Applications of elementary flux modes, extreme pathways

1. engineer a network; e.g., optimize the production of a compound
2. "attack" a network

Equilibrium fluxes can be expressed as

$$v = c_1 v_1 + c_2 v_2 + ... + c_r v_r$$

where $Sv_k = 0$ (we'll call this Eqn 1).

We start with the equation $Sv = 0$. We decompose v as

$$\begin{bmatrix} v_{rev} \\ v_{irr} \end{bmatrix}$$

where the two subvectors correspond to the reversible and irreversible reactions in the network. We are interested in solutions to Eqn 1 that satisfy

$$v_{irr} \geq 0$$

That is, we constrain solutions so that coefficients associated with irreversible reactions are positive. Furthermore, we focus on solutions of Eqn 1 of the form

$$v = \sum_{k \in rev} c_k v_k + \sum_{k \in irr} \lambda_k v_k$$

where $\lambda_k \geq 0$ and $c_k \in \mathbb{R}$.

A *flux mode* is all vectors of the form

$$\lambda v^*$$

where v^* satisfies the 3 conditions just described.

1. $Sv^* = 0$
2. $v^*_{irr} \geq 0$
3. $\lambda > 0$

An *elementary flux mode* is a flux mode that cannot be further decomposed as a sum of other flux modes (not a proper basis since they are not necessarily linearly independent).

An *extreme pathway* is an elementary flux mode where all reversible reactions are decomposed to two irreversible reactions, increasing the dimensionality of the solution space and constraining it to the non-negative space.