Eventual Reaction Time in General Bio-Molecular Networks

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We consider a novel model of general bio-molecular networks, where a number of different classes of the molecules are involved. And among each class there is a number of different types of the molecules. Without loss of the generality, we assume there is a total number of fundamental re-actions in this network. With this general description of the network, we may include many existing sub-networks as specials. The proposed bio-molecular network basically consists of four organizational control layer: Layer 1- Genome (genes); Layer 2- Transcriptome (RNAs - mRNA, rRNA, tRNA); Layer 3-Proteome (proteins); Layer 4- Metabolome (metabolites). The biomolecular network interacts with it's environment through multiple mechanisms - chemical, photo, thermal, vibrational. In general, there are mainly four types of the element molecules, i.e., Genes, mRNA, Protein, Metabolite and plus a general environment (it is too clear) where sometimes the proteins and metabolite. Since there are normally some molecules, which are a joint molecule combined with another one etc., we will then call those molecules as complex molecules. Now, let $\boldsymbol{X}(t)$ be the state variable of this network on the state space Ω..We assume there are total M fundamental chemical reactions in the network, say $R_1, R_2, \cdots, R_M$. Each reaction changes the population of at least one class of molecules and a population change of any classes comes from a reaction. Mathematically speaking, reaction R_k is characterized by a reaction constant c_k . A fundamental hypothesis of chemical reaction kinetics is that the rate of each reaction R_k can be specified in terms of a so-called propensity function $a_k(\boldsymbol{x})$ depending on the reaction constant and the current state $\boldsymbol{x}$ of the cell network. The change in numbers of molecules of the cell network is described by the state-change vector, $\boldsymbol{v}_k = (\boldsymbol{v}_{1,k}, \boldsymbol{v}_{2,k}, \cdots, \boldsymbol{v}_{10,k})$, where $\boldsymbol{v}_{i,k} = (v_{i,1,k}, v_{i,2,k}, \cdots, v_{i,N_i,k})$, and $v_{i,j,k}$ = the change of number of (i,j) molecule produced by reaction R_k , for the reasonable i, j and k. In general, propensity functions and state-change vectors together will completely characterize all reaction channels. Mathematically speaking, they also characterize the stochastic process $\boldsymbol{X}$(t) as follows: $P[\boldsymbol{X}(t+dt) = \boldsymbol{x} + \boldsymbol{v}_k | \boldsymbol{X}(t) = \boldsymbol{x}] = a_k(\boldsymbol{x})dt$. In this network, we consider an interesting problem, which is called is the eventual reaction time (ERT). This measure is defined as the time interval beginning from the time when the network is in a special state of the network to the time when another special state of the network appears after a series of reactions. An example of ERT may include the time interval beginning from the time when one is detected to have only one cancel molecule in the body to the time when this cancel molecule grows up to 20 molecules. Mathematically speaking, if at time t_0, there is a number of $x_{i_0, j_0}(t_0)$ of (i_0, j_0) molecule, we are interested in the problem of the time interval of the eventual reaction time when there is firstly a number x_{i_1, j_1} of (i_1, j_1) molecule after a series of reactions. Now, denote by x_0 a specific state where the number of (i_0, j_0) molecule is x_{i_0, j_0} , we obtain the following exact result:

<u>Theorem</u>. The probability density function of the eventual reaction time is

$$p(t) = \sum_{n=1}^{\infty} b_n^E(\boldsymbol{x_0}) \frac{t^{n-1}}{(n-1)!}, \quad t \geq 0,$$

where $b_n^E(\boldsymbol{x_0})$ is given in terms of the propensity functions and state change vectors as follows:

$$b_1^E(\boldsymbol{x_0}) = -a_0(\boldsymbol{x_0}) + \sum_{k=1}^{M^E} a_k(\boldsymbol{x_0}),$$

$$b_n^E(\boldsymbol{x_0}) = -a_0(\boldsymbol{x_0}) b_{n-1}^E(\boldsymbol{x_0}) + \sum_{k=1}^{M^E} a_k(\boldsymbol{x_0}) b_{n-1}^E(\boldsymbol{x_0} + \boldsymbol{v_k}), \quad \text{for n} = 2, \cdots ,$$

where M^E is the number of different reactions in a state set consisting of only those states in which the number of (i_1, j_1) molecule is not x_{i_1, j_1} .