

# Analysis of Markovian Population Models

## Dissertation Defense

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# Motivation

- ▶ Example
- ▶ list other applications: queueing, metabolic networks, switches etc.

# Markovian Population Models

## Semantics

- ▶ counting agents / population size
- ▶ continuous time
- ▶ exponential jump times / CTMC dynamics
- ▶ example: birth-death process

# Markovian Population Models

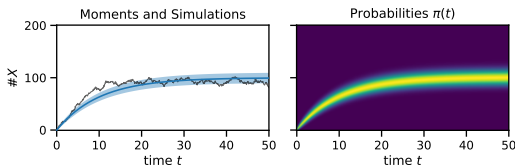
## Stationary Distribution – Foster-Lyapunov Functions

- ▶ ergodic chains converge to unique distribution
- ▶ how does this distribution look like for infinite state-spaces?
- ▶ use Foster-Lyapunov function to bound sets
- ▶ locally augment functions for tighter sets / bounds

# Markovian Population Models

## Moment Dynamics

- ▶ alternative approach: look at moments instead of states
- ▶ expected values, e.g.  $E(X)$ ,  $E(X^2)$



- ▶ Moment formula

$$\frac{d}{dt} E(f(X_t)) = \sum_{j=1}^{n_R} E((f(X_t + v_j) - f(X_t)) \alpha_j(X_t))$$

- ▶ ODE system not closed

# Markovian Population Models

## Martingale Process

- ▶ multiply time-weighting:  $w(t) = t^k$ ,  $k \in \mathbb{N}$  or  $w(t) = \exp(\lambda t)$
- ▶ analytic integration and resulting martingale process

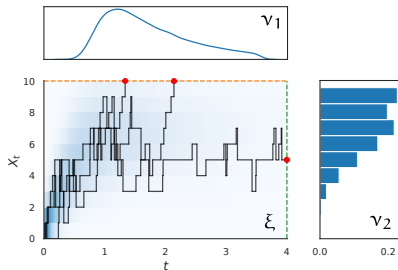
$$\begin{aligned} Z_T := & w(T)f(X_T) - w(0)f(X_0) - \int_0^T \frac{dw(t)}{dt} f(X_t) dt \\ & - \sum_{j=1}^{n_R} \int_0^T w(t) (f(X_t + v_j) - f(X_t)) \alpha_j(X_t) dt \end{aligned}$$

- ▶ known expectation:  $E(Z_T) = 0$ ,  $\forall T \geq 0$

# Bounding Mean First-Passage Times

## Martingale Process and Linear Moment Constraints

- ▶ expected occupation time and exit measures (in relation to expectation of the martingale)



- ▶  $0 = E(Z_T)$  is a linear moment constraint constraint on  $\nu_1$ ,  $\nu_2$ , and  $\xi$  ( $w(t) = t^k$ ) (TODO: integrate moms and figure)

(Backenköhler, Bortolussi, and Wolf 2020)

# Bounding Mean First-Passage Times

## Moment Matrices and Semi-Definite Programs

- ▶ semi-definite moment constraints (positive variance as example)
- ▶ hint at localizing matrices

(Backenköhler, Bortolussi, and Wolf 2020)



# Bounding Mean First-Passage Times

## Results and Practical Issues

- ▶ moment problems are inherently stiff
- ▶
- ▶ some examples

(Backenköhler, Bortolussi, and Wolf 2020)

# Bounding Mean First-Passage Times

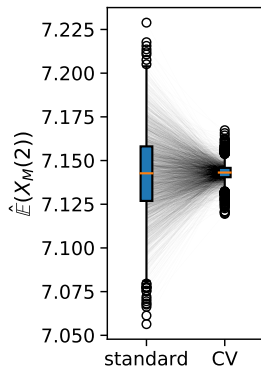
## Hausdorff Constraints and Linear Programs

- ▶ linear constraints possible if domains (time and space) are finite
- ▶ 1D visualization of Hausdorff constraints

# Linear Control Variates

## Using Correlated RVs with Known Expected Value

- ▶ segue: use the same martingale constraints to enhance MC estimation
- ▶  $E(X_T) = E(X_T) + bE(Z_T)$
- ▶ use correlations between target RV and martingales (linear regression, i.e. control variates)



(Backenköhler, Bortolussi, and Wolf 2019)

# Linear Control Variates

## Finding Efficient Sets of Control Variates

- ▶ time-weighting has a large influence on the correlation
- ▶ Infinitely many possibilities (cost needs to be controlled though)
- ▶ variates can be highly redundant (correlated) and incur an additional cost
- ▶ Alg. 1: Tighten an initial proposal set
- ▶ Alg. 2: Re-sample promising candidates

(Backenköhler, Bortolussi, and Wolf 2019, 2022)

# Linear Control Variates

## Selection Algorithms

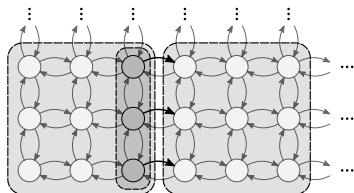
# Linear Control Variates

## Results

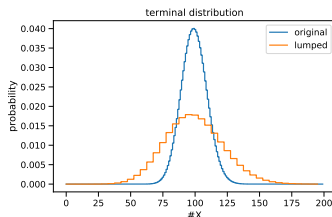
- ▶ best example?

# State-Space Aggregation

Treating Hyper-Cubes of States as One



- ▶ hyper-cube macro-states
- ▶ *assumption*: uniform dist. within
- ▶ closed-form transition rates



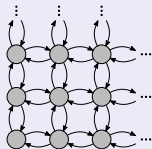
- ▶ resulting distribution more “flat”
- ▶ locate main probability mass

(Backenköhler, Bortolussi, Großmann, et al. 2021a,b)

# Stationary Distribution

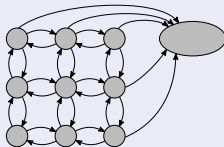
## Finite-Space Projection

### Original



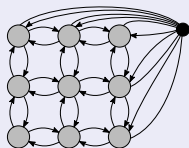
- ▶ infinite

### Sink state



- ▶ transient analysis
- ▶ keep track of approx. error

### Redirection



- ▶ stationary dist.
- ▶ dependent on redirection

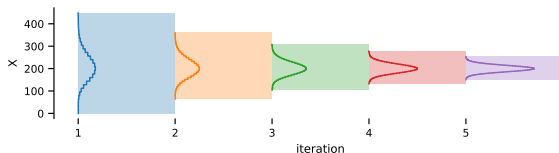


# Stationary Distribution

## Iterative Refinement Algorithm

A simple refinement based on approximate solutions:

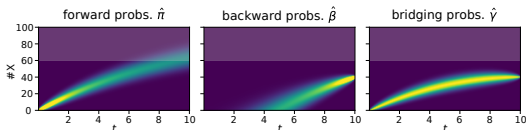
1. start with macro-states of size  $2^k$
2. compute approximate distribution
3. remove states with low probability
4. split the remaining states
5. go to step 2



(Backenköhler, Bortolussi, Großmann, et al. 2021a,b)

# Bridging Problem

## Dynamical Analysis Under Initial *and* Terminal Constraints



### Forward Probabilities

How the process evolves with time:  $\Pr(X_t = x \mid X_0 = 0)$

### Backward Probabilities

Probability of ending up in a given state:  $\Pr(X_T = 40 \mid X_t = x)$

### Bridging Probabilities

In between:  $\Pr(X_t = x \mid X_0 = 0, X_T = 40)$

(Backenköhler, Bortolussi, Großmann, et al. 2021a)

# Bridging Problem




## Refinement

(backenkoehler2020analysis)

# Importance Sampling

# Conclusions and Future Directions

# References I

-  Backenköhler, Michael, Luca Bortolussi, and Verena Wolf (2020). “Bounding Mean First Passage Times in Population Continuous-Time Markov Chains”. In: *17th International Conference on Quantitative Evaluation of SysTems*. Vol. 12289. Lecture Notes in Computer Science. Springer, pp. 155–174.
-  — (2019). “Control Variates for Stochastic Simulation of Chemical Reaction Networks”. In: *17th International Conference on Computational Methods in Systems Biology*. Vol. 11773. Lecture Notes in Computer Science. Springer, pp. 42–59.
-  — (2022). “Variance Reduction in Stochastic Reaction Networks using Control Variates”. In: *Principles of Systems Design – Essays Dedicated to Thomas A. Henzinger on the Occasion of His 60th Birthday*. Vol. 13660. Lecture Notes in Computer Science. Springer.

# References II



Backenköhler, Michael, Luca Bortolussi, Gerrit Großmann, et al. (2021a). “Analysis of Markov Jump Processes under Terminal Constraints”. In: *27th International Conference on Tools and Algorithms for the Construction and Analysis of Systems*. Vol. 12651. Lecture Notes in Computer Science. Springer, pp. 210–229.



— (2021b). “Abstraction-Guided Truncations for Stationary Distributions of Markov Population Models”. In: *18th International Conference on Quantitative Evaluation of SysTems*. Vol. 12846. Lecture Notes in Computer Science. Springer, pp. 351–371.