Asymptotic Genealogies of Sequential Monte Carlo Algorithms

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State space models

Hidden process $X_0, \ldots, X_T \in \mathcal{X}$
Observable process $Y_0, \ldots, Y_T \in \mathcal{Y}$

$$\begin{tikzcd}
 & Y_{t-1} & Y_t & \\
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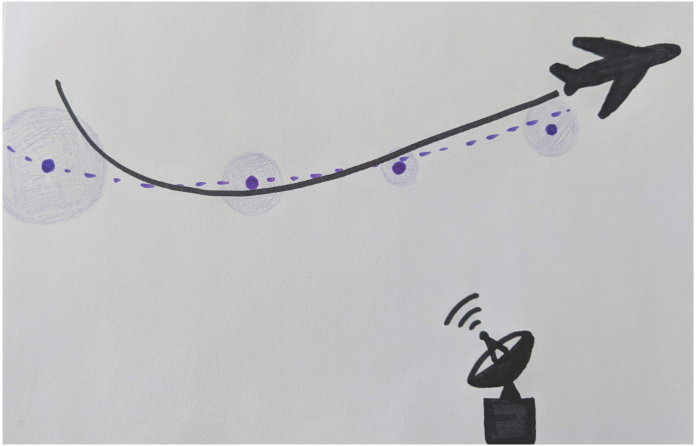
Target tracking



use noisy radar data to infer position/trajectory of aircraft:

- f models how aircraft moves
- g models uncertainty in radar measurements

Inference problems

Filtering: where is it now? $p(x_t|y_{0:t})$

Prediction: where will it go next? $p(x_{t+1}|y_{0:t})$

Smoothing: where has it been? $p(x_{0:t}|y_{0:t})$

Smoothing is "harder" than filtering/prediction [1].

Deterministic solutions

Kalman filter [2]

Under a linear Gaussian model:

$$\begin{aligned} X_0 &\sim \mathcal{N}(0, \Sigma_0) \\ X_{t+1} \mid (X_t = x_t) &\sim \mathcal{N}(Ax_t, \Sigma_x) \\ Y_t \mid (X_t = x_t) &\sim \mathcal{N}(Bx_t, \Sigma_y) \end{aligned}$$

we can recursively compute filtering distributions. Then a backward pass of RTS smoother [3] provides smoothing distributions.

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Unscented Kalman filter [5]

For highly non-linear Gaussian models, replace the prediction step of Kalman filter by propagating a representative set of points through f.

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Sequential Monte Carlo (SMC) provides general-purpose (stochastic) methods that do not require a tractable model.

Only requires sampling from $f(\cdot|x)$, and pointwise evaluation of $g(y|x)$ up to a normalising constant for each y.

Sequential Monte Carlo

Prior: $p(x_{0:t}) = \mu(x_0) \prod_{i=1}^{t} f(x_i | x_{i-1})$

Likelihood: $p(y_{0:t} | x_{0:t}) = \prod_{i=0}^{t} g(y_i | x_i)$

Posterior: $p(x_{0:t} | y_{0:t}) \propto \mu(x_0) g(y_0 | x_0) \prod_{i=1}^{t} f(x_i | x_{i-1}) g(y_i | x_i)$

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- Represent posterior distribution at time t with N particles.
- Posterior factorises sequentially, avoiding increase of dimension with T.

Sequential Monte Carlo

Algorithm

After initialisation, iterate these steps:

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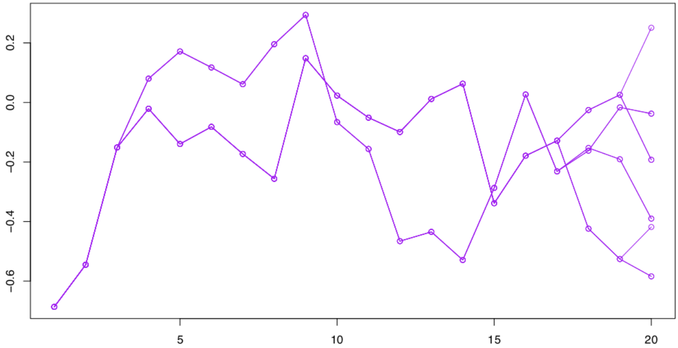
Approximate posterior distribution $p(dx_{0:t}|y_{0:t})$ by the empirical measure of the particles:

$$\hat{p}(dx_{0:t}|y_{0:t}) = \frac{1}{N}\sum_{i=1}^{N}\delta_{X_{0:t}^{(i)}}(dx_{0:t})$$

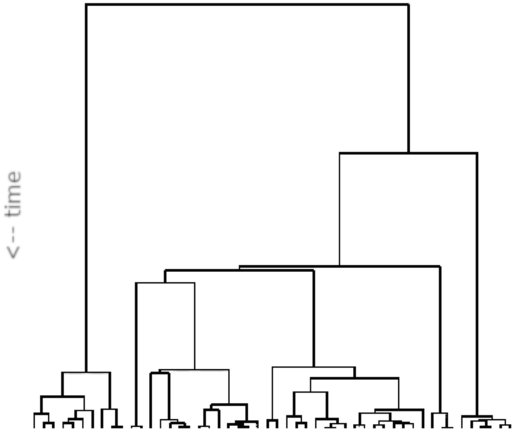
Ancestral degeneracy

For smoothing we need a sample of trajectories.

Resampling means that trajectories of time T particles coalesce backwards in time.



Kingman's coalescent



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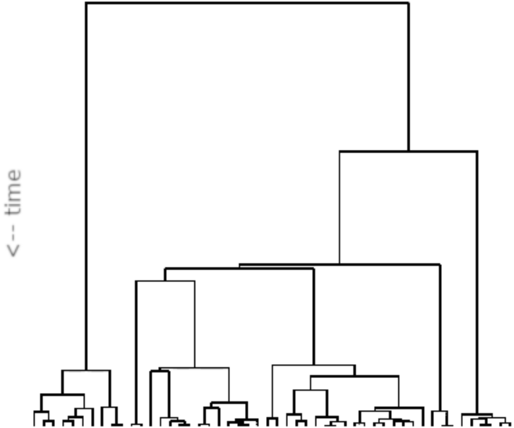

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This is the limiting coalescent process in many population models as $N \to \infty$ [7, 8].

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- Analysing the coalescent can help us to understand the performance of various SMC algorithms.
- The limiting coalescent of an SMC algorithm may depend on the resampling mechanism.
- For multinomial resampling, the limiting coalescent is a scaled Kingman coalescent [9].
- What about other (more used) resampling schemes?

Resampling

Requirements:

- The total number of particles N remains fixed.
- The particles after resampling are equally weighted.
- The resampling scheme is unbiased; that is, the expected number of offspring of each particle i is equal to $Nw_t^{(i)}$.

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- Residual resampling yields lower Monte Carlo variance than multinomial resampling [11].
- Residual resampling is widely used by practitioners.
- Analysing the coalescent for residual resampling is a work in progress.

Particle Gibbs [12]

Hidden Markov model where transition depends on a hyperparameter θ:

$$
\begin{aligned}
&\theta \sim \nu(\cdot) \\
&X_0 \sim \mu(\cdot) \\
&X_{t+1} \mid (X_t = x_t) \sim f_\theta(\cdot|x_t) \qquad t = 0, \ldots, T-1 \\
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Gibbs sampler: alternately sample from $p(\theta|x_{0:t}, y_{0:t})$ and $p(x_{0:t}|\theta, y_{0:t})$.

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- SMC is an appropriate method for sampling from $p(x_{0:t}|\theta, y_{0:t})$
- To target the correct posterior distribution, need to use *conditional SMC*.

Conditional SMC

- One “immortal” trajectory is conditioned to survive all of the resampling steps.
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- But we have this result:

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- Intuition: as $N \to \infty$, there is zero probability that an arbitrary sample of fixed size n contains the immortal particle.

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- Proved: conditional SMC (with multinomial resampling) $\Rightarrow$ Kingman coalescent.
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- In progress: analysis of residual resampling (and other resampling schemes).

References I

[1] Neil J Gordon, David J Salmond, and Adrian FM Smith. Novel approach to nonlinear/non-Gaussian Bayesian state estimation. In *IEE Proceedings F (Radar and Signal Processing)*, volume 140, pages 107–113. IET, 1993.

[2] Rudolph Emil Kalman. A new approach to linear filtering and prediction problems. *Journal of Basic Engineering*, 82(1):35–45, 1960.

[3] Herbert E Rauch, CT Striebel, and F Tung. Maximum likelihood estimates of linear dynamic systems. *AIAA Journal*, 3(8):1445–1450, 1965.

[4] Andrew H Jazwinski. *Stochastic Processes and Filtering Theory*. Courier Corporation, 2007.

[5] Eric A Wan and Rudolph Van Der Merwe. The unscented Kalman filter for nonlinear estimation. In *Proceedings of the IEEE 2000 Adaptive Systems for Signal Processing, Communications, and Control Symposium*, pages 153–158. IEEE, 2000.

[6] Paolo Vidoni. Exponential family state space models based on a conjugate latent process. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 61(1):213–221, 1999.

References II

[7] John Kingman. The coalescent. *Stochastic Processes and Their Applications*, 13(3):235–248, 1982.

[8] Martin Möhle. Robustness results for the coalescent. *Journal of Applied Probability*, 35(2):438–447, 1998.

[9] Jere Koskela, Paul A Jenkins, Adam M Johansen, and Dario Spanò. Asymptotic genealogies of interacting particle systems with an application to sequential Monte Carlo. *arXiv preprint arXiv:1804.01811*, 2018.

[10] Jun S Liu and Rong Chen. Sequential Monte Carlo methods for dynamic systems. *Journal of the American Statistical Association*, 93(443):1032–1044, 1998.

[11] Randal Douc, Olivier Cappé, and Eric Moulines. Comparison of resampling schemes for particle filtering. In *Image and Signal Processing and Analysis, 2005. ISPA 2005. Proceedings of the 4th International Symposium on*, pages 64–69. IEEE, 2005.

[12] Christophe Andrieu, Arnaud Doucet, and Roman Holenstein. Particle Markov chain Monte Carlo methods. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 72(3):269–342, 2010.