

K-FIT: An accelerated kinetic parameterization algorithm using steady-state fluxomics data

Background

- Robust parameterization of predictive organism-level kinetic models remains an open challenge due to long parameterization times and poor tractability of existing methods

Approach

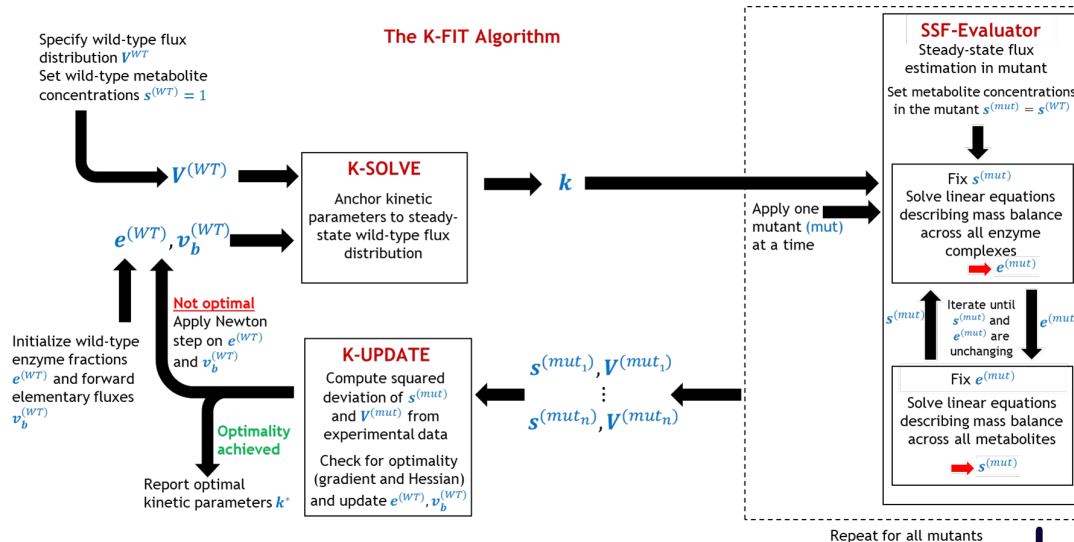
- Decomposition of underlying system of equations describing conservation of mass into two systems of linear equations was completed. Steady-state conditions were evaluated by iterating between the two systems of equations until quantities are unchanging.
- Parameter were updated using gradients evaluated from steady-state sensitivities

Outcome

- K-FIT offers a 1,000-fold accelerated parameterization compared to existing techniques
- Acceleration is due to robust steady-state evaluation and efficient traversal of feasible parameter space using gradients

Significance

- Rapid estimation of *in vivo* kinetic parameters fill knowledge gaps and inform meaningful metabolic engineering strategies
- Easy sensitivity evaluation will enable uncertainty quantification and aid design of experiments for precise parameter estimation



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