

Exchangeable Particle Gibbs for Markov Jump Processes

Lanya Yang

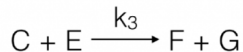
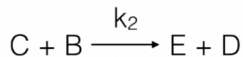
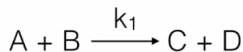
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Reaction networks

Reaction mechanism



Reaction network

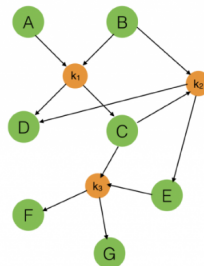


Figure 1: An example of a simple reaction mechanism

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),

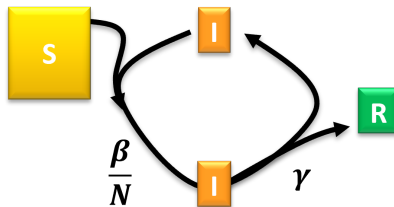


Figure 2: SIR model

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}_i :

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

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

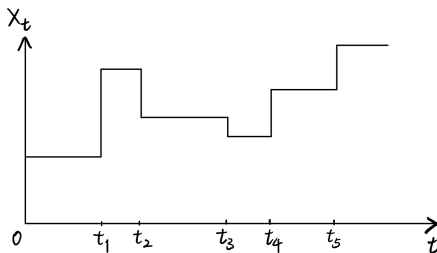


Figure 3: A Markov jump process

Hidden Markov Model (HMM)

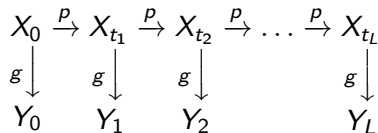


Figure 4: A hidden Markov model with states $X_{t_{0:L}}$ and observations $Y_{0:L}$

Hidden Markov Model (HMM)

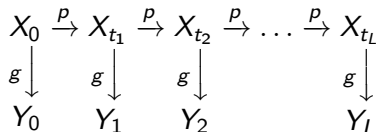


Figure 4: A hidden Markov model with states $X_{t_{0:L}}$ and observations $Y_{0:L}$

The mathematical form of the Hidden Markov model is given by

$$\begin{aligned}
 X_0 &\sim p_0(\cdot \mid \theta), \\
 X_{t_\ell} \mid (x_{[0,t_\ell-1]}, y_{0:\ell-1}, \theta) &\sim p(\cdot \mid x_{t_\ell-1}, \theta), \quad \ell = 1, \dots, L \\
 Y_\ell \mid (x_{[0,t_\ell]}, y_{0:\ell-1}, \theta) &\sim g(\cdot \mid x_{t_\ell}, \theta).
 \end{aligned}$$

Bayesian Inference

Given:

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

Goal:

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

$$p(x_{t_{0:L}}, \theta \mid y_{0:L})$$

Inference methods

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

Particle Filter

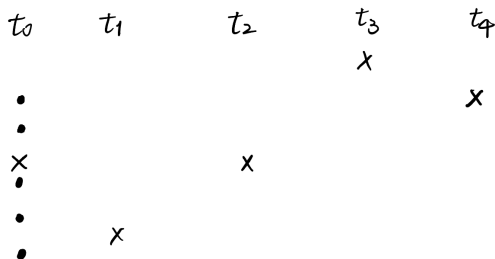


Figure 5: particle filter

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

Particle Filter

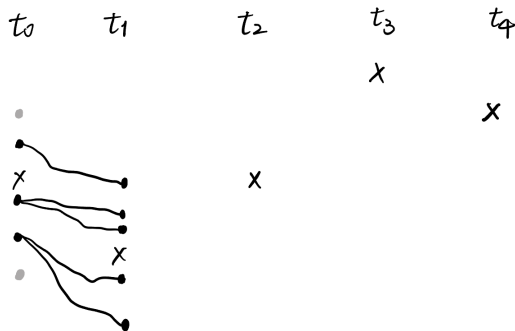


Figure 6: particle filter

Particle Filter

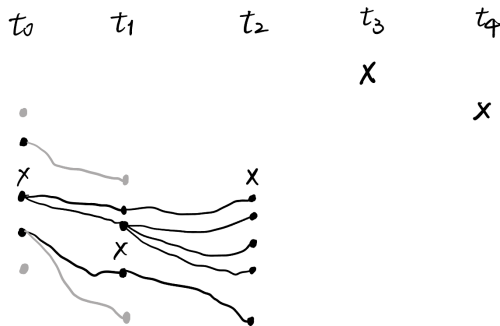


Figure 7: particle filter

Particle Filter

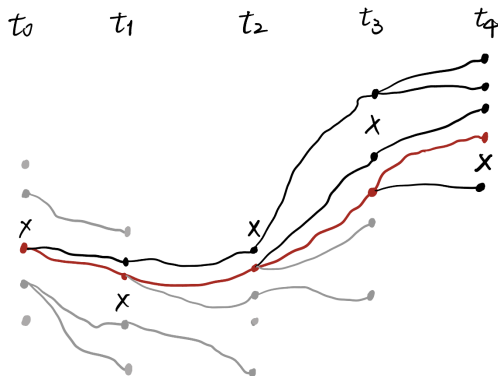


Figure 8: particle filter

Conditional Particle filter

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

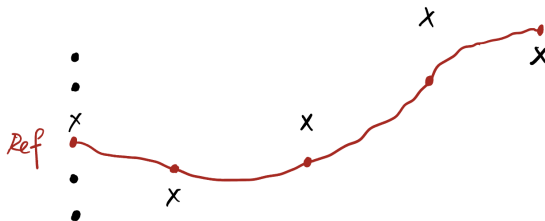


Figure 9: conditional particle filter

Conditional Particle filter

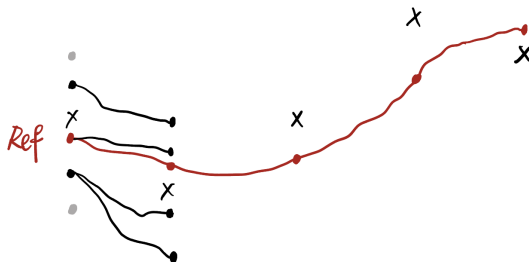


Figure 10: conditional particle filter

Conditional Particle filter

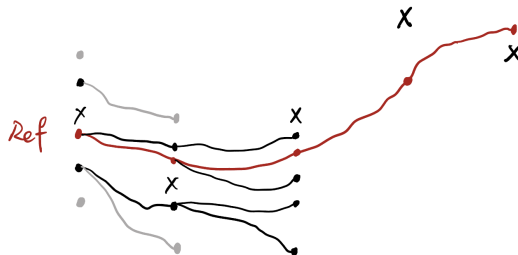


Figure 11: conditional particle filter

Conditional Particle filter

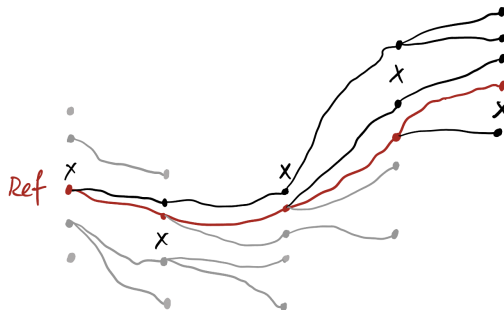


Figure 12: conditional particle filter

Particle Gibbs (PG)

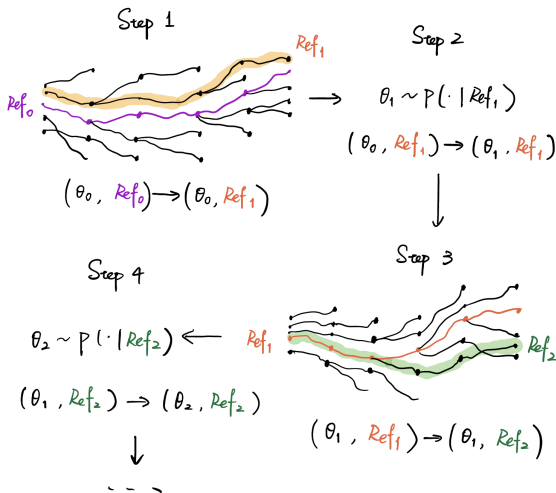


Figure 13: Particle Gibbs sampler

Particle degeneracy

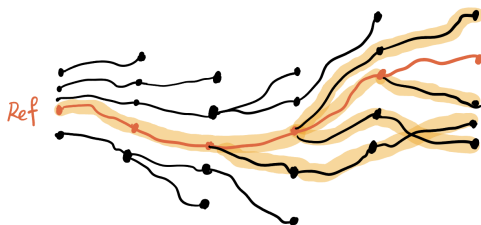


Figure 14: Particle degeneracy

Particle degeneracy

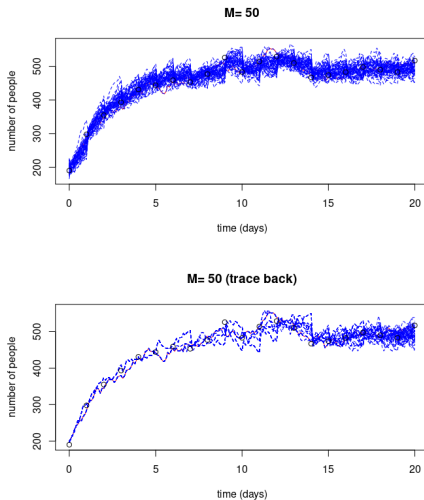
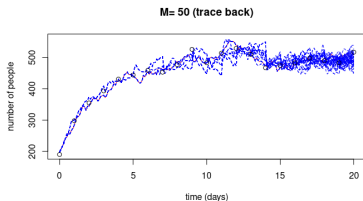
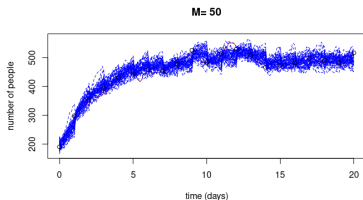


Figure 15: A run of conPF on the SIS model with $\lambda = 1.2$ and $\mu = 0.6$

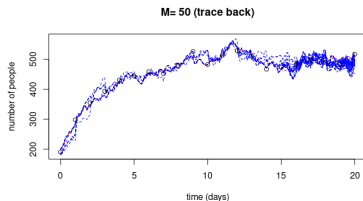
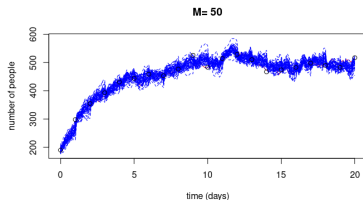
Methods for addressing particle degeneracy issue

- 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



conPF run



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)

Algorithm 1 Tau-leap method

- 1: Choose a step size τ 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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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)

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

xPG

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

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

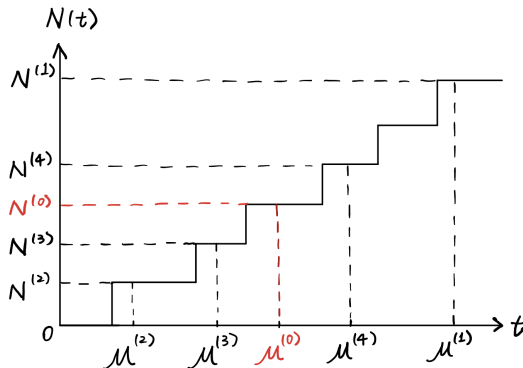


Figure 17: Sample path of a Poisson process $N(t)$ with rate 1

xPG

We introduce a tuning parameter δ 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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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 thinning and Poisson update sequentially

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

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

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

Experiment results

SIS model

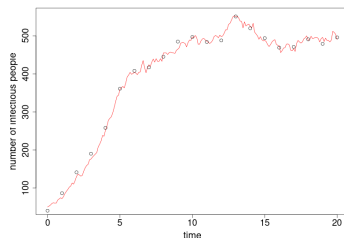
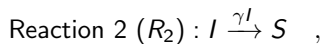
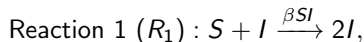
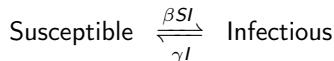


Figure 18: One simulated trajectory of the number of infectious individuals in the SIS model with 21 observations, using $\beta = 1.2$ and $\gamma = 0.6$

SIS models

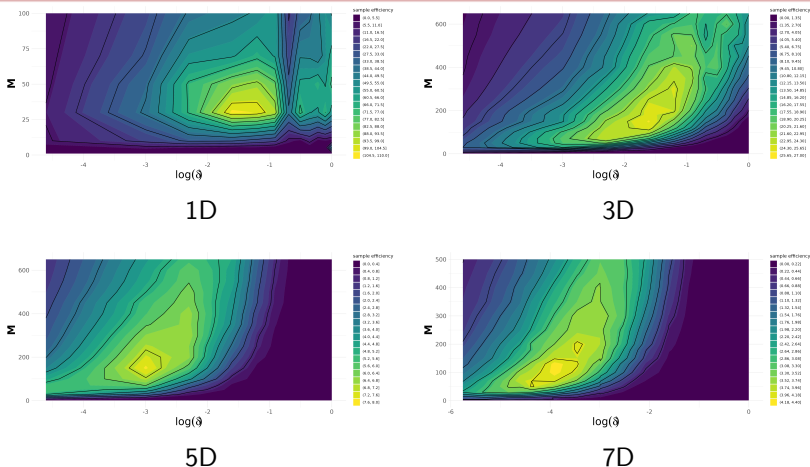


Figure 19: Contour plots of $\text{ESS}(X_0)/M$ after 10^5 iterations in 1D, 3D, 5D, and 7D; latent states are products of SIS models with shared parameters $\beta = 1.2$ and $\gamma = 0.6$.

SIR models

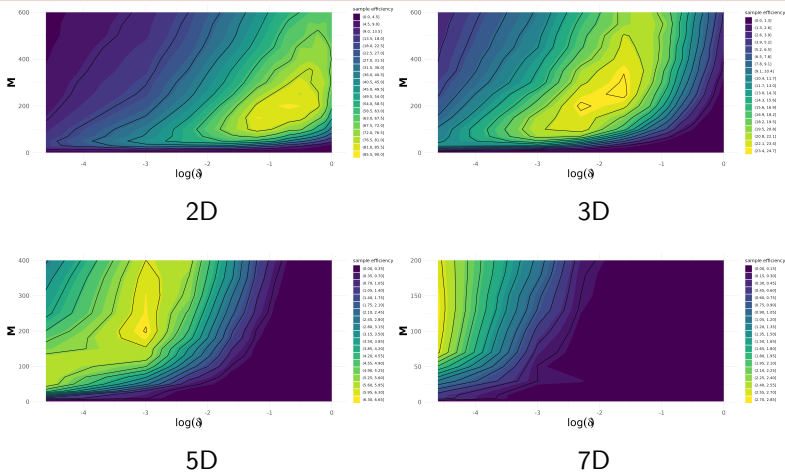
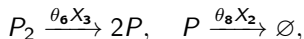
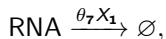
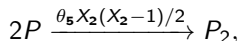
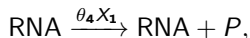
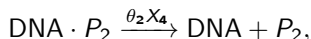
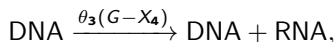
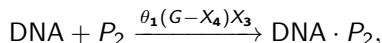


Figure 20: Contour plots of the $\text{ESS}(X_0)/M$ after 10^5 iterations in 2D, 3D, 5D and 7D; the true latent states are product of SIR models with shared model parameters $\beta = 0.6$ and $\gamma = 0.2$.

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 $\text{DNA} \cdot P_2$, respectively.

Autoregulatory model

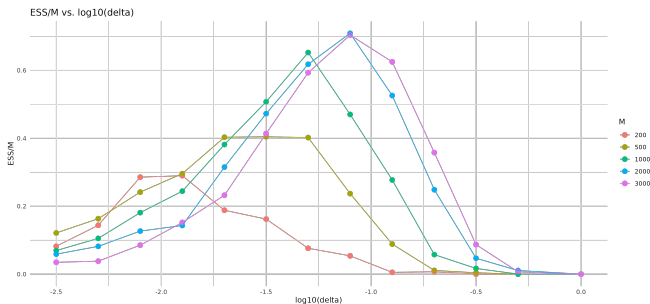


Figure 21: The efficiency of xPG against $\log_{10} \delta$ after 2×10^5 iterations, with each curve corresponding to a different value of M , $M = 200, 500, 1000, 2000, 3000$

Tuning parameters M and δ

Tuning Parameters M and δ

- α_{ref} : expected probability of accepting a path that has not coalesced with the reference path at time 0.
- α_{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 δ is fixed,

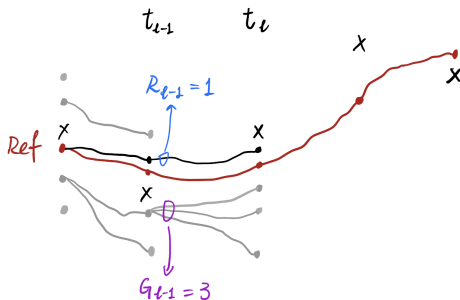
$$\text{Eff} = \frac{\text{ESS}(X_0)}{M} \propto \frac{\alpha_{\text{val}}}{M}.$$

Tuning parameters M and δ

- **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_l be the number of good particles **after resampling** at time t_l , and let R_l be the number of bad particles. Since all particles are either good or bad,

$$G_l + R_l = M.$$



Tuning parameters M and δ

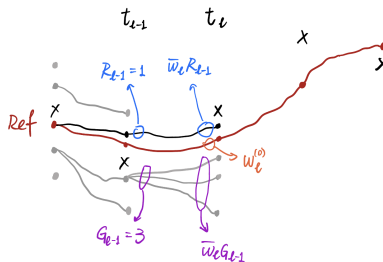
Assumption 1. For $l = 1, \dots, L$, we assume that

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

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 α_{ref} to a value of **0.368**.



Tuning parameters M and δ

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_*^δ 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 δ ; larger values of δ correspond to smaller p_*^δ .

Tuning parameters M and δ

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

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

$$l = 0, 1, \dots, L \quad (4)$$

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 δ

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

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

Tuning parameters M and δ

Therefore, the acceptance rate α_{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 α_{ref} is given by

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

If we fix δ 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 α_{ref} is given by

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

Tuning parameters M and δ

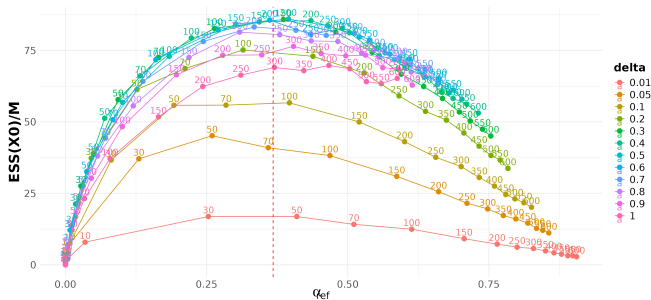


Figure 24: $\text{ESS}(X_0)/M$ against α_{ref} ; the vertical red dashed line represents $\alpha_{\text{ref}} = 0.368$; the true latent process is the product of two independent SIR models with shared model parameters $\beta = 0.6$ and $\gamma = 0.2$.

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 δ , denoted by \hat{M}_δ , from equation 7 by

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

Tuning strategy

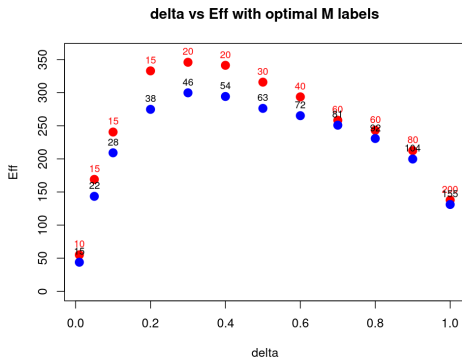


Figure 25: The blue dots are $\delta \in \{0.01, 0.05, (1 : 10) \times 0.1\}$ versus $\text{Eff} = \text{ESS}(X_0) / \hat{M}_\delta$ with the \hat{M}_δ labeled; $\text{ESS}(X_0)$ is obtained by running xPG with (δ, \hat{M}_δ) ; the red dots represent the maximum efficiency attained for each δ , with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

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Particle Filter

Given:

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

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)

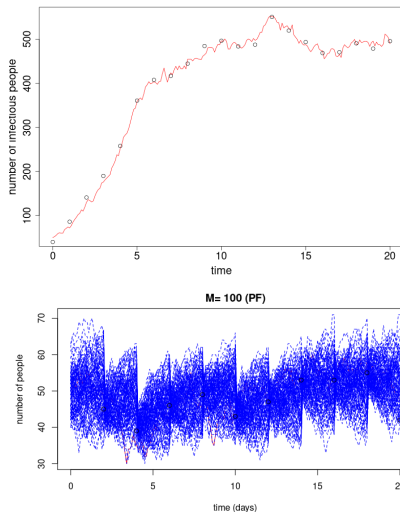


Figure 26: A single run of PF on the SIS model, with $M = 100$, $\lambda = 0.8$ and $\mu = 0.4$.

Conditional PF within the Framework of the τ -Leap

Algorithm 2 conditional PF within the Framework of the τ -Leap

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

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

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

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

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.