

Minimization of Stochastic Dynamical Systems A Comparison of Models & Methods

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Modelling of Complex Self-Organizing Systems Group, 10.03.2020

Motivation

Differential Equations (DE) are omni-present in natural science:

Physics & Chemistry

- electrodynamics
- thermodynamics & diffusion
- fluid dynamics & plasma physics
- classical mechanics
- celestial motion & general relativity
- nuclear physics & quantum mechanics
- Chemical reactions

Biology

- Population dynamics
- wound healing
- epidemiology
- blood flow
- reaction-diffusion equations
- Hodgkin Huxley model
- capillary pressure

Engineering & Economics

- optimal control
- optimization techniques
- electrical engineering
- signal processing
- traffic flow
- mean field game theory
- advertising effects
- economic growth
- price evolution

Motivation

- Dynamical processes describe everything that changes
- DEs are the most common modelling tool in natural sciences
- Automata are the underlying computational model in current hardware and software systems
- Automata also describe dynamical processes (paths/traces) i.e the flow of computation
- Continuous time Markov chains e.g. for chemical reaction networks, quantum automata, . . .
- Those models are extremely complex when all degrees of freedom taken into account

Why Stochastic Dynamical Systems?

Laplace's demon:

An intellect which would know all forces that set nature in motion, and all positions of all items of which nature is composed, if this intellect were also vast enough to submit these data to analysis, it would embrace in a single formula the movements of the greatest bodies of the universe and those of the tiniest atom; for such an intellect nothing would be uncertain and the future just like the past would be present before its eyes.

- Pierre-Simon Laplace, [1]

- Only the universe itself exists since its' beginnings \Rightarrow initial condition problem
- Thermodynamic and quantum mechanical irreversability \Rightarrow Cannot certainly infer past
- Chaos Theory: Butterfly effect

Research Questions

1. How to model stochastic dynamics universally and exactly?
2. How do automata and DE models relate?
3. How do reduction, approximation and minimization methods relate?
4. Is it possible to automatically combine bounded-error approximations, minimizations, reductions of order, ... to achieve minimal computational effort?

TL;DR: What's the most exact, interpretable, computationally fastest and memory-greediest approach of modelling arbitrary stochastic dynamical systems and **why** is that so?

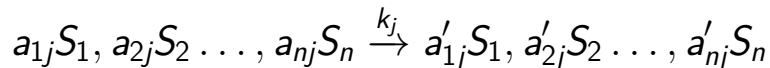
Example: Chemical Reaction Networks

Taken from [2] with support of [3].

Let the chemical reaction network CRN be a 2-tuple (S, R) with

$$S = \{S_1, S_2, \dots, S_n\}$$

the set of distinct species and $R = \{R_1, R_2, \dots, R_k\}$ the set of reactions in the form



where a_j is called to consumption vector, a'_j the production vector, k_j the reaction rate constant and

$$\nu_j = a'_j - a_j$$

the change vector of R_j

Classical chemical kinetics

- Continuous, deterministic ODE-based model.
- Assumes constant pressure and temperature, well-stirredness.
- Based on concentrations rather than particles.

Let $s_0 = (s_1, s_2, \dots, s_n)$ be an initial state. The deterministic reaction rate is given by

$$\lambda_j(s_i) = k_j \prod_{i=1}^n s_i^{a_{ij}}$$

and the model by the solution of n coupled non-linear ODEs

$$\frac{d}{dt}s_i(t) = \sum_{j=1}^k \nu_{ij} \lambda_j(s_i(t))$$

Problem: Can not explain variations present in reality

Stochastic chemical kinetics I

- Discrete, stochastic CTMC-based model.
- Assumption: Thermal equilibrium, well-stirred
- Based on particles.
- Transient probability distribution is measure of interest

Let $x_0 = (x_1, x_2, \dots, x_n)$ be an initial state. The stochastic reaction rate for each reaction is given by

$$\tilde{\lambda}_j(x) = c_j \prod_{i=1}^n \binom{x_i}{a_{ij}}$$

Stochastic chemical kinetics II

The model is defined by the CTMC X_t over the states

$$S = \{x \mid x \text{ reachable from } x_0\}$$

with $p_0(x_0) = 1$ and the generator matrix

$$w(x, y) = \sum_{j=1}^k \lambda_j(x) 1_{y=x-\nu_j}$$

Transient probability distributions can then be obtained by solving the chemical master equation (CME)

$$\frac{d}{dt} p^{(t)}(x) = \sum_{x-\nu_j \in S} \sum_{j=1}^k \lambda_j(x-\nu_j) p^{(t)}(x-\nu_j) - \sum_{j=1}^k \lambda_j(x) p^{(t)}(x)$$

- Instead of solving the CME, do dynamic MCMC approximation on the CTMC
- stochastic simulation algorithm (SSA)

To summarize:

- classical chem. kin. use coupled ODEs to approx. stochastic model in the limit of species and volume to infinity at constant concentrations
- Continuous Markov Process (CMP) models stochastic chem. kin.
- solving Master Equation provides transient probability distribution
- which is in turn approx. by MCMC on the CTMC def'd by the CMP






Questions:

- Are Monte Carlo methods on automata always cheaper than numerical solution of high dimension & order DEs?
- Is there always an automaton that can approximate the DE?
- If reducing the complexity in either the CTMC (minimization) or the DE (reduction of order, fwd/bwd eq., QSSA), how does the counterpart change if existent?
- When only interested in certain quantities: How do we adapt the models?

Goals

1. Implement minimization algorithm for weighted automata [4].
2. Implement model reduction algorithm for ODEs [5].
3. Develop reproducible benchmarks
4. Write report including
 - formal description of models, properties, specializations
 - connections & discords of models
 - Description of dimensionality reductions, minimizations, approximations, reduction to partial models for each
 - compare reduction, minimization and approximation techniques
 - compare 1. & 2. quantitatively by results 3.

Bibliography

-  P.-S. Laplace, *Philosophical Essay on Probabilities: Translated from the fifth French edition of 1825*. Springer Science & Business Media, 1998, vol. 13.
-  T. Petrov, “Markov chain aggregation and its application to rule-based modelling”, *CoRR*, vol. abs/1812.09774, 2018. arXiv: 1812.09774. [Online]. Available: <http://arxiv.org/abs/1812.09774>.
-  N. G. Van Kampen, *Stochastic processes in physics and chemistry*. Elsevier, 1992, vol. 1.
-  S. Kiefer, A. S. Murawski, J. Ouaknine, B. Wachter, and J. Worrell, “On the complexity of equivalence and minimisation for q-weighted automata”, *Logical Methods in Computer Science*, vol. 9, 2013.
-  L. Cardelli, M. Tribastone, M. Tschaikowski, and A. Vandin, “Maximal aggregation of polynomial dynamical systems”, *Proceedings of the National Academy of Sciences of the United States of America*, vol. 114 38, pp. 10 029–10 034, 2017.