

05/22/2014

Biochemical Reaction Network Models

Reference. Anderson + Kurtz. Continuous time Markov chain models for chemical reaction networks.

$\mathcal{S}$: finite set of species (e.g. $\{A_1, \dots, A_n\}$ or $\{A, B, C, \dots, M\}$ or $\{S_1, \dots, S_n\}$).

$\mathcal{C}$: finite set of complexes. A complex is the left or right side of a reaction.

e.g. $A_1 + A_2 \rightarrow A_3$. $A_1 + A_2$ is a complex & so is A_3 .

Represent these by n -dimensional vectors where i^{th} component of such a vector is the # of molecules of species i in the complex. $A_1 + A_2: v_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$. $A_3: v_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

$\mathcal{R}$: finite set of reactions of the form $v \rightarrow v'$ where $v, v' \in \mathcal{C}$. (Suppose $\mathcal{R}$ has K elements.)

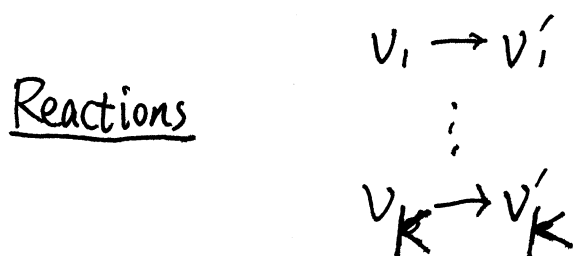
Stoichiometric matrix $S_{n \times K}$.

Cols. correspond to reactions. k^{th} column is $v'_k - v_k$ if k^{th} reaction is $v_k \rightarrow v'_k$.

$v'_k - v_k$ is the change in # of molecules of each species.

Microscopic Stochastic Model for Dynamics of Biochemical Reaction Network

For each species i , let $X_i(t)$ be the # of molecules of species i in system at time t . Let $X = (X_1, \dots, X_n)$. Assume X is a Markov chain. When k^{th} reaction occurs at time t and it's the only reaction that occurs then, $X(t) = X(t-) + v'_k - v_k$.



Rate of 1st reaction = $\frac{1}{\text{mean waiting time}} = \lambda_1(x)$, where $x = (x_1, \dots, x_n)$ is the # of molecules of each type currently in system.

Representation for X (Poisson integral representation)

$$X(t) = X(0) + \sum_{k=1}^K (v'_k - v_k) \cdot R_k(t),$$

where $R_k(t)$ is the # of times the k^{th} reaction has occurred by time t . Let $N_1, \dots, N_K$ be independent rate 1 Poisson processes.

$$R_k(t) = N_k \left(\int_0^t \lambda_k(X(s)) ds \right).$$

$$X(t) = X(0) + SR(t), \quad R(t) = \begin{pmatrix} R_1(t) \\ \vdots \\ R_K(t) \end{pmatrix}.$$