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.

\[
\frac{d}{dt} \mathbb{E}(X(t)) = \sum_i \mathbb{E}((X_t + i \mu_i) - X(t)) \nu_i(X(t))
\]

**Weighting & integration**

Multiply a time-weighting \( w(t) = t^\alpha \) and integrate symbolically.

\[
w(t) = t^\alpha \Rightarrow \mathbb{E}(X(t)) = \int_0^t t^\alpha \mathbb{E}(X(t) \mid t) dt
\]

**Finding a martingale**

The expectation implies a process

\[
x_t = x_t^{(0)} + \int_0^\tau X_t^{(0)} \mu(X_t) dt + \sum_i \int_0^\tau X_t^{(i)} \nu_i(X_t) dt
\]

\( \forall \tau \geq 0, \mathbb{E}(x_t) = 0 \)

**Linear constraints**

By Doob's theorem

\[
\mathbb{E}(x_t) = 0
\]

for stopping times \( \tau \) under mild conditions.

Defining appropriate measures

We define three measures \( \nu_1, \nu_2, \mu \) restricted to distinct subsets of the state-space \( \mathcal{X} \times \mathcal{S} \). In the relaxation the domain restrictions are expressed through semi-definite constraints.

**A semi-definite relaxation**

We can formulate constraints on the moments of the measures \( \nu_1, \nu_2, \mu \).

- In particular, the moment matrix of all measures must be positive semi-definite.

\[
M(y) = \begin{pmatrix} y_1 & y_2 & y_3 \\
                      y_2 & y_4 & y_5 \\
                      y_3 & y_5 & y_6 \end{pmatrix} \quad \mathbb{E}(X(t)) = y_6
\]

- A matrix \( M \) is positive semi-definite if

\[
\forall y \in \mathbb{R}^n, y^T M y \geq 0
\]

- The maximum / minimum 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**

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

**Transient analysis**

**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.