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Kinetic Diagram Analysis: A Python Library for Algebraic Solutions for Steady-State Observables of Kinetic Networks NIKOLAUS AWTREY, OLIVER BECKSTEIN, Arizona State University — T.L. Hill's development of biochemical cycle kinetics can be used to calculate steady-state observables and construct analytic solutions [Terrell L. Hill. Free Energy Transduction and Biochemical Cycle Kinetics. en. New York: Springer-Verlag, 1989.doi:10.1007/978-1-4612-3558-3.1]. His theory focuses on constructing diagram representations of distinct-state systems with coupled chemical reactions. Hill shows how these diagrams yield rational algebraic expressions for steady-state cycle fluxes and state probabilities. Despite the benefits of his method, these problems are typically solved using ODE solvers or matrix methods due to their simplicity. Kinetic Diagram Analysis (https://github.com/Becksteinlab/kda) is a Python library that takes aim at this issue, bringing Hill's methods forward without the learning curve of his diagrammatic method. KDA leverages the NetworkX library to create diagrams and generate related directional and flux diagrams. It uses the SymPy library to simplify functions, make algebraic and calculus manipulations, and convert the output into Python lambda functions for rapid calculation. This is demonstrated using examples from Hill's book.

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