plots namely pdf, png or none (pdf)
<code>showStats</code>	flag to enable writing of curve statistics on plots (T)
<code>excludeEarly</code>	exclude peaks before main peak (T)
<code>earlyCutoff</code>	spacing required for exclusion (3 deg C)

excludeLate	exclude peaks after main peak (F)
lateCutoff	spacing required for exclusion (3 deg C)
includeShoulders	include premature shoulders in rising curve (T)
shoulderCutoff	fractional height at which to start inclusion (0.1)
showFlorSmooth	flag to enable drawing of smoothing curve for Florescence plot (F)
showDFlorSmooth	flag to enable drawing of smoothing curve for dFlorescence plot (T)
useLasso	flag to indicate whether to use regression model to filter bad data files (T)
t1Cutoff	delta temp that Theta 1 must be exceeded for T1 candidates (1 deg C)
t2Cutoff	delta temp that Theta 2 must be exceeded for T2 candidates (1 deg C)
t1SlopeWindow	Interval used to approximate slope at T1 (1 deg C)
t2SlopeWindow	Interval used to approximate slope at T2 (1 deg C)
scoreFile	DivMelt score file to compare against
dataFile	output file for DivMelt scores
modelFile	Alternate Lasso model file saved as an R object
rejectsFile	File to which to write names of Lasso rejected samples ("rejected.csv")
statsFile	File to which to write statistics like mean, max, etc. - used to help make a Lasso model training set
xrangeOverride	Option to override x-axis range (FALSE)
xrangemin	Value to use as override to x-axis min (75)
xrangemax	Value to use as override to x-axis min (100)
progressFunc	Optional function to call during processing passing it the fraction complete as a real

Author(s)

David Swan <dswan@fhcrc.org>

statDivMelt

Statistical Output for the Diversity Assay Analysis Tool

Description

statDivMelt uses various passed input, output and analysis parameters to performing a statistical analysis of the data from an HIV Diversity Assay. The data consists of fluorescence measures, the analysis identifies characteristics such as minimum, maximum and average fluorescence and dFluorescence. These statistics can be used to generate training data for a linear regression model which can be used in order to reject bad data files in future analysis. Parameters are listed below (default values are in parenthesis).

Usage

```
statDivMelt(dir,
singleFile,
selectList,
theta1=50,
theta2=30,
excludeEarly,
earlyCutoff,
excludeLate,
lateCutoff,
includeShoulders,
shoulderCutoff,
t1Cutoff,
t2Cutoff,
t1SlopeWindow,
t2SlopeWindow,
statsFile)
```

Arguments

dir	directory containing desired ABT/FLO files (required)
singleFile	a single file in that directory (for just one file)
selectList	a list of samples to plot (searched for in the file or files above), the default is to do all
theta1	T1 cutoff angle (50 deg)
theta2	T2 cutoff angle as absolute value (30 deg)
excludeEarly	exclude peaks before main peak (T)
earlyCutoff	spacing required for exclusion (3 deg C)
excludeLate	exclude peaks after main peak (F)
lateCutoff	spacing required for exclusion (3 deg C)
includeShoulders	include premature shoulders in rising curve (T)
shoulderCutoff	fractional height at which to start inclusion (0.1)
t1Cutoff	delta temp that Theta 1 must be exceeded for T1 candidates (1 deg C)
t2Cutoff	delta temp that Theta 2 must be exceeded for T2 candidates (1 deg C)
t1SlopeWindow	Interval used to approximate slope at T1 (1 deg C)
t2SlopeWindow	Interval used to approximate slope at T2 (1 deg C)
statsFile	File to which to write statistics like mean, max, etc. - used to help make a Lasso model training set

Author(s)

David Swan <dswan@fhcrc.org>

training

Training data for Linear regression model

Description

This data represents a the training set used to generate the "model" Linear regression model used by default with the DivMelt package. The training set contains sets of acceptable and unacceptable input samples. The samples are characterized in terms of average, minimum and maximum fluorescence and dfluorescence as well as other measures. It was generated using the statDivMelt function in the DivMelt package. This file serves as input to the glmnet function located in the R package by that same name.

Format

CSV

Index

*Topic **datasets**

model, [2](#)

training, [11](#)

*Topic **interface**

DivMelt_gui, [2](#)

*Topic **programming**

plotPDF, [4](#)

plotPNG, [6](#)

processDivMelt, [7](#)

statDivMelt, [9](#)

*Topic **utilities**

modelDivMelt, [3](#)

DivMelt_gui, [2](#)

model, [2](#)

modelDivMelt, [3](#)

plotPDF, [4](#)

plotPNG, [6](#)

processDivMelt, [7](#)

statDivMelt, [9](#)

training, [11](#)