Efficient MCMC for Continuous Time Discrete State Systems

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Overview

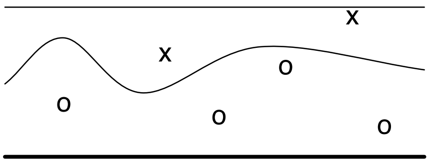
- Continuous time discrete state systems: applications in physics, chemistry, genetics, ecology, neuroscience etc.
- The simplest example: the Poisson process on the real line.
- Generalizations: renewal processes, Markov jump processes, continuous time Bayesian networks etc.
- These relate back to the basic Poisson process via the idea of *uniformization*.
- We use this connection to develop tractable models and efficient MCMC sampling algorithms.

Thinning

Uniformization generalizes the idea of 'thinning'.

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

- Sample from a Poisson process with rate $\Omega > \lambda(t)\ \forall t$.
- Thin or reject each point with probability $1 - \frac{\lambda(t)}{\Omega}$.



Follows from the *complete randomness* of the Poisson process.

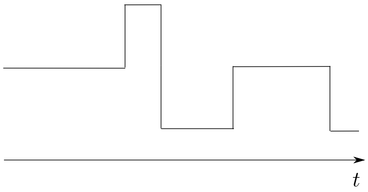
Markov jump processes or renewal processes are *not* completely random: *Uniformization*—thin points by running a *Markov chain*.

Uniformization (at a high level)

- Draw from a Poisson process with rate Ω.
- Ω is larger than the fastest rate at which 'events occur'.
- Construct a 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. $\mathcal{S} = \{1, 2, ...n\}$. It is parametrized by an *initial distribution* π and a *rate matrix* A.



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

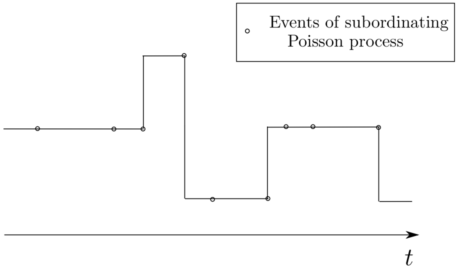
A_{ij} : rate of leaving state i for j

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

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

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 $[t_{start}, t_{end}]$.
- Run a discrete time Markov chain with initial distribution π 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]

Lemma

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 π and rate matrix A.

Auxiliary variable Gibbs sampler

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

Observations can include:

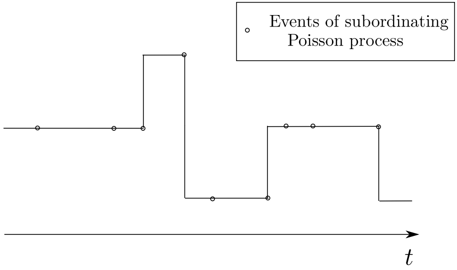
- State values at the end points of an interval.
- Observations $x(t) \sim F(\mathbf{S}(t))$ at a finite set of times t.
- More complicated likelihood functions that depend on the entire trajectory, e.g. Markov modulated Poisson processes and continuous time Bayesian networks (see later).

State space of Gibbs sampler consist of:

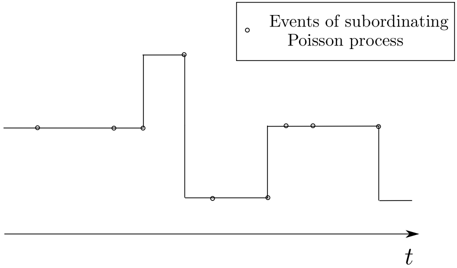
- Trajectory of MJP $\mathbf{S}(t)$.
- Auxiliary set of points rejected via self-transitions.

[Rao and Teh, 2011a]

Auxiliary variable Gibbs sampler

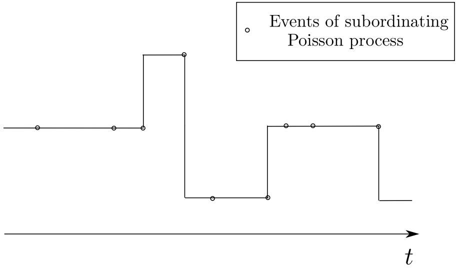


Auxiliary variable Gibbs sampler



- 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 Ω Poisson process with probability $1 + \frac{A_{\mathsf{S}(t)\mathsf{S}(t)}}{\Omega}$,
  - thus, distributed according to a inhomogeneous Poisson process with piecewise constant rate $(\Omega + A_{\mathsf{S}(t)\mathsf{S}(t)})$.

Auxiliary variable Gibbs sampler



- 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

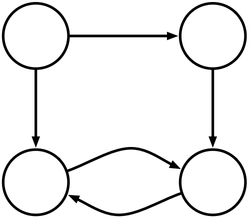
- Complexity: $O(n^2 P)$, where P is the (random) number of points.
- Can take advantage of sparsity in transition rate matrix A.
- Only dependence between successive samples is via the transition times of the trajectory.
- Increasing Ω reduces this dependence, but increases computational cost.
- Sampler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

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).

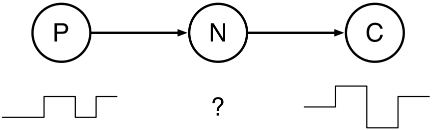
Continuous-time Bayesian networks (CTBNs)



- 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.

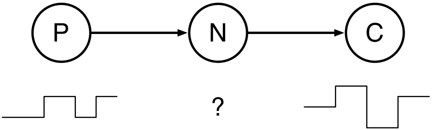
[Nodelman et al., 2002]

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.

Gibbs sampling CTBNs via uniformization



- Sample candidate transition times from a Poisson process with rate $\Omega > A^P_{ii}$.
- Between two successive Poisson events, N remains in a constant state.
  - This state must account for the likelihood of children nodes' 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

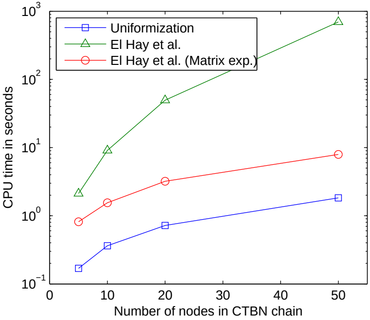


Figure: CPU time vs length of CTBN chain.

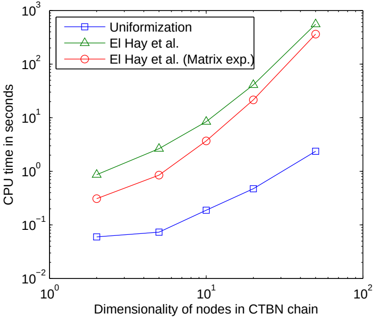


Figure: CPU time vs number of states of CTBN nodes.

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

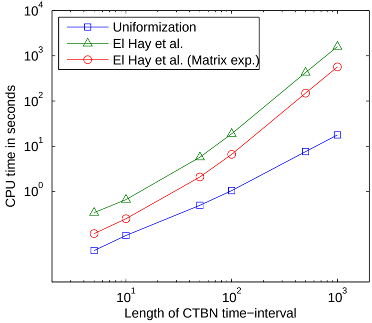


Figure: CPU time vs time interval of CTBN paths.

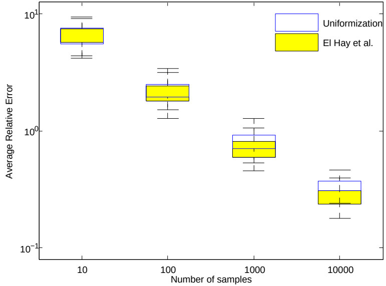
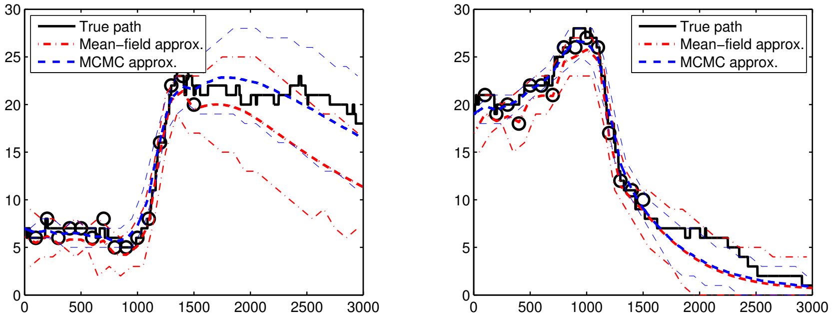


Figure: Average relative error vs number of samples

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 [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).

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.

Our contribution: modulated renewal processes:

- Nonstationarity: allow external time-varying factors to modulate the inter-event distribution.
- We place a (transformed) Gaussian process prior on the intensity function.

[Rao and Teh, 2011b]

Modulated renewal processes

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

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

- 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, $h(\tau, t) = h(\tau)\lambda(t)$.
- Another interaction function is additive $h(\tau, t) = h(\tau) + \lambda(t)$.

Modulated renewal processes (continued)

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

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

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

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

$$\exists\,\Omega \geq \max_{t,\tau} h(\tau)\lambda(t)$$

- Sample $E = \{E_0 = 0, E_1, E_2, \ldots\}$ from a Poisson process with rate Ω.
- Let $\{Y_0 = 0, Y_1, Y_2, \ldots\}$ be an integer-valued Markov chain on the times in E, where each Y_i either equals Y_{i-1} or i.
    - $Y_i = Y_{i-1} \rightarrow$ reject E_i,
    - $Y_i = i \rightarrow$ keep E_i.
- $E_i - E_{Y_i}$: time since the last accepted event. For $i > j \geq 0$, define

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

- Define $G = \{E_i \in E \text{ s.t. } Y_i = i\}$.

Sampling via uniformization

Lemma

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

Sampling via uniformization

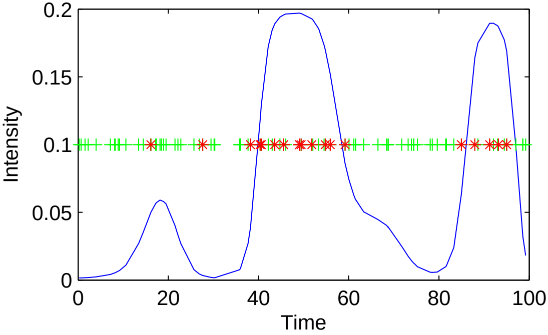


Figure: Green: rejected events, Red: sample for a Gamma(3) modulated renewal process.

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:

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

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

Inference

Given a set of event times G, obtain sample 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 G and the intensity function, and then the intensity function given G and rejected events.

Inference

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

In the interval (G_{i-1}, G_i), events from a rate Ω Poisson process were rejected with probability:

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

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

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

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Catch: we know $\lambda(t)$ only at a discrete set of times. Use thinning method of GP Cox processes [Adams et al., 2009].

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Catch: we know $\lambda(t)$ only at a discrete set of times. Use thinning method of GP Cox processes [Adams et al., 2009].

We resample the GP on the events and the rejected points using elliptical slice sampling [Murray et al., 2010].

Computational considerations

- Complexity: $O(N^3)$, where $N = |G| + 2|E|$, $|G|$ is the number of observations and $|E|$ is the number of rejected points.
- For large G, we must resort to approximate inference for Gaussian processes [Rasmussen and Williams, 2006].
- Question: how do these approximations compare with time-discretized approximations like [Cunningham et al., 2008]?

Experiments

Three synthetic datasets generated by modulating a Gamma(3) renewal process.

- $\lambda_1(t) = 2\exp(t/5) + \exp(-((t-25)/10)^2, t \in [0, 50]$: 44 events
- $\lambda_2(t) = 5\sin(t^2) + 6, t \in [0, 5]$: 12 events
- $\lambda_3(t)$: a piecewise linear function, $t \in [0, 100]$: 153 events

Three settings of our model and a strawman:

- with the shape parameter fixed to 1 (MRP Exp),
- with the shape parameter fixed to 3 (MRP Gam3),
- with a hyperprior on the shape parameter (MRP Full),
- an approximate discrete time sampler on a regular grid covering the interval, all intractable integrals were approximated numerically.

Experiments

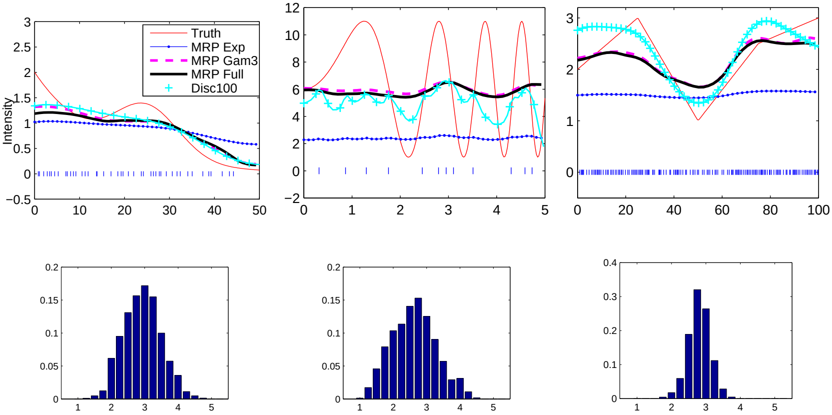

Figure: Synthetic datasets 1-3: Posterior mean intensities (top) and Gamma shape posteriors (bottom). Results from 5000 MCMC samples after a burn-in of 1000 samples.

Experiments

	MRP Exp	MRP Gam3	MRP Full	Disc25	Disc100
l_2 error	7.85	3.19	2.55	4.09	**2.43**
log pred.	-47.55	-38.07	**-37.37**	-41.65	-41.02
l_2 error	141.01	**56.22**	58.44	91.32	57.9
log pred.	-3.70	**-2.95**	-3.28	-5.25	-3.85
l_2 error	82.03	**11.42**	13.44	122.34	38.05
log pred.	-89.88	**-48.28**	-48.57	87.17	-55.80

Table: l_2 distance from the truth and mean log predictive probabilities of test sets for synthetic datasets 1 (top) to 3 (bottom).

Experiments

Dataset: the coal mine disaster dataset, recording the dates of a series of 191 coal mining disasters (each of which killed ten or more men [Jarrett, 1979]).

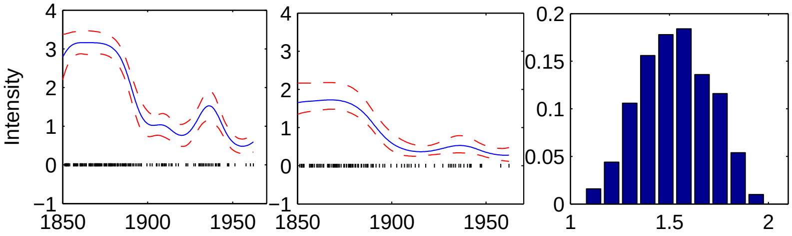

Figure: Left: posterior mean of the intensity function. The posterior for shape parameter was close to 1. Middle and right: results after deleting every alternate event.

Experiments

Dataset: neural spike train recorded from grasshopper auditory receptor cells [Rokem et al., 2006].

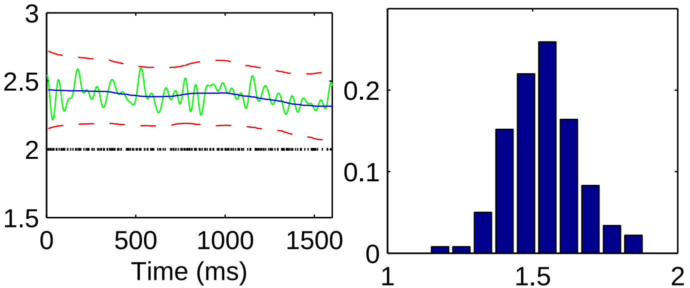

Figure: Left: Posterior mean intensity for neural data with 1 standard deviation error bars. Superimposed is the log stimulus (scaled and shifted). Right: Posterior over the gamma shape parameter.

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 ± 6.91	50.94 ± 5.21	77.85
MH	56.37 ± 10.30	19.34 ± 11.55	345.44
	Coalmine dataset		
	Mean ESS	Minimum ESS	Time(sec)
Gibbs	53.54 ± 8.15	24.87 ± 7.38	282.72
MH	47.83 ± 9.18	18.91 ± 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.

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 can look into extending the models we discussed here:
  - renewal processes with unbounded hazard rates,
  - semi-Markov jump processes,
  - inhomogeneous MJPs, MJPs with infinite state spaces etc.
- Other applications we wish to study, such as survival analysis, queuing systems etc.

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

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

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

1: Sample $A \subset [0, T]$ from a Poisson process with rate Ω.

2: Sample $l_A | l_{G\cup\tilde{G}_{prev}}$.

3: Thin A, keeping element $a \in A \cap [G_{i-1}, G_i]$ with probability $\left(1 - \frac{\hat{\lambda}\sigma(l(a))h(a-G_{i-1})}{\Omega}\right)$.

4: Let $\tilde{G}_{new}$ be the resulting set and $l_{\tilde{G}_{new}}$ be the restriction of l_A to this set. Discard $\tilde{G}_{prev}$ and $l_{\tilde{G}_{prev}}$.

5: Resample $l_{G\cup\tilde{G}_{new}}$ using, for example, elliptical slice sampling.