MathIOmica Guide

MathIOmica is an omics analysis package for Mathematica, designed to facilitate method development for the analysis of multiple omics in the Wolfram Language, particularly for dynamics (time series/longitudinal data). MathIOmica provides a collection of functions for importing mapped omics data from text files to created collated analysis objects. The data may be normalized, filtered, and classified to reveal trends. Additionally MathIOmica offers visualization with combined dendrogram/heatmap plots based on cluster results, representation on biological pathways, and a mass spectrometry spectral viewer. Finally, MathIOmica offers basic enrichment analysis and annotation for Gene Ontology (GO) and biological pathways.

Reference

Data Importing

DataImporter — graphical interface to import data from files

DataImporterDirect — import data as an **OmicsObject** directly from files

OmicsObjectCreator — create an **OmicsObject** for use with MathIOmica

OmicsObject — structured data used by MathIOmica

DataImporterDirectLabeled ▪ **FileSelector**

Data Processing of an OmicsObject

Applier — apply functions to an **OmicsObject**

ApplierList — apply a function to a list of lists from the values across an **OmicsObject**

EnlargeInnerAssociation — combining a list of **OmicsObject** elements by enlarging the inner associations

EnlargeOuterAssociation — combine a list of **OmicsObject** elements by enlarging the outer associations

FilteringFunction — filters an **OmicsObject**'s data by a chosen comparison to a cutoff

FilterMissing — filters out data from **OmicsObject** if across the datasets a *percentage* of data points is missing.

LowValueTag — tag low values in an **OmicsObject** and tag values in specified position as Missing [ ] based on a provided value cutoff.

Returner — substitute data in an **OmicsObject**

MeasurementApplier ▪ **ConstantAssociator** ▪ **OmicsObjectUniqueMassConverter** ▪ **OmicsObjectMerge** ▪ **OmicsObjectPairedMerge**

Data Processing of a Series

CreateTimeSeries — creates a time series list across an OmicsObject using outer keys

TimeExtractor — extract a list of sorted times from an OmicsObject's outer keys

ConstantSeriesClean — removes constant list series from an association of lists

SeriesApplier — apply a function to an association of lists, masking for Missing values

SeriesCompare — merges the values of two associations of series by pointwise operation on the values of each matching pair of keys

SeriesInternalCompare — compare each value in each list of an association of lists to an internal reference value in the list

Miscellaneous Data Processing

JoinNestedAssociations — merges a nested association list by joining inner associations

MissingDataCreator — fill in Missing tags in a paired dataset for which the first component is not a member of a given sample list

StandardizeExtended — standardize data that may include Missing values

Data Transformations

BoxCoxTransform — computes the Box-Cox transformation for a given parameter λ

ApplyBoxCoxTransform — compute the Box-Cox transformation at the maximum likelihood λ parameter

QuantileNormalization — perform quantile normalization of data

Spectral Analysis

Autocorrelation — calculate the normalized autocorrelation for a time series using a Lomb-Scargle based approach

LombScargle — calculate the Lomb-Scargle power spectrum for time series data

InverseAutocovariance

Classification and Clustering

BootstrapGeneral — perform a resampling of an OmicsObject's data with replacement

QuantileEstimator — obtain the quantile estimator following bootstrap for time series

TimeSeriesClassification — identify classes of temporal behavior in time series

TimeSeriesClusters — perform two-tiered clustering of time series data

MatrixClusters — perform hierarchical clustering in both dimensions a matrix

TimeSeriesSingleClusters

Annotation and Enrichment

GetGeneDictionary — creates an ID/accession dictionary from a UCSC search

GeneTranslation — Convert gene identities across different annotations/accessions

GOAnalysis — Gene Ontology (GO) enrichment analysis

KEGGAnalysis — KEGG: Kyoto Encyclopedia of Genes and Genomes pathway enrichment analysis

KEGGDictionary — create a dictionary from KEGG: Kyoto Encyclopedia of Genes and Genomes terms

OBOGODictionary — create an Open Biomedical Ontologies (OBO) Gene Ontology (GO) vocabulary dictionary

GOAnalysisAssigner ▪ **KEGGAnalysisAssigner** ▪ **EnrichmentReportExport** ▪ **MassDictionary** ▪ **MassMatcher** ▪ **UCSCBrowserSQL**

Multiple Hypothesis Testing

BenjaminiHochbergFDR — calculate the Benjamini Hochberg approach false discovery rates (FDR) from a list of p-values

Visualization

MatrixDendrogramHeatmap — generate dendrograms and heatmap plot for a matrix

MatrixDendrogramsHeatmaps — generate multiple dendrograms and heatmap plots for a matrix with many classifications

TimeSeriesDendrogramHeatmap — generate a dendrogram and heatmap plot for time series data clusters

TimeSeriesDendrogramsHeatmaps — generate multiple dendrograms and heatmap plots for multiple classified classes of time series data clusters

KEGGPathwayVisual — representation for a KEGG: Kyoto Encyclopedia of Genes and Genomes pathway

MSViewer — view spectra for mass spectrometry from .mzXML or .mzML files

Heatmapper ▪ TimeSeriesSingleDendrogramHeatmap ▪ TimeSeriesSingleDendrogramsHeatmaps

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Related Links

- MathIOmica website
- MathIOmica on github
- MathIOmica on twitter (@mathiomica)
- G Mias Lab website