Bounding Mean First Passage Times in Stochastic Reaction Networks

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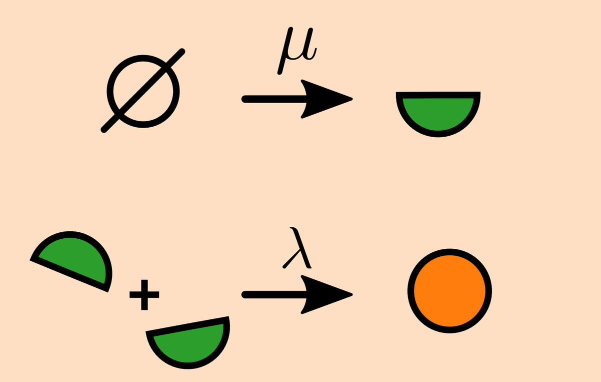
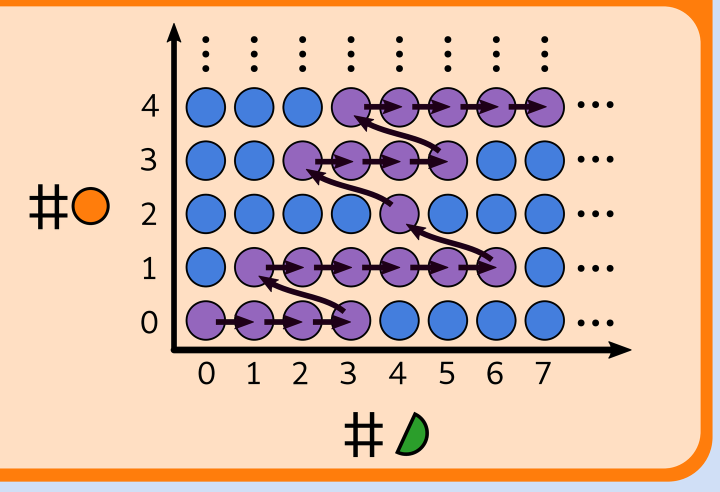
Background and Goal

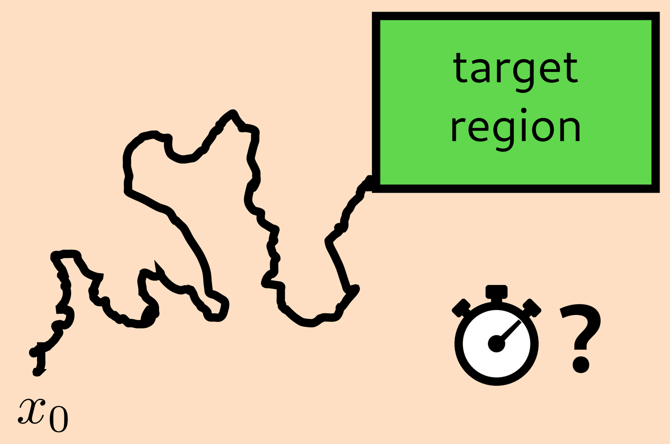
Reaction network



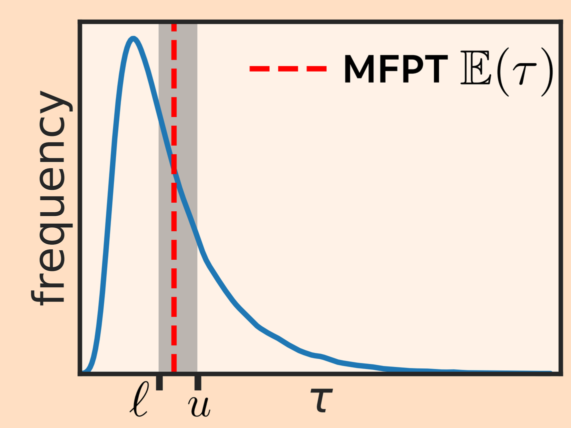
CTMC semantics



First-passage times



Finding bounds



Method

Moment dynamics

Derive the dynamics of statistical moments from the CME.

$$\frac{d}{dt}\mathbb{E}(X_t^m) = \sum_j \mathbb{E}\left(((X_t+v_j)^m - X_t^m)\,\alpha_j(X_t)\right)$$

→

Weighting & integration

Multiply a time-weighting $w(t) = t^s$ and integrate symbolically.

no moment closure

→

Finding a martingale

The expectation implies a process

$$Z_t = t^k X_t^m - t_0^k X_0^m + \sum_i c_i \int_0^t s^{m_i} X_s^{m_i}\, ds$$

$$\forall t \geq 0.\ \mathbb{E}(Z_t) = 0$$

→

Linear constraints

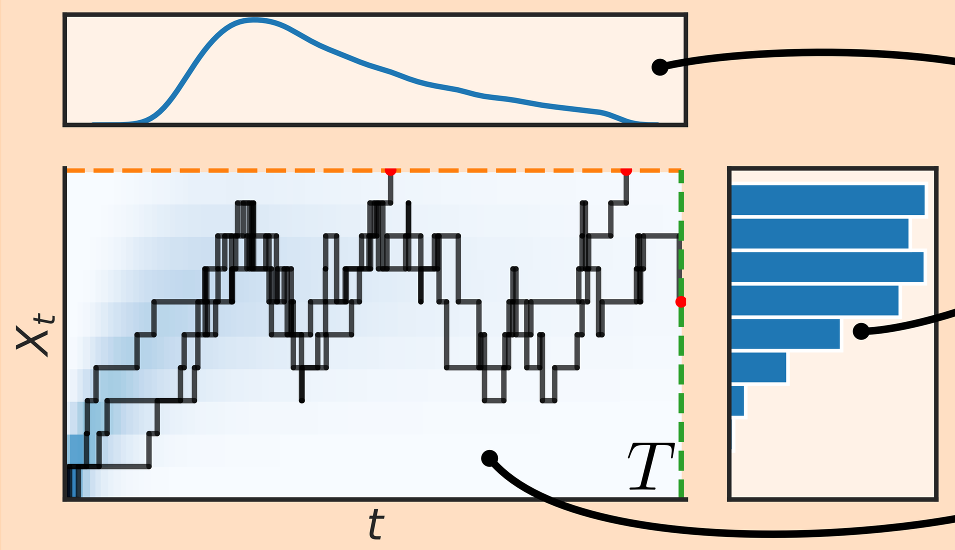
By Doob's theorem

$$\mathbb{E}(Z_\tau) = 0$$

for stopping times τ under mild conditions.

Defining appropriate measures

We define three measures ν_1, ν_2 and μ restricted to distinct subsets of the state-time space $[0,T] \times \mathcal{S}$. In the relaxation the domain restrictions are expressed through semi-definite constraints.



First-passage time distribution
$\nu_1(C) = \Pr(\tau \in C, \tau < T)$

Exit location probability
$\nu_2(B) = \Pr(X_T \in B, \tau = T)$

Expected occupation measure
$\mu(B \times C) = \mathbb{E}\left(\int_{[0,\tau]\cap C} 1_B(X_s)\, ds\right)$

A semi-definite relaxation

We can formulate constraints on the moments of the measures ν_1, ν_2 and μ. In particular, the **moment matrix** of all measures must be **positive semi-definite.**

Moment matrix

$$M(\vec{y}) = \begin{pmatrix} y_0 & y_1 & y_2 \\ y_1 & y_2 & y_3 \\ y_2 & y_3 & y_4 \end{pmatrix}$$

$y_n = \mathbb{E}(X^n)$

Positive semi-definite

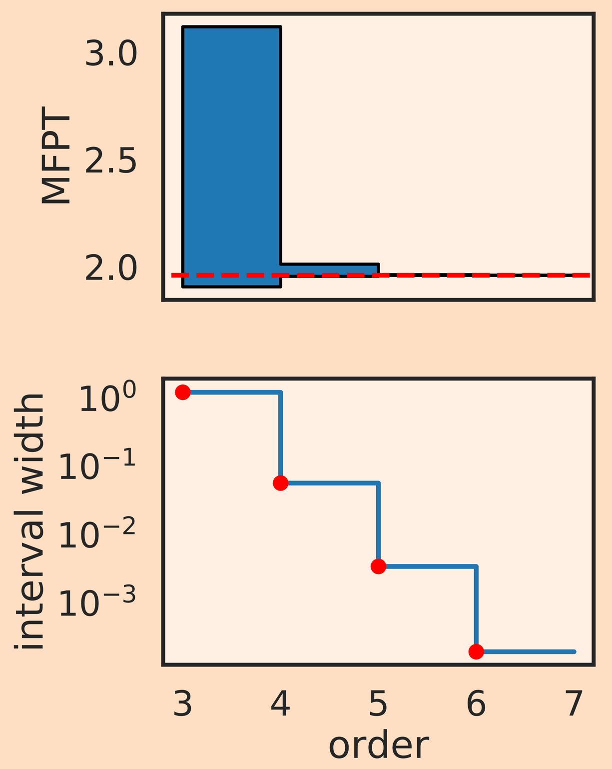
A matrix M is positive semi-definite iff.

$\forall v \in \mathbb{R}^n.\ v^\top M v \geq 0.$

max / min 0-th moment of EOM ($\sim \mathbb{E}(\tau)$)
such that **linear moment constraints** hold
moment matrices are psd
proper measure domains

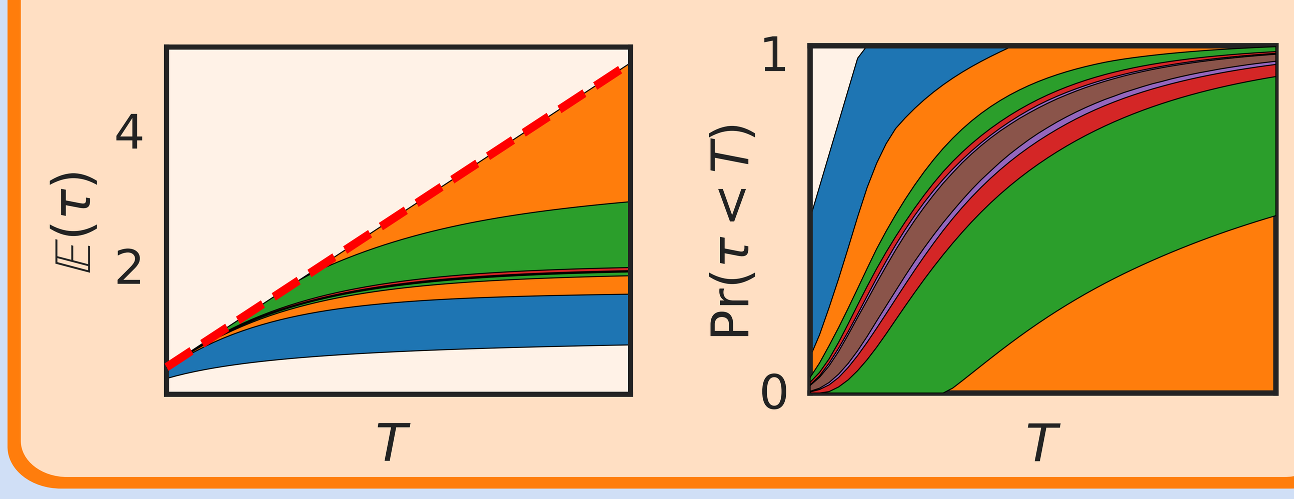
Results and Challenges

Convergence



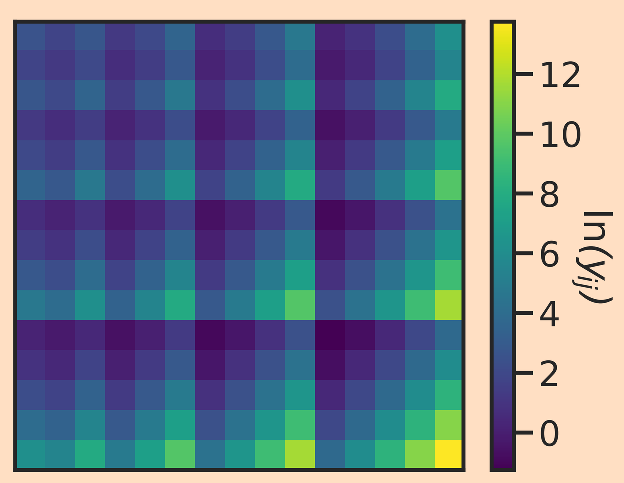
Transient analysis

We can vary the time horizon T and compute bounds on the MFPT and the probability of reaching the target region before T.



Challenges / Future work

Vastly different orders of magnitude lead to numerical difficulties for the SDP solver.



Re-scale the state-space to reduce the differences in the moment matrices.

Modify linear constraints such that low and high order moments become independent.

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