

## Author Information

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## Ebook Details

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### 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

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### [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](#)

## *Foundations of Computational Biology with MATLAB*

- 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
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### **Chapter 4**

- The fundamental theorem of linear algebra
- Practice Assignment
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### **Chapter 5**

- Projections
- Practice Assignment
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### **Chapter 6**

- Least squares
- Special Topics:
  - Information and precision matrix
  - Multiple Linear regression and regularization techniques
- Practice Assignment
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- [Practice Assignment Solution](#)

### **Chapter 7**

- Duality, Optimization and Minimum Principles
- Special Topics:

## *Foundations of Computational Biology with MATLAB*

- Taylor series
- Newton-Raphson
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### **Chapter 8**

- Non-linear least squares
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### **Chapter 9**

- Eigenvalues and eigenvectors
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### **Chapter 10**

- Principal component analysis
- Special Topics:
  - Rotational ambiguity of eigenvector basis in PCA
  - Norms and Condition Number
  - Independent Component Analysis
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### **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

## *Foundations of Computational Biology with MATLAB*

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### **Chapter 13**

- Simulation of chemical reactions
- Special Topics:
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  - Molecular dynamics and the leapfrog/velocity Verlet algorithm
  - Topology and dynamics of a network of reactions
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### **Chapter 14**

- Simulation and analysis of Binding Reactions
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### **Chapter 15**

- Simulation and analysis of Enzymatic Reactions
- Practice Assignment
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### **Chapter 16**

- Dynamic simulation of a network of chemical reactions, Metabolic Control Analysis (MCA), Pharmacokinetics/Pharmacodynamics (PKPD)
- Practice Assignment
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### **Chapter 17**

- Unconstrained minimization
- [Chapter Code](#)

### **Chapter 18**

## *Foundations of Computational Biology with MATLAB*

- 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](#)
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### **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*

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[SimBiology](#)

[Pharmacokinetics/Pharmacodynamics\(PK/PD\)](#)

[Computational Biology](#)



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