Time Series and Sequence Learning

Lecture 6 – Learning of State Space Models

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Summary of Lecture 5: 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 5: 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

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

Summary of Lecture 5: 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:

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

Summary of Lecture 5: 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,

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

Summary of Lecture 5: ARMA model in state space form

State space formulation of ARMA: Consider the ARMA(p, q) model,

$$y_t = \sum_{j=1}^{p} a_j y_{t-j} + \sum_{j=1}^{q} b_j \eta_{t-j} + \eta_t.$$

Let $d = \max(p, q+1)$ and define $a_j = 0$ for $j > p$ and $b_j = 0$ for $j > q$. Then, an equivalent **state space form** is given by

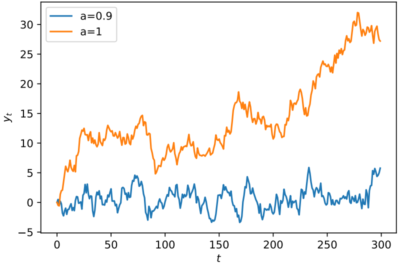
$$\alpha_t = \begin{bmatrix} a_1 & a_2 & \cdots & a_{d-1} & a_d \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix} \alpha_{t-1} + \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \eta_t,$$

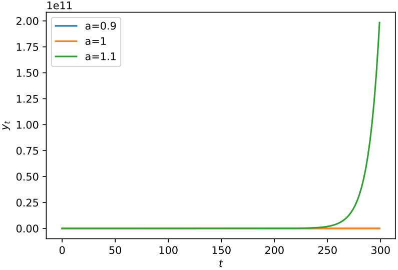
$$y_t = \begin{bmatrix} 1 & b_1 & \cdots & b_{d-2} & b_{d-1} \end{bmatrix} \alpha_t$$

Stability of state space models

ex) Simulation of AR(1)

Simulation of $y_t = ay_{t-1} + \varepsilon_t$





The AR(1) model is:

- Stable if $|a| < 1 \Rightarrow$ converges to stationary
- Marginally stable if $|a| = 1 \Rightarrow$ linear drift
- Unstable if $|a| > 1 \Rightarrow$ exponential explosion

Stability of state space model

Can this be generalized to an LGSS model?

AR(1): $y_t = ay_{t-1} + \varepsilon_t$

LGSS: $\alpha_t = T\alpha_{t-1} + R\eta_t$

Intuitively, the state process is unstable if "size(T)" > 1.

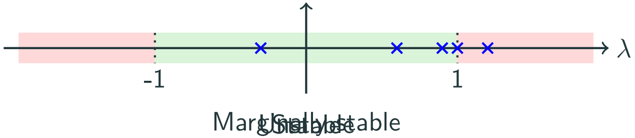
Stability of state space model

Thm. A state space model of dimension $d = \dim(\alpha_t)$ is:

- Stable iff $|\lambda_j| < 1, \quad j = 1, \ldots, d,$
- Marginally stable iff $|\lambda_j| \leq 1, \quad j = 1, \ldots, d,$
- Unstable iff $|\lambda_j| > 1$ for any $j = 1, \ldots, d,$

where λ_j, $j = 1, \ldots, d$ are the **eigenvalues of T.**

If all eigenvalues are real numbers,

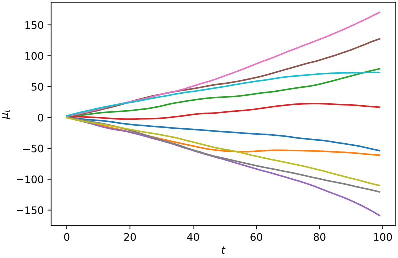


ex) Eigenvalues of linear trend model

Linear trend model:

$$\alpha_t = \overbrace{\begin{bmatrix} 2 & -1 \\ 1 & 0 \end{bmatrix}}^{F} \alpha_{t-1} + \overbrace{\begin{bmatrix} 1 \\ 0 \end{bmatrix}}^{R} \zeta_t$$

$$\mu_t = \underbrace{\begin{bmatrix} 1 & 0 \end{bmatrix}}_{Z} \alpha_t$$



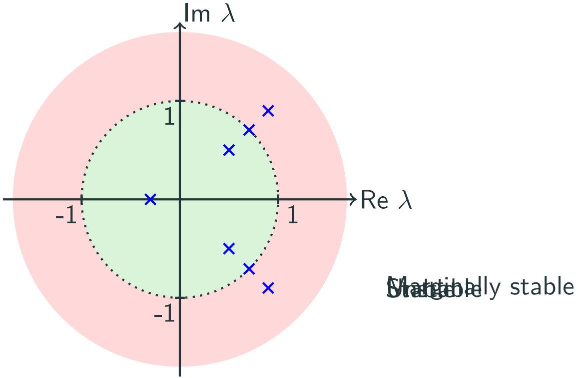
Check for stability by computing the eigenvalues

$$\text{eig}(F) \Rightarrow \lambda_1 = \lambda_2 = 1.$$

The trend model is **marginally stable!**

Note. The eigenvalues can be complex numbers in general. Thus, the stability condition reads

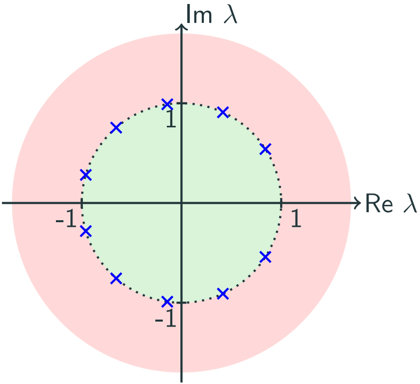
all eigenvalues of T are within the unit circle in the complex plane.



ex) Eigenvalues of seasonal model

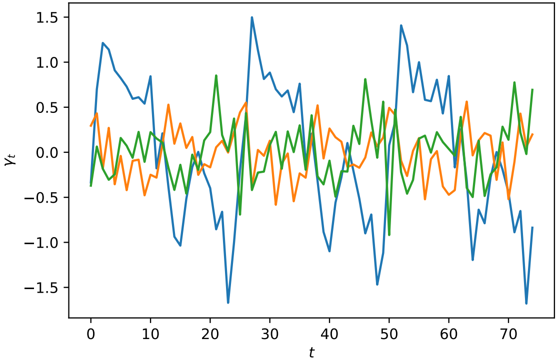
Seasonal model:

$$T = \begin{bmatrix} -1 & -1 & \cdots & -1 & -1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$



The seasonal model is **marginally stable!**

ex) Sample trajectories for seasonal model



Stability of structural time series

The structural time series models that we have proposed are

designed to be marginally stable!

Marginal stability results in desirable properties:

- Real eigenvalues $\lambda_j = 1 \Rightarrow$ polynomial drift/trend.
- Complex eigenvalues with $|\lambda_j| = 1 \Rightarrow$ periodicity/seasonality.

Likelihood estimation

Recap: The log-likelihood of the local level model

The Local Level Model given by

$$y_t = \mu_t + \varepsilon_t, \qquad \varepsilon_t \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma_\varepsilon^2)$$

$$\mu_{t+1} = \mu_t + \eta_{t+1}, \qquad \eta_{t+1} \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma_\eta^2)$$

and initial distribution $\mu_1 \sim \mathcal{N}(a_1, P_1)$

Log-Likelihood Given a sequence $y_{1:n}$ the **log-likelihood** is given by

$$\begin{aligned} \ell(\theta) &= \log p_\theta(y_1) + \sum_{t=2}^{n} \log p_\theta(y_t \mid y_{1:t-1}) \\ &= -\frac{n}{2} \log 2\pi - \frac{1}{2} \sum_{t=1}^{n} \left(\log F_{t \mid t-1}(\theta) + \frac{(y_t - \hat{\mu}_{t \mid t-1}(\theta))^2}{F_{t \mid t-1}(\theta)} \right) \end{aligned}$$

Log-likelihood of general SSM

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

As in the local level model we write,

$$\ell(\theta) = \log p_\theta(y_1) + \sum_{t=2}^{n} \log p_\theta(y_t \mid y_{1:t-1})$$

Remains to find the distribution $y_t \mid y_{1:t-1}$.

Calculating the log-likelihood

We again need to look at the distribution of $y_t \mid y_{1:t-1}$.

Gaussian distribution $\Rightarrow$ find mean and variance.

$$
\begin{aligned}
\mathbb{E}[y_t \mid y_{1:t-1}] &= \mathbb{E}[Z\alpha_t + \varepsilon_t \mid y_{1:t-1}] = Z\hat{\alpha}_{t|t-1} = \hat{y}_{t|t-1} \\
\mathrm{Var}[y_t \mid y_{1:t-1}] &= \mathrm{Var}[Z\alpha_t + \varepsilon_t \mid y_{1:t-1}] \\
&= Z\,\mathrm{Var}[\alpha_t \mid y_{1:t-1}]Z^\mathsf{T} + \sigma_\epsilon^2 \\
&= ZP_{t|t-1}Z^\mathsf{T} + \sigma_\epsilon^2 = F_{t|t-1}
\end{aligned}
$$

This gives us

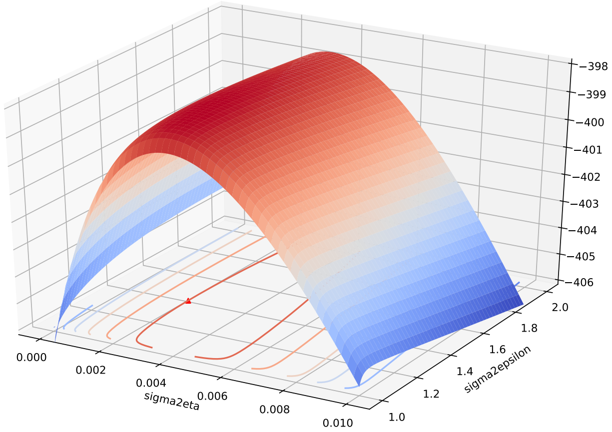
$$
\log p_{\theta}(y_t \mid y_{1:t-1}) = \text{const} - \frac{1}{2}\left(\log|F_{t|t-1}| + (y_t - \hat{y}_{t|t-1})^\mathsf{T} F_{t|t-1}^{-1}(y_t - \hat{y}_{t|t-1})\right)
$$

and

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

ex) Maximum likelihood in local level model

We return to the example of lecture 4.



Maximum found for $\sigma_\varepsilon^2 = 1.37$ and $\sigma_\eta^2 = 0.002$.

Expectation-Maximization

Another approach to parameter estimation

- Calculating the derivatives of $\ell(\theta)$ is a hard problem.
- If we had access to $\alpha_{1:n}$ it would be much easier.

$$\log p_{\theta}(\alpha_{1:n}, y_{1:n}) = \text{const.} - \frac{1}{2}\sum_{i=1}^{n}[\log|\sigma_{\epsilon}^2| + \log|Q| \\ + (y_i - Z\alpha_i)^{\mathsf{T}}\sigma_{\varepsilon}^{-2}(y_i - Z\alpha_i) \\ + (\alpha_i - T\alpha_{i-1})^{\mathsf{T}}RQ^{-1}R^{\mathsf{T}}(\alpha_i - T\alpha_{i-1})]$$

$$\log p_{\theta}(\alpha_{1:n}, y_{1:n}) = \text{const.} - \frac{1}{2}\sum_{i=1}^{n}[\log|\sigma_{\epsilon}^2| + \log|Q| \\ + \varepsilon_i^{\mathsf{T}}\sigma_{\varepsilon}^{-2}\varepsilon_i + \eta_i^{\mathsf{T}}Q^{-1}\eta_i]$$

$$\varepsilon_i = y_i - Z\alpha_i$$

$$\eta_i = R^{\mathsf{T}}(\alpha_i - T\alpha_{i-1})$$

- Easy to take derivatives of this and maximize.
- Unfortunately we don't know $\alpha_{1:t}$, so can't use this directly.

Expectation-Maximization

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

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

We have that, (using $\mathbb{E}[x^\top A x] = \mathrm{tr}[A\Sigma] + m^\top A m$ when $x \sim \mathcal{N}(m, \Sigma)$)

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

where $\hat{\varepsilon}_{t|n}, \mathrm{Var}[\varepsilon_t \mid y_{1:n}], \hat{\eta}_{t|n}$, and $\mathrm{Var}[\eta_t \mid y_{1:n}]$ are the **smoothed** mean and variances of ε_t and η_t.

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

One Slide on the Proof

The Smoothing Distribution

The smoothing distribution

- **State smoothing** refers to the problem of estimating $\alpha_t \mid y_{1:n}$ for $t < n$.
- Often separated into three classes:
  - **Fixed-interval smoothing**, when n is fixed.
  - **Fixed-point smoothing**, when t is fixed and $n = t+1, t+2, \ldots$.
  - **Fixed-lag smoothing**, when $t = n - \ell$.
- In our case we are interested in the distributions

$$\eta_t \mid y_{1:n} \qquad \varepsilon_t \mid y_{1:n},$$

  this is known as **disturbance smoothing**.
- In the LGSS model the distributions will be **Gaussian**.

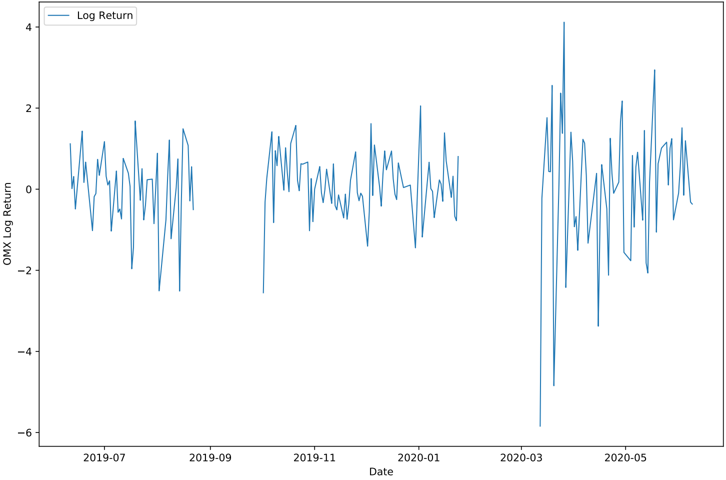
State smoothing

- Smoothing is typically a **two-step** algorithm.
  1. A **filter** is run in the forward direction $(t = 1, 2, \ldots, n)$
  2. A **smoother** is run in the backward direction $(t = n, n-1, \ldots, 1)$
- During the backward pass we will "correct" the filter distributions to the smoothing distributions.
- For $\hat{\alpha}_{t|n}$ we get,

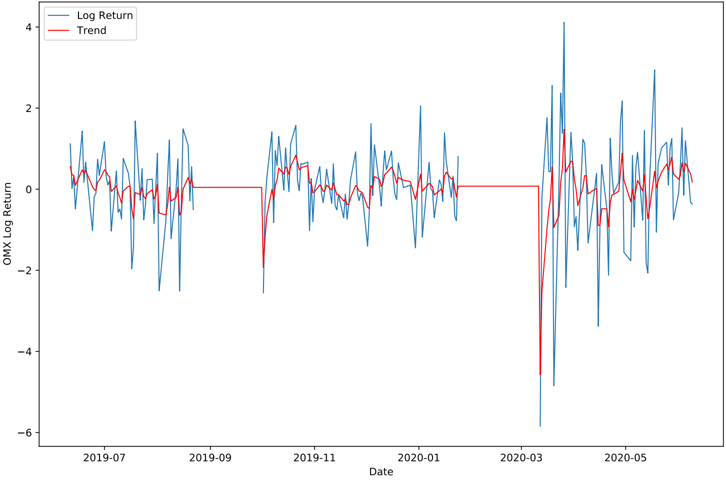
$$
\begin{aligned}
L_t &= T - TK_tZ \\
r_{t-1} &= Z^\top F_{t|t-1}^{-1}(y_t - \hat{y}_{t|t-1}) + L_t^\top r_t \\
\hat{\alpha}_{t|n} &= \hat{\alpha}_{t|t-1} + P_{t|t-1} r_t.
\end{aligned}
$$

Initialized using $r_n = 0$

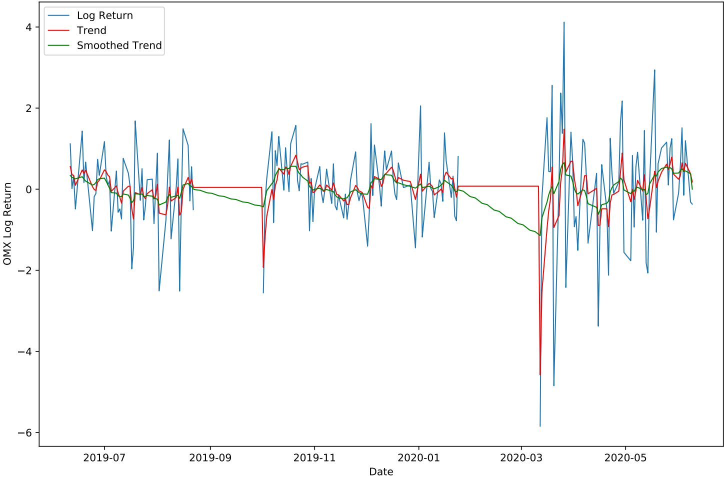
ex) Filter vs. Smoothing distribution



ex) Filter vs. Smoothing distribution



ex) Filter vs. Smoothing distribution



Kalman filter:

1. **Initialize:** Set $\hat{\alpha}_{1|0} = a_1$ and $P_{1|0} = P_1$.
2. **for** $t = 1, 2, \ldots$
   (a) **Measurement update:** // Skip if y_t is unavailable

   · Predict y_t:
   $$\begin{cases} \hat{y}_{t|t-1} = Z\hat{\alpha}_{t|t-1}, \\ F_{t|t-1} = ZP_{t|t-1}Z^\mathsf{T} + \sigma_\varepsilon^2 \end{cases}$$

   · Kalman gain:
   $$K_t = P_{t|t-1}Z^\mathsf{T}F_{t|t-1}^{-1}$$

   · Update filter:
   $$\begin{cases} \hat{\alpha}_{t|t} = \hat{\alpha}_{t|t-1} + K_t(y_t - \hat{y}_{t|t-1}), \\ P_{t|t} = (I - K_tZ)P_{t|t-1} \end{cases}$$

   (b) **Measurement update:**

   · Predict α_t:
   $$\begin{cases} \hat{\alpha}_{t+1|t} = T\hat{\alpha}_{t|t}, \\ P_{t+1|t} = TP_{t|t}T^\mathsf{T} + RQR^\mathsf{T} \end{cases}$$

State smoothing for general SSM

State smoother:

1. **Initialize:** Run the **Kalman Filter** and save the Kalman gains and the predictive distributions.
2. **Initialize:** Set $r_n = 0$ and $N_n = 0$
3. **for** $t = n, n-1, \ldots 1$

· Calculate:

$$\begin{cases} L_t = T - TK_tZ \\ r_{t-1} = Z^{\mathsf{T}} F_{t|t-1}^{-1}(y_t - \hat{y}_{t|t-1}) + L_t^{\mathsf{T}} r_t \\ N_{t-1} = Z^{\mathsf{T}} F_{t|t-1}^{-1} Z + L_t^{\mathsf{T}} N_t L_t \end{cases}$$

· State smoothing:

$$\begin{cases} \hat{\alpha}_{t|n} = \hat{\alpha}_{t|t-1} + P_{t|t-1} r_{t-1} \\ P_{t|n} = P_{t|t-1} - P_{t|t-1} N_{t-1} P_{t|t-1} \end{cases}$$

Disturbance smoothing for general SSM

Disturbance smoother:

1. **Initialize:** Run the **Kalman Filter** and save the Kalman gains and the predictive distributions.
2. **Initialize:** Set $r_n = 0$ and $N_n = 0$
3. **for** $t = n, n-1, \ldots 1$

· Calculate:
$$\begin{cases} C_t = T^\mathsf{T} N_t T \\ D_t = F_{t|t-1}^{-1} + K_t^\mathsf{T} C_t K_t \\ u_t = F_{t|t-1}^{-1}(y_t - \hat{y}_{t|t-1}) - K_t^\mathsf{T} T^\mathsf{T} r_t \end{cases}$$

· Observation noise:
$$\begin{cases} \hat{\varepsilon}_{t|n} = \sigma_\epsilon^2 u_t \\ \mathrm{Var}[\varepsilon_t \mid y_{1:n}] = \sigma_\epsilon^2 - \sigma_\epsilon^2 D_t \sigma_\epsilon^2 \end{cases}$$

· State noise:
$$\begin{cases} \hat{\eta}_{t|n} = QR^\mathsf{T} r_t \\ \mathrm{Var}[\eta_t \mid y_{1:n}] = Q - QR^\mathsf{T} N_t R Q \end{cases}$$

· Time update:
$$\begin{cases} r_{t-1} = Z^\mathsf{T} u_t + T^\mathsf{T} r_t \\ N_{t-1} = Z^\mathsf{T} D_t Z + C_t - Z^\mathsf{T} K_t^\mathsf{T} C_t - C_t K_t Z \end{cases}$$

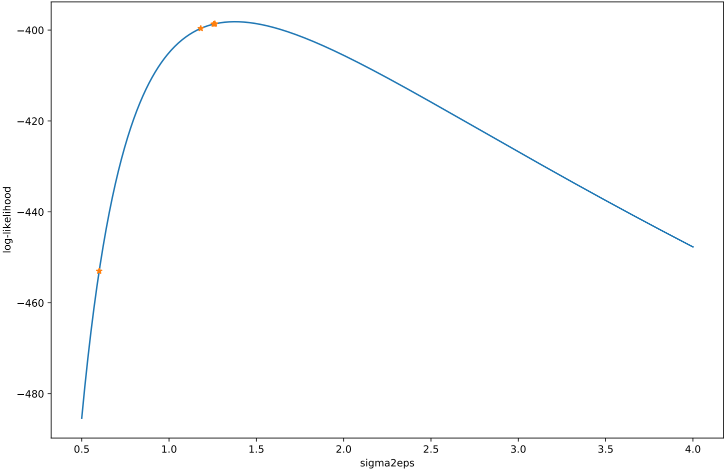
The EM algorithm

- Set an initial parameter value θ_0.
- For $k = 0, 1, \ldots$ do:
    1. Calculate the smoothing distribution using the **disturbance smoother** with the current parameter value θ_k.
    2. Set $\theta_{k+1} = \arg\max \mathcal{Q}(\theta, \theta_k)$.

  Until convergence.

ex) The EM algorithm

Let's look at σ_ε^2 for the local level model.



Summary

A few concepts to summarize lecture 6:

- **Stability:** Results in a stationary state process (possibly after an initial transient). Corresponds to all eigenvalues of T being strictly within the unit circle.
- **Marginal stability:** Results in a state process that grows polynomially and/or shows a non-diminishing periodic pattern. Corresponds to some eigenvalues of T being *on* the unit circle.
- **Log-likelihood:** The log-likelihood for a LGSS can be calculated using the Kalman filter.
- **Expectation-Maximization:** Algorithm for maximum likelihood estimation. Iterates two steps, the **E-step** and **M-step**.
- **State Smoothing:** When estimating the hidden state α_t conditioned on data $y_{1:n}$ for $n > t$.
- **Disturbance Smoothing:** Estimation of the *noise variables* η_t and ε_t conditioned on $y_{1:n}$ for $n > t$.