

PML session 4. Sequential Monte Carlo

Probabilistic Machine Learning Reading Group

Mario Chacón-Falcón

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Institute of Mathematical Sciences (ICMAT-CSIC)

Logistics for the upcoming sessions

- Next session:
 - **Special session: VI + MCMC**
 - January 14th, 2026
 - *Max Hird (PostDoc @ University of Waterloo)*
- Following section:
 - **Bayesian Neural Networks (Ch. 17)**
 - January 21st, 2026
 - *Daniel Corrales (PhD @ Institute of Mathematical Sciences)*
- After that:
 - Every other week (so 4/2, 18/2, 4/3, ...)

Contents

- Introduction
- State Space Models
- Sequential Monte Carlo for SSMs
- Sequential Monte Carlo for sampling
- Conclusions

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Sequential Monte Carlo for sampling

Conclusions

Sequential Monte Carlo (SMC): Estimating a Sequence of Distributions

- Goal of SMC: approximate a sequence of related distributions

$$\pi_t(z_{1:t}) = \frac{1}{Z_t} \tilde{\gamma}(z_{1:t})$$

for $t = 1 : T$.

- Such sequences arise in:
 - **State Space Models (SSMs)**: $\pi_t(z_{1:t}) \propto p(z_{1:t}|y_{1:t})$
 - **SMC Samplers**: tempered or bridging distributions between prior π_0 and posterior π_T .
- We focus on:
 1. SMC for inference in SSMs (particle filtering)
 2. SMC samplers for general Bayesian inference

Applications of Sequential Monte Carlo

1. SMC for SSMs

- **Object Tracking:** Estimating position/velocity of aircraft or animals using noisy radar or GPS data.
- **Stocks:** Stochastic volatility modelling for option pricing.

2. SMC Samplers

- **Epidemiology:** Inferring transmission rates for disease outbreaks (e.g., COVID-19) using complex simulators.
- **Reinforcement Learning:** Policy search and planning in sparse-reward environments.
- **Climate:** Calibrating parameters of large-scale climate models.

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State Space Models (SSMs)

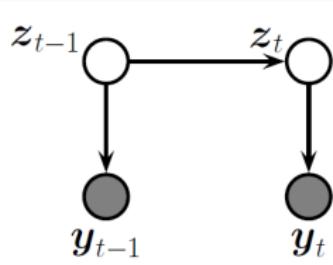
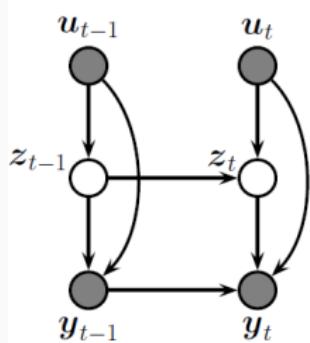
A SSM can be represented as a probabilistic model of the form:

$$p(z_t | z_{t-1}, u_t) = p(z_t | f(z_{t-1}, u_t)) \quad (\text{Transition model})$$

$$p(y_t | z_t, u_t, y_{1:t-1}) = p(y_t | h(z_t, u_t, y_{1:t-1})) \quad (\text{Observation model})$$

We focus on a simplified case:

$$p(z_{1:T}, y_{1:T}) = p(z_1) \prod_{t=2}^T p(z_t | z_{t-1}) \prod_{t=1}^T p(y_t | z_t)$$



Bayesian Filtering equations

We want to compute the belief state $p(z_t | y_{1:t})$ given the prior belief from the previous step, $p(z_{t-1} | y_{1:t-1})$:

Prediction step (Chapman-Kolmogorov equation):

$$p(z_t | y_{1:t-1}) = \int p(z_t | z_{t-1}) p(z_{t-1} | y_{1:t-1}) dz_{t-1}$$

Bayesian Filtering equations

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$$p(z_t | y_{1:t-1}) = \int p(z_t | z_{t-1}) p(z_{t-1} | y_{1:t-1}) dz_{t-1}$$

Update step (Bayes' rule):

$$p(z_t | y_{1:t}) = \frac{p(y_t | z_t) p(z_t | y_{1:t-1})}{p(y_t | y_{1:t-1})}$$

Linear–Gaussian State Space Models

A **linear dynamical system** is a special case of an SSM where both the transition and observation models are linear with Gaussian noise:

State transition model

$$z_t = F_t z_{t-1} + b_t + \varepsilon_t, \quad \varepsilon_t \sim \mathcal{N}(0, Q_t)$$

Observation model

$$y_t = H_t z_t + d_t + \eta_t, \quad \eta_t \sim \mathcal{N}(0, R_t)$$

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Equivalently,

$$p(z_t | z_{t-1}) = \mathcal{N}(F_t z_{t-1} + b_t, Q_t), \quad p(y_t | z_t) = \mathcal{N}(H_t z_t + d_t, R_t).$$

Key property: If $p(z_{t-1} | y_{1:t-1})$ is Gaussian, then $p(z_t | y_{1:t})$ is also Gaussian

This closure property enables **exact Bayesian filtering**.

Kalman Filter: Predict and Update

Assume the filtering distribution at time $t - 1$ is Gaussian:

$$p(z_{t-1} \mid y_{1:t-1}) = \mathcal{N}(\mu_{t-1|t-1}, \Sigma_{t-1|t-1})$$

Predict step (time update)

$$\mu_{t|t-1} = F_t \mu_{t-1|t-1} + b_t$$

$$\Sigma_{t|t-1} = F_t \Sigma_{t-1|t-1} F_t^\top + Q_t$$

Kalman Filter: Predict and Update

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Update step (measurement update)

$$\hat{y}_t = H_t \mu_{t|t-1} + d_t$$

$$S_t = H_t \Sigma_{t|t-1} H_t^\top + R_t$$

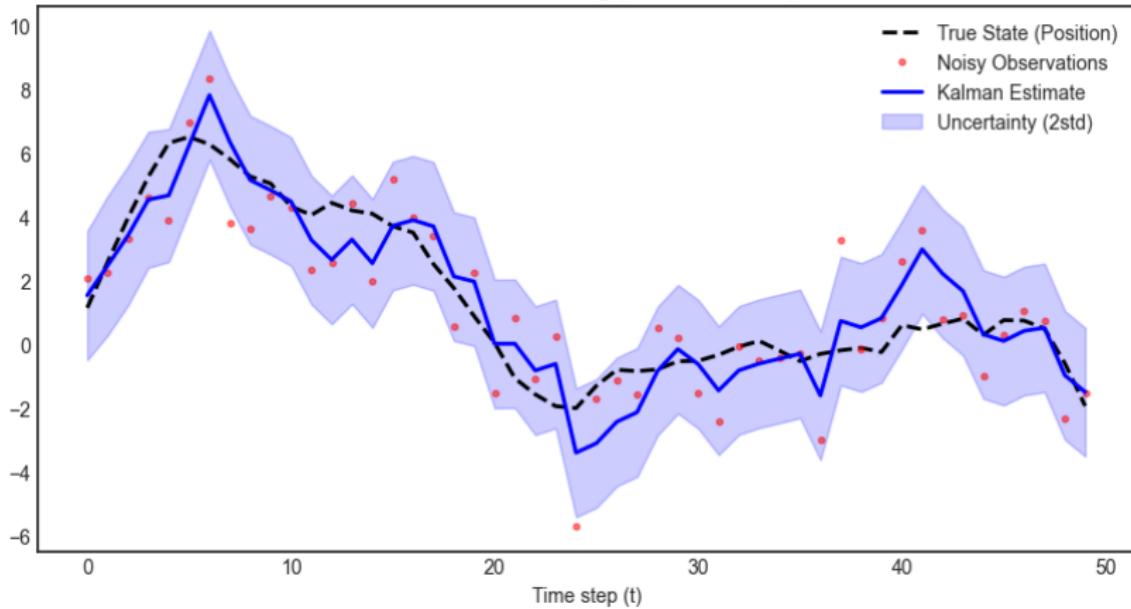
$$K_t = \Sigma_{t|t-1} H_t^\top S_t^{-1}$$

$$\mu_{t|t} = \mu_{t|t-1} + K_t (y_t - \hat{y}_t)$$

$$\Sigma_{t|t} = \Sigma_{t|t-1} - K_t S_t K_t^\top$$

Linear Gaussian Case: Example

Kalman Filter Tracking (Exact Inference)



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Importance Sampling (Self-Normalized IS)

Goal: estimate expectations under a target distribution π_t :

$$\mathbb{E}_{\pi_t}[\varphi_t(z_{1:t})] = \int \varphi_t(z_{1:t}) \pi_t(z_{1:t}) dz_{1:t}, \quad \pi_t(z_{1:t}) = \frac{\tilde{\gamma}_t(z_{1:t})}{Z_t}.$$

Using a proposal $q_t(z_{1:t})$, with $\text{supp}(\pi) \subseteq \text{supp}(q)$, we can rewrite:

$$\mathbb{E}_{\pi_t}[\varphi_t(z_{1:t})] = \frac{\int \left[\frac{\tilde{\gamma}(z_{1:t})}{q(z_{1:t})} \varphi_t(z_{1:t}) \right] q(z_{1:t}) dz_{1:t}}{\int \left[\frac{\tilde{\gamma}(z_{1:t})}{q(z_{1:t})} \right] q(z_{1:t}) dz_{1:t}}$$

Importance Sampling (Self-Normalized IS)

Drawing $z_{1:t}^{(i)} \sim q_t(z_{1:t})$, $i = 1, \dots, N_s$, we estimate

$$\mathbb{E}_{\pi_t} [\varphi_t(z_{1:t})] \approx \sum_{i=1}^{N_s} W_t^{(i)} \varphi_t(z_{1:t}^{(i)}),$$

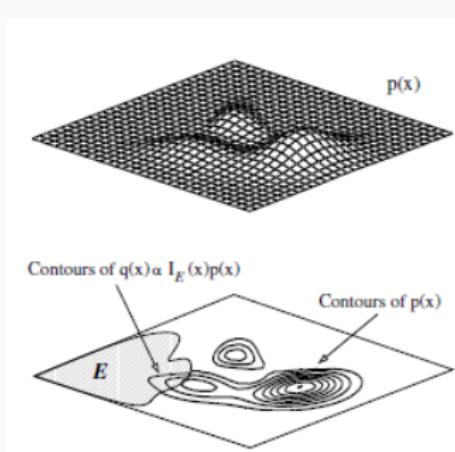
Where:

$$\tilde{w}_t^{(i)} = \frac{\tilde{\gamma}_t(z_{1:t}^{(i)})}{q_t(z_{1:t}^{(i)})}, \quad W_t^{(i)} = \frac{\tilde{w}_t^{(i)}}{\sum_j \tilde{w}_t^{(j)}}, \quad \hat{Z}_t = \frac{1}{N_s} \sum_{i=1}^{N_s} \tilde{w}_t^{(i)}.$$

Importance Sampling (Self-Normalized IS)

To approximate the target distribution:

$$\pi_t(z_{1:t}) \approx \sum_{i=1}^{N_s} W_t^{(i)} \delta(z_{1:t} - z_{1:t}^{(i)}).$$



Sequential Importance Sampling (SIS)

Key idea: exploit the autoregressive (online) structure of the problem.

Autoregressive proposal:

$$q_t(z_{1:t}) = q_{t-1}(z_{1:t-1}) q_t(z_t \mid z_{1:t-1})$$

Given particles $\{z_{1:t-1}^{(i)}\}$, extend each trajectory by sampling

$$z_t^{(i)} \sim q_t(z_t \mid z_{1:t-1}^{(i)}).$$

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Given particles $\{z_{1:t-1}^{(i)}\}$, extend each trajectory by sampling

$$z_t^{(i)} \sim q_t(z_t \mid z_{1:t-1}^{(i)}).$$

Recursive weight update:

$$\tilde{w}_t(z_{1:t}) = \frac{\tilde{\gamma}_t(z_{1:t})}{q_t(z_{1:t})} = \tilde{w}_{t-1}(z_{1:t-1}) \cdot \underbrace{\frac{\tilde{\gamma}_t(z_{1:t})}{\tilde{\gamma}_{t-1}(z_{1:t-1}) q_t(z_t \mid z_{1:t-1})}}_{\text{incremental importance weight } \alpha_t(z_{1:t})}$$

Sequential Importance Sampling (SIS)

Special case: State Space Models

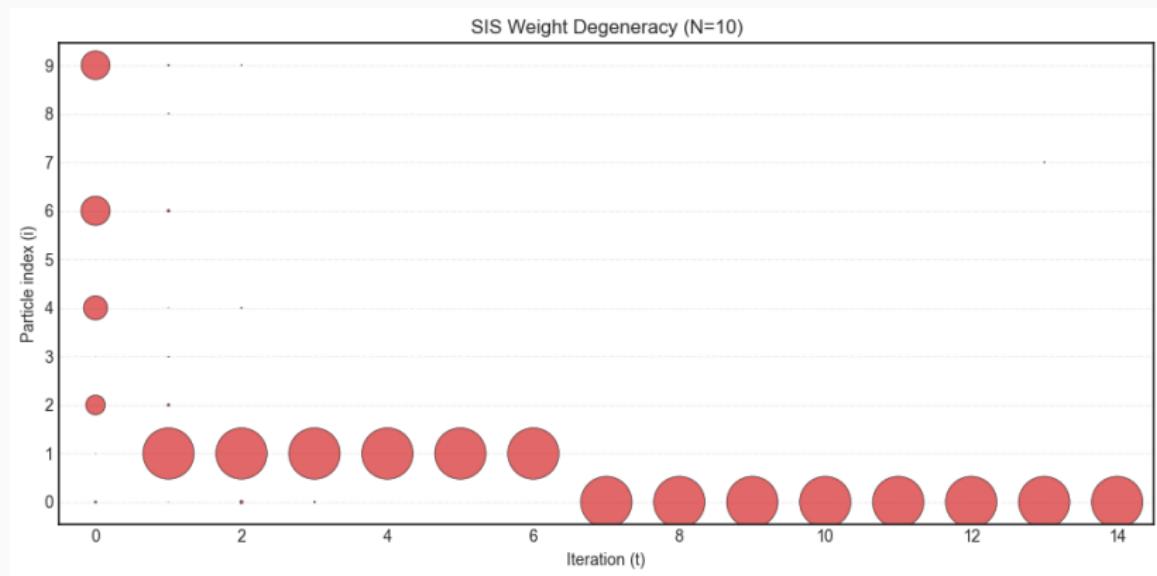
$$\tilde{\gamma}_t(z_{1:t}) = p(z_{1:t}, y_{1:t}) = \color{orange}p(y_t \mid z_{1:t})\color{black} p(z_t \mid z_{1:t-1}) \tilde{\gamma}_{t-1}(z_{1:t-1})$$

Hence,

$$\alpha_t(z_{1:t}) = \frac{\color{orange}p(y_t \mid z_{1:t})\color{black} p(z_t \mid z_{1:t-1})}{q_t(z_t \mid z_{1:t-1})}.$$

Sequential Importance Sampling (SIS)

Limitation: Weight degeneracy



Sequential Importance Sampling with Resampling (SISR)

SIS proposal:

$$q_t^{\text{SIS}}(z_{1:t}) = q_{t-1}(z_{1:t-1}) q_t(z_t \mid z_{1:t-1}),$$

SISR proposal:

$$q_t^{\text{SISR}}(z_{1:t}) = \hat{\pi}_{t-1}(z_{1:t-1}) q_t(z_t \mid z_{1:t-1}),$$

where $\hat{\pi}_{t-1}(z_{1:t-1}) = \sum_i W_{t-1}^{(i)} \delta(z_{1:t-1} - z_{1:t-1}^{(i)})$.

Sequential Importance Sampling with Resampling (SISR)

SIS proposal:

$$q_t^{\text{SIS}}(z_{1:t}) = q_{t-1}(z_{1:t-1}) q_t(z_t \mid z_{1:t-1}),$$

SISR proposal:

$$q_t^{\text{SISR}}(z_{1:t}) = \hat{\pi}_{t-1}(z_{1:t-1}) q_t(z_t \mid z_{1:t-1}),$$

where $\hat{\pi}_{t-1}(z_{1:t-1}) = \sum_i W_{t-1}^{(i)} \delta(z_{1:t-1} - z_{1:t-1}^{(i)})$.

How resampling works (selection step):

- Resample N_s samples from $z_{1:t-1}^{(a_i)} \sim \hat{\pi}_{t-1}(z_{1:t-1})$.
- Reset weights: $\tilde{w}_{t-1}^{(i)} = 1$.

Propagation:

$$z_t^{(i)} \sim q_t(z_t \mid z_{1:t-1}^{(a_i)}), \quad z_{1:t}^{(i)} = (z_{1:t-1}^{(a_i)}, z_t^{(i)}).$$

Sequential Importance Sampling with Resampling (SISR)

Weight update:

$$\tilde{w}_t^{(i)} = \alpha_t(z_{1:t}^{(i)}) = \frac{\tilde{\gamma}_t(z_{1:t}^{(i)})}{\tilde{\gamma}_{t-1}(z_{1:t-1}^{(a_i)}) q_t(z_t^{(i)} \mid z_{1:t-1}^{(a_i)})}.$$

(Same incremental weights as SIS.)

Resampling methods: Inverse cdf, multinomial resampling, stratified resampling, systematic resampling.

Bootstrap filter

Bootstrap filter: Special case where the model is an SSM and the proposal equal to the dynamical prior:

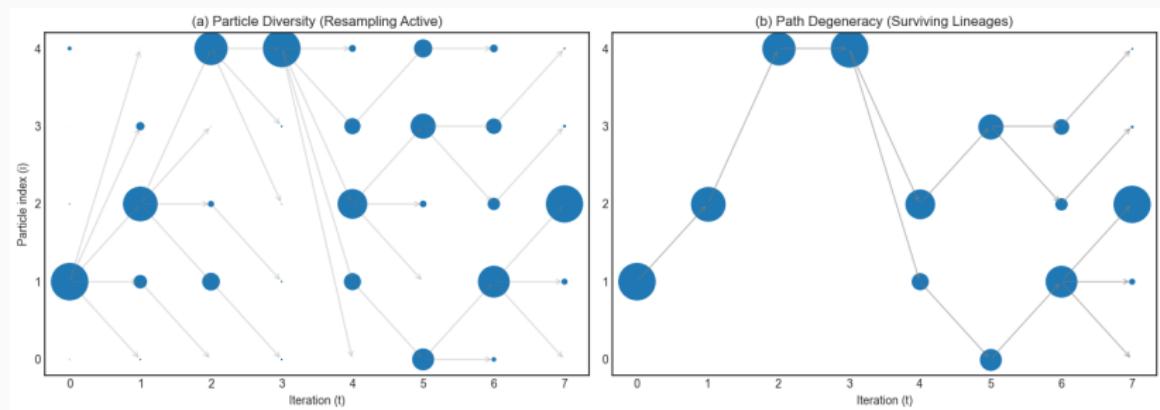
$$q_t(z_t | z_{1:t-1}) = p(z_t | z_{1:t-1})$$

Hence,

$$\alpha_t(z_{1:t}) = \frac{p(y_t | z_{1:t})p(z_t | z_{1:t-1})}{q_t(z_t | z_{1:t-1})} = p(y_t | z_{1:t})$$

Bootstrap filter

Limitation: Path degeneracy



Adaptive Resampling

Key trade-off:

- **No resampling** \Rightarrow SIS:
 - severe *weight degeneracy*
 - few particles effectively contribute
- **Resample at every step:**
 - avoids weight collapse
 - increases *path degeneracy* (loss of diversity in ancestry)

Adaptive Resampling

Key trade-off:

- **No resampling** \Rightarrow SIS:
 - severe *weight degeneracy*
 - few particles effectively contribute
- **Resample at every step:**
 - avoids weight collapse
 - increases *path degeneracy* (loss of diversity in ancestry)

Adaptive resampling: resample only when particle diversity becomes too low.

Effective Sample Size (ESS):

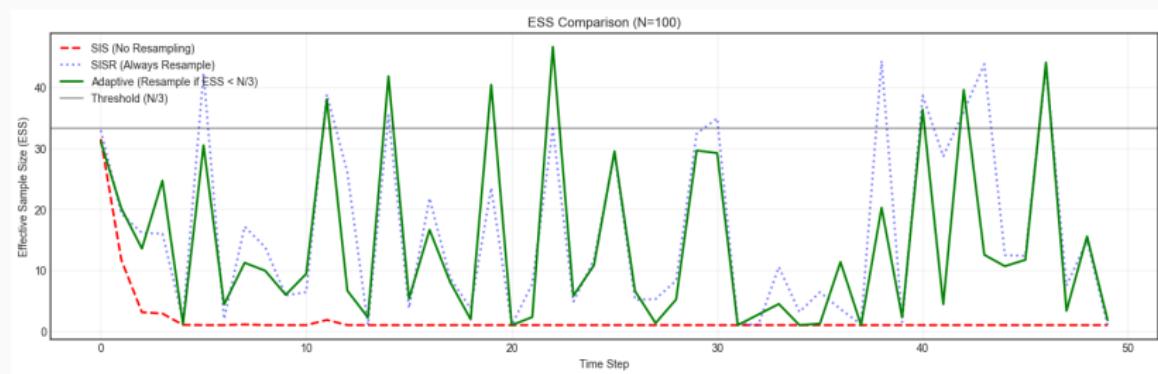
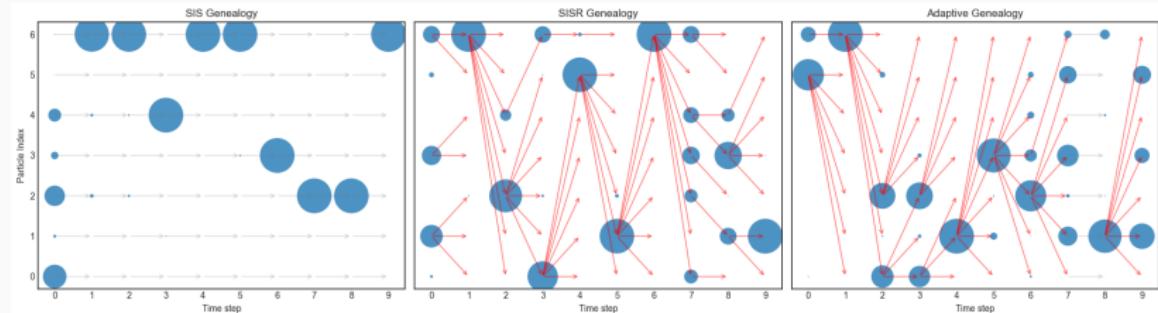
$$\text{ESS}(W_{1:N}) = \frac{1}{\sum_{n=1}^N W_n^2}, \quad \text{ESS}(\tilde{w}_{1:N}) = \frac{\left(\sum_{n=1}^N \tilde{w}_n\right)^2}{\sum_{n=1}^N \tilde{w}_n^2}.$$

Algorithm: SISR with Adaptive Resampling

Algorithm 1 SISR with adaptive resampling (generic SMC)

```
1: Initialization:  $\tilde{w}_0^{1:N_s} = 1$ ,  
2: for  $t = 1 : T$  do  
3:   for  $i = 1 : N_s$  do  
4:     Sample particle:  $z_t^{(i)} \sim q_t(z_t | z_{1:t-1}^{(i)})$   
5:     Compute incremental weight:  $\alpha_t^{(i)} = \frac{\tilde{\gamma}_t(z_{1:t}^{(i)})}{\tilde{\gamma}_{t-1}(z_{1:t-1}^{(i)}) q_t(z_t^{(i)} | z_{1:t-1}^{(i)})}$   
6:     Compute unnormalized weight:  $\tilde{w}_t^{(i)} = \tilde{w}_{t-1}^{(i)} \alpha_t^{(i)}$   
7:   end for  
8:   if  $\text{ESS}(\tilde{w}_{t-1}^{1:N_s}) < \text{ESS}_{\min}$  then  
9:     Compute ancestors:  $a_{1:N_s} = \text{resample}(\tilde{w}_{t-1}^{1:N_s})$   
10:    Select particles:  $z_{1:t}^{(i)} \leftarrow z_{1:t}^{(a_i)}$   
11:    Reset weights:  $\tilde{w}_t^{(i)} = 1/N_s$   
12:   end if  
13:   Normalize weights:  $W_t^{(i)} = \frac{\tilde{w}_t^{(i)}}{\sum_j \tilde{w}_t^{(j)}}$   
14:   Posterior approximation:  $\hat{\pi}_t(z_{1:t}) = \sum_{i=1}^{N_s} W_t^{(i)} \delta(z_{1:t} - z_{1:t}^{(i)})$   
15: end for
```

Comparing SIS and SISR



Proposal distributions

The locally optimal proposal distribution $q^*(z_t|z_{1:t-1})$ is the one that minimizes:

$$D_{KL}(\pi_{t-1}(z_{1:t-1})q_t(z_t|z_{1:t-1})\|\pi_t(z_{1:t})),$$

which is:

$$q^*(z_t|z_{1:t-1}) = \pi_t(z_t|z_{1:t-1}) = \frac{\tilde{\gamma}(z_{1:t})}{\tilde{\gamma}(z_{1:t-1})}.$$

Usually intractable. Some approximations are:

- Proposals based on extended and unscented Kalman filter.
- Laplace approximations.
- Nested SMC.

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Goal: sample from a *generic* target distribution

$$\pi(z) = \frac{\tilde{\gamma}(z)}{Z},$$

SMC samplers provide an alternative to MCMC, with:

- estimation of the normalizing constant Z ,
- natural adaptivity,
- easy parallelization.

Key idea: define a sequence of intermediate distributions

$$\pi_t(z_t) = \frac{\tilde{\gamma}_t(z_t)}{Z_t}, \quad t = 0, \dots, T,$$

interpolating between an easy distribution π_0 and the target
 $\pi_T = \pi$.

Path construction via forward and backward kernels:

- **Forward kernel** $M_t(z_t \mid z_{t-1})$: a Markov kernel that leaves π_t invariant. Used to propagate particles forward.
- **Backward kernel** $L_{t-1}(z_{t-1} \mid z_t)$: defines a joint path distribution

$$\pi_t(z_{1:t}) = \pi_t(z_t) \prod_{s=1}^{t-1} L_s(z_s \mid z_{s+1}),$$

satisfying $\sum_{z_{1:t-1}} \pi_t(z_{1:t}) = \pi_t(z_t)$.

Incremental importance weight:

$$\alpha_t = \frac{\pi_t(z_{1:t})}{\pi_{t-1}(z_{1:t-1}) M_t(z_t \mid z_{t-1})} \propto \frac{\tilde{\gamma}_t(z_t)}{\tilde{\gamma}_{t-1}(z_{t-1})} \frac{L_{t-1}(z_{t-1} \mid z_t)}{M_t(z_t \mid z_{t-1})}.$$

Key condition (time-reversal): choose L_{t-1} such that

$$\pi_t(z_t) L_{t-1}(z_{t-1} \mid z_t) = \pi_t(z_{t-1}) M_t(z_t \mid z_{t-1}),$$

which simplifies the weight update to

$$\alpha_t \propto \frac{\tilde{\gamma}_t(z_t)}{\tilde{\gamma}_{t-1}(z_{t-1})}$$

Likelihood Tempering (Geometric Path)

Geometric path of targets

$$\tilde{\gamma}_t(z) = \tilde{\gamma}_0(z)^{1-\lambda_t} \tilde{\gamma}(z)^{\lambda_t}, \quad 0 = \lambda_0 < \dots < \lambda_T = 1.$$

Bayesian parameter inference

$$\tilde{\gamma}_0(\theta) \propto \pi_0(\theta), \quad \tilde{\gamma}(\theta) = \pi_0(\theta) p(D | \theta),$$

$$\tilde{\gamma}_t(\theta) = \pi_0(\theta) p(D | \theta)^{\lambda_t} = \pi_0(\theta) \exp[-\lambda_t E(\theta)], \quad E(\theta) = -\log p(D, \theta)$$

Incremental importance weights

Let $\lambda_t = \lambda_{t-1} + \delta_t$. Then

$$\alpha_t(\theta) = \frac{\tilde{\gamma}_t(\theta)}{\tilde{\gamma}_{t-1}(\theta)} = \exp[-\delta_t E(\theta)].$$

Adaptive choice of δ_t

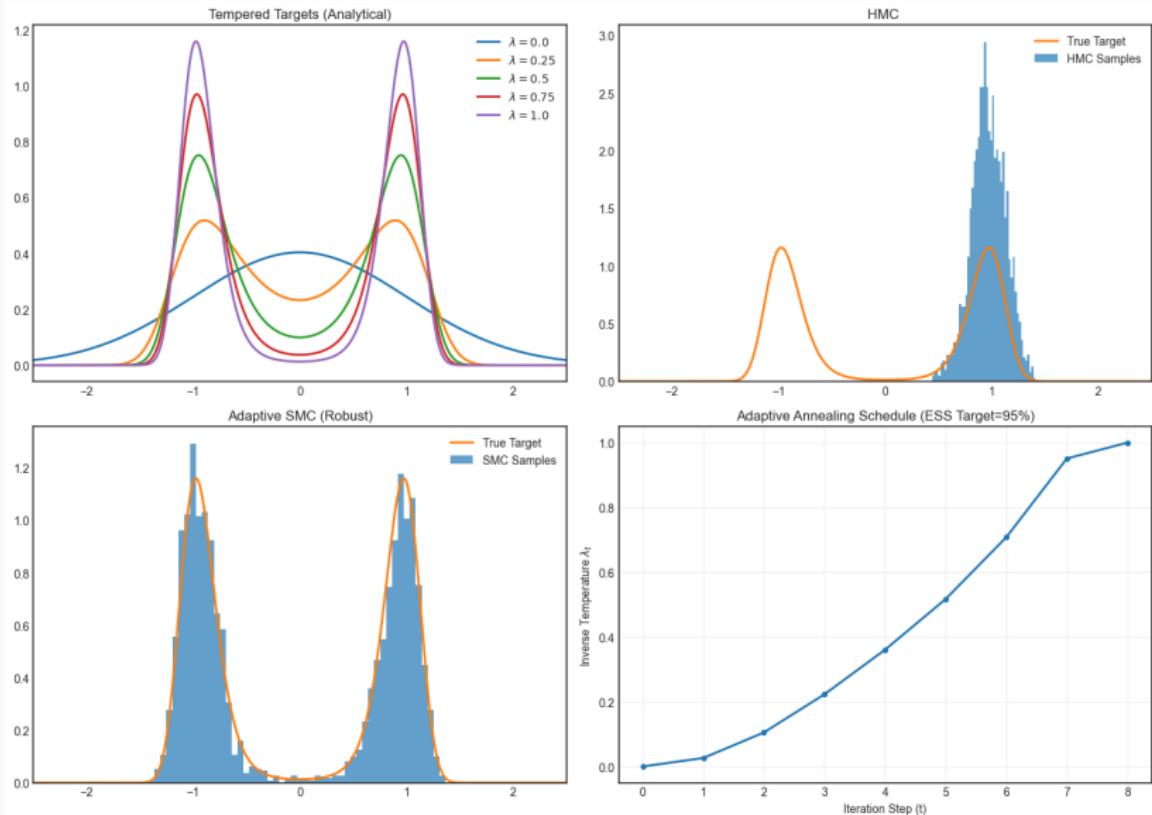
Choose δ_t such that

$$\delta_t = \operatorname{argmin}_{\delta \in [0, 1 - \lambda_{t-1}]} (\text{ESSLW}(\{-\delta E(\theta_t^n)\}) - \text{ESS}_{\min})$$

typically $\text{ESS}_{\min} \approx 0.5 N$.

- Ensures successive targets are approximately equidistant
- Prevents weight degeneracy
- If there is no such δ_t , set $\delta_t = 1 - \lambda_{t-1}$

Example



Data Tempering

Intermediate target distributions

Given iid observations $y_{1:T}$, define

$$\tilde{\gamma}_t(\theta) = p(\theta) p(y_{1:t} \mid \theta), \quad t = 1, \dots, T.$$

- Prior: $\tilde{\gamma}_0(\theta) = p(\theta)$
- Final target: $\tilde{\gamma}_T(\theta) = p(\theta \mid y_{1:T})$

Incremental importance weights Using the SMC sampler weight update,

$$\alpha_t(\theta) = \frac{\tilde{\gamma}_t(\theta)}{\tilde{\gamma}_{t-1}(\theta)} = \frac{p(\theta)p(y_{1:t} \mid \theta)}{p(\theta)p(y_{1:t-1} \mid \theta)} = p(y_t \mid y_{1:t-1}, \theta).$$

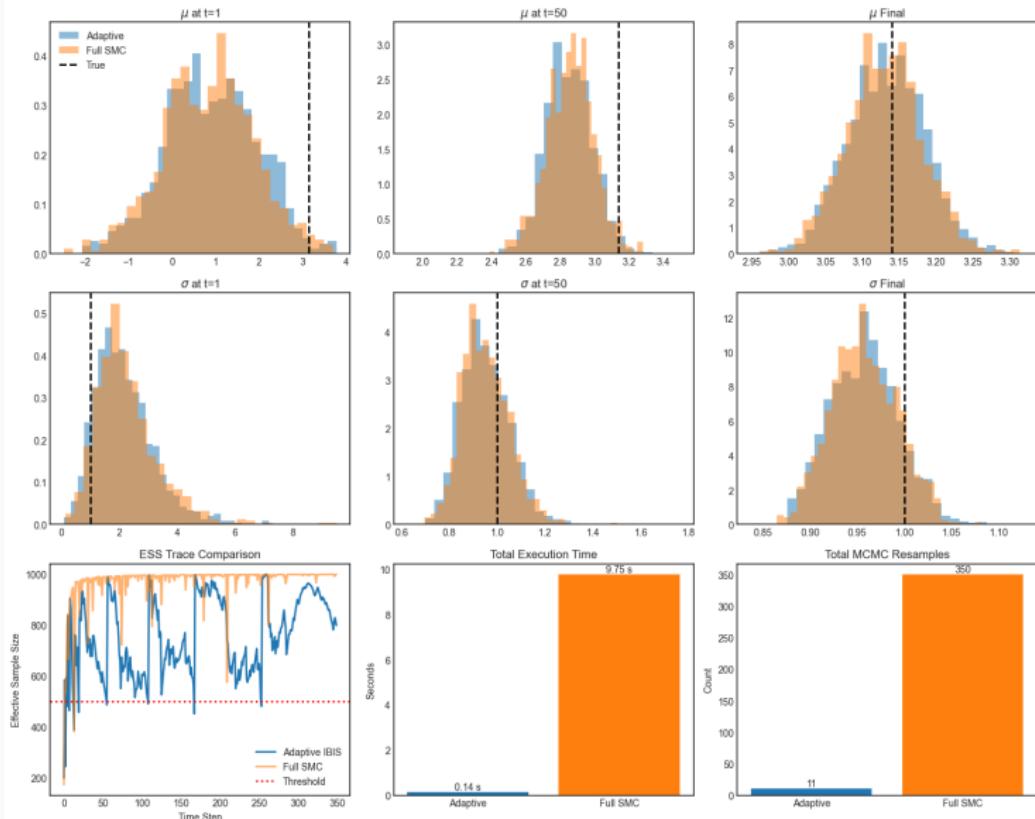
Computational considerations

- Evaluating MCMC at every step is expensive.

IBIS (Iterated Batch Importance Sampling)

- Only apply MCMC step when ESS drops below a threshold
- Otherwise, propagate particles deterministically ($\theta^{(i)} = \theta^{(i-1)}$)

Example



Sampling Rare Events:

- Goal: sample from $\pi_0(\theta)$ conditioned on a rare event $S(\theta) > \lambda^*$, where $S(\theta)$ is a score or fitness function.
- Approach: SMC with gradually increasing thresholds:

$$\pi_t(\theta) = \frac{1}{Z_t} \mathbb{I}(S(\theta) \geq \lambda_t) \pi_0(\theta), \quad \lambda_0 < \dots < \lambda_T = \lambda^*.$$

- We may use likelihood tempering with the “likelihood” at each step being:

$$G_t(\theta) = \mathbb{I}(S(\theta) \geq \lambda_t)$$

Likelihood-Free Inference (SMC-ABC):

- Consider models where the likelihood $p(y|\theta)$ is **intractable** but we can **simulate data** $y \sim p(\cdot|\theta)$.
- Approximate Bayesian Computation (ABC) samples (θ, y) such that simulated data is close to observed data:

$$d(y, y^*) < \epsilon$$

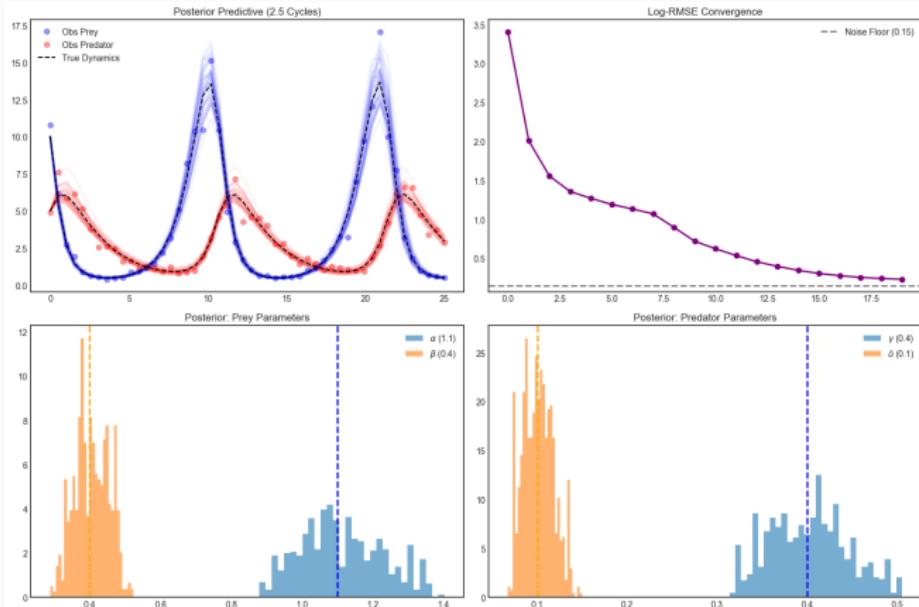
or for summary statistics $s(y)$: $d(s(y), s(y^*)) < \epsilon$.

- SMC-ABC gradually decreases ϵ over iterations:

$$\pi_t(\theta, y) = \frac{1}{Z_t} \pi_0(\theta) p(y|\theta) \mathbb{I}(d(y, y^*) < \epsilon_t), \quad \epsilon_0 > \dots > \epsilon_T$$

- This is analogous to rare-event SMC, but the “likelihood” is evaluated in **data space**.

Example



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Conclusions

- We motivated **Sequential Monte Carlo (SMC)** as a general framework for approximating sequences of complex distributions. Specifically, we
- Studied SMC for **State Space Models**, including:
 - Sequential Importance Sampling (SIS).
 - Sequential Importance Sampling with Resampling (SISR).
 - Adaptive resampling.
- Presented **SMC samplers** as a flexible alternative to MCMC:
 - likelihood tempering.
 - Data tempering.
 - likelihood free inference.

References i

- [DGA00] Arnaud Doucet, Simon Godsill, and Christophe Andrieu. “**On sequential Monte Carlo sampling methods for Bayesian filtering**”. In: *Statistics and Computing* (2000).
- [DJ09] Arnaud Doucet and Adam Johansen. “**A Tutorial on Particle Filtering and Smoothing: Fifteen Years Later**”. In: *Handbook of Nonlinear Filtering* 12 (Jan. 2009).
- [DMDJ12] Pierre Del Moral, Arnaud Doucet, and Ajay Jasra. “**An Adaptive Sequential Monte Carlo Method for Approximate Bayesian Computation**”. In: *Statistics and Computing* (2012).

Questions?

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Upcoming sessions

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