Particle Filtering for Data-Driven Simulation and Optimization

John R. Birge
The University of Chicago Booth
School of Business

Includes joint work with Nicholas Polson.
Themes

• Particle filters can provide an efficient way to analyze and *to simulate* complex systems
• Sequential Monte Carlo methods provide an approach to obtain samples from complicated distributions *including optima*
• Combining these approaches leads to new methods that can defeat (in some cases) the curse of dimensionality
Outline

• Basic problem
• Particle filtering 001
• Sequential methods for simulation
• Optimizing by simulating (an old idea in a new light)
• Additional applications
• Extensions
Start of Particle Methods

• Origin: estimating values (distributions) in a hidden Markov model
• Example: We begin with inventory $x_0$ (which may be uncertain)
• We make observations $y_1, \ldots, y_T$ based on reported sales and new inputs
• What is the distribution of actual inventory $x_t$ at any time $t$?
Special Case: LQG

- Linear, quadratic Gaussian (LQG) Model
- Implications: All of the distributions are normal
- Simple updating formulas from Kalman filter:
  \[
  y_t = H x_t + v_t; \quad x_t = F x_{t-1} + u_t; \quad v \sim N(0, Q); \quad u \sim N(0, R)
  \]

  Iterations:
  \[
  w_t = y_t - H x_t'; \quad S = H P' H^T + R;
  \]
  \[
  K = P' H S^{-1}; \quad x_{t'} = x_t' + K w_t
  \]
  \[
  P'' = (I - KH) P'; \quad x_t' = F x_{t-1}'; \quad P' = F P'' F^T + Q
  \]
Kalman Prediction

Inventory over 10 periods:
- Actual (*)
- Observed (+)

Kalman estimate:
\[ x_t \sim N(x''_t, P''_t) \]

Here:
\[ x_{10} \sim N(13.8, 0.62) \]
Bayesian Interpretation

• Suppose a distribution on $x_0$: $f(x_0)$
• Assume some transition: $p(x_t|x_{t-1})$
• Observations: $q(y_t|x_t)$
• Goal: find $P(x_t|y_1,\ldots,y_t (\ldots y_T))$
• Idea: Use Bayes Rule to find the conditional probability:

$$P(x_t|y^t) = P(x_t,y^t)/P(y^t) \propto \Pi_s q(y_s|x_s)p(x_s|x_{s-1})f(x_0)$$
General Processes

• If the observation and transition functions, $q$ and $p$ are quite general, then

$$P(x_t \mid y_t)$$ may not be available analytically.

(E.g., no sales if stocked out, maximum limit, bulky demand)

• Alternatives:
  – Markov chain Monte Carlo (MCMC)
  – Particle methods
Particle Methods

- Idea: Keep a limited number \( (N) \) of particles in each period
- Propagate forward to obtain new points
- Re-sample (re-weight) backwards to get consistent weights
- Re-balance if weights are low

Method Structure

Propagate:
- $w_t^1, x_t^1$
- $w_t^2, x_t^2$
- ...
- $w_t^N, x_t^N$

Re-sample:
- $x_{t+1}^1$
- $x_{t+1}^2$
- $y_{t+1}$
- ...
- $x_{t+1}^N$
- $w_t^1$
- $w_t^2$
- ...
- $w_t^N$
Sequential Importance Resampling (SIR) Method
Cum. Results

- $N=50$
- Compare to Kalman Cumulative
Particle Frequency

- $N=50$
- Particle (+)
- Kalman (*)
Other Uses of Particles

- Particle filtering: finding $x_t$ from $y_t=(y_1,\ldots,y_t)$
- Particle smoothing: finding $x_t$ from $y_T=(y_1,\ldots,y_T)$
- Particle learning: (Polson et al.) Find parameters $\theta_t$ at the same time to explain the model.
- Simulation
Particle Filter in Simulation

• Interpretation:
  – Usage is a form of sequential importance sampling
  – Use $q(x_t|x_{t-1})$ to draw
  – Many more samples to draw in area of interest (e.g., tail of distribution)

• Example: Find the probability of a 50% loss over 5 periods for a portfolio with 1-period mean=5%, st. dev.=20%
Loss Probabilities

- Compare crude MC to SIS
- Use $q$ to match target
- Reduces std. deviation in half
Earlier in Optimization


• Pincus (1968): 2 ideas
  – Can use expectation to optimize
  – Can find the expectation with Markov chain
Using Simulation for Optimization

• Pincus results:
• Model: $\min F(x)$
• Create a distribution $P_\lambda(x) = \exp(-\lambda F(x))$
• Then:

$$\lim_{\lambda \to \infty} E_{P_\lambda}(x) = x^*$$
Markov Chain Simulation

- From $x_t$ to $x_{t+1}$
- Sample over
  \[ \exp(-\lambda F(\mu x_t + (1-\mu) x_{t+1})) \]
- Choose directions to obtain mixing in the region
Example

• Rosenbrock function:
Test for Rosenbrock

• $T=5000$ iterations
• $N=500$ replications
• Re-sample when:
  Effective Sample Size $<250$
• $\kappa=2, 10, 100$
Rosenbrock Graphs

$\kappa = 2$  10  100
Other Examples: Rastigrin

![Rastigrin: kappa=0.1](image1)

![Rastigrin: kappa=0.5](image2)

![Rastigrin: kappa=1](image3)

![Rastigrin: kappa=5](image4)
Himmelblau

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Shubert

Shubert: \(\kappa = 0.1\)

Shubert: \(\kappa = 0.5\)

Shubert: \(\kappa = 1\)

Shubert: \(\kappa = 5\)
Combine Particles and Simulation

• Suppose \( N \) particles are used

• Consider a 2-stage problem

• \( f(x, \xi) = c(x) + Q(x, y, \xi) \)

• Distribution on \( x, y_i, \xi \):

\[
P(x, y_1, \ldots y_N, \xi) = \Pi_{i=1}^{N} (c(x) + Q(x, y_i, \xi_i))
\]

Result: \( E_P (x) \rightarrow x^* \)
Implementation

• Propagation forward on y’s:

\[ q( \xi_j | x_1 ) \propto \left\{ c(x) + Q( \xi_j, y_j, x) \right\} p( \xi_j ) \]

where \( y_j = \text{argmin}(c(x) + Q( \xi_j, y_j, x)) \)

• \( p( x | \xi_1, y_1, ..., \xi_N y_N ) \)

\[ \propto \prod_{j=1}^{N} \left\{ c(x) + Q(\xi_j, y_j, x) \right\} p( \xi_j ) \]

The particles concentrate the distribution on \( x^* \) as in the deterministic optimization.
Example

• From B/Louveaux, Chapter 1 (Farmer):
Example: Linear-Quadratic Gaussian

• All distributions are available in closed form

\[ x_t = Ax_{t-1} + B_t u_{t-1} + v_t \]

• All normal distributions with risk-sensitive objective:

\[ -\log E(\exp(- (\theta/2)(x_2^T Q x_2 + u_1^T R u_1))) \]

where \( u_1 \) is control in the first period

• Now, all can be found in closed form
Results for LQG

• Mean of \( u \): \( m_{u_1} \)
• \( m_{u_1} = L_1(\theta) x_1 \),
where \( L_1 \) is the result from the Kalman filter
• Variance of \( u \): \( V_u(N) \) where
\( V_{u_1}(N) \rightarrow 0 \) as \( N \rightarrow \infty \)
\( m_{u_1}(\theta) \rightarrow u_1^\ast \) as \( \theta \rightarrow 0 \)
where \( u_1^\ast \) is the two-stage risk-neutral solution.
Extensions to T Stages

• Can derive $S^\theta_t$ recursively to show that:

$$p(x_t|x^{t-1}, u^{t-1}) = K \exp\left(-\frac{1}{2} \times \left( \sum_{s=1}^{t-1} (x_t^T Q_s x_s + u_s^T R_s u_s) + x_t^T S^\theta_t x_t \right) + (x_t - Ax_{t-1} - Bu_{t-1})^T V_{t-1} (x_t - Ax_{t-1} - Bu_{t-1}) \right)$$

For particle methods, $j=1 \ldots N$:

Each $x_j$ drawn consistently from this distribution
General Method Structure

Propagate:
• $w_t^1, x_t^1$
  $u_t^1$
• $w_t^2, x_t^2$
  $u_t^2$
• $\ldots$
• $w_t^N, x_t^N$
  $u_t^N$

Re-sample:
• $w_t'^1, x_t^1$
  $u_t'^1$
• $w_t'^2, x_t^2$
  $u_t'^2$
• $\ldots$
• $w_t'^N, x_t^N$
  $u_t'^N$
General Result

• If the propagation step is unbiased, then
\[ E(u_i) \rightarrow u_i^* \]

• The unbiased result is possible in LQG from the recursive structure.

• Harder to obtain in more general systems (without additional future sampling)
Generalizing Objectives

- **Direct:** risk-sensitive exponential utility:
  \[ \exp(-\theta Q(x,y,\xi)) - Q \text{ quadratic} \]
- **Objective:**
  \[ e^{-\theta |y-d|} \]
  
  \[ E_{\lambda} \left[ \exp\left(\frac{-\theta^2}{2\lambda_j}(y_j - d)^2\right) \right] \]
  where \( \lambda \sim \text{Exp}(2) \)

  Also, use:
  \[ E[ e^{-\theta |y-d|} ] \approx 1 + \theta |y-d| + O(1) \]
Further Generalizations

• Use objective approximations that preserve normal forms
• Extend LQG-like results to this general framework
• Find other frameworks where unbiased future samples are available
• Obtain sensitivity results on bias from “imperfect” future sampling
• Use optimization to pick ML instead
Conclusions

• Estimation models have many similar aspects to optimization models (e.g., often MLE)
• Particle methods allow for general forms of estimation in time series when analytical results are not available
• Simulation on a larger distribution including decision variables can combine the methods
• Key feature to remember is the backward step of updating controls with observations
Other Questions to Consider

• How can learning and parameter estimation be combined with optimization?
• What is the range of problems that can be approached in this manner?
• What are the best uses of optimization technology as part of this process?
Thank you!

• Questions?