

# Statistical Model Checking of High-Dimensional Cyber-Controlled Systems

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# Investigators



Geir Dullerud



Mahesh Viswanathan



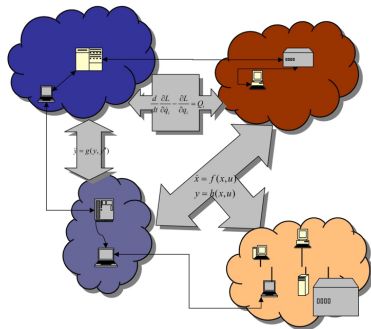
Matt West

***Project Start date: October 1, 2013; Breakthrough.***

# Automated Cyberphysical System Verification

Many modern systems are constructed from physical process interacting with discrete computer processes via communication channels.

- ▶ physical processes modeled by PDEs, SDEs, ODEs.
- ▶ computer algorithms/software have discrete-state models.
- ▶ in this sense direct models are usually hybrid, containing two distinct state types.

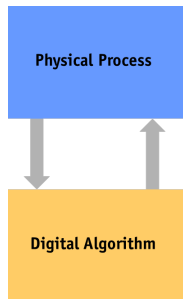


**Motivation:** Development of automated verification methods that can accommodate complex dynamics and specifications.

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**Motivation:** Development of automated verification methods that can accommodate complex dynamics and specifications.

## Technical Approach: Two Main Components

- ▶ Probabilistic models and specifications.
- ▶ Large-scale computation: stochastic simulation.

# Accomplishments

## Year 1:

- ▶ Stochastic simulation for continuous time Markov chains:
  - ▶ Maginness, West, Dullerud, “Exact Simulation of Continuous Time Markov Jump Processes with Anticorrelated Variance Reduced Monte Carlo Estimation”, IEEE CDC; to appear 2014.
- ▶ Modeling with complex specifications:
  - ▶ Wang, Roohi, West, Viswanathan, Dullerud, “Statistical Verification of Nonlinear Systems”, submitted.
- ▶ Summer engineering camp for high-school girls.

## Next Steps:

- ▶ Correlated sampling methods for verifying algorithms.
- ▶ Expanding class of models.

# G-BAM (Girls Building Awesome Machines)



Prosthetic limb prototypes



Wind turbine prototypes

## Synopsis

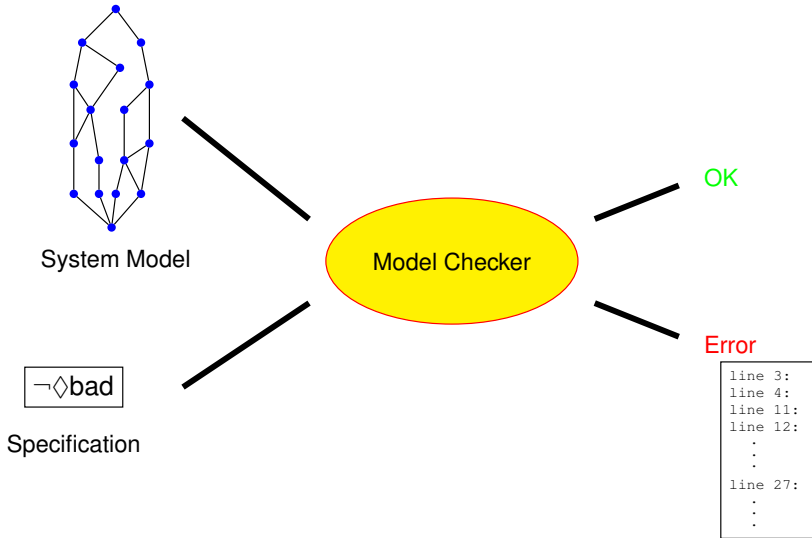
- ▶ 1 week residential engineering camp on campus.
- ▶ High-school girls (9th to 12th grade): 16 in 2013, 24 in 2014.
- ▶ Girls work with women mentors (students, alumni) on creative, team-based design projects.
- ▶ By end of camp: 90% intend to study mechanical engineering.
- ▶ New mechatronics accelerometer-design activity added this year.

## Technical Approach: Two Main Components

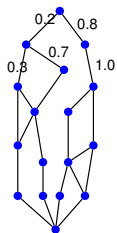
- ▶ **Probabilistic models and specifications.**
- ▶ Large-scale computation: stochastic simulation.



# Model Checking



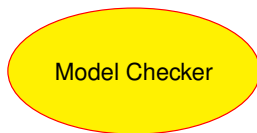
# Probabilistic Model Checking



System Model

$$P_{<0.5}(\diamond \text{bad})$$

Specification

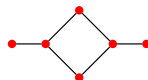


Model Checker

OK

Quantitative  
Results

Error



# What is Probabilistic Model Checking?

## Overview

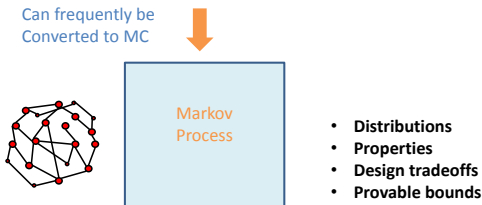
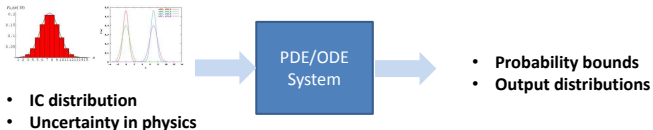
Probabilistic model checking is a **automatic, formal** verification technique for analysing systems that exhibit **stochastic** behavior.

- ▶ Systems modeled by (finite state) Markov Chains, Markov Decision Process, Continuous Time Markov Chains
- ▶ Properties reason over the measure space of **executions**. Allow one to quantify reliability, performance, security. Examples include “probability of shutdown is less than 0.02”, “the expected energy consumption is 15mW”

## Algorithmic Approaches

- ▶ **Exact Methods:** Iterative algorithms that rely on techniques such as linear programming, and numerical integration.
- ▶ **Statistical:** Simulate the system, and statistically estimate the correctness of the system based on the sample executions drawn, using hypothesis testing

# Probability Propagation in Physics-based Models



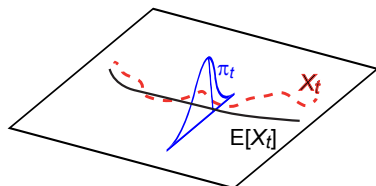
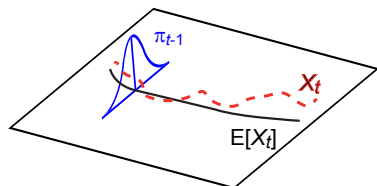
Poster yesterday; conference paper submitted 2014.

## Technical Approach: Two Main Components

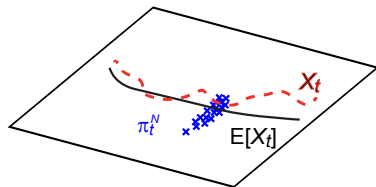
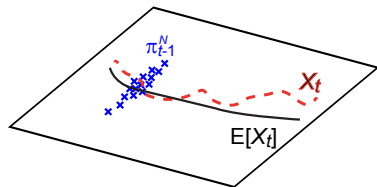
- ▶ Probabilistic models and specifications.
- ▶ **Large-scale computation: stochastic simulation.**

# Stochastic Simulation

Evolution of random processes through system dynamics

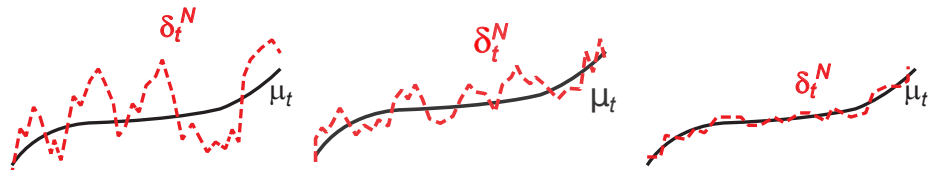


Numerical approximation via simulation



P. A. Maginnis, M. West, G. E. Dullerud, "Exact Simulation of Continuous Time Markov Jump Processes with Anticorrelated Variance Reduced Monte Carlo Estimation", IEEE CDC; to appear 2014.

## Example: Mean Estimators



Suppose  $X$  is a process under consideration with mean behavior  $\mu := \mathbb{E}[X]$ . Define a mean estimator  $\delta^N$ , a random variable such that  $\delta^N \rightarrow \mu$  as  $N \rightarrow \infty$ . Observe:

$$\begin{aligned} \mathbb{E} [\|\delta^N - \mu\|] &\leq \mathbb{E} [\|\delta^N - \mathbb{E}[\delta^N]\|] + \|\mathbb{E}[\delta^N] - \mu\| \\ &\leq \sqrt{\text{tr Cov}(\delta^N)} + \|\mathbb{E}[\delta^N] - \mu\| \end{aligned}$$

So, in some sense, error scales with an estimator's variance and bias.

# Overview

1. Stochastic Simulation and Poisson Variance Reduction
2. Finite Channel Markov Processes and  $\tau$ -Leaping
3. Continuous Process Variance Reduction



# Motivation

- ▶ Stochastic simulation: Applicable to problems from physical modeling to control and estimation.
- ▶ Classic problem is estimation of the mean behavior based on random samples. Convergence of  $n$  averaged estimates is sure but slow  $\mathcal{O}(\frac{1}{\sqrt{n}})$ .
- ▶ How to reduce costs? Variance reduction: 2 orders of magnitude reduction in error of 1000 particle simulation.
- ▶ Property of method:
  - ▶ samples are fair draws;
  - ▶ ensemble members correlated.
- ▶ Tau-leaping: a fast, cheap algorithm to discretely approximate Markov processes.
- ▶ We apply variance reduction to the Poisson samples used to “tau-leap”.

# Motivation

Consider the nonlinear evolution of a continuous-time stochastic process, given by:

$$X(t) = X(0) + \sum_{i=1}^I Y^i \left( \int_0^t \rho^i(s, X(s)) ds \right) \zeta^i,$$

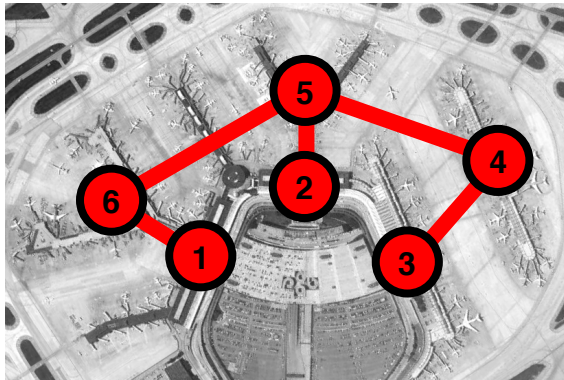
where  $Y^i$  is a random process. Numerical integration  $\implies$  corresponding discrete-time stochastic process:

$$\tilde{X}_{\ell+1} = \tilde{X}_{\ell} + \sum_{i=1}^I S_{\ell}^i \left( \rho^i(t_{\ell}, \tilde{X}_{\ell}) \tau \right) \zeta^i,$$

where  $S_{\ell}^i$  is also random.

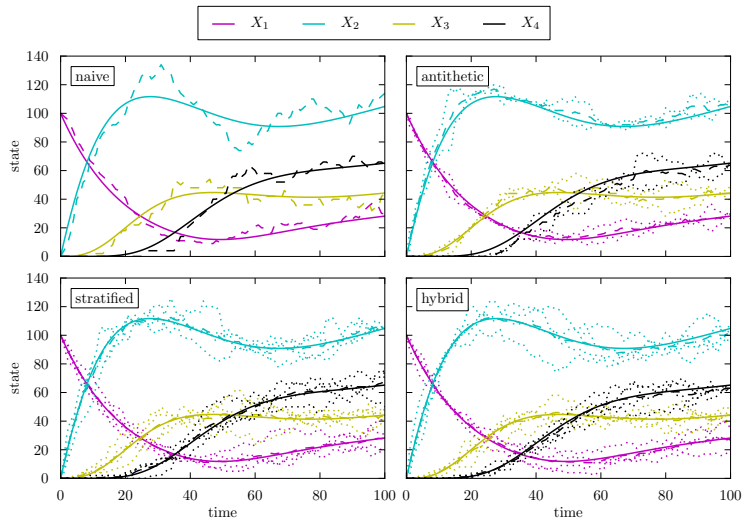
- ▶ Mean pathwise behavior? Analytical solution is impossible.
- ▶ Estimation by simulation.

# Example: Building Population Dynamics



**Figure:** Six node graph of O'Hare International Airport's domestic terminals. State  $X_t \in \mathbb{R}^6$  is the population of each node.

# Sample Paths - Chemistry Model



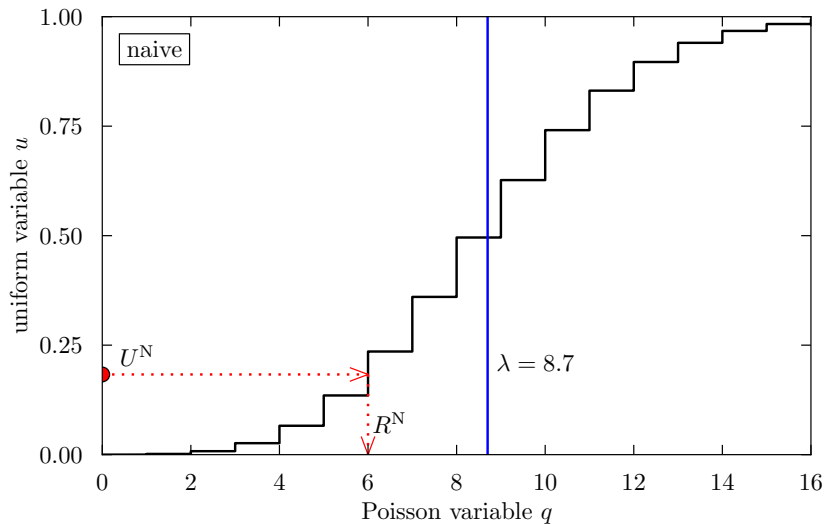
# Basic Approach Illustrated: Poisson Random Variables

- ▶ Poisson distribution  $\text{Pois}(\lambda)$  takes real parameter  $\lambda > 0$ .
- ▶ If  $X \sim \text{Pois}(\lambda)$  then  $\mathbb{P}(X = q) = \frac{e^{-\lambda}\lambda^q}{q!}$ .  $\mathbb{E}[X] = \text{Var}(X) = \lambda$ . Defines Poisson process: number of arrivals in a unit of time if arrivals occur at rate  $\lambda$  and are independent of the time since the last arrival.
- ▶ Define the generalized inverse of the CDF of a Poisson random variable with parameter  $\lambda$  to be

$$F_{\lambda}^{-1}(u) := \mathbb{I}_{\{q:F_{\lambda}(q)>u\}}$$

- ▶  $F_{\lambda}^{-1}(U) \sim \text{Pois}(\lambda)$  if  $U \sim \text{Unif}(0, 1)$ .

# Poisson Sampling



# Poisson Mean Estimation

Let's construct the naive Monte Carlo Poisson mean estimator:

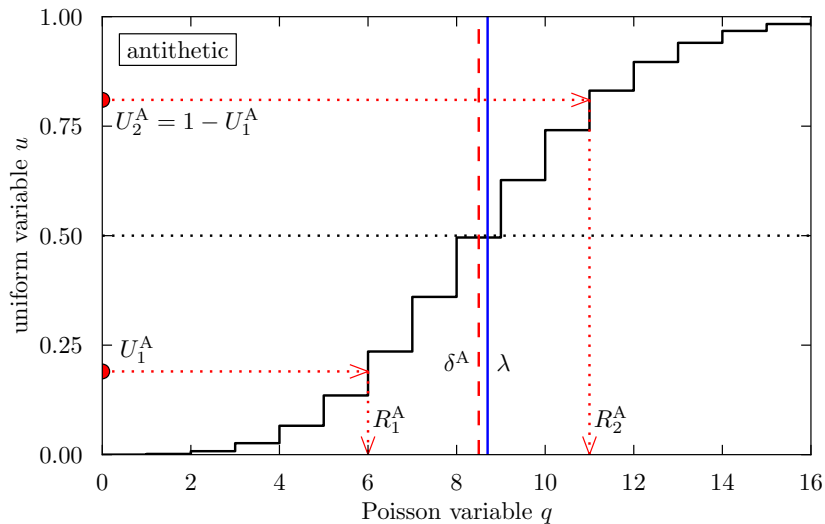
$$U_k^N \stackrel{\text{i.i.d.}}{\sim} \text{Unif}(0, 1)$$

$$R_k^N := F_\lambda^{-1}(U_k^N)$$

$$\delta^{N,n} := \frac{1}{n} \sum_{k=1}^n R_k^N.$$

- ▶ Strong Law of Large Numbers:  $\lim_{n \rightarrow \infty} \delta^{N,n} = \lambda$
- ▶  $\text{Var}(\delta^{N,n}) = \frac{1}{n} \text{Var}(R_k^N) = \frac{\lambda}{n}$
- ▶ Can we do better? Is i.i.d. sampling a necessary condition?

# Antithetic





# Antithetic

The antithetic Poisson mean estimator can be defined:

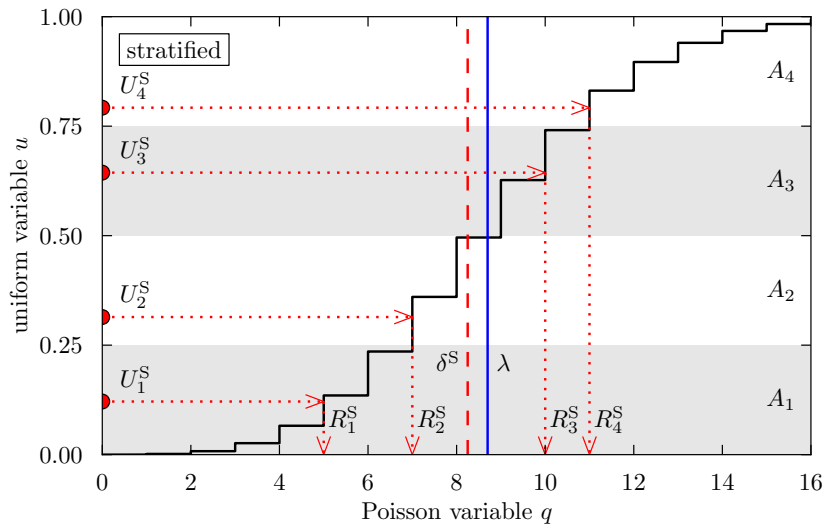
$$\begin{aligned}U_k^A &\stackrel{\text{i.i.d.}}{\sim} \text{Unif}(0, 1) \\R_{k,1}^A &:= F_\lambda^{-1}(U_k^A) \\R_{k,2}^A &:= F_\lambda^{-1}(1 - U_k^A) \\\delta^{A,2n} &:= \frac{1}{2n} \sum_{k=1}^n (R_{k,1}^A + R_{k,2}^A).\end{aligned}$$

- ▶ Observe that  $R_{k,1}^A, R_{k,2}^A$  are not independent.
- ▶  $\text{Cov}(R_{k,1}^A, R_{k,2}^A) \leq 0$ .

Motivated by

$$\text{Var}\left(\frac{X+Y}{2}\right) = \frac{1}{4} \text{Var}(X) + \frac{1}{4} \text{Var}(Y) + \frac{1}{2} \text{Cov}(X, Y).$$

# Stratified



# Stratified

Construct the stratified Poisson mean estimator by partitioning  $[0, 1)$  into  $A_j := [\frac{j-1}{M}, \frac{j}{M})$  for  $j = 1, \dots, M$ :

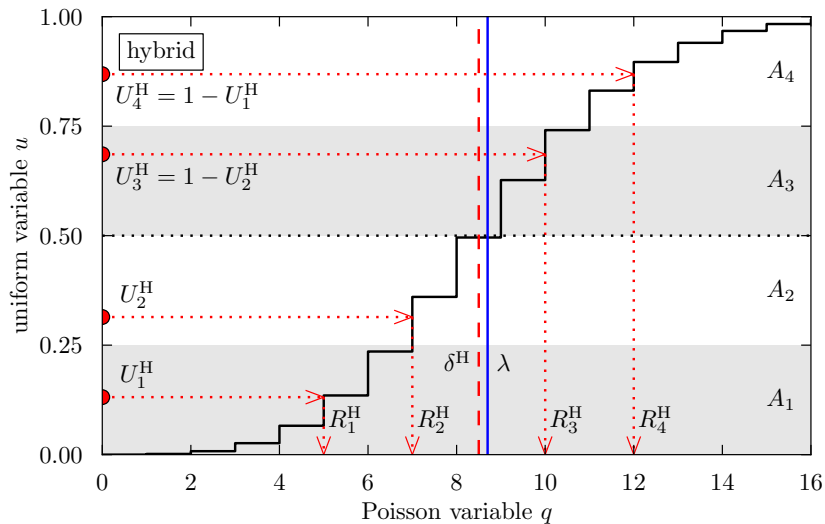
$$U_{k,j}^S \stackrel{\text{i.i.d.}}{\sim} \text{Unif}(A_j) \text{ for } j = 1, \dots, M$$

$$R_{k,j}^S := F_\lambda^{-1}(U_{k,j}^S) \text{ for } j = 1, \dots, M$$

$$\delta_M^{S, Mn} := \frac{1}{Mn} \sum_{k=1}^n \sum_{j=1}^M R_{k,j}^S.$$

- ▶ Observe that  $R_{k,1}^S \not\sim R_{k,2}^S \not\sim \dots \not\sim R_{k,M}^S$ .
- ▶ Here  $\frac{1}{M} \sum_{j=1}^M R_{k,j}^S$  serves as our point estimate to be averaged.

# Hybrid



# Hybrid

Finally, we combine the antithetic and stratified techniques to construct the hybrid Poisson mean estimator for an even number  $M$  of strata:

$$U_{k,j}^H \stackrel{\text{i.i.d.}}{\sim} \text{Unif}(A_j) \text{ for } j = 1, \dots, \frac{M}{2}$$

$$U_{k,j}^H := 1 - U_{k,M-j+1}^H \text{ for } j = (\frac{M}{2} + 1), \dots, M$$

$$R_{k,j}^H := F_\lambda^{-1}(U_{k,j}^H) \text{ for } j = 1, \dots, M$$

$$\delta_M^{H,Mn} := \frac{1}{Mn} \sum_{k=1}^n \sum_{j=1}^M R_{k,j}^H.$$

- ▶  $R_{k,j_1}^H, R_{k,j_2}^H$  are not independent iff  $j_1 + j_2 = M + 1$ .
- ▶  $R_{k,j}^H \sim R_{k,j}^S$

# Analytical Results

## Theorem

*Our estimators are unbiased and consistent.*

## Theorem

*For  $\lambda < \ln 2$ ,*

$$\text{Var}(\delta^{A,2n}) = \frac{1}{n} \left( \frac{\lambda}{2} - \frac{\lambda^2}{2} \right).$$

*For  $\lambda < \ln \frac{M}{M-1}$ ,*

$$\text{Var}(\delta_M^{S,Mn}) = \frac{1}{n} \left( \frac{\lambda}{M} - \frac{M-1}{M} \lambda^2 \right).$$

# Analytical Results

## Theorem

For every Poisson parameter  $\lambda > 0$  and even number of strata  $M \geq 2$ ,

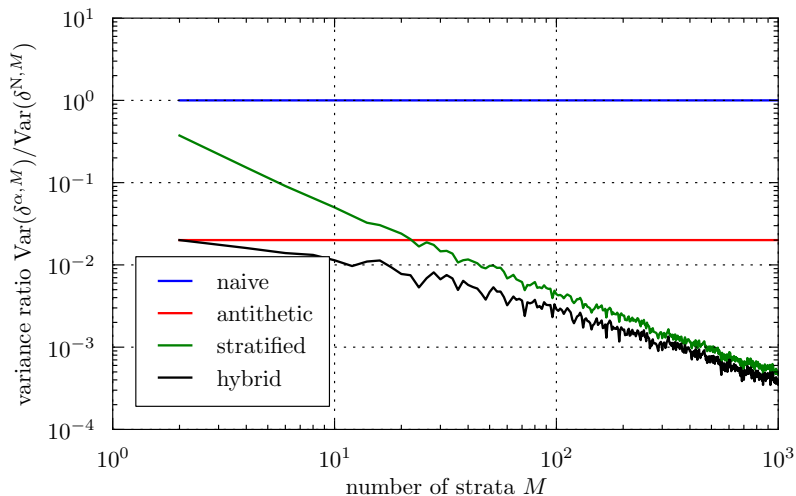
$$\text{Var}(\delta_M^{H,M}) \leq \text{Var}(\delta^{A,M}) \leq \text{Var}(\delta^{N,M}),$$

$$\text{Var}(\delta_M^{H,M}) \leq \text{Var}(\delta_M^{S,M}) \leq \text{Var}(\delta^{N,M}).$$

- ▶ Stratified and antithetic sampling perform better in different regimes of  $\lambda$  and  $M$ .
- ▶ Result proves that regardless of operating parameters, a single method will always perform better than either.
- ▶ Useful in applications where Poisson parameter not known *a priori*.

# Numerical Results

Estimator Variance Ratio versus Number of Strata,  $\lambda = 20$





# Overview

1. Stochastic Simulation and Poisson Variance Reduction
2. Finite Channel Markov Processes and  $\tau$ -Leaping
3. Continuous Process Variance Reduction

# Random Time-Change Representation for Markov Processes

We may represent a Markov process  $X(t) \in \mathbb{R}^D$  with  $I$  event channels that produce transitions  $\zeta^i$  at rates given by rate functions  $\rho^i(t, X(t))$ , as:

$$X(t) = X(0) + \sum_{i=1}^I Y^i \left( \int_0^t \rho^i(s, X(s)) ds \right) \zeta^i,$$

where  $Y^i$  is a unit-rate Poisson process and  $t \in [0, T]$ .

- ▶ Can be simulated exactly, often via Gillespie's (1975) stochastic simulation algorithm (SSA).
- ▶ Simulation is costly when transitions occur frequently.

## Example System: Chemical Reactions

Consider the chemical reactions



with appropriate propensities. This can be represented via the Markov process  $X \in \mathbb{R}^4$  starting from  $X_0 = [N \ 0 \ 0 \ 0]^\top$  with  $I = 4$  reaction channels, defined by:

$$\begin{array}{ll} \zeta^1 = [-1 \ 2 \ 0 \ 0]^\top & \rho^1(t, X) = 0.05X_1 \\ \zeta^2 = [0 \ -2 \ 2 \ 0]^\top & \rho^2(t, X) = 0.01N^{-1}X_2(X_2 - 1) \\ \zeta^3 = [0 \ 0 \ -2 \ 2]^\top & \rho^3(t, X) = 0.05N^{-1}X_3(X_3 - 1) \\ \zeta^4 = [2 \ 0 \ 0 \ -2]^\top & \rho^4(t, X) = 0.02N^{-1}X_4(X_4 - 1), \end{array}$$

where  $N$  is the representative system size (number of particles scale).

# Tau-Leaping Approximation

Gillespie (2001): approximate SSA by discretizing time. For time-step increment  $\tau$ , let  $t_\ell = \ell\tau$  and  $\tilde{X}_\ell \approx X(t_\ell)$  for  $\ell \in \{0, \dots, L\}$ , where  $L := \max\{\ell : t_\ell \leq T\}$ . Then  $\tilde{X}_\ell$  evolves via:

$$\tilde{X}_{\ell+1} = \tilde{X}_\ell + \sum_{i=1}^I S_\ell^i \left( \rho^i(t_\ell, \tilde{X}_\ell) \tau \right) \zeta^i,$$

where  $S_\ell^i(\lambda) \sim \text{Pois}(\lambda)$ .

For compactness, define  $\lambda_\ell^i = \rho^i(t_\ell, \tilde{X}_\ell) \tau$  and denote  $S_\ell^i(\lambda_\ell^i)$  by  $S_\ell^i$ .

# Pathwise Mean Estimators

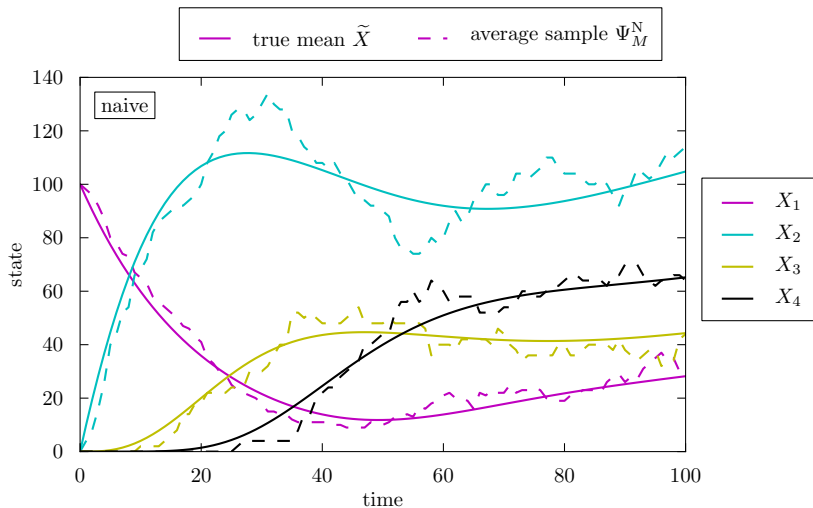
- ▶ We'd like estimates of the mean Pathwise behavior of the approximate Markov process.
- ▶ Naive Pathwise Monte Carlo:

$$\Psi_M^N := \frac{1}{M} \sum_{r=1}^M \tilde{X}_r,$$

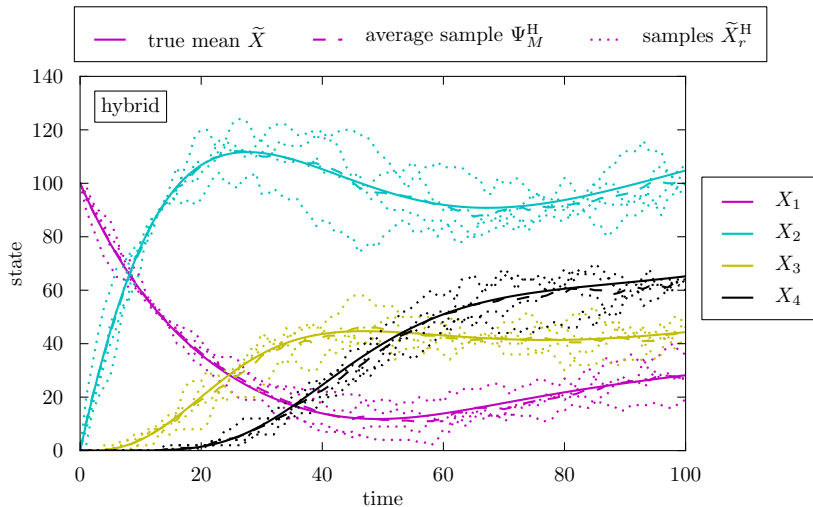
where  $\tilde{X}_r$  are i.i.d. sample paths from the tau-leaping model.

- ▶  $\tilde{X}_{r,\ell}$ : state of the  $r$ th path at time  $\ell$
- ▶  $\Psi_{M,\ell}^N$ : value of the estimator at time  $\ell$
- ▶ Can we reduce the variance (error) of these estimates?

# Naive Monte Carlo Pathwise Mean Estimation



# Hybrid Pathwise Mean Estimation



# Variance Reduced Pathwise Mean Estimators

For any variance reduction technique  $\alpha \in \{A, S, H\}$ , define the variance reduced pathwise mean estimator

$$\Psi_M^\alpha := \frac{1}{M} \sum_{r=1}^M \tilde{X}_r^\alpha.$$

Define the pathwise Mean Square Error (MSE) of an estimation method to be

$$\text{MSE}(\Psi_M^\alpha) = \mathbb{E} \left[ \sum_{\ell=0}^L \left\| \Psi_{M,\ell}^\alpha - \mathbb{E}[\Psi_{M,\ell}^\alpha] \right\|^2 \right],$$

where  $\|x\|^2 = x^\top x$ .



## Case: State Independent Rates

In general, the Poisson parameter  $\lambda_{r,\ell}^{\alpha,i}$  of  $S_{r,\ell}^{\alpha,i}$  depends on current state  $\tilde{X}_{r,\ell}^{\alpha}$ . Thus it depends on past inputs for each reaction channel. But state-independent rates  $\implies \lambda_{r,\ell}^{\alpha,i} = \lambda_{\ell}^i = g^i(t_{\ell})$ .

- ▶ Decouples Poisson variables in time.
- ▶ Allows for extension of pure Poisson estimation results to pathwise estimation. Namely:

### Theorem

*If propensity rates are state-independent, then*

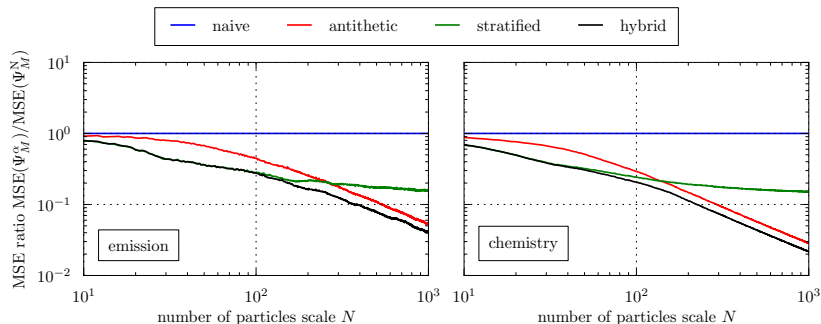
$$\text{MSE}(\Psi_M^H) \leq \text{MSE}(\Psi_M^A) \leq \text{MSE}(\Psi_M^N)$$

$$\text{MSE}(\Psi_M^H) \leq \text{MSE}(\Psi_M^S) \leq \text{MSE}(\Psi_M^N)$$

*for every even number of strata  $M$ .*

# Numerical Results

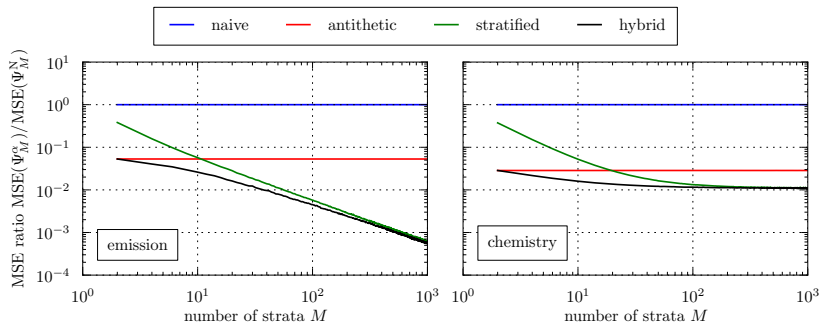
MSE Ratio versus Number of Particles Scale  $N$ , with  $M = 4$



- Typical Poisson parameter  $\lambda$  used in simulation roughly follows  $\lambda \propto N$ .

# Numerical Results (con.)

MSE Ratio versus Number of Strata  $M$ , with  $N = 10^3$



- Only qualitative deviation from Poisson case.

# Overview

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# Motivation

We develop algorithms for the simulation of continuous sample paths of Markov jump processes that introduce negative correlation between samples as a variance reduction technique.

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- ▶ Leverage pointwise techniques for pathwise variance reduction in continuous time.
- ▶ Applicable beyond tau-leaping context.
- ▶ No error due to time discretization, unbiased, consistent.

# Motivation

We develop algorithms for the simulation of continuous sample paths of Markov jump processes that introduce negative correlation between samples as a variance reduction technique.

- ▶ Leverage pointwise techniques for pathwise variance reduction in continuous time.
- ▶ Applicable beyond tau-leaping context.
- ▶ No error due to time discretization, unbiased, consistent.

Note: for ease of illustration all variance reduction techniques are taken to be antithetic, though extension to stratified and hybrid are straightforward.

# Markov Jump Process Model

Recall, the random time-change representation of a Markov jump process

$$X(t) = X(0) + \sum_{i=1}^I Y^i \left( \int_0^t \rho^i(s, X(s)) ds \right) \zeta^i,$$

where  $\rho$  is some rate function and  $\zeta^i$  characterize the transition of a single reaction channel. All random input to sample path due to unit rate Poisson processes  $Y^i$ .



# Markov Jump Process Model

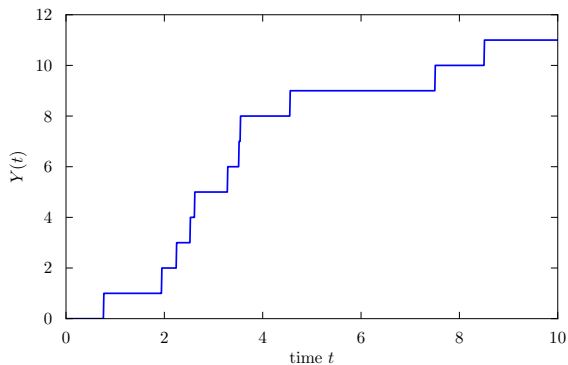
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How do we anticorrelate Poisson process sample paths?

# Poisson Process Simulation



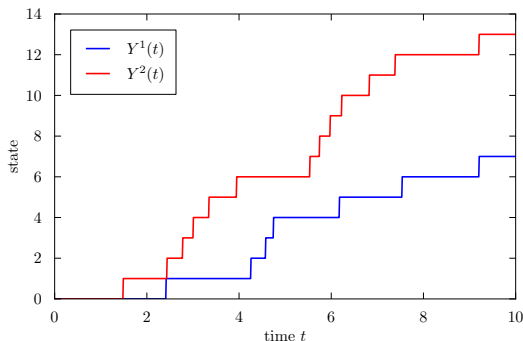
**Figure:** Sample path of a unit rate Poisson process.

Recall: For a given time  $T > 0$  and unit rate Poisson process  $Y$ ,  $Y(T) \sim \text{Pois}(T)$ . Conditioned on number of arrivals in a time interval, arrival times are uniformly distributed.

# Endpoint Technique

- ▶ Sample  $\{Y^i(T)\}$  using pointwise variance reduction techniques
- ▶ Simulate the corresponding jump times

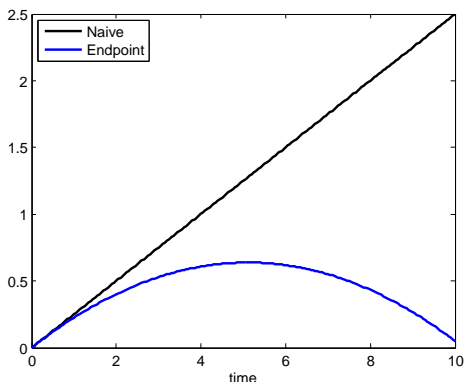
$$\tau_j^i \stackrel{\text{i.i.d.}}{\sim} \text{Unif}([0, T]), j = 1, \dots, Y^i(T).$$



**Figure:** Two sample paths of a unit rate Poisson process. In this case  $Y^1(10), Y^2(10) \sim \text{Pois}(10)$  are antithetically paired.

# Endpoint Technique Variance

Variance of the pathwise mean estimator is reduced over all of  $(0, T]$ , not just at the endpoint.



**Figure:** Variance of a 4-sample Poisson process antithetic endpoint mean estimator, compared to the naive 4-point estimator variance  $\text{Var}(\Psi_t^4)$ .

# Concatenation

Challenge: Can we improve performance (i.e. reduce variance) further in the interior?

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Challenge: Can we improve performance (i.e. reduce variance) further in the interior?

- ▶ Concatenate endpoint correlated processes to produce new increments.

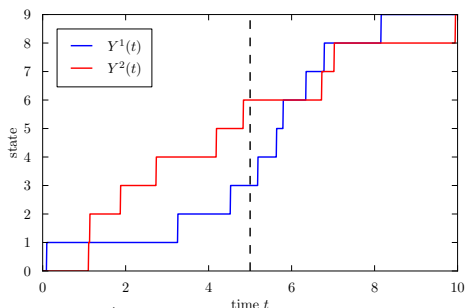


Figure: Sample  $Y^1(5), Y^2(5) \overset{\text{anti.}}{\sim} \text{Pois}(5)$  and  $(Y^1(10) - Y^1(5)), (Y^2(10) - Y^2(5)) \overset{\text{anti.}}{\sim} \text{Pois}(5)$ .

# Concatenation Technique Variance

Significant gains in neighborhood of  $t = 5$ ; slight sacrifice at  $t = 10$ .

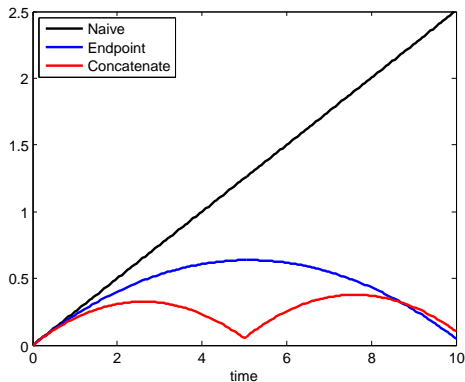


Figure: Same as above with variance of a 4-sample Poisson process 2-step concatenated antithetic mean estimator.

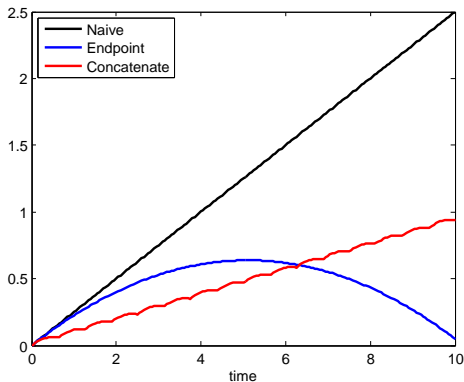
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Concatenation is not a panacea. The sum of independent, nonzero-variance random variables produces an additive drift from desired endpoint performance.



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**Figure:** Same as above with variance of a 4-sample Poisson process 16-step concatenated antithetic mean estimator.

# Binomial midpoint

Modified Challenge: Can we improve performance (i.e. reduce variance) in the interior without sacrificing endpoint performance?

- ▶ Recall:  $Y(T/2)|Y(T) \sim \text{Binom}(Y(T), 1/2)$ .
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(3a)  $\{Y^i(T/4)|Y^i(T/2)\} \stackrel{\text{anti.}}{\sim} \text{Binom}(Y^i(T/2), 1/2)$

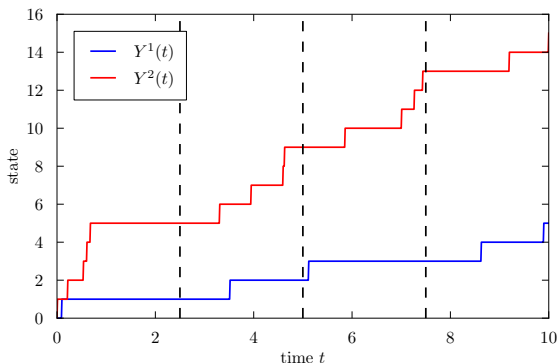
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(3b)  
 $\{Y^i(3T/4)|Y^i(T/2), Y^i(T)\} \stackrel{\text{anti.}}{\sim} \text{Binom}(Y^i(T) - Y^i(T/2), 1/2) + Y^i(T/2)$ ,  
etc.

# Binomial Midpoint

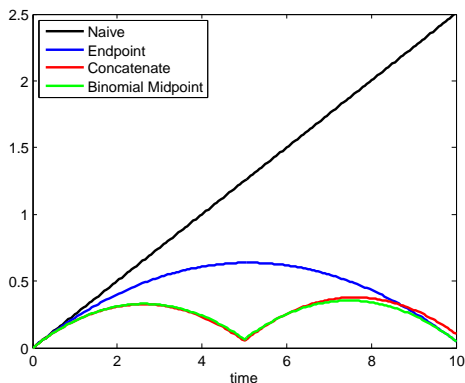
Once we sample state values at these time points, we uniformly sample jump times to produce Poisson process realizations.



**Figure:**  $Y^i(10) \stackrel{\text{anti.}}{\sim} \text{Pois}(10)$  is sampled first, then  $Y^i(5) | Y^i(10) \stackrel{\text{anti.}}{\sim} \text{Binom}(10, 1/2)$ , and finally  $Y^i(2.5) | Y^i(5) \stackrel{\text{anti.}}{\sim} \text{Binom}(5, 1/2)$  and  $Y^i(7.5) | Y^i(5), Y^i(10) \stackrel{\text{anti.}}{\sim} \text{Binom}(5, 1/2) + Y^i(5)$ . Jump times follow.

# Binomial Midpoint Variance

Same variance at  $t = 10$  as endpoint technique, comparable performance at  $t = 5$  to concatenation.

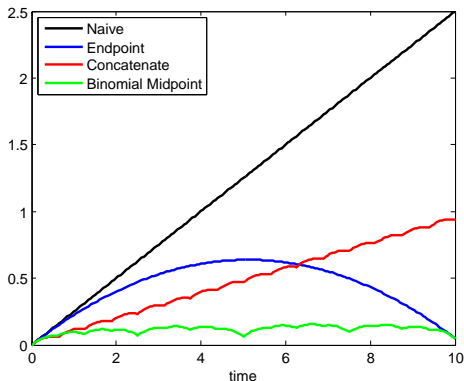


**Figure:** Same as above with variance of a 4-sample Poisson process 2-step binomial midpoint antithetic mean estimator.



# Binomial Midpoint Covariance

Scales up well as number of midpoints increases. Method saturates when midpoints become nearly constant, i.e. when  $\ll 1$  transition expected in interval.



**Figure:** Same as above with variance of a 4-sample Poisson process 16-step binomial midpoint antithetic mean estimator.

# Statistical Model Checking of High-Dimensional Cyber-Controlled Systems

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