(Last updated: 11/28/2017)

Author Information

Professor Domenico L. Gatti, MD, PhD  
School of Medicine, Wayne State University

Ebook Details

**Description**

Written for graduate students in the Chemical and Biological Sciences, *Foundations of Computational Biology with MATLAB* is a web-based ebook in which MATLAB is introduced and progressively developed as a programming and visualization tool in a variety of applications ranging from data analysis and simulation to the development of complex mathematical models in biology.

The ebook contains:

* 21 chapters
* 17 MATLAB & SimBiology Practice Assignments
* Code for all the MATLAB scripts and functions used in the book
* Code for all the Practice Assignments, with many assignments already solved
* 6 Toolboxes for specific applications described in the book
* 2 Tutorials on enzymatic and metabolic simulations

Ebook Contents

**Chapter 1**

* The fundamental ideas of linear algebra
* Special Topic: Other types of products between vectors or matrices
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 2**

* Change of basis
* Special Topics:
  + Intrinsic and extrinsic rotations
  + Covariant and Contravariant bases
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 3**

* Matrix factorization and systems of linear equations
* Special Topic: Iterative methods for systems of linear equations
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 4**

* The fundamental theorem of linear algebra
* Practice Assignment
* Chapter Code
* Practice Assignment Solution Code

**Chapter 5**

* Projections
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 6**

* Least squares
* Special Topics:
  + Information and precision matrix
  + Multiple Linear regression and regularization techniques
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 7**

* Duality, Optimization and Minimum Principles
* Special Topics:
  + Taylor series
  + Newton-Raphson
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 8**

* Non-linear least squares
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 9**

* Eigenvalues and eigenvectors
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 10**

* Principal component analysis
* Special Topics:
  + Rotational ambiguity of eigenvector basis in PCA
  + Norms and Condition Number
  + Independent Component Analysis
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 11**

* Singular Value Decomposition (SVD)
* Special Topics
  + The Trace operator
  + RMSD superposition of two conformations of a biological molecule
  + Principal Component Regression and Partial Least Squares
* Chapter Code

**Chapter 12**

* Singular Value Decomposition (SVD) of microarray data
* Special Topic: Microarray analysis by Independent Component Analysis
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 13**

* Simulation of chemical reactions
* Special Topics:
  + Conversion of a single higher order differential equation into a system of 1st order differential equations
  + Molecular dynamics and the leapfrog/velocity Verlet algorithm
  + Topology and dynamics of a network of reactions
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 14**

* Simulation and analysis of Binding Reactions
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 15**

* Simulation and analysis of Enzymatic Reactions
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 16**

* Dynamic simulation of a network of chemical reactions, Metabolic Control Analysis (MCA), Pharmacokinetics/Pharmacodynamics (PKPD)
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 17**

* Unconstrained minimization
* Chapter Code

**Chapter 18**

* Duality and Linear Programming
* Special Topic: Interior Point Method and Quadratic programming (QP)
* Chapter Code

**Chapter 19**

* Metabolic Network Reconstruction, Flux Balance Analysis
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

**Chapter 20**

* Information Theory
* Special Topic: Mutual information methods for the analysis of multiple sequence alignments
* Chapter Code

**Chapter 21**

* Nonnegative/sparse matrix factorization and Tensor decomposition
* Practice Assignment
* Chapter Code
* Practice Assignment Solution

Resources

[SimBiology](https://www.mathworks.com/products/simbiology.html)

[Pharmacokinetics/Pharmacodynamcis(PK/PD)](https://www.mathworks.com/discovery/pharmacokinetic.html)

[Computational Biology](https://www.mathworks.com/solutions/computational-biology.html)

  
This work is licensed under a [Creative Commons Attribution-ShareAlike 3.0 Unported License](http://creativecommons.org/licenses/by-sa/3.0/deed.en_US).

Learn more about MathWorks academic resources: [www.mathworks.com/academia/](http://www.mathworks.com/academia/)