

Computational Analysis and Visualization of Complex Biochemical Systems: A linear Algebra Challenge

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Relating the phenotype of an organism to its genotype is one of the 'Grand Challenges' in modern biology. For example, relating a disease such as diabetes or cancer to the causative changes (mutations) in the organisms DNA or changes in the organism's environmental insults (toxins). Our lab has developed a theoretical framework that relates the genotype and environment of an organism to the behavior of its underlying biochemical systems (the phenotype).

We also have developed a computational toolbox for analysis and visualization of these important relationships. One of the current limitations has to do with the computational linear algebra operators at the heart of the methods. There are "anomalous" cases for which we understand the underlying theory, but this theory is currently not implemented in the toolbox. The following is a list of the issues to be fixed, prioritized from the simplest to the more challenging.

- Fix an "index problem" to handle the simplest $n=1$ case
- Automate "nudge off the boundary" to avoid certain borderline issues
- Fixing values for some parameters and calculating with remaining parameters (an efficiency issue)
- Resolving issues that arise in dealing with underdetermined cases that are consistent
- Resolving issues that arise in dealing with underdetermined cases that are inconsistent.
- Faster interactive plotting (a visualization issue)
- "Graceful" halt option to avoid system crashes

We would like the assistance of computer science talent to expand the capabilities of the current toolbox, while making it more robust and user-friendly. The project involves programming in python, computational linear algebra, and visualization techniques. I would be happy to meet with any prospective team, to give a demonstration that would provide more detail, and to discuss the nature and relative importance of the algebraic and visualization challenges.