



生物信息学研究中心

Center of Bioinformatics

学术报告

题目： A Constraint for Optimal Parameter Estimation to Solve an Issue of Molecular Network Models in Systems Biology

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Abstract: One point is definitely different between network modeling in systems biology and that in other scientific fields. The point is that the models including unmeasured variables frequently emerged, so as to measure the variables under the conditions with as less perturbation to the organism as possible. To consider the point specific to systems biology, we have designed a method by symbolic-computation approach, to estimate kinetic parameter values with a high degree of accuracy [1-5]. First, we utilize differential elimination, which is an algebraic approach for rewriting a system of differential equations into another equivalent system, to derive the constraints between kinetic parameters from differential equations. Second, since its equivalent system is frequently composed of large equations, the system is further simplified by another symbolic computation. Third, we estimate the kinetic parameters introducing these constraints into an objective function, in addition to the error function of the square difference between the measured and estimated data, in the standard parameter optimization method such as the genetic algorithm (GA) and the particle swarm optimization (PSO). Here, the performance of our method for parameter accuracy improvement is illustrated by the simulation of two representative models in biology, a simple cascade model and a negative feedback model, and the actual data analysis for a signal transduction pathway, in comparison with the previous numerical methods. In addition, we will discuss the merits and pitfalls of the present method for further improvements.

References

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