

Noise Covariance Estimation for an Air Separation Plant

Travis J. Arnold



WISCONSIN
UNIVERSITY OF WISCONSIN-MADISON

Department of Chemical and Biological Engineering

Systems Seminar

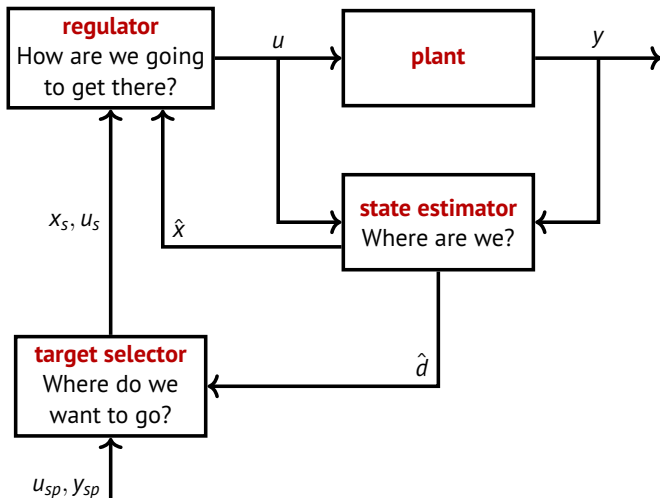
January 20, 2017



MPC Controller



MPC Controller



Motivation



Motivation



- Noise and unmodeled disturbances are ubiquitous in practice in systems and controls engineering.

Motivation



- Noise and unmodeled disturbances are ubiquitous in practice in systems and controls engineering.
- However, dynamic system modeling often focuses primarily on identifying a deterministic (input-output) model.

Motivation



- Noise and unmodeled disturbances are ubiquitous in practice in systems and controls engineering.
- However, dynamic system modeling often focuses primarily on identifying a deterministic (input-output) model.

Quantifying the noises that affect the system is necessary in order to build an optimal state estimator.

Two common assumptions

Two common assumptions

- 1 There are two distinct types of noise: process noise and measurement noise.

Two common assumptions

- 1 There are two distinct types of noise: process noise and measurement noise.
- 2 Noises can be modeled as zero-mean Gaussian random variables.

Two common assumptions

- 1 There are two distinct types of noise: process noise and measurement noise.
- 2 Noises can be modeled as zero-mean Gaussian random variables.

Under these assumptions, the task of noise model identification reduces to identifying the process and measurement noise covariance matrices.

Linear dynamic model

Linear dynamic model

$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \mathbf{B}\mathbf{u}_k + \mathbf{w}_k$$

$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{v}_k$$

$$\mathbf{w}_k \stackrel{iid}{\sim} \mathcal{N}(0, Q)$$

$$\mathbf{v}_k \stackrel{iid}{\sim} \mathcal{N}(0, R)$$

State:

$$\mathbf{x} \in \mathbb{R}^n$$

Input:

$$\mathbf{u} \in \mathbb{R}^m$$

Output:

$$\mathbf{y} \in \mathbb{R}^p$$

Process noise:

$$\mathbf{w} \in \mathbb{R}^n$$

Measurement noise:

$$\mathbf{v} \in \mathbb{R}^p$$

Linear dynamic model

$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \mathbf{B}u_k + \mathbf{w}_k$$

$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{v}_k$$

$$\mathbf{w}_k \stackrel{iid}{\sim} \mathcal{N}(0, Q)$$

$$\mathbf{v}_k \stackrel{iid}{\sim} \mathcal{N}(0, R)$$

State: $\mathbf{x} \in \mathbb{R}^n$

Input: $u \in \mathbb{R}^m$

Output: $\mathbf{y} \in \mathbb{R}^p$

Process noise: $\mathbf{w} \in \mathbb{R}^n$

Measurement noise: $\mathbf{v} \in \mathbb{R}^p$

Our goal:

Linear dynamic model

$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \mathbf{B}u_k + \mathbf{w}_k$$

$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{v}_k$$

$$\mathbf{w}_k \stackrel{iid}{\sim} \mathcal{N}(0, Q)$$

$$\mathbf{v}_k \stackrel{iid}{\sim} \mathcal{N}(0, R)$$

State:

$$\mathbf{x} \in \mathbb{R}^n$$

Input:

$$u \in \mathbb{R}^m$$

Output:

$$\mathbf{y} \in \mathbb{R}^p$$

Process noise:

$$\mathbf{w} \in \mathbb{R}^n$$

Measurement noise:

$$\mathbf{v} \in \mathbb{R}^p$$

Our goal: Given a set of of input-output data $u_{0:N-1}$ and $y_{0:N}$, estimate (Q, R) .

Innovations form



Innovations form



- Estimate the states using a stable (but not necessarily optimal) linear state estimator with gain L , giving estimates:

Innovations form



- Estimate the states using a stable (but not necessarily optimal) linear state estimator with gain L , giving estimates:

$$\hat{x}_{k+1|k} = A\hat{x}_{k|k} + Bu_k$$

$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + L(y_k - C\hat{x}_{k|k-1})$$

Innovations form



- Estimate the states using a stable (but not necessarily optimal) linear state estimator with gain L , giving estimates:

$$\begin{aligned}\hat{x}_{k+1|k} &= A\hat{x}_{k|k} + Bu_k \\ \hat{x}_{k|k} &= \hat{x}_{k|k-1} + L(y_k - C\hat{x}_{k|k-1})\end{aligned}$$

- Define the state estimate error $\varepsilon_k := x_k - \hat{x}_{k|k-1}$ and the L -innovations $\mathcal{Y}_k = y_k - C\hat{x}_{k|k-1}$. These evolve according to



Innovations form

- Estimate the states using a stable (but not necessarily optimal) linear state estimator with gain L , giving estimates:

$$\begin{aligned}\hat{x}_{k+1|k} &= A\hat{x}_{k|k} + Bu_k \\ \hat{x}_{k|k} &= \hat{x}_{k|k-1} + L(y_k - C\hat{x}_{k|k-1})\end{aligned}$$

- Define the state estimate error $\varepsilon_k := x_k - \hat{x}_{k|k-1}$ and the L -innovations $\mathcal{Y}_k = y_k - C\hat{x}_{k|k-1}$. These evolve according to

$$\begin{aligned}\varepsilon_{k+1} &= \bar{A}\varepsilon_k + \bar{G}\bar{w}_k \\ \mathcal{Y}_k &= C\varepsilon_k + v_k\end{aligned}$$

$$\blacktriangleright \bar{A} = A - AL, \quad \bar{G} = [I \quad -AL], \quad \bar{w}_k = \begin{bmatrix} w_k \\ v_k \end{bmatrix}$$



Innovations form

- Estimate the states using a stable (but not necessarily optimal) linear state estimator with gain L , giving estimates:

$$\begin{aligned}\hat{x}_{k+1|k} &= A\hat{x}_{k|k} + Bu_k \\ \hat{x}_{k|k} &= \hat{x}_{k|k-1} + L(y_k - C\hat{x}_{k|k-1})\end{aligned}$$

- Define the state estimate error $\varepsilon_k := x_k - \hat{x}_{k|k-1}$ and the L -innovations $\mathcal{Y}_k = y_k - C\hat{x}_{k|k-1}$. These evolve according to

$$\begin{aligned}\varepsilon_{k+1} &= \bar{A}\varepsilon_k + \bar{G}\bar{w}_k \\ \mathcal{Y}_k &= C\varepsilon_k + v_k\end{aligned}$$

$$\blacktriangleright \bar{A} = A - ALC, \quad \bar{G} = [I \quad -AL], \quad \bar{w}_k = \begin{bmatrix} w_k \\ v_k \end{bmatrix}$$

- $E[\mathcal{Y}_{k+j}\mathcal{Y}_k']$ is the autocovariance of the innovations at lag j .

Optimal estimators produce white innovations



Optimal estimators produce white innovations



$$A = 0.9, \quad C = 1, \quad Q = 1, \quad R = 1$$



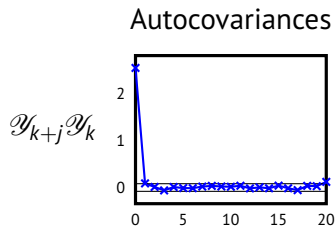
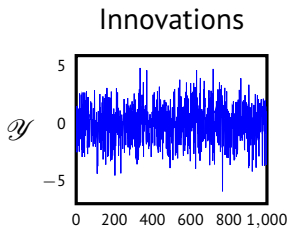
Optimal estimators produce white innovations

$$A = 0.9, \quad C = 1, \quad Q = 1, \quad R = 1$$

Estimator
parameters

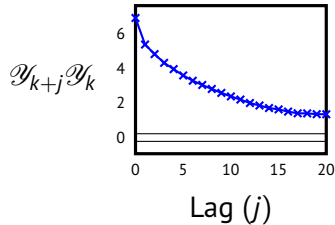
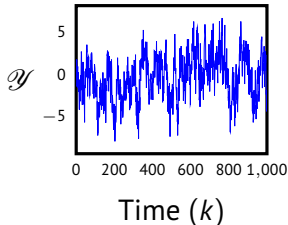
$$Q = 1$$

$$R = 1$$



$$Q = 0$$

$$R = 1$$



The autocovariance least squares (ALS) method



The autocovariance least squares (ALS) method



- Introduced by Odelson et al. (2006), improved by Rajamani and Rawlings (2009) and Zagrobelny and Rawlings (2015).

The autocovariance least squares (ALS) method



- Introduced by Odelson et al. (2006), improved by Rajamani and Rawlings (2009) and Zagrobelny and Rawlings (2015).
- Takes advantage of the linear relationship between the autocovariance matrix $\mathcal{R}_1(M)$ and (Q, R) :

The autocovariance least squares (ALS) method



- Introduced by Odelson et al. (2006), improved by Rajamani and Rawlings (2009) and Zagrobelny and Rawlings (2015).
- Takes advantage of the linear relationship between the autocovariance matrix $\mathcal{R}_1(M)$ and (Q, R) :

$$\mathcal{R}_1(M) := E \begin{bmatrix} \mathcal{Y}_k \mathcal{Y}_k' \\ \dots \\ \mathcal{Y}_{k+M-1} \mathcal{Y}_k' \end{bmatrix} = \mathcal{A} \begin{bmatrix} \text{vec } Q \\ \text{vec } R \end{bmatrix}$$

- ▶ \mathcal{A} is a constant matrix depending on A , C , and L .



The autocovariance least squares (ALS) method

- Introduced by Odelson et al. (2006), improved by Rajamani and Rawlings (2009) and Zagrobelny and Rawlings (2015).
- Takes advantage of the linear relationship between the autocovariance matrix $\mathcal{R}_1(M)$ and (Q, R) :

$$\mathcal{R}_1(M) := E \begin{bmatrix} \mathcal{Y}_k \mathcal{Y}_k' \\ \dots \\ \mathcal{Y}_{k+M-1} \mathcal{Y}_k' \end{bmatrix} = \mathcal{A} \begin{bmatrix} \text{vec } Q \\ \text{vec } R \end{bmatrix}$$

- ▶ \mathcal{A} is a constant matrix depending on A , C , and L .
- We define the ALS problem as

$$\min_{Q,R} \left\| \mathcal{A} \begin{bmatrix} \text{vec } Q \\ \text{vec } R \end{bmatrix} - \hat{\mathcal{R}}_1(M) \right\|^2$$

- ▶ $\hat{\mathcal{R}}_1(M)$ is estimated from the data.

Maximum likelihood estimation



Maximum likelihood estimation



- If we model the initial state as a Gaussian random variable $x_0 \sim \mathcal{N}(\mu, \Sigma)$, we can write down the probability density of the outputs, $p(y_{0:N}; \mu, \Sigma, Q, R)$.

Maximum likelihood estimation



- If we model the initial state as a Gaussian random variable $x_0 \sim \mathcal{N}(\mu, \Sigma)$, we can write down the probability density of the outputs, $p(y_{0:N}; \mu, \Sigma, Q, R)$.
 - ▶ This notation is used to indicate that (μ, Σ, Q, R) parameterize the density of $y_{0:N}$.

Maximum likelihood estimation



- If we model the initial state as a Gaussian random variable $x_0 \sim \mathcal{N}(\mu, \Sigma)$, we can write down the probability density of the outputs, $p(y_{0:N}; \mu, \Sigma, Q, R)$.
 - ▶ This notation is used to indicate that (μ, Σ, Q, R) parameterize the density of $y_{0:N}$.
- The maximum likelihood problem is

$$\max_{\mu, \Sigma, Q, R} p(y_{0:N}; \mu, \Sigma, Q, R)$$

Expectation maximization (EM)



Expectation maximization (EM)



- Iterative scheme for solving maximum likelihood problems.

Expectation maximization (EM)



- Iterative scheme for solving maximum likelihood problems.
- Particularly useful in situations where there are "hidden" states (these are the x 's in our case).

Expectation maximization (EM)



- Iterative scheme for solving maximum likelihood problems.
- Particularly useful in situations where there are "hidden" states (these are the x 's in our case).
- First described by Dempster et al. (1977).

Expectation maximization (EM)



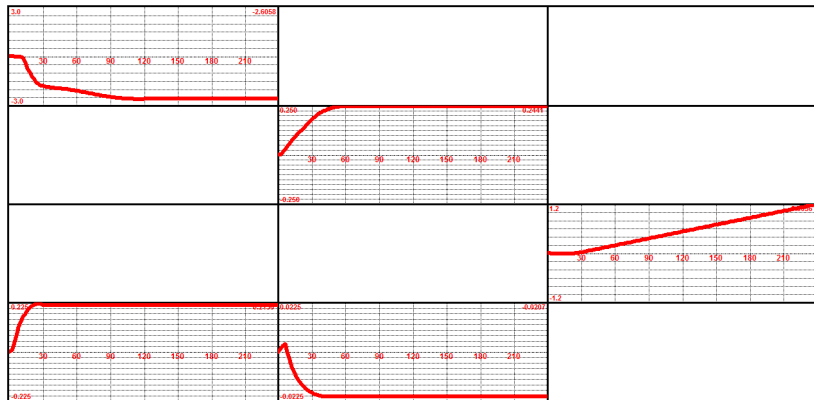
- Iterative scheme for solving maximum likelihood problems.
- Particularly useful in situations where there are "hidden" states (these are the x 's in our case).
- First described by Dempster et al. (1977).
- Shumway and Stoffer (1982) were the first to use an EM scheme to estimate Q and R . Researchers have remained interested: see Li and Badgwell (2014) for a recent example.

Case study: air separation plant





Case study: air separation plant

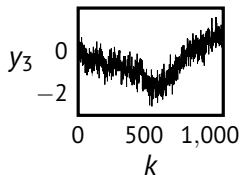
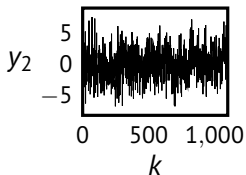
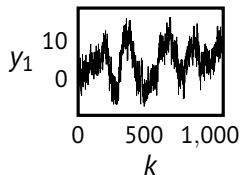
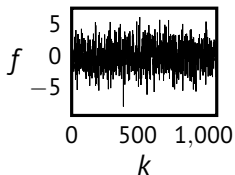
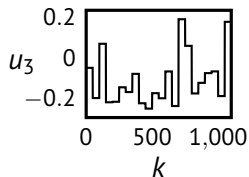
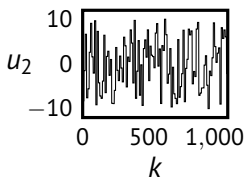
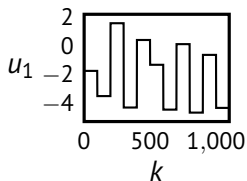


3 inputs, 1 feedforward, 3 outputs. State space realization ($n = 7$) generated with Matlab's system identification toolbox.

Simulated data plots



Simulated data plots

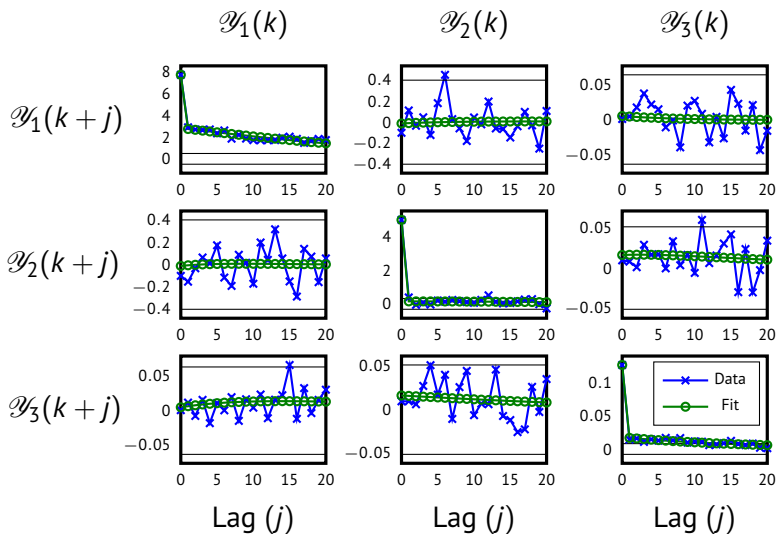


ALS results – fit





ALS results—fit

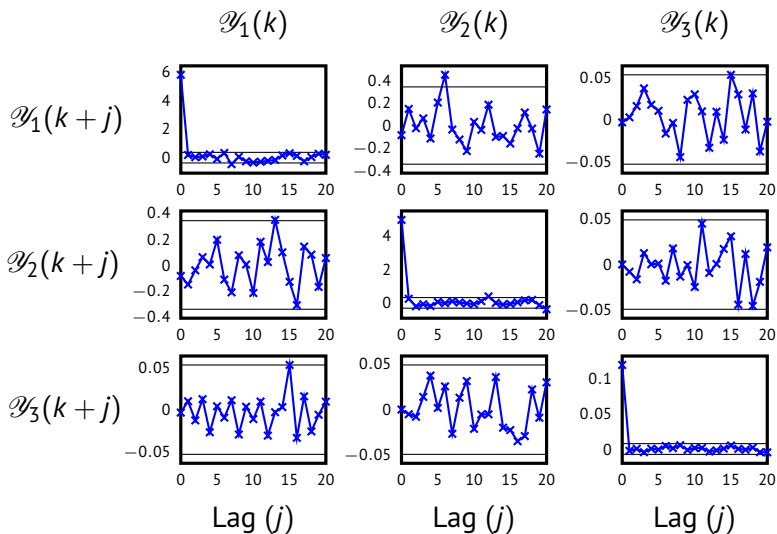


ALS results—new estimator performance





ALS results—new estimator performance



MLE results – objective function



MLE results – objective function

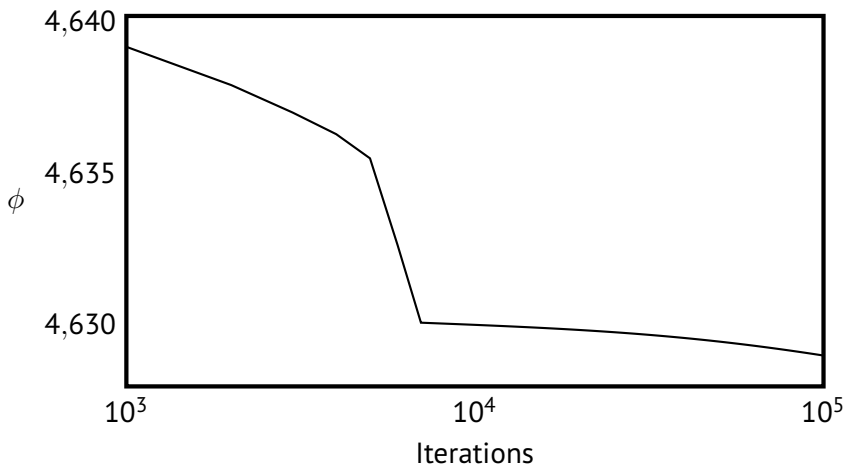


$\phi(\mu, \Sigma, Q, R) = -2 \ln p(y_{0:N}; \mu, \Sigma, Q, R)$ without the constant term.

MLE results – objective function



$\phi(\mu, \Sigma, Q, R) = -2 \ln p(y_{0:N}; \mu, \Sigma, Q, R)$ without the constant term.

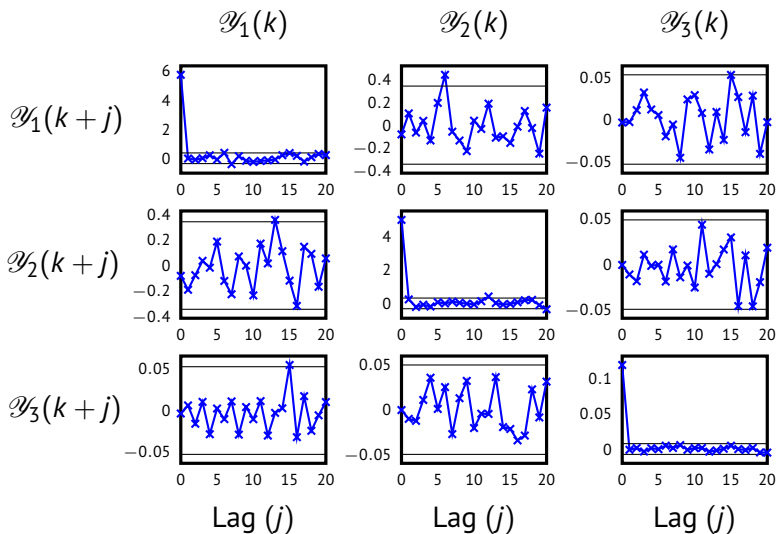


MLE results – estimator performance





MLE results—estimator performance



Comparison of ALS and MLE/EM



Comparison of ALS and MLE/EM



- ALS is a significantly faster algorithm than EM.

Comparison of ALS and MLE/EM



- ALS is a significantly faster algorithm than EM.
 - ▶ EM does not necessarily need to run to full optimality in order to give estimates of Q and R that lead to good estimator.

Comparison of ALS and MLE/EM



- ALS is a significantly faster algorithm than EM.
 - ▶ EM does not necessarily need to run to full optimality in order to give estimates of Q and R that lead to good estimator.
- $\phi(\mu, \Sigma, Q, R)$ is non-increasing with each step of EM, but this does not preclude the possibility of convergence to some stationary point other than the global minimum.

Comparison of ALS and MLE/EM



- ALS is a significantly faster algorithm than EM.
 - ▶ EM does not necessarily need to run to full optimality in order to give estimates of Q and R that lead to good estimator.
- $\phi(\mu, \Sigma, Q, R)$ is non-increasing with each step of EM, but this does not preclude the possibility of convergence to some stationary point other than the global minimum.
- It can be difficult to know when EM has converged because $\phi(\mu, \Sigma, Q, R)$ may be intractable for large data sets.

Comparison of ALS and MLE/EM



- ALS is a significantly faster algorithm than EM.
 - ▶ EM does not necessarily need to run to full optimality in order to give estimates of Q and R that lead to good estimator.
- $\phi(\mu, \Sigma, Q, R)$ is non-increasing with each step of EM, but this does not preclude the possibility of convergence to some stationary point other than the global minimum.
- It can be difficult to know when EM has converged because $\phi(\mu, \Sigma, Q, R)$ may be intractable for large data sets.
- Both algorithms can be modified to encourage the estimate of Q to be low rank:
 - ▶ ALS: Rajamani and Rawlings (2009)
 - ▶ EM: Li and Badgwell (2014)

Acknowledgments



- The authors gratefully acknowledge the financial support of the industrial members of the Texas-Wisconsin-California Control Consortium, and NSF through grant #CTS-1159088.
- Thanks to Dr. Gangshi Hu from Praxair for providing an industrial model to use.

Further reading I



- A. P. Dempster, N. M. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the EM algorithm. *J. Roy. Stat. Soc. Ser. B*, 39:1–38, 1977.
- W. Li and T. A. Badgwell. Structured covariance estimation for state prediction. In *53rd IEEE Conference on Decision and Control*, pages 296–303, Los Angeles, CA, December 15–17 2014.
- B. J. Odelson, M. R. Rajamani, and J. B. Rawlings. A new autocovariance least-squares method for estimating noise covariances. *Automatica*, 42(2):303–308, February 2006.
- M. R. Rajamani and J. B. Rawlings. Estimation of the disturbance structure from data using semidefinite programming and optimal weighting. *Automatica*, 45(1):142–148, 2009.

Further reading II



- R. H. Shumway and D. S. Stoffer. An approach to time series smoothing and forecasting using the EM algorithm. *J. Time Series Anal.*, 3:253–264, 1982.
- M. A. Zagrobelny and J. B. Rawlings. Practical improvements to autocovariance least-squares. *AIChE J.*, 61:1840–1855, 2015.

Questions?

$$y_{0:N} \sim \mathcal{N}(m, P)$$

$$m = \mathbb{A}_0 \mu + \mathbb{B} U_{0:N-1}$$

$$P = \mathbb{A}_0 \Sigma \mathbb{A}_0' + \mathbb{A} (I_M \otimes Q) \mathbb{A}' + (I_{M+1} \otimes R)$$

$$U_{0:N-1} = [u_0 \cdots u_{N-1}]$$

$$\mathbb{A}_0 = \begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^N \end{bmatrix} \quad \mathbb{A} = \begin{bmatrix} 0 & & & & \\ C & & & & \\ CA & C & & & \\ \vdots & \vdots & \ddots & & \\ CA^{N-1} & CA^{N-2} & \cdots & C \end{bmatrix}$$

$$\mathbb{B} = \begin{bmatrix} 0 & & & & \\ CB & & & & \\ CAB & CB & & & \\ \vdots & \vdots & \ddots & & \\ CA^{N-1}B & CA^{N-2}B & \cdots & CB \end{bmatrix}$$

- E-step:

$$G(\mu, \Sigma, Q, R) = E_{x_{0:N}|y_{0:N}}[\ln p(x_{0:N}, y_{0:N}; \mu, \Sigma, Q, R)]$$

Take the conditional expectation of $\ln p(x_{0:N}, y_{0:N}; \mu, \Sigma, Q, R)$ given $y_{0:N}$ where $(\hat{\mu}_n, \hat{\Sigma}_n, \hat{Q}_n, \hat{R}_n)$ determine the conditional density of $x_{0:N}$. This requires that we run the Kalman smoother.

- M-step:

$$(\hat{\mu}_{n+1}, \hat{\Sigma}_{n+1}, \hat{Q}_{n+1}, \hat{R}_{n+1}) = \arg \min_{\mu, \Sigma, Q, R} G(\mu, \Sigma, Q, R)$$