Bagging and blocking: Inference via particle filters for interacting dynamic systems

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Background

The curse of dimensionality. Particle filter (PF) methods are effective for inference on low-dimensional nonlinear partially observed stochastic dynamic systems. They scale exponentially badly.

Bagged filters. We study three algorithms that combine many non-interacting Monte Carlo processes.

- Unadapted bagged filter (UBF)
- adapted bagged filter (ABF)
- adapted bagged filter with intermediate resampling (ABF-IR)

Metapopulation dynamics. Bagged filters have theoretical and empirical scaling properties suited to collections of weakly coupled populations.

So, what about COVID-19?

- Researchers have developed many models for disease spread.
- Most of these build on the SIR (Susceptible-Infected-Removed) model that divides a population into three homogeneous classes.
- Extensions can include a latent period after infection, age structure, spatial structure, temperature, control policies.
- We may observe some fraction of cases.
- These models are partially observed stochastic dynamic systems.
- Understanding of COVID-19 epidemiology draws on analysis of previous epidemics combined with assessment of limited available data.
- Methods that fit a general class of mechanistic models assist with formulating and testing scientific hypotheses.

What is a SpatPOMP?

POMP models are partially observed Markov processes, also known as state space models or hidden Markov models

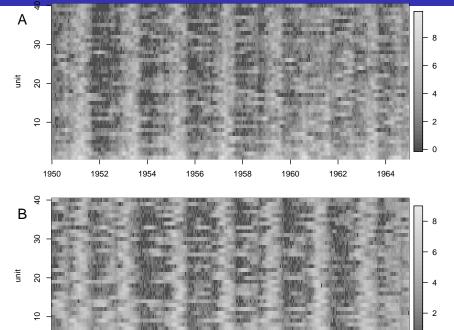
SpatPOMP models are POMP models with a unit structure

Latent Markov process: $X_{u,n} = X_u(t_n)$, $u \in 1:U$, $n \in 1:N$

Observation process: $Y_{u,n}$ depends only on $X_{u,n}$

The units could be a metapopulation, say cities in an epidemic model

U=40 units for a coupled measles SEIR model



Bagged filter inputs, outputs and implicit loops.

input:

simulator for $f_{\boldsymbol{X}_0}(\boldsymbol{x}_0)$ and $f_{\boldsymbol{X}_n|\boldsymbol{X}_{n-1}}(\boldsymbol{x}_n\,|\,\boldsymbol{x}_{n-1})$ evaluator for $f_{Y_{u,n}|X_{u,n}}(y_{u,n} \mid x_{u,n})$

number of islands. \mathcal{I} neighborhood structure, $B_{u,n}$

data, $\boldsymbol{y}_{1\cdot N}^*$ ABF and ABF-IR: particles per island, J

ABF-IR: number of intermediate timesteps, S

ABF-IR: measurement variance parameterizations, $\overset{\leftarrow}{\mathbf{v}}_{u.n}$ and $\overset{\rightarrow}{\mathbf{v}}_{u.n}$

output: Log likelihood estimate, $\ell^{\text{MC}} = \sum_{n=1}^{N} \sum_{n=1}^{U} \ell_{nn}^{\text{MC}}$ implicit loops:

ABF-IR: approximate process and observation mean functions, μ and h_{un}

u in 1:U, n in 1:N, i in 1: \mathcal{I} , j in 1:J

BIF. Unadapted bagged filter.

Simulate
$$\mathbf{A}_{0:N,i} \sim f \mathbf{X}_{0:N}(\mathbf{x}_{0:N})$$

Measurement weights, $w_{u,n,i}^M = f_{Y_{u,n}|X_{u,n}}(y_{u,n}^* \mid X_{u,n,i})$

Simulate
$$oldsymbol{X}_{0:N,i} \sim f_{oldsymbol{X}_{0:N}}(oldsymbol{x}_{0:N})$$

Prediction weights, $w_{u,n,i}^P = \prod_{(\tilde{u},\tilde{n}) \in B_{u,n}} w_{\tilde{u},\tilde{n},i}^M$

 $\ell_{u,n}^{\,\mathrm{MC}} = \log\left(\textstyle\sum_{i=1}^{\mathcal{I}} w_{u,n,i}^{M} w_{u,n,i}^{P}\right) - \log\left(\textstyle\sum_{i=1}^{\mathcal{I}} w_{u,n,i}^{P}\right)$

The basic island filter is not as naive as it may first appear

- ullet UBF seems naive. Particle filter (PF) method are well known to scale better with N than unconditional simulations.
- ullet UBF scales well with U for weakly coupled systems.
- \bullet With modern computers, large numbers of simulations are feasible even when U and N are not small.
- Initially we studied UBF as a theoretical toy. Then we found it is competitive in practice on some models of interest.

Adapted simulation: An easier problem than filtering

- We aim to make each island track the data in a weak sense that does not involve a solution to the full filtering problem.
- ullet The adapted simulation problem is to draw from $f_{m{X}_n|m{Y}_n,m{X}_{n-1}}ig(m{x}_n\,|\,m{y^*}_n,m{x}_{n-1}ig).$
- The adapted bagged filter (ABF) algorithm uses importance sampling to carry out adapted simulation on each island.
- ABF calculates the likelihood using the proper weight restricted to a neighborhood.

ABF. Adapted bagged filter.

Initialize adapted simulation: $m{X}_{0.i}^{
m A} \sim f_{m{X}_0}(m{x}_0)$

For
$$n$$
 in $1:N$

Proposals: $X_{n,i,i}^{P} \sim f_{X_{n-1}}(x_n | X_{n-1,i}^{A})$

Measurement weights: $w_{u,n,i,j}^M = f_{Y_{u,n}|X_{u,n}}(y_{u,n}^* \mid X_{u,n,i,j}^P)$

Adapted resampling weights: $w_{n,i,j}^{\mathrm{A}} = \prod_{u=1}^{U} w_{u,n,i,j}^{M}$

Resampling:
$$\mathbb{P}\big[r(i)=a\big]=w_{n,i,a}^{\mathrm{A}}\Big(\sum_{k=1}^{J}w_{n,i,k}^{\mathrm{A}}\Big)^{-1}$$

Resampling:
$$\mathbb{P}[r(i) = a] = w_{n,i,a}^{A} \left(\sum_{k=1}^{J} w_{n,i,k}^{A}\right)^{-1}$$

$$X_{n,i}^{\mathbf{A}} = X_{n,i,r(i)}^{\mathbf{P}}$$

$$w_{u,n,i,j}^{\mathbf{P}} = \prod_{\tilde{n}=1}^{n-1} \left[\frac{1}{J} \sum_{k=1}^{J} \prod_{(\tilde{u},\tilde{n}) \in B_{u,n}^{[\tilde{n}]}} w_{\tilde{u},\tilde{n},i,k}^{M} \right] \prod_{(\tilde{u},n) \in B_{u,n}^{[n]}} w_{\tilde{u},n,i,j}^{M}$$

End for

$$\ell_{u,n}^{\,\mathrm{MC}} = \log \left(\frac{\sum_{i=1}^{\mathcal{I}} \sum_{j=1}^{J} w_{u,n,i,j}^{M} w_{u,n,i,j}^{P}}{\sum_{i=1}^{\mathcal{I}} \sum_{j=1}^{J} w_{u,n,i,j}^{P}} \right)$$

Intermediate resampling

- ullet Intermediate resampling splits the time interval between observations into S subintervals.
- Reweighting and/or sampling at each subinterval uses a revised estimate
 of the anticipated measurement density at the end of the interval called a
 guide function.
- This is applicable to continuous time models.
- Intermediate resampling has useful theoretical and empirical properties (Del Moral and Murray, 2015; Park and Ionides, 2019).
- Intermediate resampling for adapted simulation within ABF gives the ABF-IR algorithm.
- Intermediate resampling within PF gives the guided intermediate resampling filter (GIRF) of Park and Ionides (2019), a generalization of the auxiliary particle filter of Pitt and Shepard (1999).

ABF-IR. ABF with intermediate resampling.

Initialize adapted simulation: $m{X}_{0.i}^{
m A} \sim f_{m{X}_0}(m{x}_0)$

For n in 1:N

Intermediate proposals: $X_{n,s,i,j}^{\text{IP}} \sim f_{X_{n,s}|X_{n,s-1}} \left(\cdot | X_{n,s-1,i,j}^{\text{IR}} \right)$ $\mu_{n,s,i,i}^{IP} = \mu(X_{n,s,i,i}^{IP}, t_{n,s}, t_n)$

 $\theta_{u,n,s,i,j} = \stackrel{\leftarrow}{\nabla}_u \left(V_{u,n,s,i,j}^{\text{meas}} + V_{u,n,s,i,j}^{\text{proc}}, \mu_{u,n,s,i,j}^{\text{IP}} \right)$

 $\ell_{u,n}^{\text{MC}} = \log \left(\frac{\sum_{i=1}^{L} \sum_{j=1}^{J} w_{u,n,i,j}^{M} w_{u,n,i,j}^{r}}{\sum_{i=1}^{L} \sum_{j=1}^{J} w_{u,n,i,j}^{P}} \right)$

End For

End for

Set $X_{n,i}^{A} = X_{n,S,i,1}^{IR}$

 $g_{n,s,i,j} = \prod_{u=1}^{U} f_{Y_{u,n}|X_{u,n}}(y_{u,n}^* \mid \mu_{u,n,s,i,j}^{\text{IP}}; \theta_{u,n,s,i,j})$

Guide weights: $w_{n,s,i,j}^G = g_{n,s,i,j}/g_{n,s-1,i,j}^R$

 $V_{u,n,s,i,j}^{\text{meas}} = \overrightarrow{v}_{u}(\theta, \mu_{u,n,s,i,j}^{\text{IP}}) , \qquad V_{u,n,s,i}^{\text{proc}} = V_{u,n,i}\left(t_{n} - t_{n,s}\right) / \left(t_{n} - t_{n,0}\right)$

Resampling: $\mathbb{P}[r(i,j)=a] = w_{n,s,i,a}^G \left(\sum_{k=1}^J w_{n,s,i,k}^G\right)^{-1}$ $X_{n,s,i,j}^{\text{IR}} = X_{n,s,i,r(i,j)}^{\text{IP}}$ and $g_{n,s,i,j}^{\text{R}} = g_{n,s,i,r(i,j)}$

Measurement weights: $w_{u,n,i,j}^M = f_{Y_{u,n}|X_{u,n}}(y_{u,n}^*|X_{u,n,i,j}^G)$ $w_{u,n,i,j}^{\mathrm{P}} = \prod_{\tilde{n}=1}^{n-1} \Big[\frac{1}{J} \sum_{a=1}^{J} \prod_{\substack{(\tilde{u},\tilde{n}) \in B_{i}^{[n]} \\ \tilde{u},\tilde{n}} \in B_{i}^{[n]}} w_{\tilde{u},\tilde{n},i,a}^{M} \Big] \prod_{\substack{(\tilde{u},n) \in B_{u,n}^{[n]} \\ \tilde{u},\tilde{n}}} w_{\tilde{u},n,i,j}^{M}$

Guide variance: $V_{u,n,i} = \text{Var}\{h_{u,n}(X_{u,n,i,j}^G), j \text{ in } 1:J\}$ $g_{n,0,i,j}^{\mathrm{R}} = 1$ and $\boldsymbol{X}_{n,0,i,j}^{\mathrm{IR}} = \boldsymbol{X}_{n-1,i}^{\mathrm{A}}$

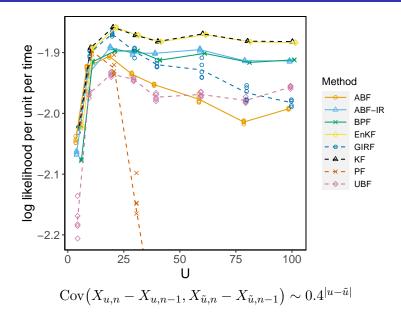
For s in 1:S

Guide simulations: $X_{n,i,j}^G \sim f_{X_n|X_{n-1}}(x_n | X_{n-1,i}^A)$

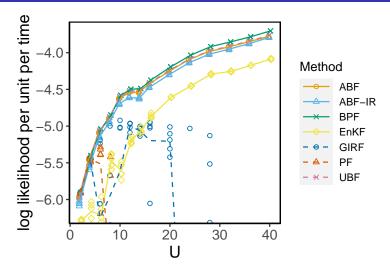
Software for SpatPOMP models

- We use the asif, asifir and girf implementations in the R package spatPomp (Asfaw et al., 2019).
- spatPomp offers a class 'spatPomp' that extends the 'pomp' class for POMP models in the R package pomp (King et al., 2016).
- All methods available in pomp can formally be applied to 'spatPomp' objects, though they may not be practically effective for spatiotemporal POMPs.

Filtering U-dimensional correlated Brownian motion

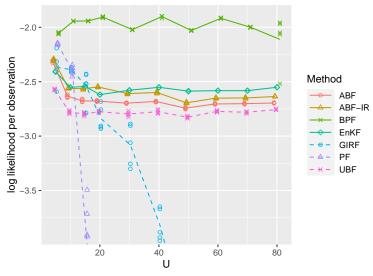


Filtering U units of a coupled measles SEIR model



Simulated data using a gravity model with geography, demography and transmssion parameters corresponding to UK pre-vaccination measles.

Filtering U units of Lorenz 96 toy atmospheric model

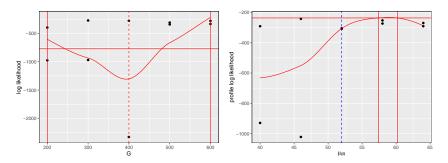


$$dX_u(t) = \{X_{u-1}(t)(X_{u+1}(t) - X_{u-2}(t)) - X_u(t) + F\}dt + \sigma dB_u(t)$$

From filtering to parameter inference

- Log likelihood evaluation in principle enables likelihood-based or Bayesian inference.
- Iterated filtering maximizes the likelihood for PF or GIRF (Ionides et al., 2015).
- Particle Markov chain Monte Carlo can be applied with any likelihood estimate (Andrieu et al., 2010). It is numerically intractable when Monte Carlo estimates are costly and noisy.
- Extending iterated filtering to island filters is future work.

Measles likelihood slices for G and μ_{IR} via ABF



- \bullet Simulating 15 year of data from U=40 cities for the measles model.
- ullet The gravitational coupling constant G is fairly weakly identified: a week of computing on a 30 core machine gives Monte Carlo error on the same scale as the statistical uncertainty.
- ullet The recovery rate μ_{IR} is well identified.

Theorem

Let ℓ^{MC} denote the Monte Carlo likelihood approximation constructed by UBF, ABF or ABF-IR. Consider a limit with a growing number of islands, $\mathcal{I} \to \infty$. Suppose regularity assumptions listed in the arXiv preprint.

There are quantities $\epsilon(U,N)=O(1)$ and $V(U,N)=O(U^2N^2)$ such that

$$\mathcal{I}^{1/2} ig[\ell^{\,\scriptscriptstyle\mathsf{MC}} - \ell - \epsilon U Nig] \xrightarrow[\mathcal{T} \to \infty]{d} \mathcal{N} ig[0,Vig],$$

where $\frac{d}{\mathcal{I} \to \infty}$ denotes convergence in distribution and $\mathcal{N}[\mu, \Sigma]$ is the normal distribution with mean μ and variance Σ . If an additional spatiotemporal mixing assumption holds, we obtain an improved variance bound

$$V(U,N) = O(UN)$$

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