Fast MCMC sampling for Markov jump processes and extensions

Vinayak Rao and Yee Whye Teh

Rao: Department of Statistical Science, Duke University
Teh: Department of Statistics, Oxford University
Work done at: Gatsby Computational Neuroscience Unit, UCL
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Hidden Markov Models

\[ p(z_{t+1} = j | z_t = i) = T_{ij} \quad p(x_t = k | z_t = i) = E_{ik} \]

- 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.

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

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

- \( A_{ij} \): 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

\[
p(R_{t+dt} = r + 1| R_t = r) = \alpha r dt
\]
\[
p(W_{t+dt} = w - 1| W_t = w) = \beta w dt
\]
\[
p(W_{t+dt} = w + 1| W_t = w, R_t = r) = \gamma w dt
\]
\[
p(R_{t+dt} = r - 1| W_t = w, R_t = r) = \delta w dt
\]

- 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 \( \exp(\lambda) \)
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 $\exp(\lambda)$

The *inhomogeneous* Poisson process process with rate $\lambda(t)$:

- the probability of an event in a small interval $dt$ is $\lambda(t)dt$
Thinning [Lewis and Shedler, 1979]

Thinning: to sample from a Poisson process with rate $\lambda(t)$. 

Choose $\Omega > \lambda(t)$ $\forall t$. Sample from a Poisson process with rate $\Omega$. Keep each point with probability $\frac{\lambda(t)}{\Omega}$, otherwise 'thin'. Follows from the complete randomness of the Poisson process. Other continuous time processes like Markov jump processes and renewal processes are not completely random. Uniformization—thin points by running a Markov chain.
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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 \textit{subordinated} to the Poisson process.
- Keep a point $t$ with probability $\lambda(t|\text{state})/\Omega$. 
Markov jump processes (MJPs)

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

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

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

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

$A_{ij}$: rate of leaving state $i$
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 $\Omega \geq \max_i |A_{ii}|$ on the interval $[t_{\text{start}}, t_{\text{end}}]$.
- 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 $x(t) \sim F(S(t))$ 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).

![Diagram of state transitions](image-url)
Auxiliary variable Gibbs sampler

Events of subordinating Poisson process

Inference via MCMC.
Auxiliary variable Gibbs sampler

Inference via MCMC.
State space of Gibbs sampler consist of:
- Trajectory of MJP $S(t)$.
- Auxiliary set of points rejected via self-transitions.

[Rao and Teh, 2011]
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 $1 - \frac{A_s(t)s(t)}{\Omega}$ (diagonal of the transition matrix $B = (I + \frac{1}{\Omega} A)$),
  - thus, distributed according to a inhomogeneous Poisson process with piecewise constant rate $(\Omega - A_s(t)s(t))$. 
Auxiliary variable Gibbs sampler

Events of subordinating Poisson process

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: $O(n^2 P)$, 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 $O(n^3 + n^2 P)$.
- 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]
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.
Sample potential jump times from a Poisson process with rate $\Omega^P - A^P_{ii}$.

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].
- When comparing running times, we measured times required to produce same effective sample sizes.
Experiments

![Graph 1: CPU time vs length of CTBN chain.](image1)

**Figure**: CPU time vs length of CTBN chain.

![Graph 2: CPU time vs number of states of CTBN nodes.](image2)

**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.

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 [Opper 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.


Bibliography II

Markoff chains as an aid in the study of Markoff processes.

Simulation of nonhomogeneous Poisson processes with degree-two exponential polynomial rate function.

Elliptical slice sampling.

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Uniformization and hybrid simulation/analytic models of renewal processes.
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:

\[ g(\tau \mid t_{\text{prev}}) = \lambda(t_{\text{prev}} + \tau) h(\tau) \exp \left( - \int_0^\tau \lambda(t_{\text{prev}} + u) h(u) du \right) \]

where \( t_{\text{prev}} \) 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: $\exists \Omega \geq \max_{t, \tau} h(\tau) \lambda(t)$
Sampling via uniformization

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- Sample $T = \{ t_0 = 0, t_1, t_2, \ldots \}$ from a rate $\Omega$ Poisson process.
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- 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 $T = \{t_0 = 0, t_1, t_2, \ldots\}$ from a rate $\Omega$ Poisson process.
- Run $\{Y_0 = 0, Y_1, Y_2, \ldots\}$, 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 $T = \{t_0 = 0, t_1, t_2, \ldots\}$ from a rate $\Omega$ Poisson process.
- Run $\{Y_0 = 0, Y_1, Y_2, \ldots\}$, 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 $X = \{t_i \in T \text{ s.t. } Y_i = i\}$. 
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].
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:

\[
\begin{align*}
    l(\cdot) & \sim \mathcal{GP}(\mu, K) \\
    \lambda(\cdot) & = \hat{\lambda} \sigma(l(\cdot)) \\
    X & \sim \mathcal{R}(\lambda(\cdot), h(\cdot))
\end{align*}
\]

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.
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
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].

<table>
<thead>
<tr>
<th></th>
<th>Synthetic dataset 1</th>
<th>Coalmine dataset</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean ESS</td>
<td>Minimum ESS</td>
</tr>
<tr>
<td>Gibbs</td>
<td>93.45 ± 6.91</td>
<td>50.94 ± 5.21</td>
</tr>
<tr>
<td>MH</td>
<td>56.37 ± 10.30</td>
<td>19.34 ± 11.55</td>
</tr>
</tbody>
</table>

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

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

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

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