Estimation of Stochastic Parameters*

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1 Introduction

Estimation of rate constants is an important problem for detailed modeling of biological systems. Most current work (reviewed in [2]) focuses on deterministic systems — systems where the number of molecules is sufficiently large that it can be approximated as a continuous quantity varying continually over time. However, many real biological systems have a small number of molecules and must be modeled as stochastic processes. There is currently no good way to measure or estimate rate constants of stochastic biological systems.

2 Results

We have developed an algorithm to estimate parameters in the stochastic ramework, given observed trajectories. In some sense, this algorithm is the inverse of the exact stochastic simulation algorithm described in [1].

Amazingly, the estimation algorithm allows one to estimate the parameter of each given reaction individually, *even though* other reactions interact with the reactants and products of the given reaction. Our method specifies how to correct for the existence of interacting reactions, without requiring complete knowledge of the other reactions. So, in principle, our method could be used *in vivo*; even though other (possibly unknown) reactions affect the reaction whose parameter is being estimated, these reactions can be de-convolved from the data to give a correct estimate of the parameter of interest. (Note that trajectories, i.e., number of molecules as a function of time, can be observed directly, whereas rate constants can not.)

As a by-product of our analysis, one can calculate the uncertainty of the estimated parameter as a function of the amount of data.

References

[1] Gibson, M. A. and Bruck, J., *Journal of Physical Chemistry A*.

[2] Gibson, M. A. and Mjolsness, E., *Computational Methods in Molecular and Cellular Biology: from Genotype to Phenotype*, Bolouri and Bower, eds., MIT Press: Cambridge, Massachusetts (in press).

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