Algorithm to find minimal media for a metabolic model

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Introduction

This is a document to describe a mixed-integer algorithm to find the minimal media for metabolic model.

Defs

Let S be an $m \in \mathcal{M}$ by $n \in \mathcal{N}$ stoichiometric matrix, where $\mathcal{M}$ and $\mathcal{N}$ are the sets of metabolites and reactions respectievely. Let v represent the vector of fluxes with some lower bound and upper bound vectors lb and ub, respectively For a subset of reactions $\mathcal{U} \in \mathcal{N}$, let $\mathcal{U}$ represent the set of uptake (or exchange reactions), and z_k represent the binary variable, where when $z_k = 1$, uptake reaction k is required for growth and $z_k = 0$, it is not. For each k, we can inforce this by imposing the following constraint:

$$l_k z_k < v_k < u_k \tag{1}$$

When $z_k = 1$, $v_k \geq lb$, otherwise $v_k \geq 0$, which means no there is no uptake flux through reaction k. If we ssume that we constrain the biomass growth rate to some min. value μ_{min}, then the full program is:

$$\begin{aligned}
\underset{v,z}{\text{minimize}} \quad & \sum_k z_k \\
\text{subject to} \quad & \sum_i s_{ij} v_i = 0, \forall j \in \mathcal{M} \\
& l_k z_k - v_k \leq 0 \forall k \in \mathcal{U} \\
& lb_i < v_i < ub_i, \forall i \in \mathcal{N} \\
& v_{\text{biomass}} > \mu_{\text{min}}
\end{aligned}$$