Designing "Particle Filters" for Particle MCMC

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Outline

- Background: SMC and PMCMC
- Beyond simple filters:
 - Iterative Lookahead Methods
 - Tempering Blocks in SMC
 - Hierarchical Particle Filters
- Conclusions

Discrete Time Filtering

Online inference for Hidden Markov Models:



• Given initial distribution $\mu_{\theta}(x_1)$, transition $f_{\theta}(x_{n-1}, x_n)$,

- and likelihood $g_{\theta}(x_n, y_n)$,
- use $p_{\theta}(x_n|y_{1:n})$ to characterize latent state, but,

$$p_{\theta}(x_n|y_{1:n}) = \frac{\int p_{\theta}(x_{n-1}|y_{1:n-1}) f_{\theta}(x_{n-1}, x_n) dx_{n-1} g_{\theta}(x_n, y_n)}{\int \int p_{\theta}(x_{n-1}|y_{1:n-1}) f_{\theta}(x_{n-1}, x'_n) dx_{n-1} g_{\theta}(x'_n, y_n) dx'_n}$$

and other densities of interest are typically intractable.

Particle Filtering

A Simple "Bootstrap" Particle Filter (Gordon et al. [10])

At n = 1:

• Sample $X_1^1, \ldots, X_1^N \sim \mu_{\theta}$.

For n > 1:

Sample

$$A_n^1, \dots, A_n^N \sim rac{\sum_{j=1}^N g_{ heta}(X_{n-1}^j, y_{n-1}) \delta_j(\cdot)}{\sum_{k=1}^n g_{ heta}(X_{n-1}^k, y_{n-1})}$$

- For *i* in 1 : *N* sample $X_n^i \sim f_{\theta}(X_{n-1}^{A_n^i}, \cdot)$.
- Approximate $p_{\theta}(dx_n|y_{1:n}), p_{\theta}(y_{1:n})$ with

$$\widehat{p_{\theta}}(\cdot|y_{1:n}) = \frac{\sum_{j=1}^{N} g_{\theta}(X_n^j, y_n) \delta_{X_n^j}}{\sum_{k=1}^{n} g_{\theta}(X_n^k, y_n)}, \frac{\widehat{p_{\theta}}(y_{1:n})}{\widehat{p_{\theta}}(y_{1:n-1})} = \frac{1}{n} \sum_{j=1}^{N} g_{\theta}(X_n^k, y_n)$$



















Various Improvements to Particle Filters

- Better Proposal Distributions:
 - ► Locally optimal (cf. Doucet et al. [6]) case $q(x_n|x_{n-1}, y_n) \propto f_{\theta}(x_{n-1}, x_n)g(x_n, y_n)$.
 - Incremental importance weights $G_n(x_{n-1}, x_n) = f(x_{n-1}, x_n)g(x_n, y_n)/q(x_{n-1}, x_n).$
- Auxiliary Particle Filters (Pitt and Shephard [15]) (see also Johansen and Doucet [13])
- Better Resampling Schemes (cf. Douc and Cappé [5])
- "Adaptive" Resampling (cf. Del Moral et al. [4])
- Resample-Move Schemes (MCMC; Gilks and Berzuini [8])
- Tempered Transitions (Godsill and Clapp [9])

All of these retain the online character of particle filtering.

Key Properties of Particle Filters

- ► Fundamentally online: can approximate p_θ(x_n|y_{1:n}) at iteration n at constant cost per iteration.
- Yield good approximations of the filtering distribution:

 $p_{\theta}(x_n|y_{1:n})$

at time n.

Can approximate the marginal likelihood

$$p_{\theta}(y_{1:n}) = \int p_{\theta}(x_{1:n}, y_{1:n}) dx_{1:n}$$

unbiasedly.

Only the last of these is critical in an offline setting...

Online Particle Filters for Offline Estimation (via PMCMC)

Particle Markov chain Monte Carlo (Andrieu et al. [2])

- Embed SMC within MCMC,
- justified via explicit auxiliary variable construction,
- or in some cases by a pseudomarginal (Andrieu and Roberts
 [1]) argument.
- Very widely applicable,
- but prone to poor mixing when SMC performs poorly for some θ (Owen et al. [14, Section 4.2.1]).
- Is valid for very general SMC algorithms.

Iterative Lookahead Methods¹: Motivation

Online algorithms can only perform so well:

$$p(x_{1:n}|y_{1:T}) = \int p(x_{1:T}|y_{1:T}) dx_{n+1:T} \neq p(x_{1:n}|y_{1:n})$$

We'd benefit from targetting the smoothing distributions:

$$\tilde{\pi}_n(x_{1:n}) = p(x_{1:n}|y_{1:T}) \propto p(x_{1:n}|y_{1:n})p(y_{n+1:T}|x_n)$$

in place of the filtering distributions:

$$\pi_n(x_{1:n}) = p(x_{1:n}|y_{1:n})$$

• But this is really hard: can we approximate $p(y_{n+1:T}|x_n)$?

¹Joint work with Pieralberto Guarniero and Anthony Lee

Twisting the HMM (complements (Whiteley and Lee [16]))

Given
$$(\mu, f, g)$$
 and $y_{1:T}$, introducing
 $\psi := (\psi_1, \psi_2, \dots, \psi_T), \psi_t \in C_b(X, (0, \infty))$ and
 $\tilde{\psi}_0 := \int_X \mu(x_1) \psi_1(x_1) dx_1 \quad \tilde{\psi}_t(x_t) := \int_X f(x_t, x_{t+1}) \psi_{t+1}(x_{t+1}) dx_{t+1}$
(and $\tilde{\psi}_T \equiv 1$) we obtain $(\mu_1^{\psi}, \{f_t^{\psi}\}, \{g_t^{\psi}\})$, with
 $\mu_1^{\psi}(x_1) := \frac{\mu(x_1)\psi_1(x_1)}{\tilde{\psi}_0}, \qquad f_t^{\psi}(x_{t-1}, x_t) := \frac{f(x_{t-1}, x_t) \psi_t(x_t)}{\tilde{\psi}_{t-1}(x_{t-1})}$

and the sequence of non-negative functions

$$g_1^{\psi}(x_1) := g(x_1, y_1) \frac{\tilde{\psi}_1(x_1)}{\psi_1(x_1)} \tilde{\psi}_0, \qquad g_t^{\psi}(x_t) := g(x_t, y_t) \frac{\tilde{\psi}_t(x_t)}{\psi_t(x_t)}.$$

Proposition

For any sequence of bounded, continuous and positive functions ψ , let

$$Z_{\psi} := \int_{X^{T}} \mu_{1}^{\psi}(x_{1}) g_{1}^{\psi}(x_{1}) \prod_{t=2}^{T} f_{t}^{\psi}(x_{t-1}, x_{t}) g_{t}^{\psi}(x_{t}) dx_{1:T}.$$

Then,
$$Z_{\psi} = p_{\theta}(y_{1:T})$$
 for any such ψ .

The (variance) optimal choice is:

$$\psi_t^*(x_t) := g(x_t, y_t) \mathbb{E}\left[\prod_{p=t+1}^T g(X_p, y_p) \left| \{X_t = x_t\}\right], \quad x_t \in \mathsf{X},$$

for $t \in \{1, \ldots, T-1\}$. Then, $Z_{\psi^*}^N = p(y_{1:T})$ with probability 1.

ψ -Auxiliary Particle Filters (Guarniero et al. [11])

ψ -Auxiliary Particle Filter

- 1. Sample $\xi_1^i \sim \mu^{\psi}$ independently for $i \in \{1, \dots, N\}$.
- 2. For $t = 2, \ldots, T$, sample independently

$$\xi_t^i \sim \frac{\sum_{j=1}^N g_{t-1}^{\psi}(\xi_{t-1}^j) f_t^{\psi}(\xi_{t-1}^j, \cdot)}{\sum_{j=1}^N g_{t-1}^{\psi}(\xi_{t-1}^j)}, \qquad i \in \{1, \dots, N\}.$$

Necessary features of ψ

1. It is possible to sample from f_t^{ψ} .

- 2. It is possible to evaluate g_t^{ψ} .
- 3. To be useful: $\mathbb{V}(Z_{\psi}^{N})$ must be small.

A Recursive Approximtion

Proposition

The sequence
$$\psi^*$$
 satisfies $\psi^*_T(x_T) = g(x_T, y_T)$, $x_T \in X$ and

$$\psi_t^*(x_t) = g(x_t, y_t) f(x_t, \psi_{t+1}^*), \quad x_t \in \mathsf{X}, \quad t \in \{1, \ldots, T-1\}.$$

Algorithm 1 Recursive function approximations

For
$$t = T, ..., 1$$
:
1. Set $\psi_t^i \leftarrow g\left(\xi_t^i, y_t\right) f\left(\xi_t^i, \psi_{t+1}\right)$ for $i \in \{1, ..., N\}$.
2. Choose ψ_t as a member of Ψ on the basis of $\xi_t^{1:N}$ and $\psi_t^{1:N}$.

Iterated Auxiliary Particle Filters (Guarniero et al. [11])

Algorithm 2 An iterated auxiliary particle filter (param's: N_0, k, τ)

1. Initialize: set $\psi_t^0 = \mathbf{1}$. $I \leftarrow 0$.

2. Repeat:

2.1 Run a ψ^{l} -APF with N_{l} particles; set $\hat{Z}_{l} \leftarrow Z_{\psi^{l}}^{N_{l}}$.

- 2.2 If l > k and $\operatorname{sd}(\hat{Z}_{l-k:l})/\operatorname{mean}(\hat{Z}_{l-k:l}) < \tau$, go to 3.
- 2.3 Compute ψ^{l+1} using Algorithm 1.
- 2.4 If $N_{l-k} = N_l$ and the sequence $\hat{Z}_{l-k:l}$ is not monotonically increasing, set $N_{l+1} \leftarrow 2N_l$. Otherwise, set $N_{l+1} \leftarrow N_l$.
- 2.5 Set $I \leftarrow I + 1$. Go to 2a.

3. Run a
$$\psi^{l}$$
-APF. Return $\hat{Z} := Z_{\psi}^{N_{l}}$.

An Elementary Implementation

Function Approximation

Numerically obtain:

$$(m_t^*, \Sigma_t^*, \lambda_t^*) = \arg \min_{(m, \Sigma, \lambda)} \sum_{i=1}^N (\mathcal{N}(x_t^i, m, \Sigma) - \lambda \psi_t^i)^2$$

Set:

$$\psi_t(x_t) := \mathcal{N}(x_t; m_t^*, \Sigma_t^*) + c(N, m_t^*, \Sigma_t^*).$$

Stopping Rule

• k = 3 or k = 5 in the following examples • $\tau = 0.5$

Resampling

• Multinomial when ESS < N/2.

A Linear Gaussian Model: Behaviour with Dimension

$$\mu = \mathcal{N}(\cdot; \mathbf{0}, I_d) \qquad f(x, \cdot) = \mathcal{N}(\cdot; Ax, I_d)$$

and $g(x, \cdot) = \mathcal{N}(\cdot; x, I_d) \qquad \text{where } A_{ij} = 0.42^{|i-j|+1},$

Box plots of \hat{Z}/Z for different dim(X) (1000 replicates; T = 100).



Linear Gaussian Model: Sensitivity to Parameters

Fixing d = 10: Bootstrap (N = 50,000) / iAPF ($N_0 = 1,000$)



Box plots of $\frac{Z}{Z}$ for different values of the parameter α using 1000 replicates.

Linear Gaussian Model: PMMH Empirical Autocorrelations



treated as unknown lower triangular matrix.

Stochastic Volatility

A simple stochastic volatility model is defined by:

$$\begin{split} \mu(\cdot) = & \mathcal{N}(\cdot; 0, \sigma^2/(1-\alpha)^2) \\ f(x, \cdot) = & \mathcal{N}(\cdot; \alpha x, \sigma^2) \\ \text{and } g(x, \cdot) = & \mathcal{N}(\cdot; 0, \beta^2 \exp(x)), \end{split}$$

where $\alpha \in (0,1)$, $\beta > 0$ and $\sigma^2 > 0$ are unknown.

Considered T = 945 observations y_{1:T} corresponding to the mean-corrected daily returns for the GBP/USD exchange rate from 1/10/81 to 28/6/85.

Estimated PMCMC Autocorrelation





Boostrap N = 1,000.iAPF $N_0 = 100.$ Comparable cost. 150,000 PMCMC iterations.





Bootstrap : $N = 1,000 / N = 10,000 / iAPF, N_0 = 100$



Bootstrap : $N = 1,000 / N = 10,000 / iAPF, N_0 = 100$



Bootstrap : $N = 1,000 / N = 10,000 / iAPF, N_0 = 100$

Block-Sampling and Tempering in Particle Filters

Tempered Transitions (Godsill and Clapp [9])

Introduce each likelihood term gradually, targetting:

 $\pi_{n,m}(x_{1:n}) \propto p(x_{1:n}|y_{1:n-1})p(y_n|x_n)^{\beta_m}$

between $p(x_{1:n-1}|y_{1:n-1})$ and $p(x_{1:n}|y_{1:n})$.

Can improve performance — but to a limited extent.

Block Sampling (Doucet et al. [7])

- Essentially uses $y_{n+1:n+L}$ in proposing x_{n+1} .
- Can dramatically improve performance,
- ▶ but requires good analytic approximation of p(x_{n+1:n+L}|x_n, y_{n+1:n+L}).

Block Sampling: An Idealised Approach

At time *n*, given $x_{1:n-1}$; discard $x_{n-L+1:n-1}$:

- Sample from $q(x_{n-L+1:n}|x_{n-L}, y_{n-L+1:n})$.
- Weight with

$$W(x_{1:n}) = \frac{p(x_{1:n}|y_{1:n})}{p(x_{1:n-L}|y_{1:n-1})q(x_{n-L+1:n}|x_{n-L},y_{1:n-L+1:n})}$$

Optimally,

$$q(x_{n-L+1:n}|x_{n-L}, y_{n-L+1:n}) = p(x_{n-L+1:n}|x_{n-L}, y_{n-L+1:n})$$
$$W(x_{1:n}) \propto \frac{p(x_{1:n-L}|y_{1:n})}{p(x_{1:n-L}|y_{1:n-1})} = p(y_n|x_{1:n-L}, y_{n-L+1:n-1})$$

Typically intractable; auxiliary variable approach in [7].

Block-Tempering (Johansen [12])

- We could combine blocking and tempering strategies.
- Run a simple SMC sampler (Del Moral et al. [3]) targetting:

$$\pi_{t,r}^{\theta}(x_{1:t\wedge T}) = \mu_{\theta}(x_{1})^{\beta_{(t,r)}^{1}} g_{\theta}(y_{1}|x_{1})^{\gamma_{(t,r)}^{1}} \cdot \prod_{s=2}^{T\wedge t} f_{\theta}(x_{s}|x_{s-1})^{\beta_{(t,r)}^{s}} g_{\theta}(y_{s}|x_{s})^{\gamma_{(t,r)}^{s}}, \qquad (1)$$

where $\{\beta_{(t,r)}^s\}$ and $\{\gamma_{(t,r)}^s\}$ are [0,1]-valued

- ▶ for $s \in \llbracket 1, T \rrbracket$, $r \in \llbracket 1, R \rrbracket$ and $t \in \llbracket 1, T' \rrbracket$, with T' = T + L
- for some $R, L \in \mathbb{N}$.
- Can be validly embedded within PMCMC:
 - Terminal likelihood estimate is unbiased.
 - Explicit auxiliary variable construction is possible.

Two Simple Block-Tempering Strategies

Tempering both likelihood and transition probabilities

$$\beta_{(t,r)}^{s} = \gamma_{(t,r)}^{s} = \left(1 \wedge \frac{R(t-s)+r}{RL}\right) \vee 0 \tag{2}$$

Tempering only the observation density

$$\beta_{(t,r)}^{s} = \mathbb{I}\{s \le t\} \qquad \gamma_{(t,r)}^{s} = \left(1 \land \frac{R(t-s)+r}{RL}\right) \lor 0, \qquad (3)$$

Tempering Only the Observation Density



Illustrative Example

Univariate Linear Gaussian SSM:

 $\begin{array}{ll} \text{transition} & f(x'|x) = \mathcal{N}(x';x,1) \\ \text{likelihood} & g(y|x) = \mathcal{N}(y;x,1) \end{array}$

- Artificial jump in observation sequence at time 75.
- Cartoon of model misspecification
- a key difficulty with PMCMC.
- ► Temper only likelihood.
- Use single-site Metropolis-Within Gibbs (standard normal proposal) MCMC moves.



True Filtering and Smoothing Distributions



Estimating the Normalizing Constant, \widehat{Z}



Relative Error in \widehat{Z} Against Computational Effort



Hierarchical Particle Filters²

 (Optimal) block sampler requires samples from (approximately)

$$p(x_{n-L+1:n}|x_{n-L}, y_{n-L+1:n})$$

and evaluations of

$$p(y_n|x_{n-L}, y_{n-L+1:n-1}) = \frac{p(y_{n-L+1:n}|x_{n-L})}{p(y_{n-L+1:n-1}|x_{n-L})}.$$

Particle filters can provide sample approximations of

$$p(x_{n-L+1:n}|x_{n-L}, y_{n-L+1:n})$$

and of

$$p(y_{n-L+1:n}|x_{n-L}).$$

Can we use particle filters hierarchically?

²Joint work with Arnaud Doucet...

SMC Distributions

Formally gives rise to the SMC Distribution:

$$\psi_{n,L}^{M}\left(\overline{\mathbf{a}}_{n-L+2:n}, \overline{\mathbf{x}}_{n-L+1:n}, \overline{k}; \mathbf{x}_{n-L}\right) = \left[\prod_{i=1}^{M} q\left(\overline{\mathbf{x}}_{n-L+1}^{i} \middle| \overline{\mathbf{x}}_{n-L}\right)\right] \prod_{p=n-L+2}^{n} \left[r(\overline{\mathbf{a}}_{p} \middle| \overline{\mathbf{w}}_{p-1}) \prod_{i=1}^{M} q\left(\overline{\mathbf{x}}_{p}^{i} \middle| \overline{\mathbf{x}}_{p-1}^{\bar{a}_{p}^{i}}\right)\right] r(\overline{k} \middle| \overline{\mathbf{w}}_{n})$$

and the conditional SMC Distribution:

$$= \frac{\widetilde{\psi}_{n,L}^{M}\left(\widetilde{\mathbf{a}}_{n-L+2:n}^{\ominus k}, \widetilde{\mathbf{x}}_{n-L+1:n}^{\ominus k}; x_{n-L} \middle| \middle| \widetilde{b}_{n-L+1:n-1}^{k}, \widetilde{x}_{n-L+1:n}^{k} \right)}{q\left(\widetilde{x}_{n-L+1}^{\widetilde{b}_{n,n-L+1}^{k}} | x_{n-L} \right) \left[\prod_{p=n-L+2}^{n} r\left(\widetilde{b}_{n,p}^{k} | \widetilde{\mathbf{w}}_{p-1} \right) q\left(\widetilde{x}_{p}^{\widetilde{b}_{n,p}^{k}} | \widetilde{x}_{p-1}^{\widetilde{b}_{n,p-1}^{n}} \right) \right] r(k|\widetilde{\mathbf{w}}_{n})}$$

Local Particle Filtering: Current Trajectories



Local Particle Filtering: PF Proposal

PF Step



Local Particle Filtering: CPF Auxiliary Proposal

CPF Step



Local SMC: Version 1

- Not just a Random Weight Particle Filter.
- Propose from:

$$\mathcal{U}_{1:M}^{\otimes n-1}(b_{1:n-2},k)p(x_{1:n-1}|y_{1:n-1})\psi_{n,L}^{M}(\overline{\mathbf{a}}_{n-L+2:n},\overline{\mathbf{x}}_{n-L+1:n},\overline{k};x_{n-L})$$

$$\widetilde{\psi}_{n-1,L-1}^{M}(\widetilde{\mathbf{a}}_{n-L+2:n-1}^{\ominus k},\widetilde{\mathbf{x}}_{n-L+1:n-1}^{\ominus k};x_{n-L}||b_{n-L+2:n-1},x_{n-L+1:n-1})$$

► Target:

$$\begin{aligned} &\mathcal{U}_{1:M}^{\otimes n}(b_{1:n-L}, \bar{b}_{n,n-L+1:n-1}^{\bar{k}}, \bar{k}) p(x_{1:n-L}, \bar{x}_{n-L+1:n}^{\bar{b}_{n,n-L+1:n}^{\bar{k}}} | y_{1:n}) \\ & \widetilde{\psi}_{n,L}^{M} \left(\overline{\mathbf{a}}_{n-L+2:n}^{\ominus \bar{k}}, \overline{\mathbf{x}}_{n-L+1:n}^{\ominus \bar{k}}; x_{n-L} \middle\| \overline{b}_{n,n-L+1:n}^{\bar{k}}, \overline{\mathbf{x}}_{n-L+1:n}^{\bar{b}_{n,n-L+1:n}^{\bar{k}}} \right) \\ & \psi_{n-1,L-1}^{M} \left(\widetilde{\mathbf{a}}_{n-L+2:n-1}, \widetilde{\mathbf{x}}_{n-L+1:n-1}, k; x_{n-L} \right). \end{aligned}$$

• Weight: $\overline{Z}_{n-L+1:n}/\widetilde{Z}_{n-L+1:n-1}$.

Local SMC: Version 2

Problems with this PF+CPF scheme:

- Expensive to run 2 filters per proposal...
- ▶ and large *M* is required...
- can't we do better?

Using a non-standard CPF/PF proposal is preferable:

- Running a CPF from time n L + 1 to n,
- and extending it's paths with a PF step to n + 1,
- invoking a careful auxiliary variable construction,
- we reduce computational cost *and* variance.
- Leads to importance weights:

$$\propto rac{\hat{p}(y_{n-L+1:n}|x_{n-L}^{b_{n-1,n-L}^k})}{\hat{p}(y_{n-L+1:n-1}|x_{n-L}^{b_{n-1,n-L}^k})}$$

Hierarchical Particle Filtering: Current Trajectories



Hierarchical Particle Filtering: CPF Proposal Component



Hierarchical Particle Filtering: PF Proposal Component



A Toy Model: Linear Gaussian HMM

Linear, Gaussian state transition:

$$f(x_t|x_{t-1}) = \mathcal{N}(x_t; x_{t-1}, 1)$$

and likelihood

$$g(y_t|x_t) = \mathcal{N}(y_t; x_t, 1)$$

► Analytically: Kalman filter/smoother/etc.

- Simple bootstrap HPF:
 - Local proposal:

$$q(x_t|x_{t-1}, y_t) = f(x_t|x_{t-1})$$

Weighting:

$$W(x_{t-1},x_t) \propto g(y_t|x_t)$$





Conclusions

- To fully realise the potential of PMCMC we should exploit its flexibility.
- Even very simple variants on the standard particle filter can significantly improve performance.
- Three particular possibilities were discussed here:
 - iAPF
 - The iAPF can improve performance substantially in some settings.
 - Extending the extent of its applicability is ongoing work.
 - In principle any function approximation scheme can be employed: provided that f^ψ_t can be sampled from and g^ψ_t evaluated.
 - Block-Tempering
 - Can significantly improve performance with misspecified models.
 - ▶ Requires MCMC kernels and introduces 2 tuning parameters
 - Hierarchical Particle Filters
 - Dramatically reduce the need for resampling.
 - Computationally rather costly.

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