

# Exchangeable Particle Gibbs for Markov Jump Processes

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# Reaction networks

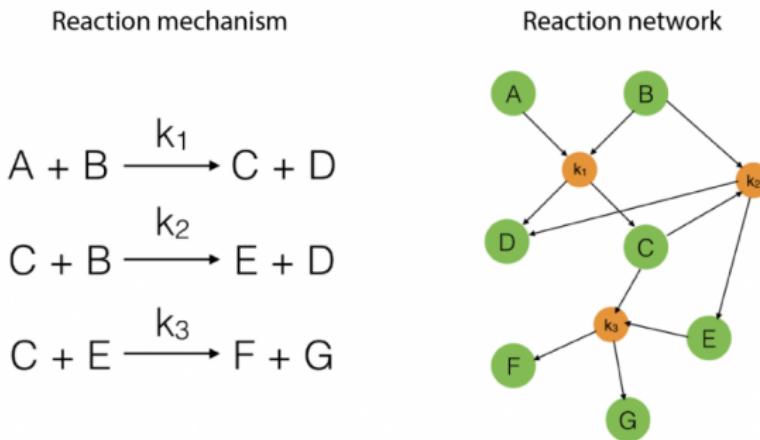


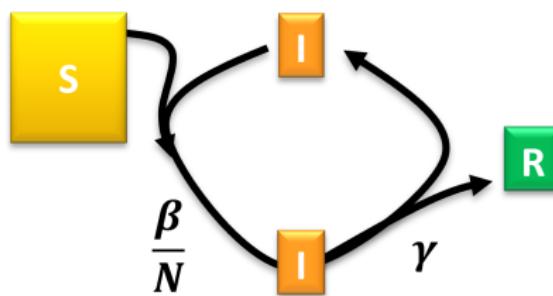
Figure 1: An example of a simple reaction mechanism

Reaction networks

Susceptible  $\xrightarrow{\beta SI}$  Infectious  $\xrightarrow{\gamma I}$  Recovered

Reaction 1 ( $R_1$ ) :  $S + I \xrightarrow{\beta SI} 2I$  (Infection),

Reaction 2 ( $R_2$ ) :  $I \xrightarrow{\gamma I} R$  (Recovery),



**Figure 2:** SIR model

## Reaction networks

## Setup:

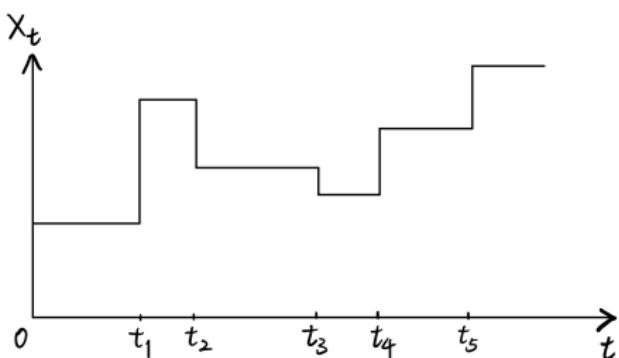
- $u$  species:  $\mathcal{X}_1, \dots, \mathcal{X}_u$
  - $v$  reactions:  $\mathcal{R}_1, \dots, \mathcal{R}_v$

**General form of reaction  $\mathcal{R}_j$ :**

$$\sum_{j=1}^u a_{ij} \mathcal{X}_j \xrightarrow{h_i} \sum_{j=1}^u b_{ij} \mathcal{X}_j$$

## Markov jump process

- Describes how a reaction network evolves over time
  - A **continuous-time, discrete-state** stochastic process
  - Each jump corresponds to the occurrence of a reaction



**Figure 3:** A Markov jump process

# Hidden Markov Model (HMM)

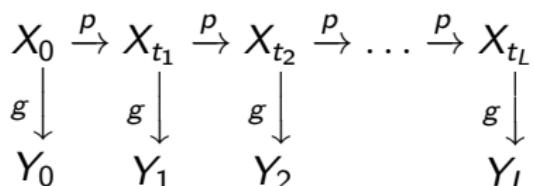
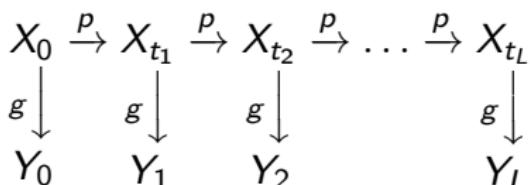


Figure 4: A hidden Markov model with states  $X_{t_{0:L}}$  and observations  $Y_{0:L}$

# Hidden Markov Model (HMM)



**Figure 4:** A hidden Markov model with states  $X_{t_{0:L}}$  and observations  $Y_{0:L}$

The mathematical form of the Hidden Markov model is given by

$$X_0 \sim p_0(\cdot | \theta),$$

$$X_{t_\ell} | (x_{[0,t_{\ell-1}]}, y_{0:\ell-1}, \theta) \sim p(\cdot | x_{t_{\ell-1}}, \theta), \quad \ell = 1, \dots, L$$

$$Y_\ell | (x_{[0,t_\ell]}, y_{0:\ell-1}, \theta) \sim g(\cdot | x_{t_\ell}, \theta).$$

# Bayesian Inference

Given:

- A sequence of observations:  $(y_0, y_1, \dots, y_L)$

Goal:

- Estimate the model parameter,  $\theta$
- Estimate the latent states  $x_{t_0}, \dots, x_{t_L}$
- Target distribution:

$$p(x_{t_0:L}, \theta | y_{0:L})$$

## Inference methods

- Approximate Bayesian Computation (ABC)
- Traditional MCMC methods
- Particle MCMC (Andrieu et al.; 2010)
  - Particle Marginal Metropolis-Hastings (PMMH)
  - **Particle Gibbs**

# Particle Filter

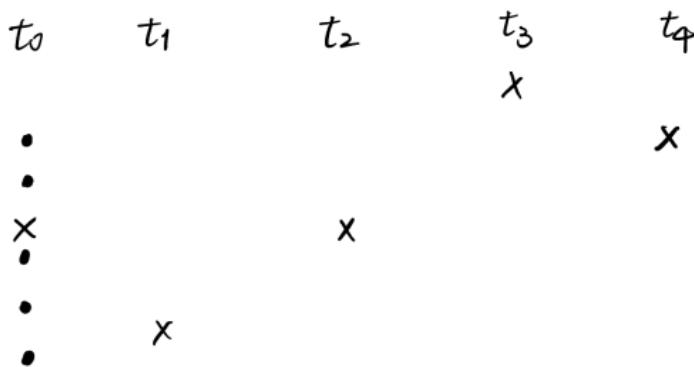


Figure 5: particle filter

The number of proposed particles at each observation time point is denoted by  $M$ . Here  $M = 5$

# Particle Filter

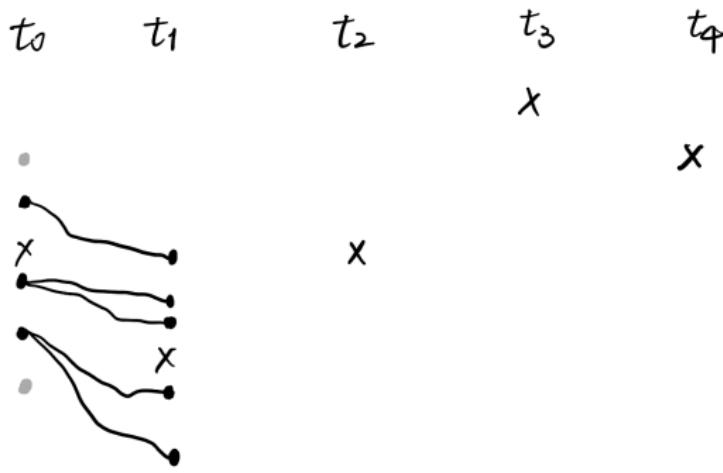


Figure 6: particle filter

# Particle Filter

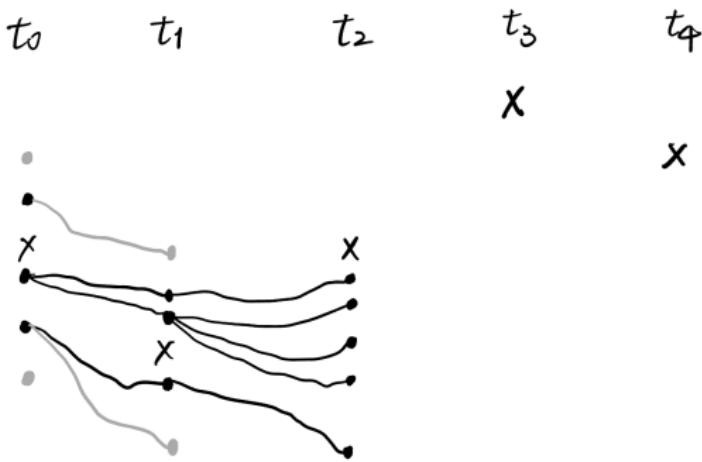


Figure 7: particle filter

# Particle Filter

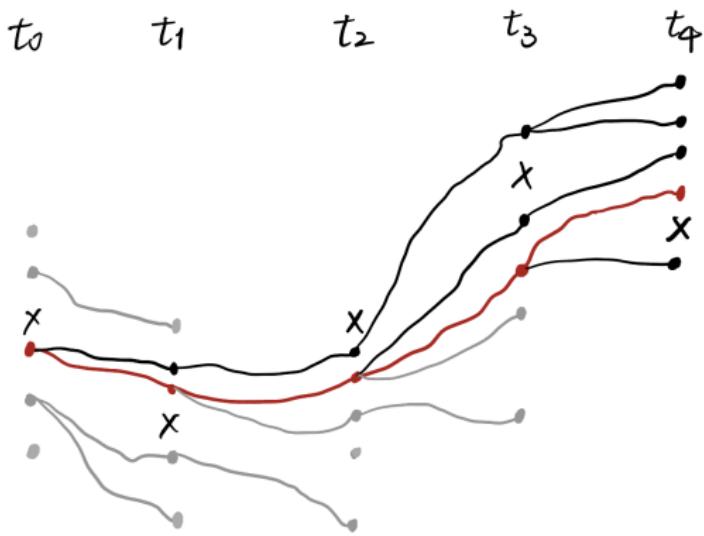


Figure 8: particle filter

# Conditional Particle filter

Suppose the number of proposed paths is  $M = 4$ ,

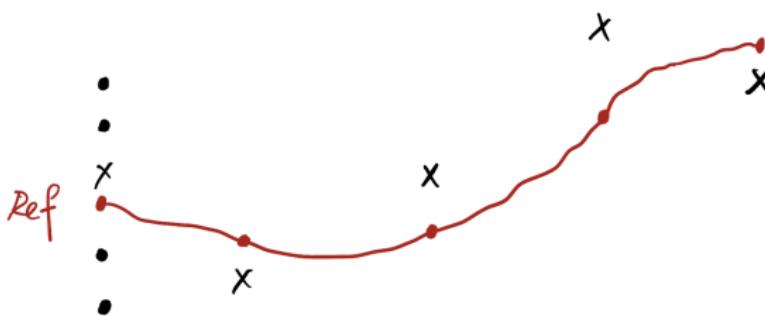


Figure 9: conditional particle filter

# Conditional Particle filter

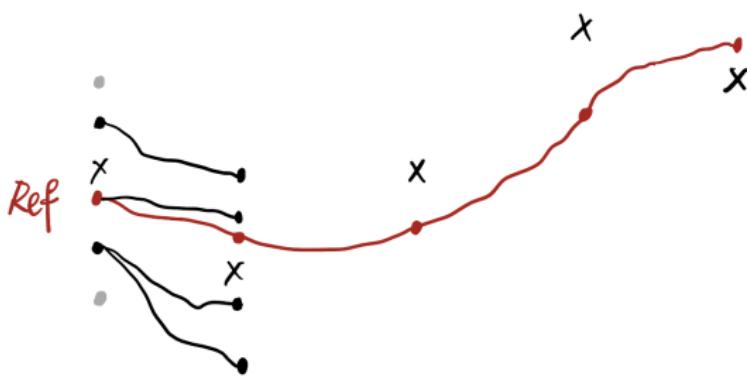


Figure 10: conditional particle filter

# Conditional Particle filter

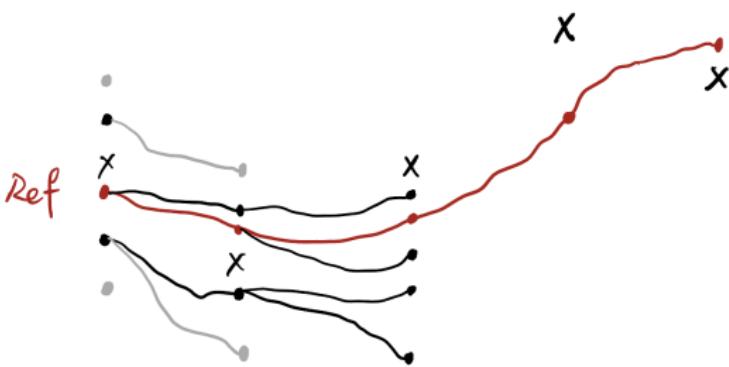
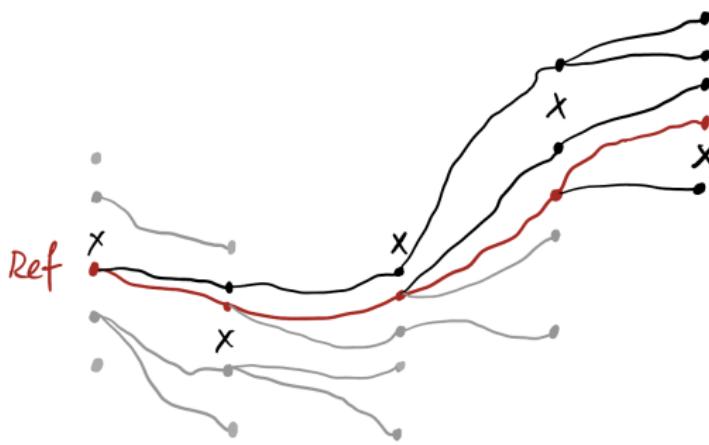


Figure 11: conditional particle filter

## Conditional Particle filter



**Figure 12:** conditional particle filter

# Particle Gibbs (PG)

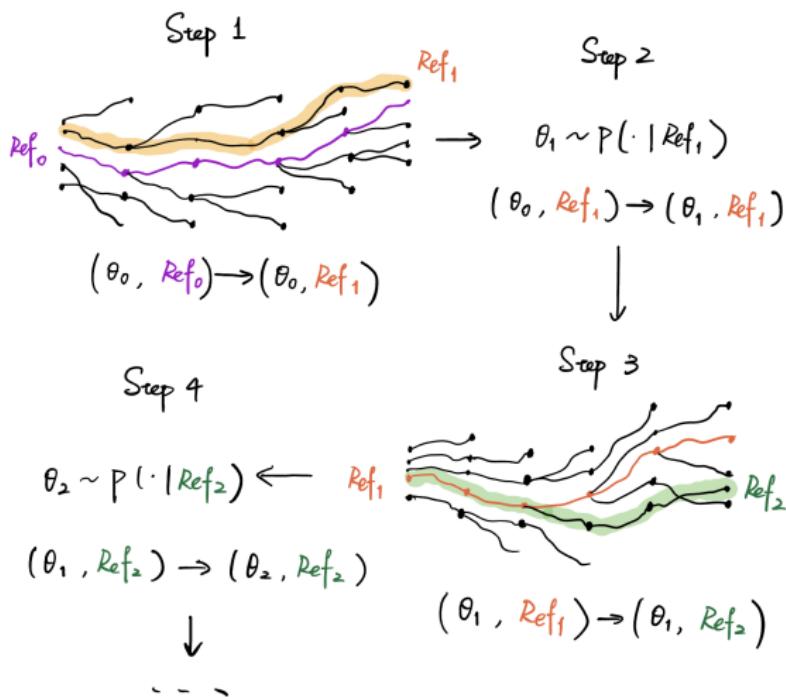


Figure 13: Particle Gibbs sampler

# Particle degeneracy

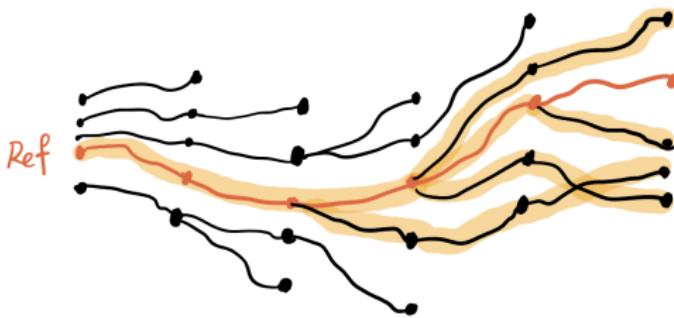


Figure 14: Particle degeneracy

# Particle degeneracy

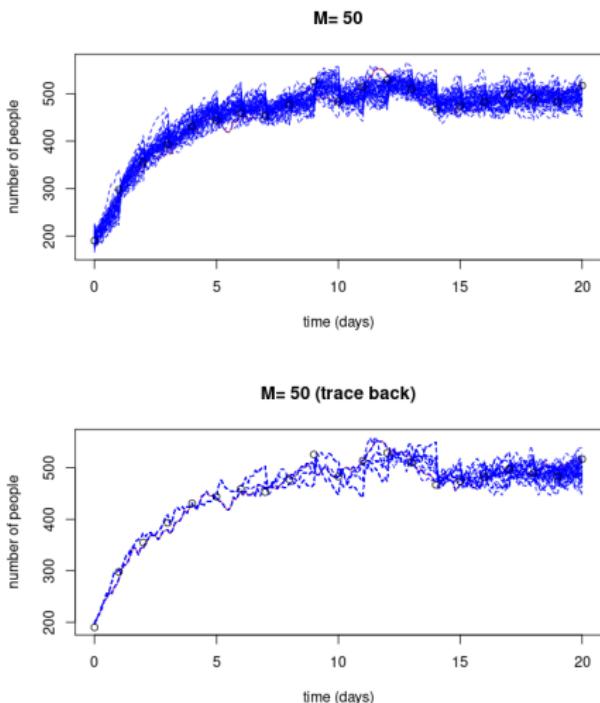
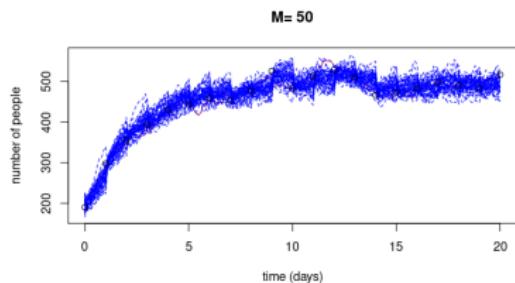


Figure 15: A run of conPF on the SIS model with  $\lambda = 1.2$  and  $\mu = 0.6$

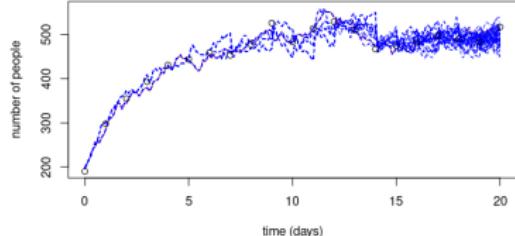
# Methods for addressing particle degeneracy issue

- Particle Gibbs with Ancestor Sampling (PGAS) (Lindsten et al.; 2014)
- Exchangeable Particle Gibbs (xPG)(Malory; 2021)
- Particle-RWM (pRWM)(Finke and Thiery; 2023)
- Particle-MALA (pMALA) (Corenflos and Finke; 2024)

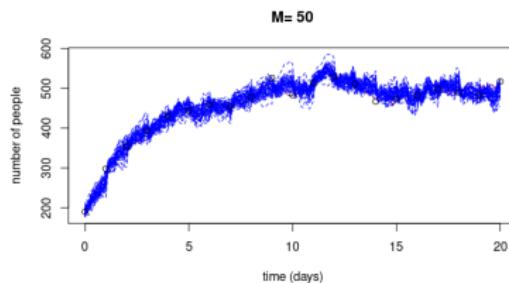
Exchangeable conditional particle filter



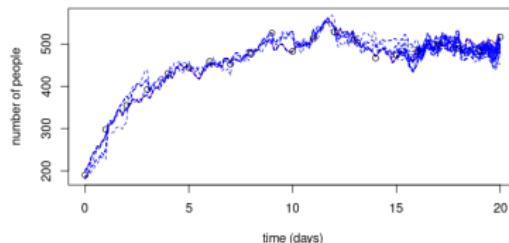
M= 50 (trace back)



## conPF run



M= 50 (trace back)



## Exchangeable conPF run

**Figure 16:** Comparison of conPF and exchangeable conPF on the SIS model with  $\lambda = 1.2$  and  $\mu = 0.6$ .

# Exchangeable Particle Gibbs (xPG)

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## Algorithm 1 Tau-leap method

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- 1: Choose a step size  $\tau$  and set initial state  $x_0$  at  $t = 0$
  - 2: **while**  $t < T$  **do**
  - 3:     Compute reaction hazards  $h_i(x_t)$ ,  $i = 1, \dots, v$
  - 4:     Sample reaction counts  $N^{\mathcal{R}_i} \sim \text{Poisson}(h_i(x_t)\tau)$
  - 5:     Update state:  $x_{t+\tau} = x_t + \sum_{i=1}^v N^{\mathcal{R}_i} S^i$
  - 6:     Advance time:  $t \leftarrow t + \tau$
  - 7: **end while**
-

## Notations:

- $X_t^{(m)}$ : state of the  $m$ -th proposed path at time  $t$
- $N_k^{(m)}$ : number of reactions in the  $m$ -th proposed path in the  $k$ -th time step

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**Step 1.** Sample the initial states for the proposed paths  $x_0^{(1:M)}$  jointly from  $\tilde{q}(\cdot | x_0^{(0)})$ , such that

$$p_0(x_0^{(0)} | \theta) \tilde{q}_0(x_0^{(1:M)} | x_0^{(0)}, \theta) = p_0(x_0^{(j)} | \theta) \tilde{q}_0(x_0^{(-j)} | x_0^{(j)}, \theta), \quad \forall j \in \{1, \dots, M\}, \quad (1)$$

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$$p_0(x_0^{(0)}|\theta)\tilde{q}_0(x_0^{(1:M)}|x_0^{(0)},\theta) = p_0(x_0^{(j)}|\theta)\tilde{q}_0(x_0^{(-j)}|x_0^{(j)},\theta), \quad \forall j \in \{1, \dots, M\}, \quad (1)$$

**Step 2.** For each  $k = 1, 2, \dots$ :

Simulate the number of reaction events of the  $k$ -th time step, i.e.,  $N_k^{(1:M)}$  jointly given the number of such events in the reference path  $N_k^{(0)}$  and Poisson means  $\mu_k^{(0:M)}$ .

$$p\left(N_k^{(0)} | \mu_k^{(0)}\right) q\left(N_k^{(1:M)} | \mu_k^{(0:M)}, N_k^{(0)}\right) = p\left(N_k^{(j)} | \mu_k^{(j)}\right) q\left(N_k^{(-j)} | \mu_k^{(0:M)}, N_k^{(j)}\right). \quad (2)$$

## Exchangeable Particle Gibbs (xPG)

Given  $N^{(0)} \sim \text{Pois}(\lambda^{(0)})$ , we want to construct  $N^{(1)} \sim \text{Pois}(\lambda^{(1)})$  such that  $N^{(0)}$  and  $N^{(1)}$  are correlated.

**Case 1:**  $\lambda^{(1)} > \lambda^{(0)}$  (Poisson update)

$$N^{(1)} = N^{(0)} + \text{Pois}(\lambda^{(1)} - \lambda^{(0)})$$

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**Case 2:**  $\lambda^{(1)} < \lambda^{(0)}$  (Binomial thinning)

$$N^{(1)} \sim \text{Bin}\left(N^{(0)}, \frac{\lambda^{(1)}}{\lambda^{(0)}}\right)$$

Suppose the number of proposed paths is  $M = 4$ . On the time interval  $[(k - 1)\tau, k\tau]$ , given  $X_{(k-1)\tau}^{(0:4)}$  and  $\theta$ , we compute the Poisson means of all paths and order them as:

$$\mu^{(2)} < \mu^{(3)} < \mu^{(0)} < \mu^{(4)} < \mu^{(1)}$$

where  $\mu^{(0)}$  is the Poisson mean of the reference path.

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For each reaction type, given the number of such events in the reference path,  $N^{(0)}$ , simulate the corresponding number of events in the proposed paths.

$$N^{(2)} \leftarrow N^{(3)} \leftarrow \mu^{(0)} \xrightarrow{+ \text{Pois}(\mu^{(4)} - \mu^{(0)})} N^{(4)} \xrightarrow{+ \text{Pois}(\mu^{(1)} - \mu^{(4)})} N^{(1)}$$

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$$N^{(2)} \xleftarrow{\text{Bin}\left(N^{(3)}, \frac{\mu^{(2)}}{\mu^{(3)}}\right)} N^{(3)} \xleftarrow{\text{Bin}\left(N^{(0)}, \frac{\mu^{(3)}}{\mu^{(0)}}\right)} N^{(0)} \rightarrow N^{(4)} \rightarrow N^{(1)}$$

$N(t)$  is a Poisson process with rate 1.

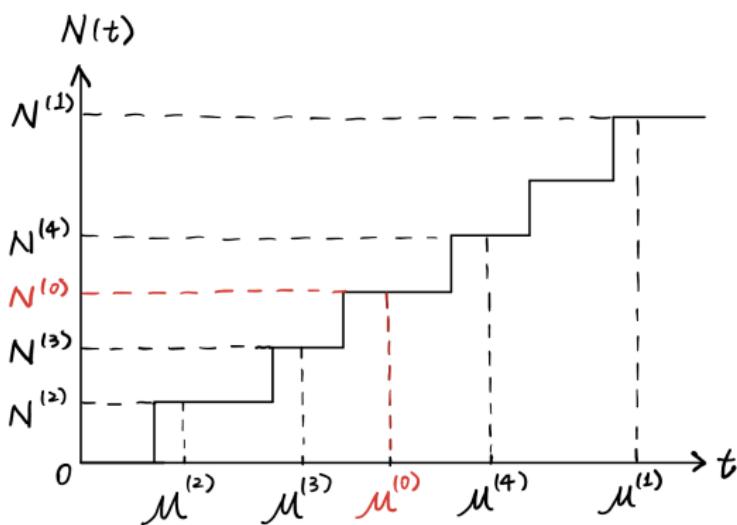


Figure 17: Sample path of a Poisson process  $N(t)$  with rate 1

We introduce a tuning parameter  $\delta$  to control the correlation between the proposed paths and the reference path. On the interval  $[(k - 1)\tau, k\tau]$ , suppose the Poisson means satisfy

$$\mu^{(2)} < \mu^{(3)} < \mu^{(0)} < \mu^{(4)} < \mu^{(1)},$$

and let  $N^{(0)}$  be the number of reaction events in the reference path. Then we proceed as follows:

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Then we proceed as follows:

1.  $\tilde{N}^{(0)} \sim \text{Bin}(N^{(0)}, 1 - \delta)$

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Then we proceed as follows:

1.  $\tilde{N}^{(0)} \sim \text{Bin}(N^{(0)}, 1 - \delta)$

2. Simulate  $\tilde{N}^{(m)}$ ,  $m = 1, \dots, 4$  using Binomial thing and Poisson update sequentially

$$\tilde{N}^{(2)} \leftarrow \tilde{N}^{(3)} \leftarrow \tilde{N}^{(0)} \xrightarrow{+ \text{Pois}\left((1-\delta)(\mu^{(4)} - \mu^{(0)})\right)} \tilde{N}^{(4)} \xrightarrow{+ \text{Pois}\left((1-\delta)(\mu^{(1)} - \mu^{(4)})\right)} \tilde{N}^{(1)}$$

$$\tilde{N}^{(2)} \xleftarrow{\text{Bin}\left(\tilde{N}^{(3)}, \frac{\mu^{(2)}}{\mu^{(3)}}\right)} \tilde{N}^{(3)} \xleftarrow{\text{Bin}\left(\tilde{N}^{(0)}, \frac{\mu^{(3)}}{\mu^{(0)}}\right)} \tilde{N}^{(0)} \rightarrow \tilde{N}^{(4)} \rightarrow \tilde{N}^{(1)}$$

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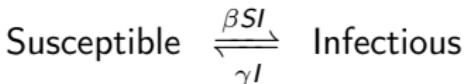
$$\tilde{N}^{(2)} \leftarrow \tilde{N}^{(3)} \leftarrow \tilde{N}^{(0)} \xrightarrow{+ \text{Pois}\left((1-\delta)(\mu^{(4)} - \mu^{(0)})\right)} \tilde{N}^{(4)} \xrightarrow{+ \text{Pois}\left((1-\delta)(\mu^{(1)} - \mu^{(4)})\right)} \tilde{N}^{(1)}$$

$$\tilde{N}^{(2)} \xleftarrow{\text{Bin}\left(\tilde{N}^{(3)}, \frac{\mu^{(2)}}{\mu^{(3)}}\right)} \tilde{N}^{(3)} \xleftarrow{\text{Bin}\left(\tilde{N}^{(0)}, \frac{\mu^{(3)}}{\mu^{(0)}}\right)} \tilde{N}^{(0)} \rightarrow \tilde{N}^{(4)} \rightarrow \tilde{N}^{(1)}$$

3.  $N^{(m)} = \tilde{N}^{(m)} + \text{Pois}(\delta\mu^{(m)})$ ,  $m = 1, \dots, 4$ .

## Experiment results

## SIS model



Reaction 1 ( $R_1$ ) :  $S + I \xrightarrow{\beta SI} 2I$ ,

Reaction 2 ( $R_2$ ) :  $I \xrightarrow{\gamma I} S$  ,

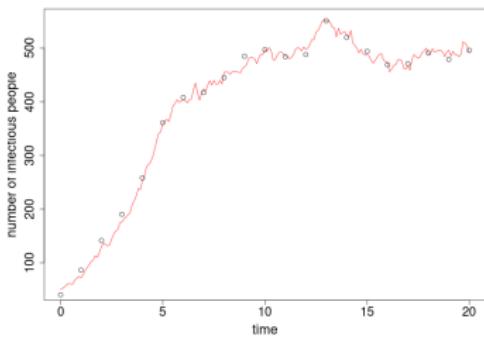
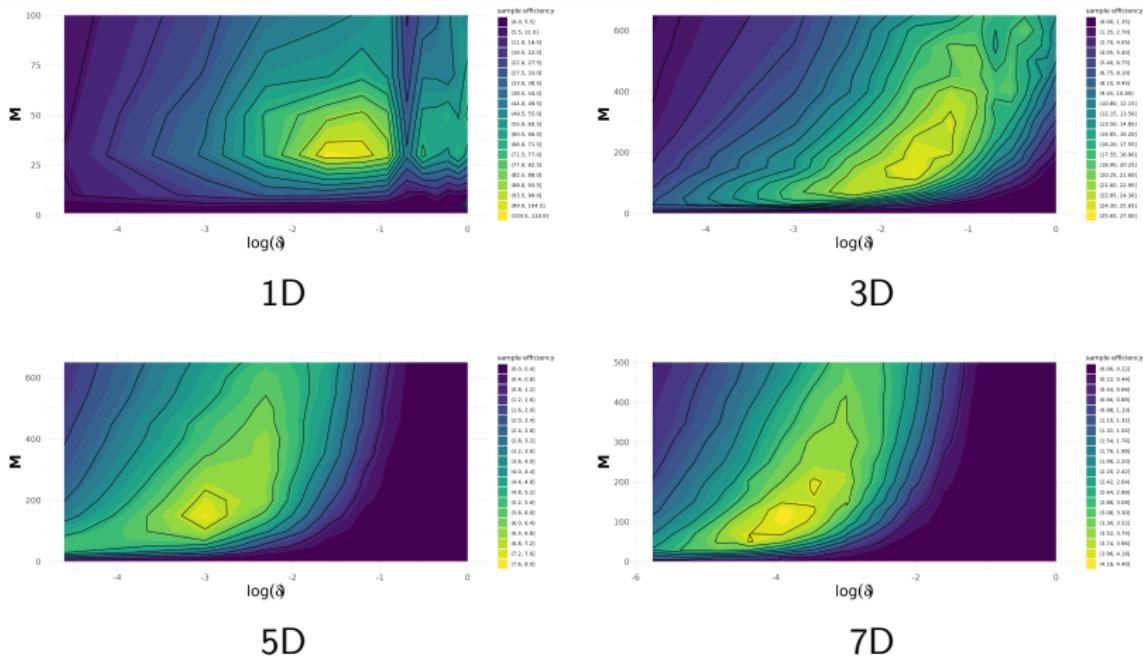


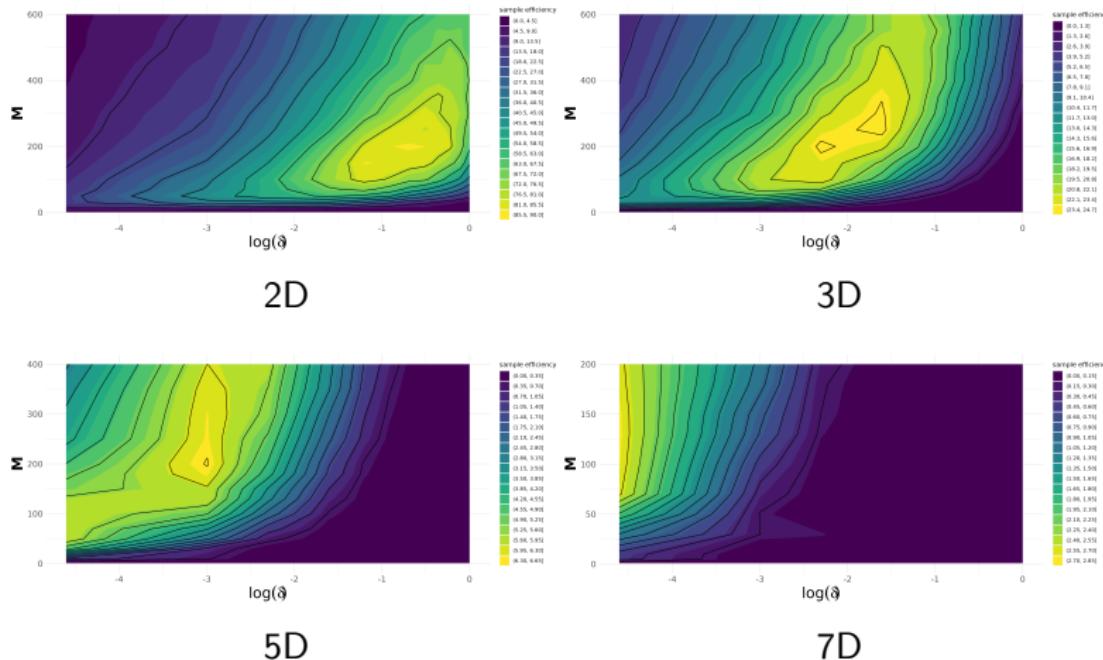
Figure 18: One simulated trajectory of the number of infectious individuals in the SIS model with 21 observations, using  $\beta = 1.2$  and  $\gamma = 0.6$

## SIS models



**Figure 19:** Contour plots of  $\text{ESS}(X_0)/M$  after  $10^5$  iterations in 1D, 3D, 5D, and 7D; latent states are products of SIS models with shared parameters  $\beta = 1.2$  and  $\gamma = 0.6$ .

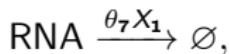
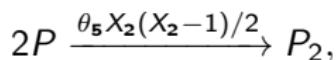
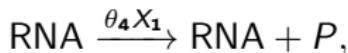
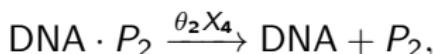
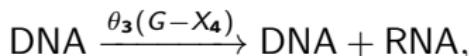
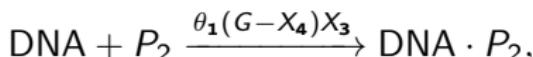
## SIR models



**Figure 20:** Contour plots of the  $\text{ESS}(X_0)/M$  after  $10^5$  iterations in 2D, 3D, 5D and 7D; the true latent states are product of SIR models with shared model parameters  $\beta = 0.6$  and  $\gamma = 0.2$ .

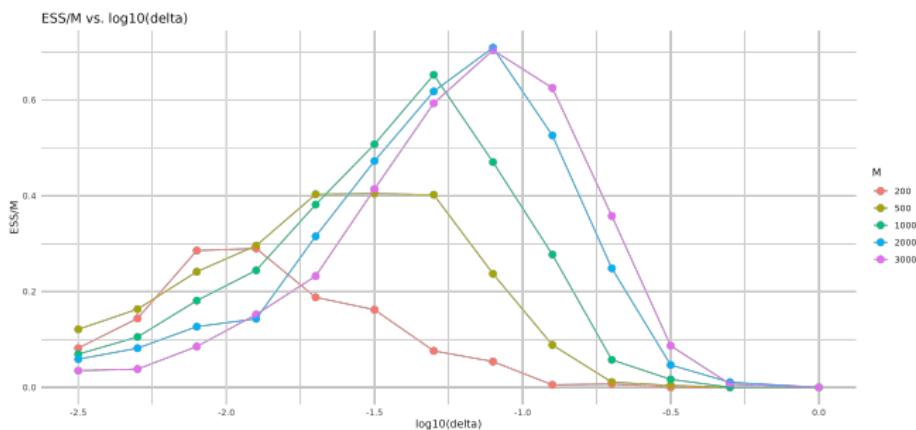
## Autoregulatory model

The total number of copies of DNA,  $G$ , is fixed, and the reactions are:



where  $X_1, X_2, X_3, X_4$  denote the counts of RNA,  $P$ ,  $P_2$ , and DNA  $\cdot$   $P_2$ , respectively.

## Autoregulatory model



**Figure 21:** The efficiency of xPG again  $\log_{10} \delta$  after  $2 \times 10^5$  iterations, with each curve corresponding to a different value of  $M$ ,  $M = 200, 500, 1000, 2000, 3000$

## Tuning parameters $M$ and $\delta$

# Tuning Parameters $M$ and $\delta$

- $\alpha_{\text{ref}}$ : expected probability of accepting a path that has not coalesced with the reference path at time 0.
- $\alpha_{\text{val}}$ : expected probability of accepting a new value for  $X_0$ .

## Key Idea

$$\text{ESS}(X_0) \approx (\text{expected squared jump distance moved}) \times \alpha_{\text{val}}.$$

For xPG, when  $\delta$  is fixed,

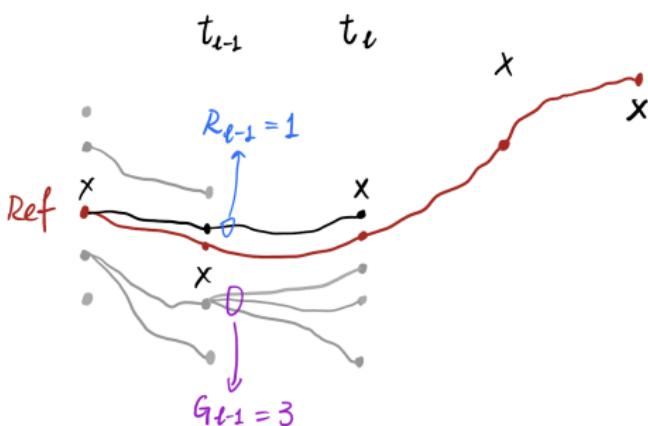
$$\text{Eff} = \frac{\text{ESS}(X_0)}{M} \propto \frac{\alpha_{\text{val}}}{M}.$$

## Tuning parameters $M$ and $\delta$

- **Good particle:** its ancestor at time 0 has a value different from  $x_0^{(0)}$
- **Bad particle:** its ancestor at time 0 has value  $x_0^{(0)}$ .

Let  $G_t$  be the number of good particles **after resampling** at time  $t$ , and let  $R_t$  be the number of bad particles. Since all particles are either good or bad,

$$G_t + R_t = M.$$



# Tuning parameters $M$ and $\delta$

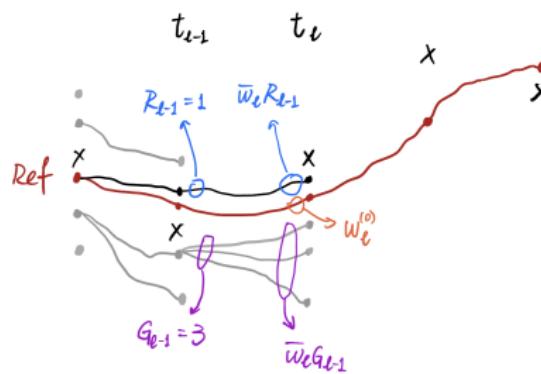
**Assumption 1.** For  $l = 1, \dots, L$ , we assume that

$$\frac{\sum_{i \in \{\text{time } 0 \text{ ancestor}=0\}} w_i^l}{R_{l-1}} = \bar{w}_l = \frac{\sum_{i \in \{\text{time } 0 \text{ ancestor} \neq 0\}} w_i^l}{G_{l-1}}, \quad (3)$$

where  $\bar{w}_l := \frac{1}{M} \sum_{m=1}^M w_\ell^{(m)}$  denotes the average weight of the proposed particles computed before the resampling at time  $t_l$ .

**Assumption 2.**  $G_{l-1}$  and  $R_{l-1}$  are independent of  $W_l^{(0)}$ .

Based on these two assumptions, the tuning suggestion is to tune the acceptance rate of the initial state  $\alpha_{\text{ref}}$  to a value of **0.368**.



## Tuning parameters $M$ and $\delta$

**Target:**  $\alpha_{\text{val}} \approx \frac{\mathbb{E}(G_L)}{M+1}$

Let  $G_{-1}$  be the number of good particles that are initially proposed particles at time zero. Its expectation is given by

$$\mathbb{E}(G_{-1}) = M(1 - p_*^\delta),$$

where  $p_*^\delta$  denotes the probability of proposing, at time zero, a particle that has the same value as the initial state of the reference path. This probability depends on  $\delta$ ; larger values of  $\delta$  correspond to smaller  $p_*^\delta$ .

## Tuning parameters $M$ and $\delta$

Therefore, at the observation times, the expected number of particles whose ancestor at time zero has a different value from  $X_0^{(0)}$  is given by

$$\mathbb{E}(G_l) = M \times \mathbb{E} \left( \frac{\bar{w}_l G_{l-1}}{\bar{w}_l M + w_l^{(0)}} \right) \approx \mathbb{E}(G_{l-1}) \times \frac{\mathbb{E}(\bar{w}_l)M}{\mathbb{E}(\bar{w}_l)M + \mathbb{E}(w_l^0)},$$
$$l = 0, 1, \dots, L \tag{4}$$

where  $w_l^{(0)}$  is the weight of the particle in the reference path at the observation time  $t_l$ . The approximations are obtained from the *strong law of large numbers*.

Tuning parameters  $M$  and  $\delta$ 

$$\begin{aligned}\mathbb{E}(G_L) &\approx (1 - p_*^\delta)M \times \prod_{l=0}^L \frac{\mathbb{E}(\bar{w}_l)M}{\mathbb{E}(\bar{w}_l)M + \mathbb{E}(w_l^0)} \\ &= (1 - p_*^\delta)M \times \prod_{l=0}^L \left(1 - \frac{\mathbb{E}(w_l^0)}{\mathbb{E}(\bar{w}_l)M + \mathbb{E}(w_l^0)}\right) \\ &\approx (1 - p_*^\delta)M \times \exp\left(-\frac{1}{M} \sum_{l=0}^L \frac{\mathbb{E}(w_l^0)}{\mathbb{E}(\bar{w}_l)}\right) \\ &= (1 - p_*^\delta)M \times \exp\left(-\frac{H}{M}\right),\end{aligned}\tag{5}$$

where  $H = \sum_{l=0}^L \frac{\mathbb{E}(w_l^0)}{\mathbb{E}(\bar{w}_l)}$ .

## Tuning parameters $M$ and $\delta$

Therefore, the acceptance rate  $\alpha_{\text{val}}$  is approximated by

$$\alpha_{\text{val}} = \frac{\mathbb{E}(G_L)}{M+1} = (1 - p_*^\delta) \frac{M}{M+1} \exp\left(-\frac{H}{M}\right). \quad (6)$$

and the actual acceptance rate  $\alpha_{\text{ref}}$  is given by

$$\alpha_{\text{ref}} = \frac{M}{M+1} \exp\left(-\frac{H}{M}\right), \quad (7)$$

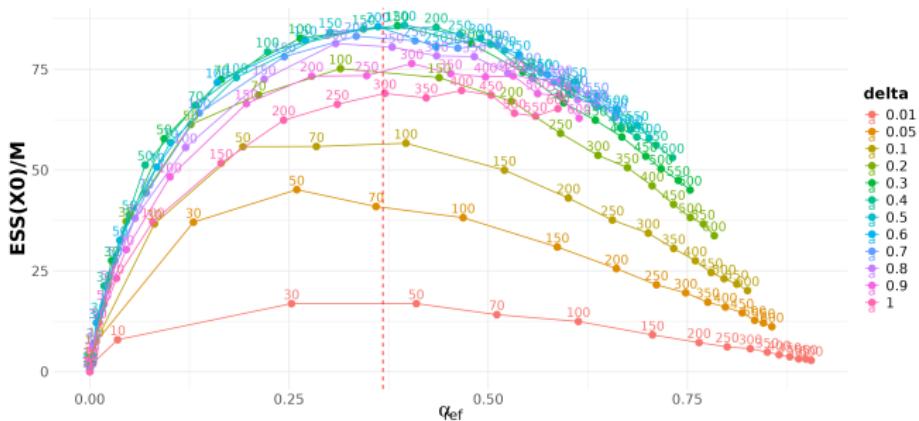
If we fix  $\delta$  for xPG, the efficiency of xPG is proportional to

$$\text{Eff} \propto \frac{\alpha_{\text{val}}}{M} \approx (1 - p_*^\delta) \frac{1}{M} \exp\left(-\frac{H}{M}\right).$$

Take derivative of Eff with respect to  $M$ , we obtain  $\hat{M} = H$ . The optimal actual acceptance rate  $\alpha_{\text{ref}}$  is given by

$$\hat{\alpha}_{\text{ref}} = e^{-1} \approx 0.368.$$

## Tuning parameters $M$ and $\delta$



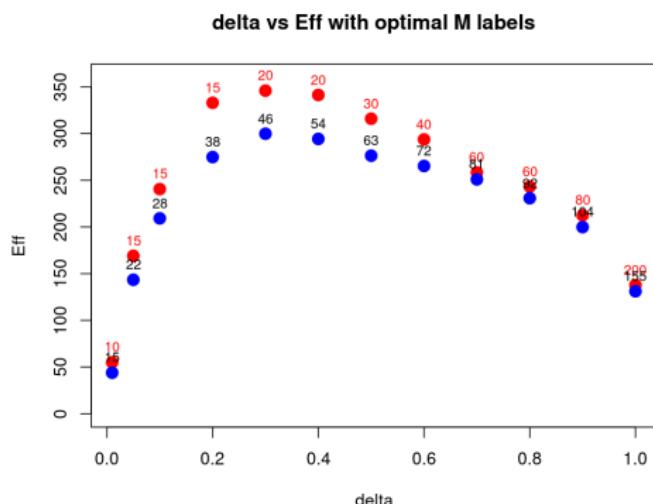
**Figure 24:**  $\text{ESS}(X_0)/M$  against  $\alpha_{\text{ref}}$ ; the vertical red dashed line represents  $\alpha_{\text{ref}} = 0.368$ ; the true latent process is the product of two independent SIR models with shared model parameters  $\beta = 0.6$  and  $\gamma = 0.2$ .

## Tuning strategy

For any  $\delta \in [0, 1]$ , we choose a large  $M = M^*$  such as  $M^* = 100$  or  $M^* = 1000$  and run the algorithm for a moderate number of iterations, noting the actual acceptance rate  $\alpha_{\text{ref}}(\delta, M^*)$ . We may then derive the optimal  $M$  for  $\delta$ , denoted by  $\hat{M}_\delta$ , from equation 7 by

$$\hat{M}_\delta = -M^* \log \left( \frac{M^* + 1}{M^*} \alpha_{\text{ref}}(\delta, M^*) \right). \quad (8)$$

# Tuning strategy



**Figure 25:** The blue dots are  $\delta \in \{0.01, 0.05, (1 : 10) \times 0.1\}$  versus  $\text{Eff} = \text{ESS}(X_0)/\hat{M}_\delta$  with the  $\hat{M}_\delta$  labeled;  $\text{ESS}(X_0)$  is obtained by running xPG with  $(\delta, \hat{M}_\delta)$ ; the red dots represent the maximum efficiency attained for each  $\delta$ , with the corresponding value of  $M$  (that achieves this maximum) shown as the label

## Additional Work and Future Directions

### Additional work completed:

- Derived an xPG algorithm for reaction networks based on **exact simulation** of the MJPs
- Found a way to apply **ancestor sampling** for the tau-leap model in some cases to enhance particle diversity.
- Apply the proposed methods to multi-dimensional state space systems where correlations exist between states across dimensions

### Future research directions:

- Extend the methodology to discrete-time **chain-binomial** epidemic model

## References

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# Particle Filter

Given:

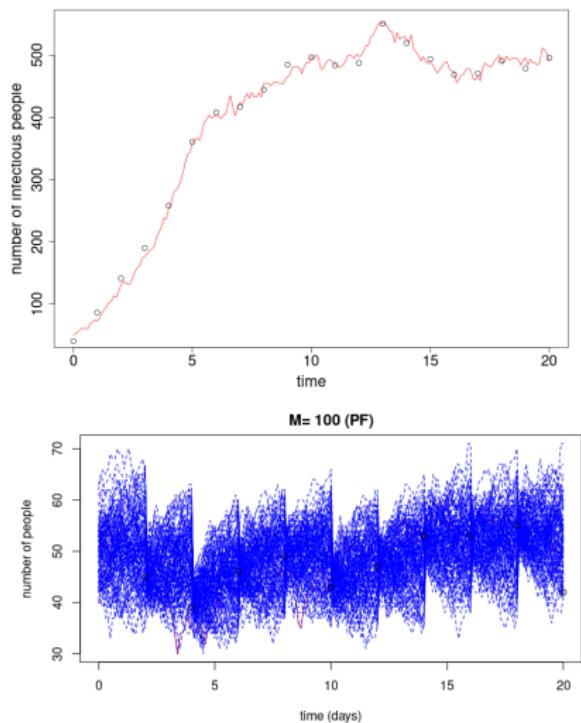
- A sequence of  $L$  observations:  $(y_{t_1}, \dots, y_{t_L})$
- Known model parameters  $\theta$

Goal:

- Infer the latent state  $X_{t_i}$ ,  $i = 1, \dots, L$ , given  $y_{t_1}, \dots, y_{t_i}$ .
- Target distribution:

$$p(X_{t_i} \mid y_{t_{1:i}}, \theta) \quad i = 1, \dots, L$$

# Particle Filter (PF)



**Figure 26:** A single run of PF on the SIS model, with  $M = 100$ ,  $\lambda = 0.8$  and  $\mu = 0.4$ .

# Conditional PF within the Framework of the $\tau$ -Leap

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## Algorithm 2 conditional PF within the Framework of the $\tau$ -Leap

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**Require:** Observations  $y = (y_{K_1\tau}, y_{K_2\tau}, \dots, y_{K_L\tau})$  and reference state process

$$(x_0^{(0)}, n_\tau^{(0)}, n_{2\tau}^{(0)}, \dots, n_{K_L\tau}^{(0)})$$

- 1: **Initialize:** Simulate  $x_0^{(1)}, \dots, x_0^{(M)}$  based on  $x_0^{(0)}$  such that  $P_0(x_0^{(0)})P(x_0^{(1:M)}|x_0^{(0)}) = P_0(x_0^{(i)})P(x_0^{(-i)}|x_0^{(i)}), i = 1, \dots, M$
  - 2: **for**  $k = 1, \dots, K_L$  **do**
  - 3:     Given  $x_{(k-1)\tau}^{(0)}, x_{(k-1)\tau}^{(1)}, \dots, x_{(k-1)\tau}^{(M)}$  and  $n_{k\tau}^{(0)}$ , simulate  $n_{k\tau}^{(1)}, \dots, n_{k\tau}^{(M)}$
  - 4:     Set  $j = 1$
  - 5:     **if**  $k = K_j$  **then**
  - 6:         Resample  $M$  particles from  $\{x_{k\tau}^{(0)}, x_{k\tau}^{(1)}, \dots, x_{k\tau}^{(M)}\}$ . The weight of particle  $x_{k\tau}^{(i)}$  is proportional to the likelihood  $g(y_{K_j\tau}|x_{k\tau}^{(i)}), i = 0, 1, \dots, M$
  - 7:         Replace  $\{x_{k\tau}^{(1)}, \dots, x_{k\tau}^{(M)}\}$  with the resampled particles
  - 8:         Set  $j = j + 1$
  - 9:     **end if**
  - 10: **end for**
  - 11: **return**  $(M + 1)$  state processes
-

## Validity of One-step xPGibbs

Imagine we now have an observation at  $y_1$  with a likelihood of  $f(y_1|x_{K\tau})$ . We have a reference path, which is  $x_0^{(0)}$  and  $x_{(1:K)\tau}^{(0)}$ . From these, we can simulate exchangeable  $X_0^{1:M}$  and  $N_{1:K}^{1:M}$ . We accept  $x_{K\tau}^{(i)}$  with a probability of

$$\alpha(0, i) = \frac{f(y_1|x_{K\tau}^{(i)})}{\sum_{j=1}^M f(y_1|x_{K\tau}^{(j)})}.$$

If  $N_{1:K}^{(0)}$  arises from their joint posterior then they have a mass function proportional to

$$f(y_1|x_{K\tau}^{(0)}) \mathbb{P}\left(X_0^{(0)} = x_0^{(0)}\right) \prod_{k=1}^K \mathbb{P}\left(N_k^{(0)} = n_k^{(0)} | x_{(k-1)\tau}^{(0)}\right),$$

where, for  $k \geq 2$ ,  $x_{(k-1)\tau}^{(0)}$  is a function of  $x_{(k-2)\tau}^{(0)}$  and  $n_{k-1}^{(0)}$ .

# Validity of One-step xPGibbs

The probability of proposing all of the other random variables is

$$\mathbb{P}(X_0^{(1:M)} = x_0^{(1:M)} | x_0^{(0)}) \prod_{k=1}^K \mathbb{P}(\tilde{N}_k^{(0)} = \tilde{n}_k^{(0)}, \tilde{N}_k^{(1:M)} = \tilde{n}_k^{(1:M)}, N_k^{(1:M)} = n_k^{(1:M)} | n_k^{(0)}, x_{(k-1)\tau}^{(0:M)}) .$$

The product of the posterior mass function and the proposal mass function can be re-written as

$$f(y_1 | x_{K\tau}^{(0)}) \mathbb{P}(X_0^{(i)} = x_0^{(i)}) \mathbb{P}(X_0^{(-i)} = x_0^{(-i)} | X_0^{(i)} = x_0^{(i)}) \\ \times \prod_{k=1}^K \mathbb{P}(N_k^{(i)} = n_k^{(i)}, \tilde{N}_k^{(i)} = \tilde{n}_k^{(i)}, \tilde{N}_k^{(-i)} = \tilde{n}_k^{(-i)}, N_k^{(-i)} = n_k^{(-i)} | x_{(k-1)\tau}^{(0:M)})$$

Multiplying this by  $\alpha(0, i)$ , where  $i \in \{0, \dots, M\}$ , gives the probability of starting from the  $i$ -th path, proposing  $M$  other paths, and then accepting path 0.