

# Fast MCMC sampling for Markov jump processes and extensions

Vinayak Rao and Yee Whye Teh

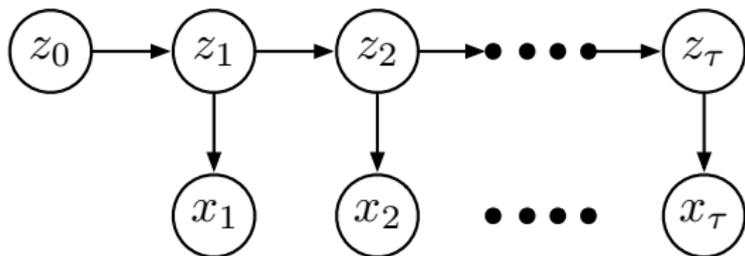
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Work done at: Gatsby Computational Neuroscience Unit, UCL

Supported by Gatsby Charitable Foundation

# Hidden Markov Models



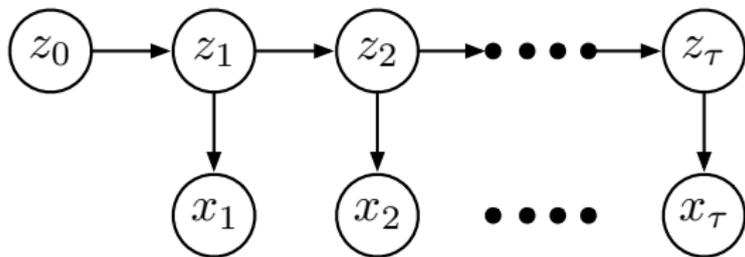
$$p(z_{t+1} = j | z_t = i) = T_{ij}$$

$$p(x_t = k | z_t = i) = E_{ik}$$

- speech recognition, time series, dynamical models, natural language processing...
- efficient inference and learning: forward-backward, Baum-Welch.

# Continuous-Time Hidden Markov Models

- Natural in models of physical, chemical and other continuous-time processes.



$$p(z_{t+dt} = j | z_t = i) = (1 - dt)\delta(i, j) + A_{ij}dt$$

$$\begin{bmatrix} -A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & -A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & -A_{nn} \end{bmatrix}$$

$A_{ij}$  : rate of leaving state  $i$  for  $j$

$$A_{ii} = \sum_{j=1, j \neq i}^n A_{ij}$$

$A_{ii}$  : rate of leaving state  $i$

# Predator-Prey (Lotka-Volterra) Model



$$p(R_{t+dt} = r + 1 | R_t = r) = \alpha r dt$$

$$p(W_{t+dt} = w - 1 | W_t = w) = \beta w dt$$

$$p(W_{t+dt} = w + 1 | W_t = w, R_t = r) = \gamma r w dt$$

$$p(R_{t+dt} = r - 1 | W_t = w, R_t = r) = \delta r w dt$$

- suppose an ecologist collects data on animal populations at certain time points.
- can she infer the likely trajectories of population sizes?
- can she estimate the parameters  $\alpha, \beta, \gamma, \delta$ ?

# Overview

- The simplest example: the Poisson process on the real line.
- Markov jump processes
- Continuous time Bayesian networks.
- These relate back to the basic Poisson process via the idea of *uniformization*.
- We use this connection to develop tractable models and efficient MCMC sampling algorithms.

# The Poisson process (on the real line)

The homogeneous Poisson process with rate  $\lambda$ :



- the probability of an event in a small interval  $dt$  is  $\lambda dt$
- time between successive events has distribution  $\exp(-\lambda t)$

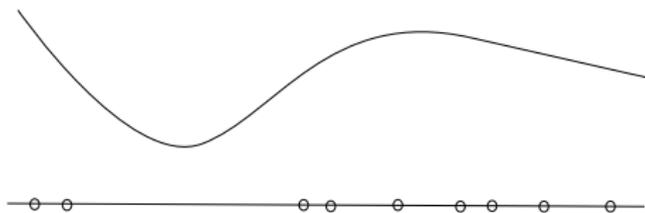
# The Poisson process (on the real line)

The homogeneous Poisson process with rate  $\lambda$ :



- the probability of an event in a small interval  $dt$  is  $\lambda dt$
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The *inhomogeneous* Poisson process with rate  $\lambda(t)$ :



- the probability of an event in a small interval  $dt$  is  $\lambda(t)dt$

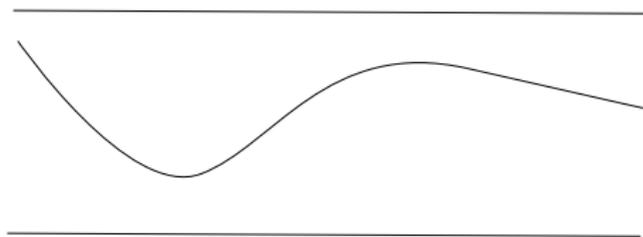
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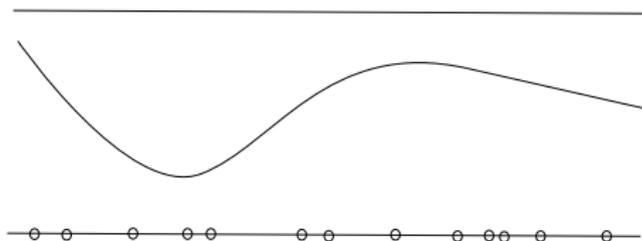
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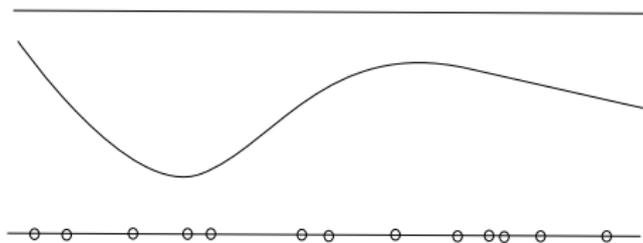
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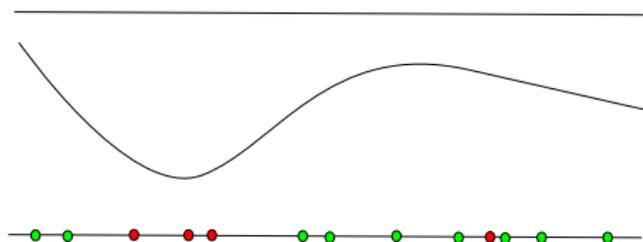
- Choose  $\Omega > \lambda(t) \forall t$ .
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- Keep each point with probability  $\frac{\lambda(t)}{\Omega}$ , otherwise 'thin'.



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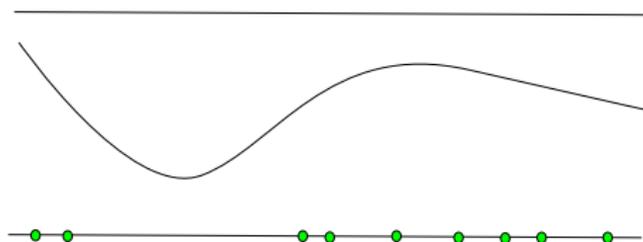
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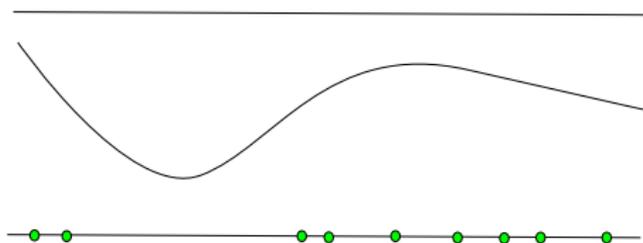
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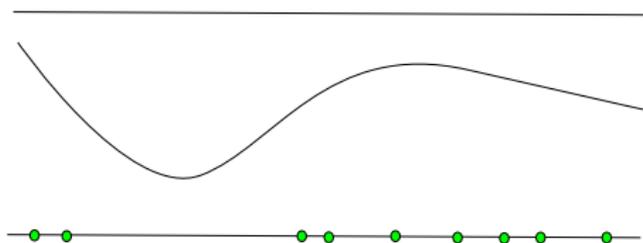


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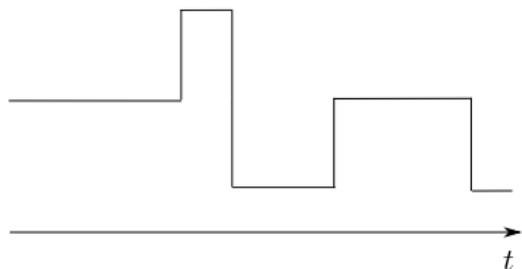
Other continuous time processes like Markov jump processes and renewal processes are *not* completely random: *Uniformization*—thin points by running a *Markov chain*.

# Uniformization (at a high level)

- Define  $\Omega$  larger than the fastest rate at which ‘events occur’.
- Draw a set of ‘potential jump times’ from a Poisson process with rate  $\Omega$ .
- Construct a discrete-time Markov chain with transition times given by the drawn point set.
- The Markov chain is *subordinated* to the Poisson process.
- Keep a point  $t$  with probability  $\lambda(t|state)/\Omega$ .

# Markov jump processes (MJPs)

An MJP  $\mathbf{S}(t)$ ,  $t \in \mathbb{R}_+$  is a right-continuous piecewise-constant stochastic process taking values in some finite space  $\mathcal{S} = \{1, 2, \dots, n\}$ . It is parametrized by an *initial distribution*  $\pi$  and a *rate matrix*  $A$ .



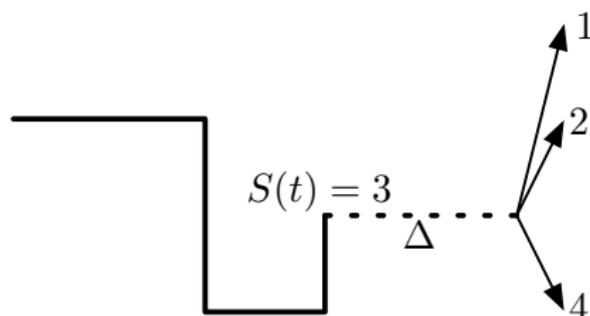
$$\begin{bmatrix} -A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & -A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & -A_{nn} \end{bmatrix}$$

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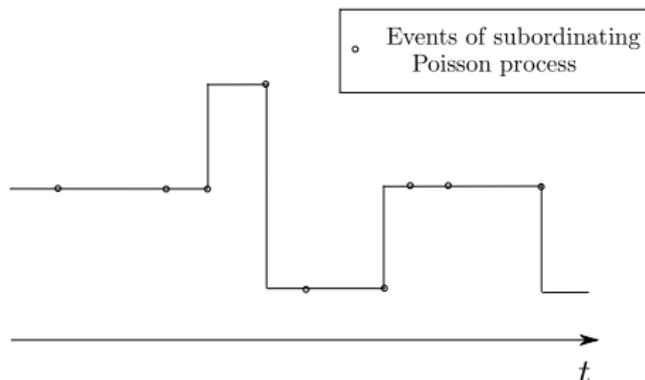
# Gillespie's Algorithm



- set  $t = 0$ .
- draw  $S(0) \sim \pi$  from the initial state distribution.
- while  $t < \tau$ :
  - ▶ set  $i = S(t)$ .
  - ▶ draw  $\Delta \sim \text{Exp}(A_{ii})$ .
  - ▶ set  $S(t') = i$  for  $t < t' < t + \Delta$ .
  - ▶ set  $t = t + \Delta$ .
  - ▶ draw  $S(t) \sim (A_{i1} \cdots A_{i,i-1}, 0, A_{i,i+1} \cdots A_{i,n}) / A_{ii}$ .

# Uniformization for MJPs

- Alternative to Gillespie's algorithm.
- Sample a set of times from a Poisson process with rate  $\Omega \geq \max_i |A_{ij}|$  on the interval  $[t_{start}, t_{end}]$ .
- Run a discrete time Markov chain with initial distribution  $\pi$  and transition matrix  $B = (I + \frac{1}{\Omega}A)$  on these times.



The matrix  $B$  allows self-transitions.

[Jensen, 1953]

# Uniformization for MJPs [Jensen, 1953]

## Proposition

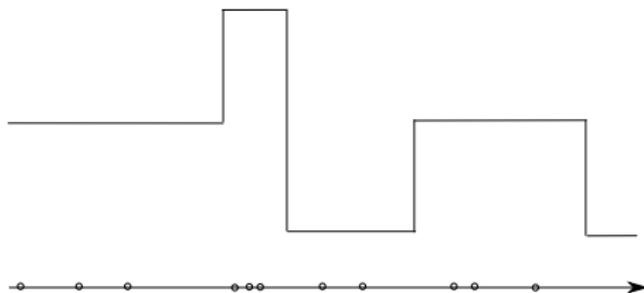
*For any  $\Omega \geq \max_i |A_{ii}|$ , the (continuous time) sequence of states obtained by the uniformized process is a sample from a MJP with initial distribution  $\pi$  and rate matrix  $A$ .*

# Posterior inference

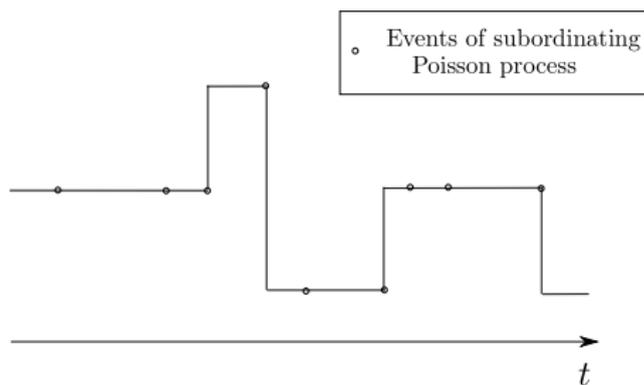
Given noisy observations of an MJP, obtain samples from the posterior.

Observations can include:

- State values at the end points of an interval.
- Observations  $x(t) \sim F(\mathbf{S}(t))$  at a finite set of times  $t$ .
- More complicated likelihood functions that depend on the entire trajectory, e.g. Markov modulated Poisson processes and continuous time Bayesian networks (later).

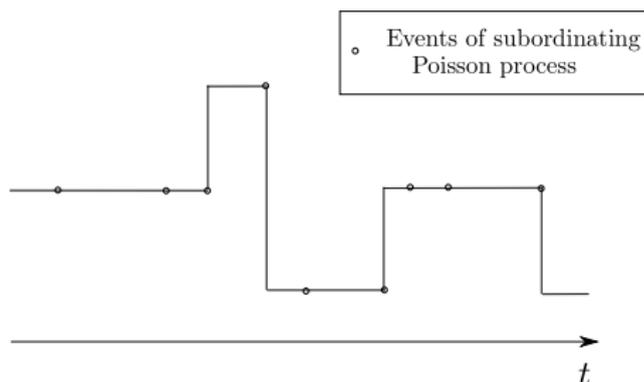


# Auxiliary variable Gibbs sampler



Inference via MCMC.

# Auxiliary variable Gibbs sampler



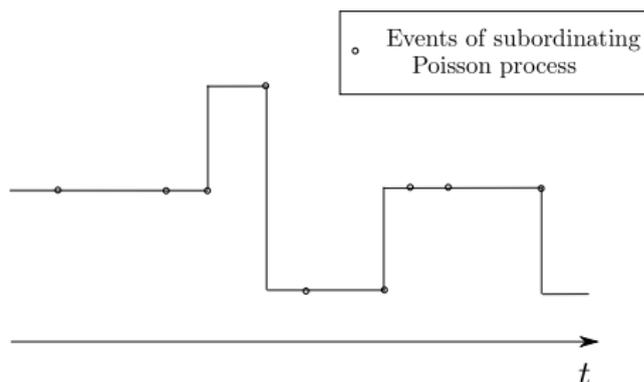
Inference via MCMC.

State space of Gibbs sampler consist of:

- Trajectory of MJP  $\mathbf{S}(t)$ .
- Auxiliary set of points rejected via self-transitions.

[Rao and Teh, 2011]

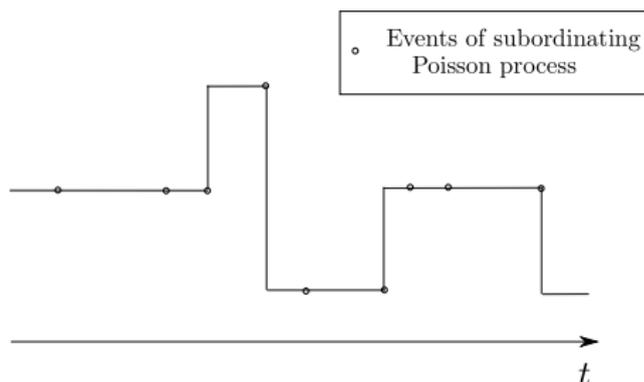
# Auxiliary variable Gibbs sampler



Inference via MCMC.

- Given current MJP path, we need to resample the set of rejected points. Conditioned on the path, these are:
  - ▶ *independent of the observations,*
  - ▶ produced by 'thinning' a rate  $\Omega$  Poisson process with probability  $1 - \frac{A_{\mathbf{s}(t)\mathbf{s}(t)}}{\Omega}$  (diagonal of the transition matrix  $B = (I + \frac{1}{\Omega}A)$ ),
  - ▶ thus, distributed according to a inhomogeneous Poisson process with piecewise constant rate  $(\Omega - A_{\mathbf{s}(t)\mathbf{s}(t)})$ .

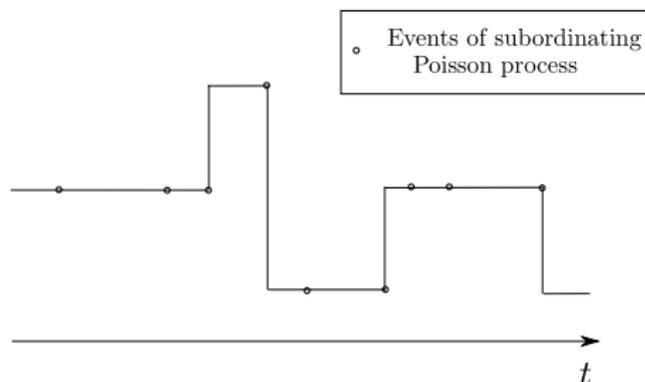
# Auxiliary variable Gibbs sampler



## Inference via MCMC.

- Given all potential transition points, the MJP trajectory is resampled using the forward-filtering backward-sampling algorithm.
- The likelihood of the state between 2 successive points must include all observations in that interval.

# Comments



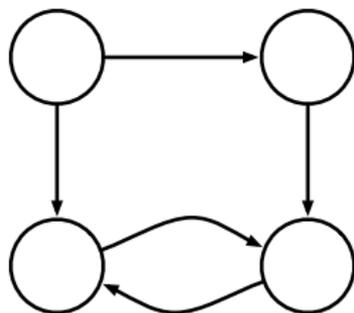
- Complexity:  $O(n^2P)$ , where  $P$  is the (random) number of points.
- Can take advantage of sparsity in transition rate matrix  $A$ .
- Sampler is ergodic for any  $\Omega > \max_i |A_{ii}|$ .
- Only dependence between successive samples is via the transition times of the trajectory.
- Increasing  $\Omega$  reduces this dependence, but increases computational cost.

## Existing approaches to sampling

[Fearnhead and Sherlock, 2006, Hobolth and Stone, 2009] produce *independent* posterior samples, marginalizing over the infinitely many MJP paths using matrix exponentiation.

- scale as  $O(n^3 + n^2P)$ .
- any structure, e.g. sparsity, in the rate matrix  $A$  cannot be exploited in matrix exponentiation.
- cannot be easily extended to complicated likelihood functions (e.g. Markov modulated Poisson processes, continuous time Bayesian networks).

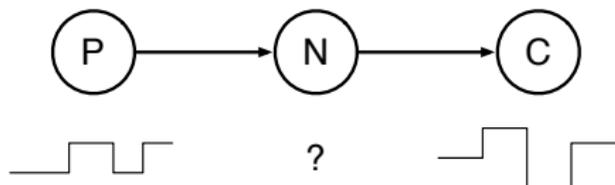
# Continuous-time Bayesian networks (CTBNs)



- Compact representations of large state space MJPs with structured rate matrices.
- Applications include ecology, chemistry, network intrusion detection, human computer interaction etc.
- The rate matrix of a node at time is determined by the configuration of its parents at that time.

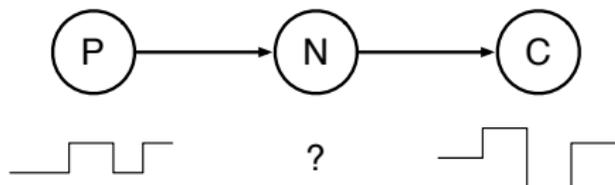
[Nodelman et al., 2002]

# Gibbs sampling CTBNs via uniformization



- The trajectories of all nodes are piecewise constant.
- In a segment of constant parent (P) values, the dynamics of N are controlled by a fixed rate matrix  $A^P$ .
- Each child (C) trajectory is effectively a *continuous-time* observation when resampling the trajectory of N.

# Gibbs sampling CTBNs via uniformization



- Sample potential jump times from a Poisson process with rate  $\Omega^P - A_{ii}^P$ .
- Between two successive potential jump times, N remains in a constant state.
  - ▶ This state must account for the likelihood of children's states.
  - ▶ The state must also explain relevant observations.
- With the resulting 'likelihood' function and transition matrix  $B = (I + \frac{1}{\Omega} A^P)$ , sample new trajectory using forward-filtering backward-sampling.

# Existing approaches to inference

[El-Hay et al., 2008] describe a Gibbs sampler involving time discretization, which is expensive and approximate.

[Fan and Shelton, 2008] uses particle filtering which can be inaccurate for long time intervals.

[Nodelman et al., 2002, Nodelman et al., 2005, Opper and Sanguinetti, 2007, Cohn et al., 2010] use deterministic approximations (mean-field and expectation propagation) which are biased and can be inaccurate.

# Experiments

- We compare our uniformization-based sampler with a state-of-the-art CTBN Gibbs sampler of [El-Hay et al., 2008]. search on the time interval.
- When comparing running times, we measured times required to produce same effective sample sizes.

# Experiments

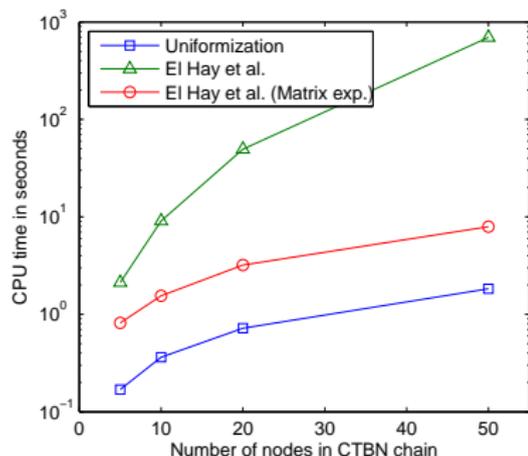


Figure: CPU time vs length of CTBN chain.

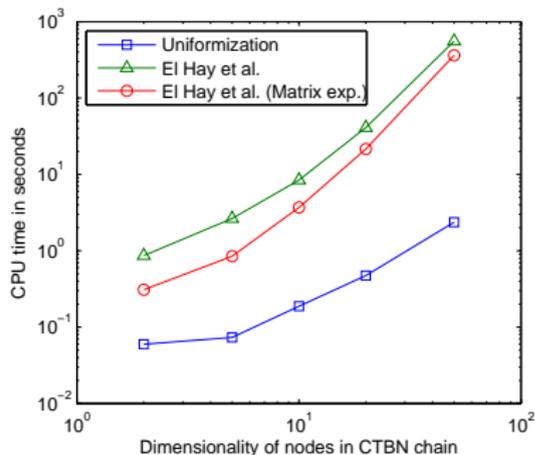


Figure: CPU time vs number of states of CTBN nodes.

The plots above were produced for a CTBN with a chain topology, increasing the number of nodes in the chain (left) and the number of states of each node (right).

# Experiments

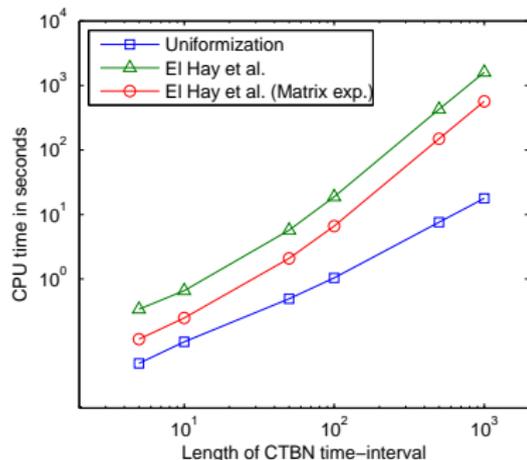


Figure: CPU time vs time interval of CTBN paths.

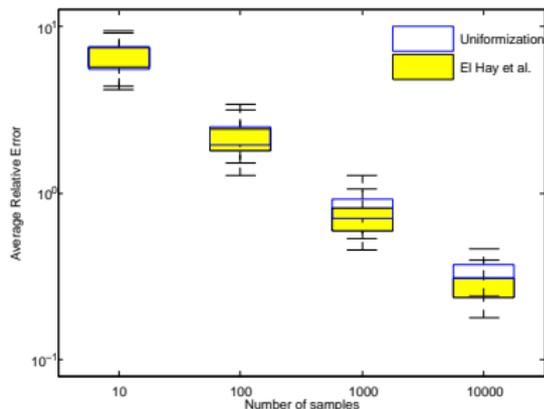


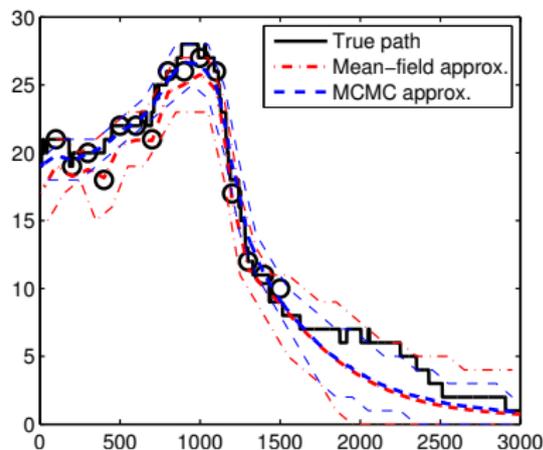
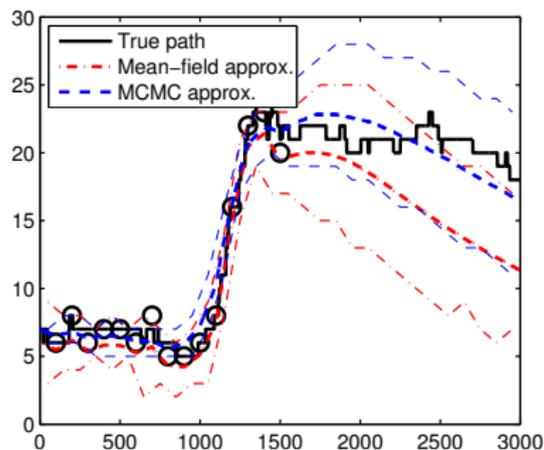
Figure: Average relative error vs number of samples

Produced for the standard 'drug network'.

Left: required CPU time as length of the time interval increases.  
Right: (normalized) absolute error in estimated parameters of the network as the (absolute) number of samples increases.

# Experiments

Compared against the mean-field approximation of [Oppen and Sanguinetti, 2007], for the predator-prey model, a CTBN describing the Lotka-Volterra equations.



Posterior (mean and 90% confidence intervals) over predator paths (observations (circles) only until 1500).

# Conclusions

- The idea of uniformization relates more complicated continuous time discrete state processes to the basic Poisson process.
- We demonstrated how this connection can be used to develop tractable models and efficient MCMC inference schemes.
- We have extended the work here in a number of directions:
  - ▶ renewal processes (Rao and Teh NIPS 2011),
  - ▶ semi-Markov jump processes (NIPS 2012),
  - ▶ Markov-modulated Poisson processes, inhomogeneous MJPs, MJPs with infinite state spaces etc (Vinayak's thesis).
- Stochastic processes are an important mathematical language for modelling many physical and biological phenomena. There is a need for effective algorithms for inference in these models.

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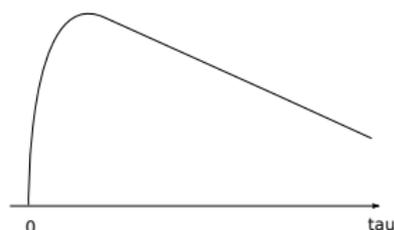
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# Renewal processes



- Renewal processes: point processes on the real line ('time').
- Inter-event times drawn i.i.d. from some *renewal density*.
- Homogeneous Poisson process: exponential renewal density.
- Can capture burstiness or refractoriness.

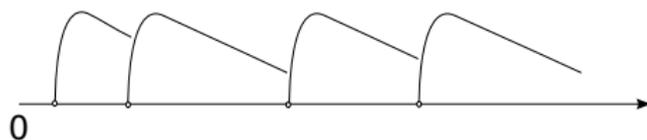
# Renewal processes



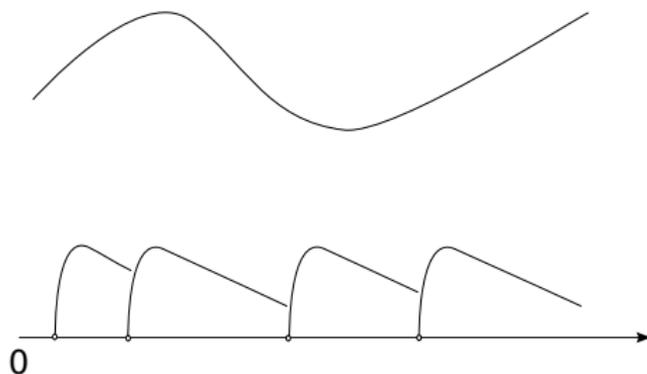
- Associated with the renewal density  $g$  is a *hazard function*  $h$ .
- For an infinitesimal  $\Delta$ ,  $h(\tau)\Delta$  is the probability of the inter-event interval being in  $[\tau, \tau + \Delta]$  conditioned on it being at least  $\tau$ :

$$h(\tau) = \frac{g(\tau)}{1 - \int_0^\tau g(u) du}$$

# Modulated renewal processes



# Modulated renewal processes



- Modulate the hazard function by some time-varying intensity function  $\lambda(t)$ :

$$h(\tau, t) \equiv m(h(\tau), \lambda(t))$$

- $m(\cdot, \cdot)$  is some *interaction function*.
- We use multiplicative interactions,  $h(\tau, t) = h(\tau)\lambda(t)$ .

# Direct sampling from prior

The modulated renewal density is:

$$g(\tau|t_{prev}) = \lambda(t_{prev} + \tau)h(\tau) \exp\left(-\int_0^\tau \lambda(t_{prev} + u)h(u)du\right)$$

where  $t_{prev}$  is the previous event time.

Naïvely, need to numerically evaluate integrals to generate samples.

- can be time consuming and introduce approximation errors.

## Sampling via uniformization

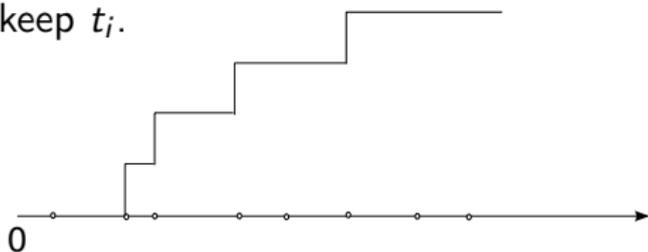
- Assume the intensity function  $\lambda(t)$  and the hazard function  $h(\tau)$  are bounded:  $\exists \Omega \geq \max_{t,\tau} h(\tau)\lambda(t)$

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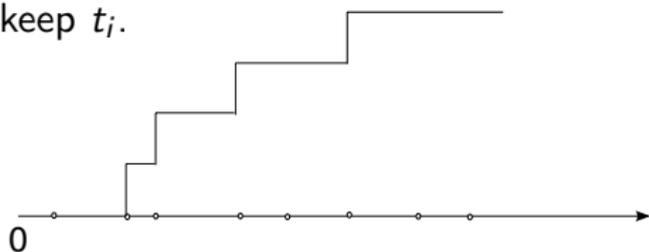
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- Sample  $T = \{t_0 = 0, t_1, t_2, \dots\}$  from a rate  $\Omega$  Poisson process.
- Run  $\{Y_0 = 0, Y_1, Y_2, \dots\}$ , an integer-valued Markov chain  $E$ 
  - ▶  $Y_i = Y_{i-1} \rightarrow$  reject  $t_i$ ,
  - ▶  $Y_i = i \rightarrow$  keep  $t_i$ .



# Sampling via uniformization

- Assume the intensity function  $\lambda(t)$  and the hazard function  $h(\tau)$  are bounded:  $\exists \Omega \geq \max_{t,\tau} h(\tau)\lambda(t)$
- Sample  $T = \{t_0 = 0, t_1, t_2, \dots\}$  from a rate  $\Omega$  Poisson process.
- Run  $\{Y_0 = 0, Y_1, Y_2, \dots\}$ , an integer-valued Markov chain  $E$ 
  - ▶  $Y_i = Y_{i-1} \rightarrow$  reject  $t_i$ ,
  - ▶  $Y_i = i \rightarrow$  keep  $t_i$ .



- For  $i > j \geq 0$ , define

$$p(Y_i = i | Y_{i-1} = j) = \frac{h(t_i - t_j)\lambda(t_i)}{\Omega}$$

- Define  $X = \{t_i \in T \text{ s.t. } Y_i = i\}$ .

# Sampling via uniformization

## Proposition

*For any  $\Omega \geq \max_{t,\tau} h(\tau)\lambda(t)$ ,  $X$  is a sample from a modulated renewal process with hazard  $h(\cdot)$  and modulating intensity  $\lambda(\cdot)$ .*

Generalizes [Shanthikumar, 1986] for the stationary case. See also [Ogata, 1981].

# Reduction to thinning of Poisson processes

For a Poisson process, the hazard function is a constant:

$$h(\tau) = h$$

Then, the transition probabilities of the Markov chain becomes:

$$p(Y_i = i | Y_{i-1} = j) = \frac{h\lambda(t_j)}{\Omega}$$

This reduces to independent thinning [Adams et al., 2009].

# Model specification

- We place a Gaussian Process prior on the intensity function  $\lambda(t)$ , transformed via a sigmoidal link function.
- The generative process is:

$$\begin{aligned}I(\cdot) &\sim \mathcal{GP}(\mu, K) \\ \lambda(\cdot) &= \hat{\lambda}\sigma(I(\cdot)) \\ X &\sim \mathcal{R}(\lambda(\cdot), h(\cdot))\end{aligned}$$

We use a gamma family for the hazard function:

$$h(\tau) = \frac{x^{\gamma-1}e^{-x}}{\int_x^\infty u^{\gamma-1}e^{-u}du}$$

where  $\gamma$  is the shape parameter.

- We place hyperpriors on  $\hat{\lambda}$ ,  $\gamma$  and the GP hyperparameters

# Inference

Given a set of event times  $X$ , obtain samples from the modulating function  $\lambda(\cdot)$  (and hyperparameters).

As before, directly sampling from the GP posterior is impossible.

Introduce the rejected events as auxiliary variables and proceed by alternately sampling the rejected events given  $X$  and the intensity function, and then the intensity function given  $X$  and rejected events.

## Inference (details)

Assume the modulating function  $\lambda(t)$  is known for all  $t$ .

In the interval  $(X_{i-1}, X_i)$ , events from a rate  $\Omega$  Poisson process were rejected with probability:

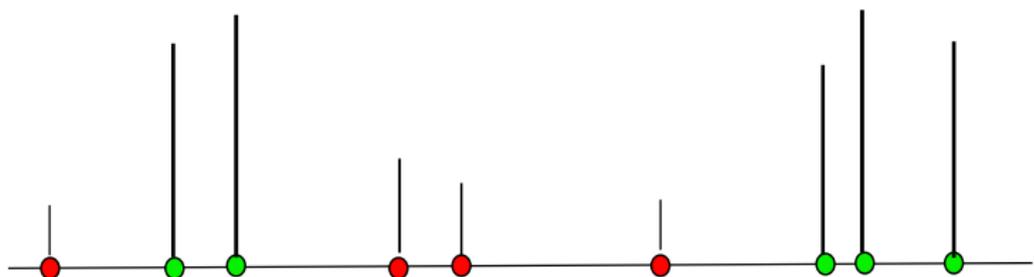
$$1 - \frac{\lambda(t)h(t - X_{i-1})}{\Omega}$$

Under the posterior, these rejected events are distributed as an inhomogeneous Poisson process with rate:

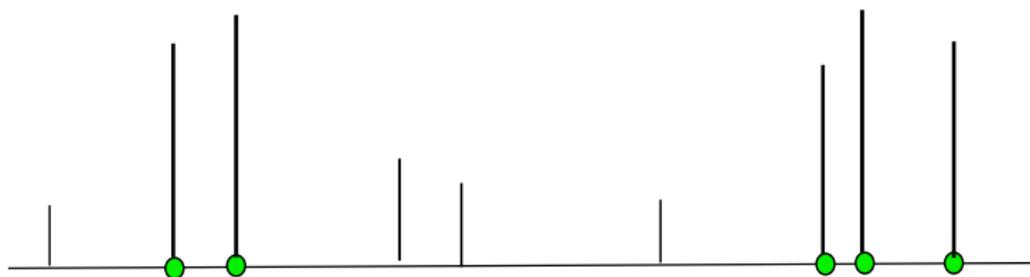
$$\Omega - \lambda(t)h(t - X_{i-1})$$

Catch: we know  $\lambda(t)$  only at a discrete set of times. Use uniformization (thinning in fact). We resample the GP on the events and the rejected points using elliptical slice sampling [Murray et al., 2010].

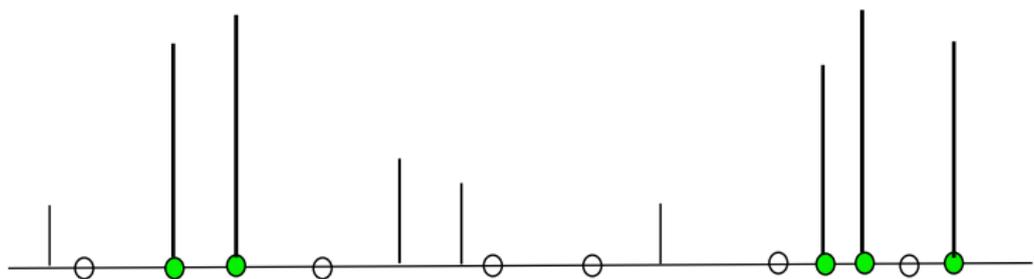
# Inference cartoon



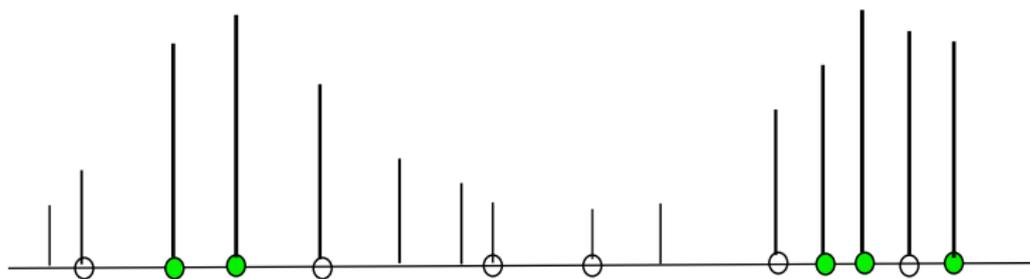
# Inference cartoon



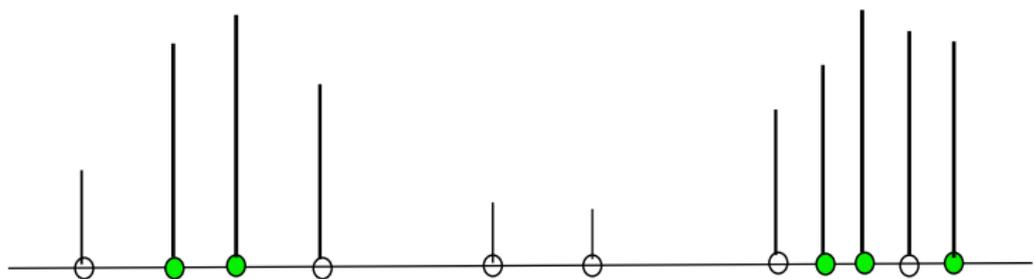
# Inference cartoon



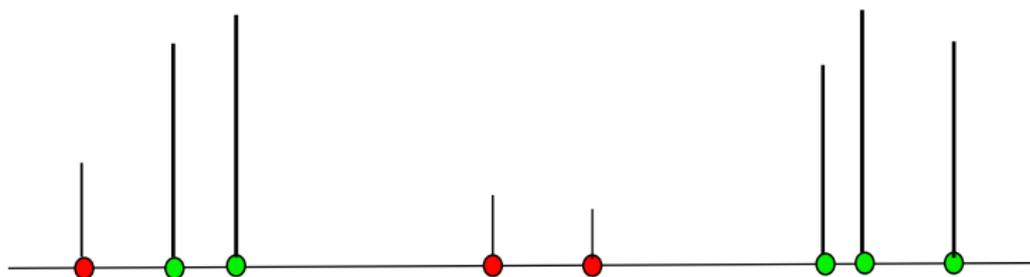
# Inference cartoon



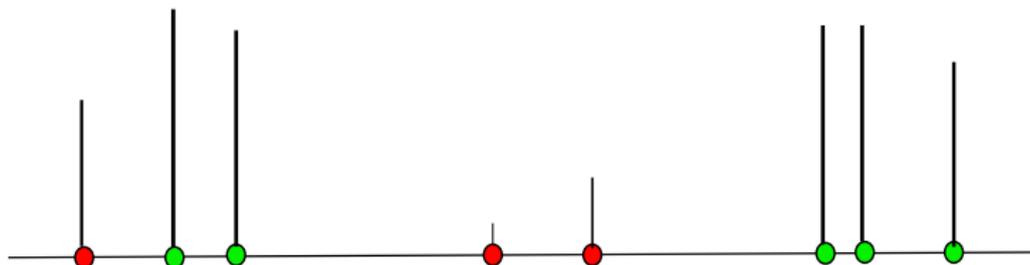
# Inference cartoon



# Inference cartoon



# Inference cartoon



# Computational considerations

- Complexity:  $O(N^3)$ , where  $N = |X| + 2|E|$ ,  $|X|$  is the number of observations and  $|E|$  is the number of rejected points.
- For large  $X$ , we must resort to approximate inference for Gaussian processes [Rasmussen and Williams, 2006].

## Experiments

We compare our uniformization based blocked Gibbs sampler with the sampler of [Adams et al., 2009].

	Synthetic dataset 1		
	Mean ESS	Minimum ESS	Time(sec)
Gibbs	$93.45 \pm 6.91$	$50.94 \pm 5.21$	77.85
MH	$56.37 \pm 10.30$	$19.34 \pm 11.55$	345.44
	Coalmine dataset		
	Mean ESS	Minimum ESS	Time(sec)
Gibbs	$53.54 \pm 8.15$	$24.87 \pm 7.38$	282.72
MH	$47.83 \pm 9.18$	$18.91 \pm 6.45$	1703

Table: Sampler comparisons. Numbers are per 1000 samples.

Besides mixing faster our sampler:

- is simpler and more natural to the problem,
- does not require any external tuning.

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**Algorithm 1** Blocked Gibbs sampler for GP-modulated renewal process on the interval  $[0, T]$ 

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Input: Set of event times  $X$ , set of thinned times  $\tilde{X}_{prev}$  and  $I$  instantiated at  $X \cup \tilde{X}_{prev}$ .

Output: A new set of thinned times  $\tilde{X}_{new}$  and a new instantiation  $I_{X \cup \tilde{X}_{new}}$  of the  $\mathcal{GP}$  on  $X \cup \tilde{X}_{new}$ .

- 1: Sample  $A \subset [0, T]$  from a Poisson process with rate  $\Omega$ .
  - 2: Sample  $I_A | I_{X \cup \tilde{X}_{prev}}$ .
  - 3: Thin  $A$ , keeping element  $a \in A \cap [X_{i-1}, X_i]$  with probability  $\left(1 - \frac{\hat{\lambda}\sigma(I(a))h(a-X_{i-1})}{\Omega}\right)$ .
  - 4: Let  $\tilde{X}_{new}$  be the resulting set and  $I_{\tilde{X}_{new}}$  be the restriction of  $I_A$  to this set. Discard  $\tilde{X}_{prev}$  and  $I_{\tilde{X}_{prev}}$ .
  - 5: Resample  $I_{X \cup \tilde{X}_{new}}$  using, for example, elliptical slice sampling.
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