FilteringChemNet README

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1 Overview

This is a README for the FilteringChemNet MATLAB package, the implementation of the algorithms described in the manuscript *State and parameter estimation from exact partial state observation in stochastic reaction networks*. These notes assume an understanding of this manuscript. Functions in `thisFont` typically refer to MATLAB scripts or functions.

2 Algorithms

2.1 State estimation - `overall_scheme.m`

We consider chemical reaction networks modeled by a discrete state and continuous in time Markov process $Z(t)$ for the vector copy number of the species. We denote the vector copy number of the observable species by $Y(t) \in Z_+^{n_2}$ and that of the rest of the (unobservable) species by $X(t) \in Z_+^{n_1}$, and our goal is to compute the conditional probability distribution

$$\pi(t, x) = P\{X(t) = x \,|\, Y(s) = y(s),\ 0 \le s \le t\}$$

for $x \in Z_+^{n_1}$.

We propose Algorithm 1, the overall scheme, in the manuscript to accomplish this task. The corresponding code is the script `overall_scheme.m`. Inside the overall scheme, crucial steps are presented as algorithms, to be specific, Algorithm 2 Continuous evolution, Algorithm 3 Jump and Algorithm 4 Offsprings. They are implemented as functions `CTMC_filter_cont.m`, `CTMC_filter_jump.m` and `resampling.m` respectively.

2.2 Parameter estimation - `Bayesian_para_scheme.m`

In general, the propensity functions a_j depend on parameters. Here we consider a Bayesian framework for inferring the parameters c from the observation $Y(s) = y(s)$ for $0 \le s \le t$. Algorithm 5, Overall scheme for Bayesian inference, describes such procedure, and it is implemented by the script `Bayesian_para_scheme.m`.

2.3 Past state estimation - `past_state_scheme.m`

We consider the estimation of the state at time t_0 with the observation made until a later time T. That is, we would like to find

$$P\{X(t_0) = x \,|\, Y(s) = y(s),\ 0 \le s \le T\}$$

with $0 \le t_0 \le T$. Algorithm 6 Past state estimation does time job and the corresponding script for that is `past_state_scheme.m`.

3 Workflow of numerical experiments

We conducted several numerical experiments to test our algorithms. In this section, we explain the workflow of the experiments.

3.1 Simulate the systems and generate the observations

All three schemes have to engage with a observation trajectory, and we could simulate the underlying systems and generate the synthetic observation trajectories using the script `CTMC_obs.m`. The result will be saved to binary files. In the manuscript, we discussed a few systems, and the specifications of these systems are provided by the functions `linprop.m`, `linprop_A.m`, `circuit.m`, `toggle.m` and `seir.m`.

3.2 State Estimation, Parameter Estimation, and Past State Estimation

Once an observation trajectory is ready, one can use the code `overall_scheme.m`, Bayesian_para_scheme.m, or `past_state_scheme.m` to obtain the conditional distribution at time t and produce the plot.

3.3 Estimation of state made at jump times of observed species

Once an observation trajectory is ready, one can use the code `traj_state_est.m` to obtain the estimation of the state at time t based on the observation on $[0, t]$ at jump times and plot the trajectory of the series of estimates along with the confidence intervals.