A Quick Guide To MATLAB Bioinformatics Toolbox

http://www.mathworks.com

This is a Quick reference Guide for MATLAB Bioinformatics Toolbox 3. MATLAB (short for "matrix laboratory") is a high-performance language for technical computing, created by *The MathWorks*. It features a family of add-on application-specific solutions called toolboxes (i.e., comprehensive collections of functions) that extend the MATLAB environment to solve particular classes of problems.

Bioinformatics Toolbox offers an integrated software environment for genome and proteome analysis. In particular, it provides access to genomic and proteomic data formats, analysis techniques, and specialized visualizations for genomic and proteomic sequence and microarray analysis. The key features of the basic categories in the Bioinformatics Toolbox will be presented in the following sections.

This guide does not replace the entire documentation provided by *The MathWorks*, but can be used as a reference for those who want to explore the essential features of the Bioinformatics Toolbox. For more information on the functions syntax you can refer to: http://www.mathworks.com/access/helpdesk/help/toolbox/bioinfo

Data formats and databases

Web-based databases

getgenbank ()	Retrieve sequence information from GenBank database	
getgenpept()	Retrieve sequence information from GenPept database	
getembl()	Retrieve sequence information from EMBL database	
getpir()	Retrieve sequence data from PIR-PSD database	
getpdb ()	Retrieve protein structure from PDB database	
getgeodata()	Get Gene Expression Omnibus (GEO) data	
gethmmalignment() Retrieve multiple aligned sequences from		
	the PFAM database	
gethmmprof()	Retrieve profile hidden Markov models from the	
	PFAM database	
gethmmtree()	Get phylogenetic tree data from PFAM database	

Raw data

scfread()	Read trace data from SCF file		
<pre>joinseq()</pre>	Join two sequences to produce the shortest		
	supersequence		
traceplot()	Draw nucleotide trace plots squares polynomial		

Reading data formats

genbankread()	Read data from a GenBank file			
genpeptread()	Read data from a GenPept file			
emblread()	Read data from EMBL file			
pirread()	Read data from PIR file			
pdbread()	Read data from PDB file			
fastaread()	Read data from FASTA report			
multialignread	() Read multiple sequence alignment file			
${\tt geosoftread}()$	Read data from a Gene Expression Omnibus			
	(GEO) SOFT file			
gprread()	Read microarray data from a GenePix Results			
	(GPR) file			
<pre>galread()</pre>	Read microarray data from a GenePix array list			
	file			
sptread()	Read data from a SPOT file			
${\tt affyread}()$	Read microarray data from Affymetrix GeneChip			
	file			

Writing data formats

fastawrite (...) Write to file with fasta format

pfamhmmread (...) Read data from a PFAM-HMM file

BLAST searches

blastncbi()	Generate a remote BLAST request
getblast()	Get BLAST report from NCBI Web site
blastread()	Read data from NCBI BLAST report

Sequence Analysis

Sequence Statistics

aacount()	Count amino acids in a sequence			
basecount()	Count the nucleotides in a sequence			
codoncount ()	Count codons in a nucleotide sequence			
ntdensity()	Plot the density of nucleotides along a sequence			
codonbias()	Calculate codon frequency for each amino acid in a DNA sequence			
$\verb"seqshoworfs"()$	Display open reading frames (ORFs) in a nucleotide sequence			
randseq()	Generate random sequence from finite alphabet			

Sequence Conversion and manipulation

nt2aa ()	Convert a nucleotide sequence to an amino acid		
	sequence		
aa2nt()	Convert amino acid sequence to nucleotide		
	sequence		
dna2rna()	Convert DNA sequence to RNA sequence		
, ,	1		
rna2dna ()	Convert RNA sequence to DNA sequence		
seqcomplement() Calculate complementary strand of		
	nucleotide sequence		
segrcomplement	() Calculate reverse complement of a nucleotide		
	sequence		
-+ ()	Determine the atomic composition of a protein		
atomiccomp()	1 1		
aminolookup()	Look up the amino acid for a codon		
molweight()	Determine the molecular weight of a protein		
<pre>isoelectric()</pre>	Estimate isoelectric point for amino acid sequence		
restrict()	Split nucleotide sequence at specified restriction		
	site		
cleave()	Cleave amino acid sequence with enzyme		
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Sequence Alignment

nwalign()	Globally align two amino acid sequences, using the Needleman-Wunsch algorithm			
swalign()	Locally align two amino acid sequences using the			
	Smith-Waterman algorithm			
multialign()	Align multiple sequences using progressive			
	method			
profalign()	Align two profiles using Needleman-Wunsch			
	global alignment			
seqdotplot()	Draw a dot plot comparing two amino acid			
	sequences			

showalignment (...) Display color-coded sequence alignment

Phylogenetic Analysis

Phylogenetic Tree Data

phytreeread()	Read phylogenetic tree file					
phytreewrite ()	Write	phylogenetic	tree	object	to	Newick
	format	ted file				
phytree()	Object	constructor for	a nhv	logenetic	c tre	e object

Create a Phylogenetic Tree

dnds ()		synonymous	and	nonsy	nonymous
dndsml ()		n rates synonymous n rates using		_	,
seqlinkage()	method Construct distances	phylogenetic	tree	from	pairwise

 seqneighjoin (...)
 Neighbor-joining method for phylogenetic tree reconstruction
 tree

 seqpdist (...)
 Calculate pairwise distance between sequences

 phytreetool (...)
 View, edit, explore phylogenetic tree data

 reroot (...)
 Change the root of a phylogenetic tree

 seqinsertgaps (...)
 Insert gaps into nucleotide or amino acid sequence

Microarray data Analysis

Microarray normalization and filtering

malowess (...) Smooth microarray data using the Lowess method

manorm (...) Normalize microarray data

geneentropyfilter (...) Remove genes the profiles of which have low entropy

genevarfilter (...) Filters out genes with small variance over time

genelowvalfilter (...) Removes genes that have very low absolute expression values

Microarray Visualization

maimage()	Display a spatial image for microarray data			
maboxplot()	Display a box plot for microarray data			
maloglog()	Create a loglog plot of microarray data			
<pre>mairplot()</pre>	Display intensity versus ratio scatter plot for microarray signals			
mapcaplot()	Create a Principal Component plot of expression profile data			
clustergram()	Create dendrogram and heat map			

Microarray utility functions

<pre>probelibraryinfo()</pre>	Extract probe set library information for
	probe results
<pre>probesetlookup()</pre>	Look up gene name for probe set
probesetvalues ()	Extract probe set values from probe results
<pre>probesetlink()</pre>	Link to NetAffx Web site
<pre>probesetplot()</pre>	Plots values for Affymetrix CHP file probe
	ant

Mass Spectrometry data Analysis

Reading raw data into MATLAB

jcampread (...)

Read JCAMP-DX formatted files (JCAMP-DX: file format for infrared, NMR, and mass spectrometry data from the Joint Committee on Atomic and Molecular Physical Data)

Preprocessing of raw data

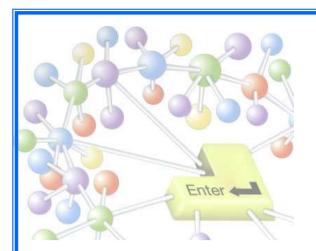
msresample()	Resample a mass spectrometry signal				
msbackadj()	Correct the baseline of a mass spectrum				
msalign()	Align peaks in mass spectrum to reference peaks				
msheatmap()	Display color image for set of spectra				
msnorm ()	Normalize set of mass spectra				
mslowess()	Smooth mass spectrum using non-parametric method				
mssgolay()	Smooth mass spectrum with least-squares polynomial				

Spectrum analysis

msviewer (...) Explore MS spectrum or set of spectra with GUI

Statistical Learning

classperf()	Evaluate performance of classifier
crossvalind()	Generate cross-validation indices
knnclassify()	Classify data using nearest neighbor method
knnimpute()	Impute missing data using nearest-neighbor
	method
optimalleaforde	r () Determine optimal leaf ordering for
	hierarchical binary cluster tree
randfeatures ()	Generate randomized subset of features
rankfeatures()	Rank key features by class separability criteria
samplealign()	Align two data sets containing sequential
	observations by introducing gaps
svmclassify()	Classify data using support vector machine
svmsmoset()	Create or edit Sequential Minimal
	Optimization (SMO) options structure
svmtrain()	Train support vector machine classifier



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