Time Series and Sequence Learning

Lecture 7 – Non-Linear/Non-Gaussian State Space Models

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Summary of Lecture 6: Structural time series

A general structural time series model

$$y_t = \mu_t + \gamma_t + \varepsilon_t$$

can be written in state space form using block matrices.

State vector: $\alpha_t = \begin{bmatrix} \mu_t & \mu_{t-1} & \cdots & \mu_{t-k+1} & \gamma_t & \gamma_{t-1} & \cdots & \gamma_{t-s+2} \end{bmatrix}^\mathsf{T}$

State space model:

$$\begin{aligned}
\alpha_t &= \begin{bmatrix} T_{[\mu]} & \\ & T_{[\gamma]} \end{bmatrix} \alpha_{t-1} + \begin{bmatrix} R_{[\mu]} & \\ & R_{[\gamma]} \end{bmatrix} \eta_t, & \eta_t &\sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma_\zeta^2 & 0 \\ 0 & \sigma_\omega^2 \end{bmatrix} \right), \\
y_t &= \begin{bmatrix} Z_{[\mu]} & Z_{[\gamma]} \end{bmatrix} \alpha_t + \varepsilon_t, & \varepsilon_t &\sim \mathcal{N}(0, \sigma_\varepsilon^2).
\end{aligned}$$

Summary of Lecture 6: Trend component

A $k-1$th order polynomial trend model $\Delta^k \mu_t = \zeta_t$ can be written as

$$\alpha_t = \begin{bmatrix} c_1 & c_2 & \cdots & c_{k-1} & c_k \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix} \alpha_{t-1} + \begin{bmatrix} 1 \\ 0 \\ 0 \\ \cdots \\ 0 \end{bmatrix} \zeta_t,$$

$$\mu_t = \begin{bmatrix} 1 & 0 & 0 & \vdots & 0 \end{bmatrix} \alpha_t,$$

where the state vector is

$$\alpha_t = \begin{bmatrix} \mu_t & \mu_{t-1} & \cdots & \mu_{t-k+1} \end{bmatrix}^\mathsf{T}$$

and $c_i = (-1)^{i+1} \binom{k}{i}$.

Summary of Lecture 6: Seasonal component

A s period seasonal model, $\sum_{j=0}^{s-1} \gamma_{t-j} = \omega_t$, can be written a

$$\alpha_t = \begin{bmatrix} -1 & -1 & \cdots & -1 & -1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix} \alpha_{t-1} + \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \omega_t$$

$$\gamma_t = \begin{bmatrix} 1 & 0 & 0 & \vdots & 0 \end{bmatrix} \alpha_t,$$

where the state vector is

$$\alpha_t = \begin{bmatrix} \gamma_t & \gamma_{t-1} & \cdots & \gamma_{t-s+2} \end{bmatrix}^\top.$$

Summary of Lecture 6: The Kalman filter

For any s, t, denote by $\hat{\alpha}_{t|s} = \mathbb{E}[\alpha_t \,|\, y_{1:s}]$ and $P_{t|s} = \mathrm{Cov}(\alpha_t \,|\, y_{1:s})$.

Thm. For an LGSS model, $p(\alpha_t \,|\, y_{1:s}) = \mathcal{N}(\alpha_t \,|\, \hat{\alpha}_{t|s}, P_{t|s})$.

Of particular interest are:

- Filtering distribution,

$$p(\alpha_t \,|\, y_{1:t}) = \mathcal{N}(\alpha_t \,|\, \hat{\alpha}_{t|t}, P_{t|t}).$$

- (1-step) Predictive distributions,

$$\begin{aligned} p(\alpha_t \,|\, y_{1:t-1}) &= \mathcal{N}(\alpha_t \,|\, \hat{\alpha}_{t|t-1}, P_{t|t-1}), \\ p(y_t \,|\, y_{1:t-1}) &= \mathcal{N}(y_t \,|\, \hat{y}_{t|t-1}, F_{t|t-1}). \end{aligned}$$

Summary of Lecture 6: Parameter Estimation

- The log-likelihood for a LGSSM is calculated using the Kalman filter

$$\ell(\theta) = \text{const} - \frac{1}{2}\sum_{t=1}^{n}\Big(\log|F_{t|t-1}| + (y_t - \hat{y}_{t|t-1})^\top F_{t|t-1}^{-1}(y_t - \hat{y}_{t|t-1})\Big)$$

- Difficult to take derivatives $\Rightarrow$ direct maximization difficult.
- For few parameters, grid the parameters and calculate the log-likelihood.

Summary of Lecture 6: Expectation-Maximization

In the Expectation Maximization (EM) algorithm we alternate two steps,

1. E-step: Calculate $\mathcal{Q}(\theta, \tilde{\theta}) = \mathbb{E}[\log p_\theta(\alpha_{1:n}, y_{1:n}) \,|\, y_{1:n}, \tilde{\theta}]$
2. M-step: Find $\theta^\star$ that maximizes $\mathcal{Q}(\theta, \tilde{\theta})$.

We have that,

$$\mathcal{Q}(\theta, \tilde{\theta}) = \text{const.} - \frac{1}{2} \sum_{t=1}^{n} \Big[\log|\sigma_\epsilon^2| + \log|Q| + \{\hat{\varepsilon}_{t|n}^2 + \mathrm{Var}[\varepsilon_t \,|\, y_{1:n}]\}\sigma_\varepsilon^{-2} + \mathrm{tr}[\{\hat{\eta}_{t|n}\hat{\eta}_{t|n}^\mathsf{T} + \mathrm{Var}[\eta_t \,|\, y_{1:n}]\}Q^{-1}]\Big],$$

where $\hat{\varepsilon}_{t|n}, \mathrm{Var}[\varepsilon_t \,|\, y_{1:n}], \hat{\eta}_{t|n}$, and $\mathrm{Var}[\eta \,|\, y_{1:n}]$ are the smoothed mean and variances of ε_t and η_t. Calculated using the current parameter values $\tilde{\theta}$.

To find the new parameter values $\theta^\star$ maximize $\mathcal{Q}(\theta, \tilde{\theta})$ by taking the derivative and set the derivative to zero.

Non-Linear State-Space Models

Limits of Linear Gaussian State-Space Models

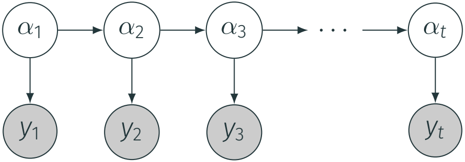
- Only allows for Gaussian observations.
  - What if we have discrete data?
- Only allows for Linear transformations.
  - What if the state moves in a non-linear fashion?
  - What if variance of the noise depends on the state?
  - What if the observation in a non-linear transformation of the states?
- To expend our models we need to work with non-linear and/or non-Gaussian models.

From LGSS model to general state-space model

Def. A Linear Gaussian State-Space (LGSS) model is given by:

$$
\begin{aligned}
\alpha_t &= T\alpha_{t-1} + R\eta_t, & \eta_t &\sim \mathcal{N}(0, Q), \\
y_t &= Z\alpha_t + \varepsilon_t & \varepsilon_t &\sim \mathcal{N}(0, \sigma_\epsilon^2),
\end{aligned}
$$

and initial distribution $\alpha_1 \sim \mathcal{N}(a_1, P_1)$.

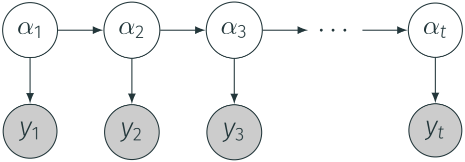


From LGSS model to general state-space model

Def. A General State-Space model is given by:

$$\alpha_t \,|\, \alpha_{t-1} \sim q(\alpha_t \,|\, \alpha_{t-1})$$
$$y_t \,|\, \alpha_t \sim g(y_t \,|\, \alpha_t)$$

and initial distribution $\alpha_1 \sim q(\alpha_1)$.



Thm. The joint-smoothing distribution is given by

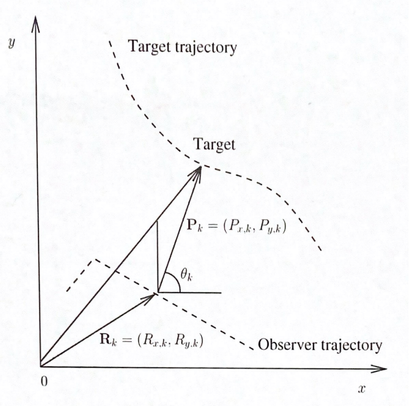
$$p(\alpha_{1:n} \,|\, y_{1:n}) = \frac{q(\alpha_1) g(y_1 \,|\, \alpha_1) \prod_{i=2}^{n} q(\alpha_i \,|\, \alpha_{i-1}) g(y_i \,|\, \alpha_i)}{L_n(y_{1:n})},$$

Example: Bearings-only Tracking

$$\alpha_k = A\alpha_{k-1} + R\eta_k,$$
$$y_k = \arctan\left(\frac{P_{y,k} - R_{y,k}}{P_{x,k} - R_{x,k}}\right) + \sigma_\varepsilon \varepsilon_k,$$

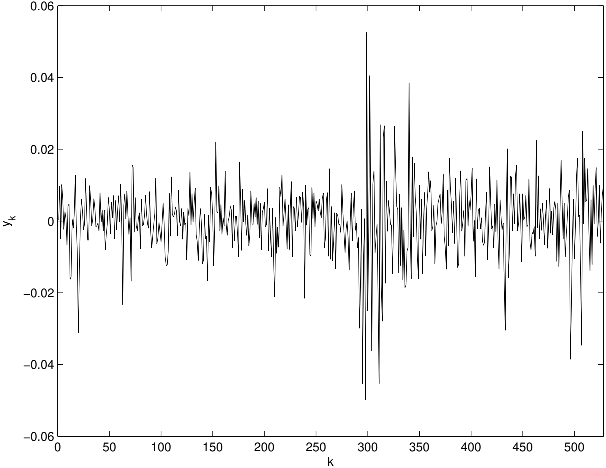
where $\alpha_k = (P_{x,k}, \dot{P}_{x,k}, P_{y,k}, \dot{P}_{y,k})^\top$
and

$$A = \begin{pmatrix} 1 & T & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & T \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad R = \begin{pmatrix} T^2/2 & 0 \\ T & 0 \\ 0 & T^2/2 \\ 0 & T \end{pmatrix}$$



Example: Stochastic Volatility

$$
\begin{aligned}
\alpha_k &= a\alpha_{k-1} + \sigma_\eta \eta_k, & \eta_k &\sim \mathcal{N}(0, \sigma_\eta^2) \\
y_k &= b \exp(\alpha_k/2)\varepsilon_k, & \varepsilon_k &\sim \mathcal{N}(0, \sigma_\varepsilon^2)
\end{aligned}
$$



Our Goal

- Given a time-series $y_{1:n}$ we are interested in:
  - Estimate the filter distributions.
  - Estimate the parameters.
- For the non-Linear models our aim is to estimate the expected values

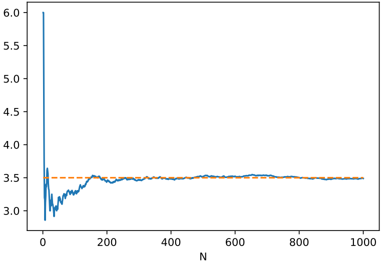
$$\mathbb{E}[h(\alpha_t) \mid y_{1:t}] = \int h(\alpha_t) p(\alpha_t \mid y_{1:t}) \mathrm{d}\alpha_t,$$

  where h is some function of interest.

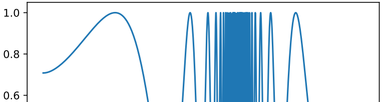
Monte Carlo and Importance Sampling

The Monte Carlo Method

- For non-linear / non-Gaussian models **exact** calculations of the filter distribution is **not possible**.
- Instead we use the Monte Carlo method:
    - Sample $x^i \sim p(x)$ for $i = 1, \ldots, N$
    - Then $\hat{h} = \frac{1}{N} \sum_{i=1}^{N} h(x^i)$ is an estimate of $\mathbb{E}[h(x)] = \int h(x)p(x)\mathrm{d}x$



1. `x = np.random.randint(1,7,size = N)`
2. `est = np.mean(x)`



Importance Sampling

- Sometimes sampling from $p(x)$ is difficult/impossible.
- It might be easier to sample form a distribution $f(x)$.
- Assume that $f(x) = 0 \Rightarrow p(x) = 0$.
- We have that

$$\mathbb{E}_p[h(x)] = \int h(x)p(x)\mathrm{d}x = \int h(x)p(x)\frac{f(x)}{f(x)}\mathrm{d}x = \mathbb{E}_f\left[h(x)\frac{p(x)}{f(x)}\right]$$

- A Monte Carlo estimator would then become:
  1. Draw $x^i \sim f(x)$, for $i = 1, \ldots, N$
  2. Calculate $\omega^i = p(x^i)/f(x^i)$
  3. Estimate $\hat{h} = \frac{1}{N}\sum_{i=1}^{N} \omega^i h(x^i)$
- Known as importance sampling

Importance Sampling

- Often $p(x)$ is only known up to a normalizing constant $p(x) = z(x)/c$ where the constant $c = \int z(x)\mathrm{d}x$ is unknown.
- We can stil perform importance sampling in the following way:
    1. Draw $x^i \sim f(x)$, for $i = 1, \ldots, N$.
    2. Calculate $\omega^i = z(x^i)/f(x^i)$
    3. Estimate $\hat{h} = \Omega^{-1} \sum_{i=1}^{N} \omega^i h(x^i)$, where $\Omega = \sum_{i=1}^{N} \omega^i$.
- Notice that:

$$\frac{1}{N} \sum_{i=1}^{N} \omega^i h(x^i) \to c \cdot \mathbb{E}_p[h(x)]$$

$$\frac{1}{N} \sum_{i=1}^{N} \omega^i \to c.$$

- We get an estimate of the normalizing constant.

Importance Sampling in SSM

Def. A General State-Space model is given by:

$$\alpha_t \,|\, \alpha_{t-1} \sim q(\alpha_t \,|\, \alpha_{t-1})$$
$$y_t \,|\, \alpha_t \sim g(y_t \,|\, \alpha_t)$$

and initial distribution $\alpha_1 \sim q(\alpha_1)$.

Thm. The joint-smoothing distribution is given by

$$p(\alpha_{1:n} \,|\, y_{1:n}) = \frac{q(\alpha_1) g(y_1 \,|\, \alpha_1) \prod_{i=2}^{n} q(\alpha_i \,|\, \alpha_{i-1}) g(y_i \,|\, \alpha_i)}{L_n(y_{1:n})},$$

where $L_n(y_{1:n}) = \int q(\alpha_1) g(y_1 \,|\, \alpha_1) \prod_{i=2}^{n} q(\alpha_i \,|\, \alpha_{i-1}) g(y_i \,|\, \alpha_i) \mathrm{d}y_{1:n}$ is the likelihood.

We wish to sample from $p(\alpha_{1:n} \,|\, y_{1:n})$ using importance sampling.

Sequential Importance Sampling

- Target this using importance sampling:
  - Assume that we have generated $(\alpha^i_{1:n})^N_{i=1}$ from $f(\alpha_{1:n})$ such that

$$\sum_{i=1}^{N} \frac{\omega^i_n}{\Omega_n} h(\alpha^i_{1:n}) \approx \mathbb{E}[h(\alpha_{1:n}) \mid y_{1:n}]$$

  - To go to $n+1$ we do the following for each $i = 1, 2, \ldots, N$:
    - Draw $\alpha^i_{n+1} \sim f(\alpha_{n+1} \mid \alpha^i_{1:n})$
    - Set $\alpha^i_{1:n+1} = (\alpha^i_{1:n}, \alpha^i_{n+1})$
    - Set $\omega^i_{n+1} = \frac{q(\alpha^i_{n+1} \mid \alpha^i_n) g(y_{n+1} \mid \alpha^i_n)}{f(\alpha^i_{n+1} \mid \alpha^i_{1:n})} \times \omega^i_n$.
- This gives us sequential importance sampling (SIS) where:

$$\sum_{i=1}^{N} \frac{\omega^i_{n+1}}{\Omega_{n+1}} h(\alpha_{1:n+1}) \approx \mathbb{E}[h(\alpha_{1:n+1}) \mid y_{1:n+1}]$$

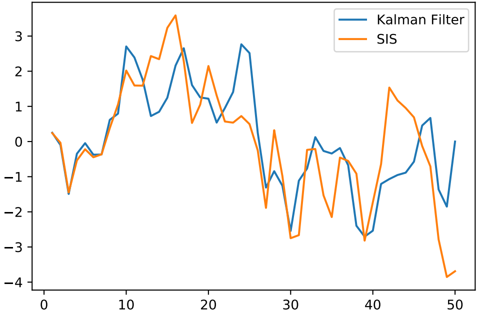
$$\frac{1}{N}\Omega_{n+1} = \frac{1}{N} \sum_{i=1}^{N} \omega^i_{n+1} \approx L(y_{1:n+1}).$$

Example: Linear Gaussian State Space Model

Def. A Linear Gaussian State-Space (LGSS) model is given by:

$$\alpha_t = T\alpha_{t-1} + R\eta_t, \qquad \eta_t \sim \mathcal{N}(0, Q),$$
$$y_t = Z\alpha_t + \varepsilon_t \qquad \varepsilon_t \sim \mathcal{N}(0, \sigma_\epsilon^2),$$

and initial distribution $\alpha_1 \sim \mathcal{N}(a_1, P_1)$.



Solving the Weight Problem

- Unfortunately, weight degeneracy is a universal problem with the sequential importance sampling algorithm.
- The degeneracy is due to the repeated multiplication used to calculate the weights.
- This drawback prevented the sequential importance sampling algorithm from being practically useful during several decades.
- We will now discuss a solution to this problem: sequential importance sampling with resampling (SISR)

Interlude: IS with resampling

- Having a weighted sample $(x^i, \omega^i)_{i=1}^N$ approximating p. We can get a **uniformly weighted sample** by **resampling**, with replacement new variables $(\tilde{x}^i)_{i=1}^N$ from $(x^i)_{i=1}^N$ according to the weights $(\omega^i)_{i=1}^N$
- We get that $\tilde{x}^i = x^j$ with probability $\frac{\omega^j}{\Omega}$.
- This does **not** add bias to the estimator.
- The resampled estimator is

$$\frac{1}{N}\sum_{i=1}^{N} h(\tilde{x}^i) \approx \mathbb{E}_p[h(x)]$$

SIS with resampling

- A simple – but revolutionary! – idea: duplicate/kill particles with large/small weights!
- The most natural such selection is to draw new particles $(\tilde{\alpha}^i_{1:n})^N_{i=1}$ among the SIS-produced $(\alpha^i_{1:n})^N_{i=1}$ with probabilities by the normalized importance weights.
- Formally, for $i = 1, 2, \ldots, N$

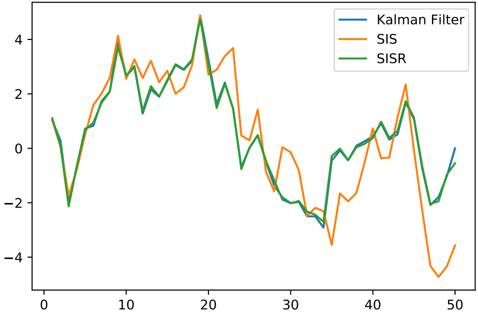
$$\tilde{\alpha}^i_{1:n} = \alpha^j_{1:n} \quad \text{w. pr.} \quad \frac{\omega^j_n}{\Omega_n}$$

Example: Linear Gaussian State Space Model

Def. A Linear Gaussian State-Space (LGSS) model is given by:

$$\alpha_t = T\alpha_{t-1} + R\eta_t, \qquad \eta_t \sim \mathcal{N}(0, Q),$$
$$y_t = Z\alpha_t + \varepsilon_t \qquad \varepsilon_t \sim \mathcal{N}(0, \sigma_\epsilon^2),$$

and initial distribution $\alpha_1 \sim \mathcal{N}(a_1, P_1)$.



Particle Filter:

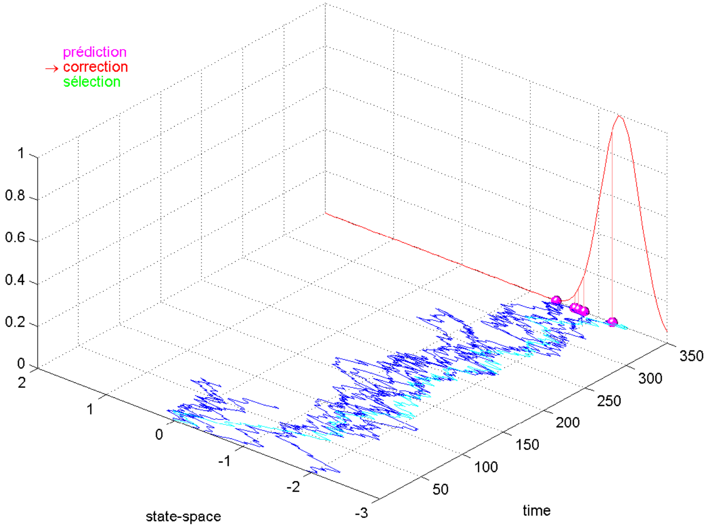
Draw $\alpha_1^i \sim f(\alpha_1)$
Set $\omega_1^i = \frac{q(\alpha_1^i)g(y_1 \mid \alpha_1^i)}{f(\alpha_1^i)}$
Set $\Omega_1 = \sum_{i=1}^N \omega_1^i$
for $t = 2, 3, \ldots, n$ **do**
  Draw $I^i = j$ w. pr. $\frac{\omega_{t-1}^j}{\Omega_{t-1}}$
  Draw $\alpha_t^i \sim f(\alpha_t \mid \alpha_{1:t-1}^{I^i})$
  Set $\omega_t^i = \frac{q(\alpha_t^i \mid \alpha_{t-1}^{I^i})g(y_t \mid \alpha_t^i)}{f(\alpha_t^i \mid \alpha_{1:t-1}^{I^i})}$
  Set $\alpha_{1:t}^i = (\alpha_{1:t-1}^{I^i}, \alpha_t^i)$
  Set $\Omega_t = \sum_{i=1}^N \omega_t^i$
end for

Algorithm: Bootstrap Particle Filter

Bootstrap Particle Filter:

Draw $\alpha_1^i \sim q(\alpha_1)$
Set $\omega_1^i = g(y_1 \mid \alpha_1^i)$
Set $\Omega_1 = \sum_{i=1}^{N} \omega_1^i$
for $t = 2, 3, \ldots, n$ **do**
    Draw $I^i = j$ w. pr. $\frac{\omega_{t-1}^j}{\Omega_{t-1}}$
    Draw $\alpha_t^i \sim q(\alpha_t \mid \alpha_{t-1}^{I^i})$
    Set $\omega_t^i = g(y_t \mid \alpha_t^i)$
    Set $\alpha_{1:t}^i = (\alpha_{1:t-1}^{I^i}, \alpha_t^i)$
    Set $\Omega_t = \sum_{i=1}^{N} \omega_t^i$
end for

Particle Filter Movie



Summary

- Non-linear/non-Gaussian components in state-space models allows for more complicated models.
- Exact calculations is **not possible**, we have to approximate instead.
- The **Monte Carlo** method is a way of approximating distribution by random numbers.
- **Importance sampling** can be used when it is hard/impossible to sample directly from the distribution.
- **Sequential importance sampling**, repeatedly applied importance sampling to a state-space model.
  - Does not work in practice.
  - Weights degenerate.
- Solution is to **resample** the particles.
- The **particle filter** works by combining the sequential importance sampler with a resampling step.
  - The **bootstrap particle filter** is the simplest version, where the particles move according to the dynamics.