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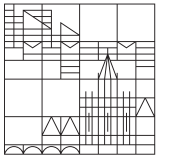

Minimization of Stochastic Dynamical Systems A Comparison of Models & Methods

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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
- Continuous time Markov chains e.g. for chemical reaction networks, quantum automata, . . .

Motivation

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

Phisics & 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
- epidemology
- blood flow
- reaction-diffusion equations
- Hodgkin Huxley model
- capiliary pressure

Engineering & Economics
- optimal control
- optimization techniques
- electrial engineering
- signal processing
- trafic flow
- mean field game theory
- advertising effects
- economic growth
- price evolution

Why Stochastic Dynamical Sytems?

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

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

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

$$a_{1j}S_1, a_{2j}S_2 \ldots, a_{nj}S_n \xrightarrow{k_j} a'_{1j}S_1, a'_{2j}S_2 \ldots, a'_{nj}S_n$$

where a_j is called to consumption vector, a'_j the production vector, k_j the reaction rate contant 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 then particles.

Let $s_0 = (s_1, s_2, \ldots, s_n)$ 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 $x_0 = (x_1, x_2, \ldots, x_n)$ 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 def'ed by the CTMC X_t over the states

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

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

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

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'ed 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 reducting the complexity in either the CTMC (minimization) or the DE (reduction of order, fwd/bwd eq., QSSA), how does the counterpart change if existant?
- 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. quantitively by results 3.

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