

Efficient Steady State Solution of Stochastic Systems Chemical Reactions

Aminisharifabad, M., Wolf, V., Spieler, D. Computer Science Department ,Saarland University ALMA Analysis of Markovian Models

Introduction

Stochastic Process:

The complexity of living systems has led to a rapidly increasing interest in modeling and analysis of biochemically reacting systems. Since biochemical reactions occur randomly, we need kind of stochastic process. Markov chain is stochastic model which at any time t one can see current state of system by defining appropriate parameters of our model.

Example from Systems Biology:







Continuous-time

Markov Chain (CTMC)

Methods

In chemical reactions modeling because of discreetness of system, state space is too large and computing of steady states is too computing expensive or almost impossible .Aggregation method is one way for fast computing of steady sate solution of stochastic systems.

Aggregation :

Markov chain defined by *P* with state space $i \in I$ can be aggregated to a Markov chain with a smaller state space $A_s \in \Delta$ and a transition matrix *R*

Normal Steady state computing :

 $\pi j = \lim_{t \to \infty} \pi j(t) = \lim_{t \to \infty} p i j(t) \qquad \qquad \pi.Q=0 \text{ or } P. \pi = \pi$





We should say that different patterns have different maximum errors and maximum times. Time and error are trade-off



Number of partition

Future Works

Idea: A good aggregation should group fast subsystems and slow transition between them, which is exactly clustering problem , so

one can finding optimal aggregation pattern using spectral or markov clustering .



Adding dummy state to markov chain as a reprehensive of other state s which already ignored. To direct border state's transition to the dummy state and redirect to one of the states in our boundary.







Original system's transition matrix

Aggregated transition matrix

Aggregated steady state solution

- 1. compute of each macro state independently using normal steady state formulas
- 2. Cpmpute Q for macto-state Markov chain , steady state solution for this markov chain
- 3. Consider final steady state of each state as multiply of corresponding marcro-state and its own steady state from (1)

With aggregation one for sure would have error but by choosing right states in one partition the solution is not far from exact one.

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