The topological logic of optimal solution spaces of genome-scale stoichiometric models of metabolism

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Conclusions

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Results

1) Unique set of vertices
2) Vertices are
   1: Elementary flux modes (EFMs)
   2: Convex combinations of original EFMs
   3) No linealities (but more rays!)

What if we make each reaction irreversible?

Maximize $\mathcal{Z}_{\text{obj}} = \mathcal{J}^{19}$
subject to,

$\mathcal{R} \cdot \mathcal{J} = 0$

$-\infty \leq J_i \leq \infty$, $J_i$ in reversible reactions

$0 \leq J_i \leq 1$, $J_i$ in irreversible reactions

FBA outcome $Z = 0.5$

Optimal solution is not a vertex; its a convex combination of 2 vertices

1) Changes the solution space
2) Increases the number of vertices
3) Makes sure that the secondary optimization is linear (since all $J_i$ are positive)
4) The optimum is always on a vertex