Sequential Monte Carlo methods

Lecture 9 – Maximum likelihood parameter estimation

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Outline – Lecture 9

Aim: Open up for using the particle filter to learn parameters θ (and not only states X_t) in state-space models.

Outline:

1. The particle filter as likelihood estimator
2. Maximum likelihood estimation of state-space models
    a. Direct optimization
    b. Non-standard μ on quasi-Newton methods
    c. Expectation maximization

State-space models

From lecture 2:

$$X_t = f(X_{t-1}, \theta) + V_t,$$
$$Y_t = g(X_t, \theta) + E_t,$$

where X_t are the states and θ the model parameters.

Only (but important!) **difference: X_t depends on t, whereas θ does not.**

The particle filter assumes θ is known and computes $p(X_t \mid y_{1:T}, \theta)$.

The likelihood function

The particle filter assumes θ is known and computes $p(x_t \mid y_{1:T}, \theta)$.

Learning θ requires

$$p(\theta \mid y_{1:T}) \textit{ (Posterior; Bayesian inference)}$$

or

$p(y_{1:T} \mid \theta)$ *(Likelihood function; Fisherian inference/maximum likelihood).*

$$p(\theta \mid y_{1:T}) = \frac{p(y_{1:T} \mid \theta)p(\theta)}{p(y_{1:T})}$$

This lecture: Focus on maximum likelihood. More on the Bayesian setting in later lectures.

Maximum likelihood parameter inference

Maximum likelihood problem: Select θ such that the observed data $y_{1:T}$ is as likely as possible to have been observed, i.e.,

$$\widehat{\theta} = \arg\max_{\theta} \, p(y_{1:T} \mid \theta)$$

Particle filter as likelihood estimator

$$
\begin{aligned}
p(y_{1:T} \mid \theta) &= \prod_{t=1}^{T} p(y_t \mid y_{1:t-1}, \theta), \\
p(y_t \mid y_{1:t-1}, \theta) &= \int p(y_t, x_t \mid y_{1:t-1}, \theta) dx_t \\
&= \int p(y_t \mid x_t, \theta) \underbrace{p(x_t \mid y_{1:t-1}, \theta)}_{\overset{\text{bPF}}{\approx} \sum_{i=1}^{N} \frac{1}{N} \delta_{x_t^i}(x_t)} dx_t \\
&\approx \frac{1}{N} \sum_{i=1}^{N} p(y_t \mid x_t^i, \theta) = \frac{1}{N} \sum_{i=1}^{N} \widetilde{w}_t^i \\
\Rightarrow p(y_{1:T} \mid \theta) &\approx \prod_{t=1}^{T} \left(\frac{1}{N} \sum_{i=1}^{N} \widetilde{w}_t^i \right)
\end{aligned}
$$

(w_t^i are the *unnormalized* weights)

Reminder: The bootstrap particle filter

Algorithm 1 Bootstrap particle filter (for $i = 1, \ldots, N$)

1. **Initialization ($t = 0$):**
   (a) Sample $x_0^i \sim p(x_0 \mid \theta)$.
   (b) Set initial weights: $w_0^i = 1/N$.
2. **for** $t = 1$ **to** T **do**
   (a) Resample: sample ancestor indices $a_t^i \sim \mathcal{C}(\{w_{t-1}^j\}_{j=1}^N)$.
   (b) Propagate: sample $x_t^i \sim p(x_t \mid x_{t-1}^{a_t^i}, \theta)$.
   (c) Weight: compute $\widetilde{w}_t^i = p(y_t \mid x_t^i, \theta)$ and normalize $w_t^i = \widetilde{w}_t^i / \sum_{j=1}^N \widetilde{w}_t^j$.

$$p(y_{1:T} \mid \theta) \approx \prod_{t=1}^{T} \left(\frac{1}{N} \sum_{i=1}^{N} \widetilde{w}_t^i \right)$$

Log-weights: an important practical aspect

For realistic problems, $\widetilde{w}_t^i$ might be smaller than machine precision $\rightarrow \widetilde{w}_t^i = 0$ on your computer.

Use **shifted log-weights** v_t^i!

$$v_t^i = \log \widetilde{w}_t^i - c_t, \quad c_t = \max\{\log \widetilde{w}_t^1, \dots, \log \widetilde{w}_t^N\}$$

Implement using shifted log-weights! Store $\{v_t^i\}_{i=1}^N$ and c_t.

From this, the likelihood estimate is obtained

$$\prod_{t=1}^{T} \left(\frac{1}{N} \sum_{i=1}^{N} \widetilde{w}_t^i \right) = \prod_{t=1}^{T} \exp\left(c_t + \log \sum_{i=1}^{N} e^{v_t^i} - \log N \right)$$

Also the normalized weights $\{w_t^i\}_{i=1}^N$ are available from $\{v_t^i\}_{i=1}^N$,

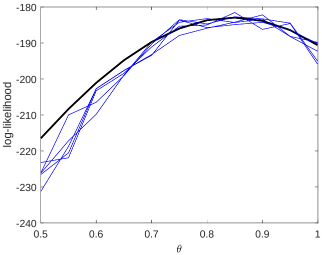
$$w_t^i = \frac{\widetilde{w}_t^i}{\sum_{j=1}^N \widetilde{w}_t^j} = \frac{e^{v_t^i + c_t}}{\sum_{j=1}^N e^{v_t^j + c_t}} = \frac{e^{v_t^i}}{\sum_{j=1}^N e^{v_t^j}}$$

ex) Numerical illustration

Simple LG-SSM,

$$
\begin{aligned}
X_t &= \theta X_{t-1} + V_t, & V_t &\sim \mathcal{N}(0,1), \\
Y_t &= X_t + E_t, & E_t &\sim \mathcal{N}(0,1).
\end{aligned}
$$

Task: estimate $p(y_{1:100} \mid \theta)$ for a simulated data set. True $\theta^\star = 0.9$.



Black line – true likelihood computed using the Kalman filter.

Blue thin lines – 5 different likelihood estimates $\widehat{p}^N(y_{1:100} \mid \theta)$ computed using a bootstrap particle filter with $N = 100$ particles.

The particle filter as likelihood estimator

- **Good news:** Each run of the particle filter returns an estimate of $p(y_{1:T} \mid \theta)$
  — in addition to the state estimates!
- **Challenge:** The particle filter contains randomness $\rightarrow$ the estimate of $p(y_{1:T} \mid \theta)$ contains randomness or ‘noise’.
- More on its stochastic properties in the next lecture.

Direct optimization

$$\widehat{\theta} = \arg\max_{\theta} \, p(y_{1:T} \mid \theta)$$

Can we use standard optimization routines?

Say, `scipy.optimize.minimize(fun=-my_BPF_function,x0 = .2)`

No. The evaluation of the cost function is 'noisy'.

Solution: Use (or design) **stochastic optimization** methods that can work with noisy cost functions.

Estimating likelihood gradients

We can also get noisy approximations for the gradient of the likelihood.

Fisher's identity states that
$\nabla_\theta \log p(y_{1:T} \mid \theta) = \mathbb{E}_\theta[\nabla_\theta \log p(x_{1:T}, y_{1:T} \mid \theta) \mid y_{1:T}]$,

where

$$\nabla_\theta \log p(x_{1:T}, y_{1:T} \mid \theta) = \sum_{t=1}^{T} \nabla_\theta \log p(x_t \mid x_{t-1}, \theta) + \nabla_\theta \log p(y_t \mid x_t, \theta),$$

$$\Rightarrow \nabla_\theta \log p(y_{1:T} \mid \theta) =$$
$$\sum_{t=1}^{T} \int [\nabla_\theta \log p(x_t \mid x_{t-1}, \theta) + \nabla_\theta \log p(y_t \mid x_t, \theta)]\, p(x_{t-1:t} \mid y_{1:T}, \theta) \mathrm{d}x_{t-}$$

Here, $p(x_{t-1:t} \mid y_{1:T}, \theta)$ requires a particle *smoother*. Several SMC-based alternative exists.

Stochastic optimization (very brief)

Quasi-Newton – A non-standard take

Our problem is of the form

$$\min_{\theta} f(\theta)$$

Idea underlying (quasi-)Newton methods: Learn a local quadratic model $q(\theta_k, \delta)$ of the cost function $f(\theta)$ around the current iterate θ_k

$$q(\theta_k, \delta) = f(\theta_k) + g(\theta_k)^\mathsf{T}\delta + \frac{1}{2}\delta^\mathsf{T} H(\theta_k)\delta$$

$$g(\theta_k) = \nabla f(\theta)\big|_{\theta=\theta_k}, \qquad H(\theta_k) = \nabla^2 f(\theta)\big|_{\theta=\theta_k}, \qquad \delta = \theta - \theta_k.$$

We have measurements of

- the cost function $f_k = f(\theta_k)$,
- and its gradient $g_k = g(\theta_k)$.

Useful basic facts

Line segment connecting two adjacent iterates θ_k and θ_{k+1}:

$$r_k(\tau) = \theta_k + \tau(\theta_{k+1} - \theta_k), \qquad \tau \in [0, 1].$$

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1. The **fundamental theorem of calculus** states that
$$\int_0^1 \frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) \mathrm{d}\tau = \nabla f(r_k(1)) - \nabla f(r_k(0)) = \underbrace{\nabla f(\theta_{k+1})}_{g_{k+1}} - \underbrace{\nabla f(\theta_k)}_{g_k}.$$
2. The **chain rule** tells us that
$$\frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) = \nabla^2 f(r_k(\tau)) \frac{\partial r_k(\tau)}{\partial \tau} = \nabla^2 f(r_k(\tau))(\theta_{k+1} - \theta_k).$$

$$\underbrace{g_{k+1} - g_k}_{=y_k} = \int_0^1 \frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) \mathrm{d}\tau = \int_0^1 \nabla^2 f(r_k(\tau)) \mathrm{d}\tau (\underbrace{\theta_{k+1} - \theta_k}_{s_k}).$$

Result – the quasi-Newton integral

With the definitions $y_k \triangleq g_{k+1} - g_k$ and $s_k \triangleq \theta_{k+1} - \theta_k$ we have

$$y_k = \int_0^1 \nabla^2 f(r_k(\tau)) \mathrm{d}\tau s_k.$$

Interpretation: The difference between two consecutive gradients (y_k) constitute a **line integral observation of the Hessian**.

Problem: Since the Hessian is unknown there is no functional form available for it.

Two different solutions

1. Recover existing quasi-Newton algorithms by assuming the Hessian to be constant

$$\nabla^2 f(r_k(\tau)) \approx H_{k+1}, \qquad \tau \in [0, 1],$$

implying the following approximation of the integral (**secant condition**)

$$y_k = H_{k+1} s_k.$$

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2. Recall that the problem is **stochastic** and **nonlinear**. Use a flexible nonlinear model.

Idea: Represent the Hessian using a **Gaussian process** learnt from data.

Adrian G. Wills and Thomas B. Schön. **Stochastic quasi-Newton with line-search regularization.** *Automatica*, 127:109503, 2021.

Expectation Maximization

EM idea

As an alternative to direct optimization of $p(y_{1:T} \mid \theta)$, we can use **Expectation Maximization** (EM).

Dempster, Arthur P., Nan M. Laird, and Donald B. Rubin. **Maximum likelihood from incomplete data via the EM algorithm.** *Journal of the Royal Statistical Society: Series B (Methodological)*, 39.1 (1977): 1-22..

$$\text{(E)} \quad \mathcal{Q}(\theta, \theta_{k-1}) = \int \log p(y_{1:T}, x_{0:T} \mid \theta) p(x_{0:T} \mid y_{1:T}, \theta_{k-1}) d x_{0:T}$$

$$\text{(M)} \quad \text{Solve } \theta_k \leftarrow \operatorname{argmax}_\theta \ \mathcal{Q}_k(\theta, \theta_{k-1})$$

Iterate until convergence.

Note: Does not make use of the particle filter as a likelihood estimator, but uses a particle smoother.

Computing $\mathcal{Q}$

Inserting

$$\log p(x_{0:T}, y_{1:T} \mid \theta) = \log \left(\prod_{t=1}^{T} p(y_t \mid x_t, \theta) \prod_{t=1}^{T} p(x_t \mid x_{t-1}, \theta) p(x_0 \mid \theta) \right)$$

$$= \sum_{t=1}^{T} \log p(y_t \mid x_t, \theta) + \sum_{t=1}^{T} \log p(x_t \mid x_{t-1}, \theta) + \log p(x_0 \mid \theta)$$

into the expression for $\mathcal{Q}(\theta, \theta_k)$ results in

$$\begin{aligned}\mathcal{Q}(\theta, \theta_k) = &\int \sum_{t=1}^{T} \log p(y_t \mid x_t, \theta) p(x_t \mid y_{1:T}, \theta_k) \mathrm{d}x_t \\ &+ \int \sum_{t=1}^{T} \log p(x_t \mid x_{t-1}, \theta) p(x_{t-1:t} \mid y_{1:T}, \theta_k) \mathrm{d}x_{t-1:t} \\ &+ \int \log p(x_0 \mid \theta) p(x_0 \mid y_{1:T}, \theta_k) \mathrm{d}x_0.\end{aligned}$$

Final EM algorithm

Inserting particle smoothing approximations now allows for straightforward approximation of $\mathcal{Q}(\theta, \theta_k)$,

$$\widehat{\mathcal{Q}}(\theta, \theta_k) = \sum_{t=1}^{T} \sum_{i=1}^{N} \log p(y_t \mid x^i_{t \mid T}, \theta) + \sum_{t=1}^{T} \sum_{i=1}^{N} \log p(x^i_{t \mid T} \mid x^i_{t-1 \mid T}, \theta) + \mathrm{lo}$$

1. Initialize θ_0 and run a particle smoother conditional on θ_0.
2. Use the result from previous step to compute $\widehat{\mathcal{Q}}(\theta, \theta_0)$.
3. Solve $\theta_1 = \arg\max_{\theta} \widehat{\mathcal{Q}}(\theta, \theta_0)$.
4. Run a particle smoother conditional on θ_1.
5. ....

Requires $N \to \infty$ **and** infinitely many iterations. There are more intricate solutions.

Further reading

Fairly recent survey/tutorial papers:

Anna Wigren, Johan Wågberg, Fredrik Lindsten, Adrian Wills and Thomas B. Schön. **Nonlinear system identification – Learning while respecting physical models using Sequential Monte Carlo.** *IEEE Control Systems Magazine*, 2022. (accepted for publication).

Nikolas Kantas, Arnaud Doucet, Sumeetpal S. Singh, Jan Maciejowski and Nicolas Chopin. **On particle methods for parameter estimation in general state-space models.** *Statistical Science*, 30(3):328-351, 2015.

Maximum likelihood inference using stochastic optimization:

Adrian G. Wills and Thomas B. Schön. **Stochastic quasi-Newton with line-search regularization.** *Automatica*, 127:109503, 2021.

Maximum likelihood inference using EM:

Thomas B. Schön, Adrian G. Wills and Brett Ninness. **System identification of nonlinear statespace models.** *Automatica*, 47(1):39-49, January, 2011.

Andreas Lindholm and Fredrik Lindsten. **Learning dynamical systems with particle stochastic approximation EM.** *arXiv:1806.09548*, 2018.