

Provides a tutorial on the computational tools that use mathematical optimization concepts and representations for the curation, analysis and redesign of metabolic networks

Analysis and redesign of metabolic networks often requires the calculation of product yield, gene essentiality prediction, identification of network gaps in the model, resolution of discrepancies with experimental data and identification of network modifications that increase product yield. The main goal of *Optimization Methods in Metabolic Networks* is to apply the language and tools of mathematical programming to describe and solve such frequently occurring tasks.

Topics covered in this book start with a formal treatment of the relevant optimization problem class followed by relevant metabolic network applications. The class of optimization problems becomes progressively more complex, starting with linear programming (LP) and mixed-integer linear programming (MILP) problems and concluding with nonlinear programming (NLP) and mixed-integer nonlinear programming (MINLP) problems.

Optimization Methods in Metabolic Networks:

- Organizes, for the first time, the fundamentals of mathematical optimization in the context of metabolic network analysis
- Reviews the foundational principles of different classes of optimization problems including LP, MILP, NLP and MINLP
- Explains how to formulate a metabolic network analysis or redesign task using mathematical optimization
- Reviews a variety of problems in metabolic network curation, analysis and redesign with an emphasis on the details of the optimization formulations
- Provides a detailed treatment of bilevel optimization techniques for computational strain design and other relevant applications
- Provides input files for examples presented on an accompanying website
- Includes problems and exercises for helping to reinforce the introduced concepts

Optimization Methods in Metabolic Networks can be used to introduce students with the knowledge of metabolism to formal mathematical treatments of core computational tasks in metabolic networks or alternatively expose students with a mathematical programming background to metabolism. The hope is that this book will serve as a starting point for more in-depth investigations of relevant techniques and concepts found in the cited literature.

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