Introduction to Sequential Monte Carlo Methods

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- We focus here on *Applications of SMC to Hidden Markov Models* (HMM) for pedagogical reasons...
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- In the HMM framework, SMC are also widely known as Particle Filtering/Smoothing methods.

Organization of the Lectures

- Filtering, smoothing and parameter estimation in HMM.

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- Filtering, smoothing and parameter estimation in HMM.
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- Advanced SMC for HMM.
- Recent Developments and Open Problems.

Markov Models

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- $\{X_k\}_{k \geq 1}$ is characterized by its *initial density*

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and its *transition density*

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- We introduce the notation $x_{i:j} = (x_i, x_{i+1}, ..., x_j)$ for $i \leq j$. We have by definition

$$\begin{aligned} p(x_{1:n}) &= p(x_1) \prod_{k=2}^{n} p(x_k | x_{1:k-1}) \\ &= \mu(x_1) \prod_{k=2}^{n} f(x_k | x_{k-1}) \end{aligned}$$

Tracking Example

- Assume you want to track a target in the XY plane then you can consider the 4-dimensional state

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- The so-called constant velocity model states that

$$X_k = AX_{k-1} + W_k, \;\; W_k \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \Sigma),$$

$$A = \begin{pmatrix} A_{CV} & 0 \\ 0 & A_{CV} \end{pmatrix}, A_{CV} = \begin{pmatrix} 1 & T \\ 0 & 1 \end{pmatrix},$$

$$\Sigma = \sigma^2 \begin{pmatrix} \Sigma_{CV} & 0 \\ 0 & \Sigma_{CV} \end{pmatrix}, \; \Sigma_{CV} = \begin{pmatrix} T^3/3 & T^2/2 \\ T^2/2 & T \end{pmatrix}$$

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- We obtain that

$$f(x_k | x_{k-1}) = \mathcal{N}(x_k; Ax_{k-1}, \Sigma).$$

Speech Enhancement

- A basic model for speech signals consists of modelling them as autoregressive (AR) processes; i.e.

$$S_k = \sum_{i=1}^{d} \alpha_i S_{k-i} + V_k, \;\; V_k \overset{\text{i.i.d.}}{\sim} \mathcal{N}\left(0, \sigma_s^2\right)$$

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- If we write $U_k = \left(S_k, ..., S_{k-d}\right)^{\mathsf{T}}$ then we have equivalently

$$U_k = AU_{k-1} + BV_k$$

where

$$A = \begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_d \\ 1 & & & \\ & \ddots & & \\ & & 1 & \end{pmatrix}, \;\; B = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

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- We have

$$f_U\left(u_k \middle| u_{k-1}\right) = \mathcal{N}\left(u_k; \left(Au_{k-1}\right)_1, \sigma_s^2\right) \delta_{\left(u_{k-1}\right)_{1:d-1}}\left(\left(u_k\right)_{2:d}\right)$$

- This model could be not flexible enough and we might want additionally to make the AR coefficient time-varying.

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$$\alpha_k = \alpha_{k-1} + W_k \text{ where } W_k \overset{\text{i.i.d.}}{\sim} \mathcal{N}\left(0, \sigma_\alpha^2 I_d\right)$$

which implies that

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- The process $X_k = (\alpha_k, U_k)$ is Markov with transition density

$$\begin{aligned} f\left(x_k \middle| x_{k-1}\right) &= \mathcal{N}\left(\alpha_k; \alpha_{k-1}, \sigma_\alpha^2 I_d\right) \mathcal{N}\left(u_k; \left(A_k u_{k-1}\right)_1, \sigma_s^2\right) \\ &\quad \times \delta_{\left(u_{k-1}\right)_{1:d-1}}\left(\left(u_k\right)_{2:d}\right) \end{aligned}$$

where $(A_k)_1 = \alpha_k$.

Econometrics

- The (simplified) Heston model (1993) is used to described the dynamics of an asset price S_t using the following model for $X_t = \log(S_t)$
$$dX_t = \mu dt + dW_t + dZ_t$$
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$$X_{t+\delta} = X_t + \delta\mu + W_{t+\delta,t} + Z_{t+\delta,t}.$$

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$$X_{t+\delta} = X_t + \delta\mu + W_{t+\delta,t} + Z_{t+\delta,t}.$$
- Similar discretization schemes are used for biochemichal networks (e.g. D. Wilkinson, Stochastic modelling for systems biology, CRC, 2006), disease dynamics (e.g. E.L. Ionides, PNAS, 2006) or population dynamics.

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- Formally this means that

$$p\,(y_{1:n}|\,x_{1:n}) = \prod_{k=1}^{n} g\,(y_k|\,x_k)\,.$$

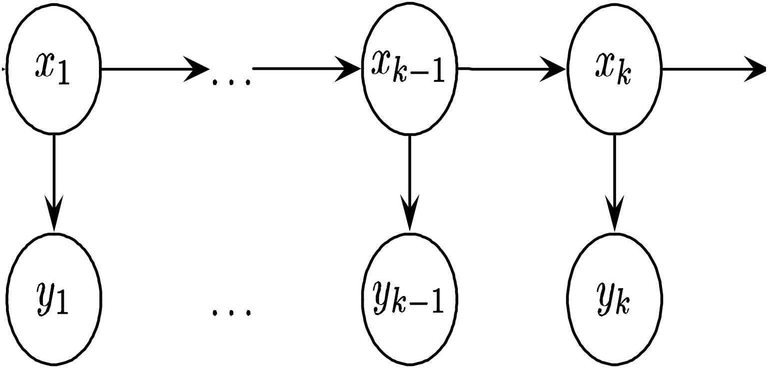

Figure: Graphical model representation of HMM

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- *Simple case*

$$Y_k = CX_k + DE_k, \; E_k \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \Sigma_e)$$

so

$$g(y_k | x_k) = \mathcal{N}(y_k; Cx_k, \Sigma_e).$$

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- *Complex realistic case* (Bearings-only-tracking)

$$Y_k = \tan^{-1}\left(\frac{X_{k,2}}{X_{k,1}}\right) + E_k,\ \ E_k \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2)$$

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Stochastic Volatility

- We have the following standard model

$$X_k = \phi X_{k-1} + V_k, \;\; V_k \overset{\text{i.i.d.}}{\sim} \mathcal{N}\left(0, \sigma^2\right)$$

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- We observe

$$Y_k = \beta \exp\left(X_k / 2 \right) W_k, \;\; W_k \overset{\text{i.i.d.}}{\sim} \mathcal{N}\left(0, 1\right)$$

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Inference in HMM

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- Using Bayes' rule, we obtain

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

where the marginal likelihood is given by

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    where the marginal smoothing distribution is

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  - We have also the minimum mean square estimate

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$$\mathbb{E}\left[X_k \middle| y_{1:n}\right] = \int x_k \, p\left(x_k \middle| y_{1:n}\right) dx_k.$$

- Conceptually, there is no problem whatsoever.

Sequential Inference in HMM

- In particular, we will focus here on the *sequential estimation* of $p(x_{1:n}|\, y_{1:n})$ and $p(y_{1:n})$; that is at each time n we want update our knowledge of the hidden process in light of y_n.

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- There is a simple recursion relating $p(x_{1:n-1}|y_{1:n-1})$ to $p(x_{1:n}|y_{1:n})$ given by

$$p(x_{1:n}|y_{1:n}) = p(x_{1:n-1}|y_{1:n-1}) \frac{f(x_n|x_{n-1})\, g(y_n|x_n)}{p(y_n|y_{1:n-1})}$$

where

$$p(y_n|y_{1:n-1}) = \int g(y_n|x_n)\, f(x_n|x_{n-1})\, p(x_{n-1}|y_{1:n-1})\, dx_{n-1:n}.$$

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- We will also simply write

$$p(x_{1:n}|y_{1:n}) \propto p(x_{1:n-1}|y_{1:n-1})\, f(x_n|x_{n-1})\, g(y_n|x_n).$$

- The "proof" is trivial and only involves rewriting

$$\begin{aligned} p\left(x_{1:n}\middle|\, y_{1:n}\right) &= \frac{p\left(x_{1:n}\middle|\, y_{1:n}\right)}{p\left(x_{1:n-1}\middle|\, y_{1:n-1}\right)} p\left(x_{1:n-1}\middle|\, y_{1:n-1}\right) \\ &= \frac{p\left(x_{1:n}, y_{1:n}\right) / p\left(y_{1:n}\right)}{p\left(x_{1:n-1}, y_{1:n-1}\right) / p\left(y_{1:n-1}\right)} p\left(x_{1:n-1}\middle|\, y_{1:n-1}\right) \end{aligned}$$

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$$\begin{aligned} p(x_{1:n}|\, y_{1:n}) &= \frac{p(x_{1:n}|\, y_{1:n})}{p(x_{1:n-1}|\, y_{1:n-1})} p(x_{1:n-1}|\, y_{1:n-1}) \\ &= \frac{p(x_{1:n}, y_{1:n}) / p(y_{1:n})}{p(x_{1:n-1}, y_{1:n-1}) / p(y_{1:n-1})} p(x_{1:n-1}|\, y_{1:n-1}) \end{aligned}$$

- Now we have

$$\frac{p(x_{1:n}, y_{1:n})}{p(x_{1:n-1}, y_{1:n-1})} = f(x_n|\, x_{n-1})\, g(y_n|\, x_n)$$

and

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

and the result follows.

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- *Prediction Step*

$$
\begin{aligned}
p(x_n|y_{1:n-1}) &= \int p(x_{n-1:n}|y_{1:n-1})\,dx_{n-1} \\
&= \int p(x_n|x_{n-1}, y_{1:n-1})\,p(x_{n-1}|y_{1:n-1})\,dx_{n-1} \\
&= \int f(x_n|x_{n-1})\,p(x_{n-1}|y_{1:n-1})\,dx_{n-1}.
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- *Prediction Step*

$$\begin{aligned} p\left(x_n \mid y_{1:n-1}\right) &= \int p\left(x_{n-1:n} \mid y_{1:n-1}\right) dx_{n-1} \\ &= \int p\left(x_n \mid x_{n-1}, y_{1:n-1}\right) p\left(x_{n-1} \mid y_{1:n-1}\right) dx_{n-1} \\ &= \int f\left(x_n \mid x_{n-1}\right) p\left(x_{n-1} \mid y_{1:n-1}\right) dx_{n-1}. \end{aligned}$$

- *Updating Step*

$$p\left(x_n \mid y_{1:n}\right) = \frac{g\left(y_n \mid x_n\right) p\left(x_n \mid y_{1:n-1}\right)}{p\left(y_n \mid y_{1:n-1}\right)}$$

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- *Prediction Step*

$$\begin{aligned} p(x_n|y_{1:n-1}) &= \int p(x_{n-1:n}|y_{1:n-1})\,dx_{n-1} \\ &= \int p(x_n|x_{n-1},y_{1:n-1})\,p(x_{n-1}|y_{1:n-1})\,dx_{n-1} \\ &= \int f(x_n|x_{n-1})\,p(x_{n-1}|y_{1:n-1})\,dx_{n-1}. \end{aligned}$$

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- Although we will not use directly the filtering recursion for SMC, the filtering distributions will also prove useful.

(Marginal) Likelihood Evaluation

- We have seen that

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- We also have the following decomposition

$$p\left(y_{1:n}\right)=p\left(y_{1}\right)\prod_{k=2}^{n}p\left(\left.y_{k}\right|y_{1:k-1}\right)$$

where

$$\begin{aligned}p\left(\left.y_{k}\right|y_{1:k-1}\right) &= \int p\left(y_{k},\left.x_{k}\right|y_{1:k-1}\right)dx_{k}\\ &= \int g\left(\left.y_{k}\right|x_{k}\right)p\left(\left.x_{k}\right|y_{1:k-1}\right)dx_{k}\\ &= \int g\left(\left.y_{k}\right|x_{k}\right)f\left(\left.x_{n}\right|x_{n-1}\right)p\left(\left.x_{k-1}\right|y_{1:k-1}\right)dx_{k-1}\end{aligned}$$

(Marginal) Likelihood Evaluation

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$$\begin{aligned} p(y_k | y_{1:k-1}) &= \int p(y_k, x_k | y_{1:k-1}) \, dx_k \\ &= \int g(y_k | x_k) \, p(x_k | y_{1:k-1}) \, dx_k \\ &= \int g(y_k | x_k) \, f(x_n | x_{n-1}) \, p(x_{k-1} | y_{1:k-1}) \, dx_{k-1} \end{aligned}$$

- We have “broken" an high dimensional integral into the product of lower dimensional integrals.

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- Remark: Surprisingly, this recursion is almost never used for finite state-space HMM.

- Proof.

$$
\begin{aligned}
p\left(x_k \mid y_{1:n}\right) &= \int p\left(x_k, x_{k+1} \mid y_{1:n}\right) dx_{k+1} \\
&= \int p\left(x_k \mid x_{k+1}, y_{1:n}\right) p\left(x_{k+1} \mid y_{1:n}\right) dx_{k+1} \\
&= \int p\left(x_k \mid x_{k+1}, y_{1:k}\right) p\left(x_{k+1} \mid y_{1:n}\right) dx_{k+1} \\
&= \int \frac{f\left(x_{k+1} \mid x_k\right) p\left(x_k \mid y_{1:k}\right)}{p\left(x_{k+1} \mid y_{1:k}\right)} p\left(x_{k+1} \mid y_{1:n}\right) dx_{k+1}
\end{aligned}
$$

Two-Filter Smoothing

- An alternative approach consists of noting that

$$p\left(x_k \mid y_{1:n}\right) = \frac{p\left(x_k \mid y_{1:k}\right) p\left(y_{k+1:n} \mid x_k\right)}{p\left(y_{k+1:n} \mid y_{1:k}\right)}$$

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- In this case, the smoothing distribution is the combination of the standard forward filter and the so-called backward information filter given by

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- We can have $\int p(y_{k+1:n} | x_k) \, dx_k = \infty$, this has led to numerous wrong algorithms in the literature.

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- We can have $\int p(y_{k+1:n}|\, x_k)\, dx_k = \infty$, this has led to numerous wrong algorithms in the literature.
- Remark: The two-filter smoother is known as the forward-backward smoother for finite state-space HMM!

Parameter Estimation for HMM

- In most applications of interest, we have the initial distribution $\mu(x_1)$, the transition density $f(x_k|x_{k-1})$ and observation density $g(y_k|x_k)$ dependent on some hyperparameters θ and we write $\mu_\theta(x_1)$, $f_\theta(x_k|x_{k-1})$ and $g_\theta(y_k|x_k)$.

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- For example, in the tracking example, the variances of both the dynamic noise and observation noise might be unknown.
- In a *full Bayesian framework*, we set a prior $p(\theta)$ on θ. If we define the extended state $Z_k = (Z_k^1, Z_k^2) = (\theta, X_k)$, we can rewrite everything as a standard HMM where

$$Z_1 \sim p(z_1^1)\, \mu_{z_1^1}(z_1^2),$$

$$Z_k|(Z_{k-1} = z_{k-1}) \sim \delta_{z_{k-1}^1}(z_k^1)\, f_{z_k^1}(z_k^2|z_{k-1}^2),$$

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$$Y_k | (Z_k = z_k) \sim g_{z_k^1}\left(y_k | z_k^2\right).$$

- Conceptually, this solution is correct. Practically, the degeneracy of the transition kernel of $\{Z_k\}_{k\geq 1}$ can cause serious numerical problems for approximation methods.

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$$\theta_{ML} = \arg\max \ \log p_\theta \left(y_{1:n} \right)$$

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- These algorithms can work decently but it can be difficult to scale the components of the gradients.

Expectation-Maximization for HMM

- We can use as an alternative the popular Expectation-Maximization algorithm

$$\theta^{(i)} = \arg\max \; Q\left(\theta^{(i)}, \theta\right)$$

where

$$\begin{aligned} Q\left(\theta^{(i)}, \theta\right) &= \int \log p_\theta\left(x_{1:n}, y_{1:n}\right) . p_{\theta^{(i-1)}}\left(x_{1:n} \middle| y_{1:n}\right) dx_{1:n} \\ &= \int \log\left(\mu\left(x_1\right) g\left(y_1 \middle| x_1\right)\right) . p_{\theta^{(i-1)}}\left(x_1 \middle| y_{1:n}\right) dx_1 \\ &+ \sum_{k=2}^{n} \int \log\left(f\left(x_k \middle| x_{k-1}\right) g\left(y_k \middle| x_k\right)\right) . p_{\theta^{(i-1)}}\left(x_{k-1:k} \middle| y_{1:n}\right) dx_{k-1:k}. \end{aligned}$$

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$$+ \sum_{k=2}^{n} \int \log\left(f\left(x_k \middle| x_{k-1}\right) g\left(y_k \middle| x_k\right)\right) . p_{\theta^{(i-1)}}\left(x_{k-1:k} \middle| y_{1:n}\right) dx_{k-1:k} .$$
- Implementing this algorithm requires being able to compute expectations with respect to the smoothing distributions $p_{\theta^{(i-1)}}\left(x_{k-1:k} \middle| y_{1:n}\right)$.

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  - A whole reverse engineering literature exists for closed-form solutions in alternative cases...
- In many cases of interest, it is impossible to compute the solution in closed-form and we need approximations,

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- Most approximation methods are not 'asymptotically consistent' and they might work better for a fixed computational complexity.

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- Standard discretization of the space is expensive and difficult to implement in high-dimensional scenarios.

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- This article introduces a simple method which relies neither on a functional approximation nor a deterministic grid.
- This paper was ignored by most researchers for a few years until its rediscovery in 1996 by Isard & Blake in the field of computer vision.