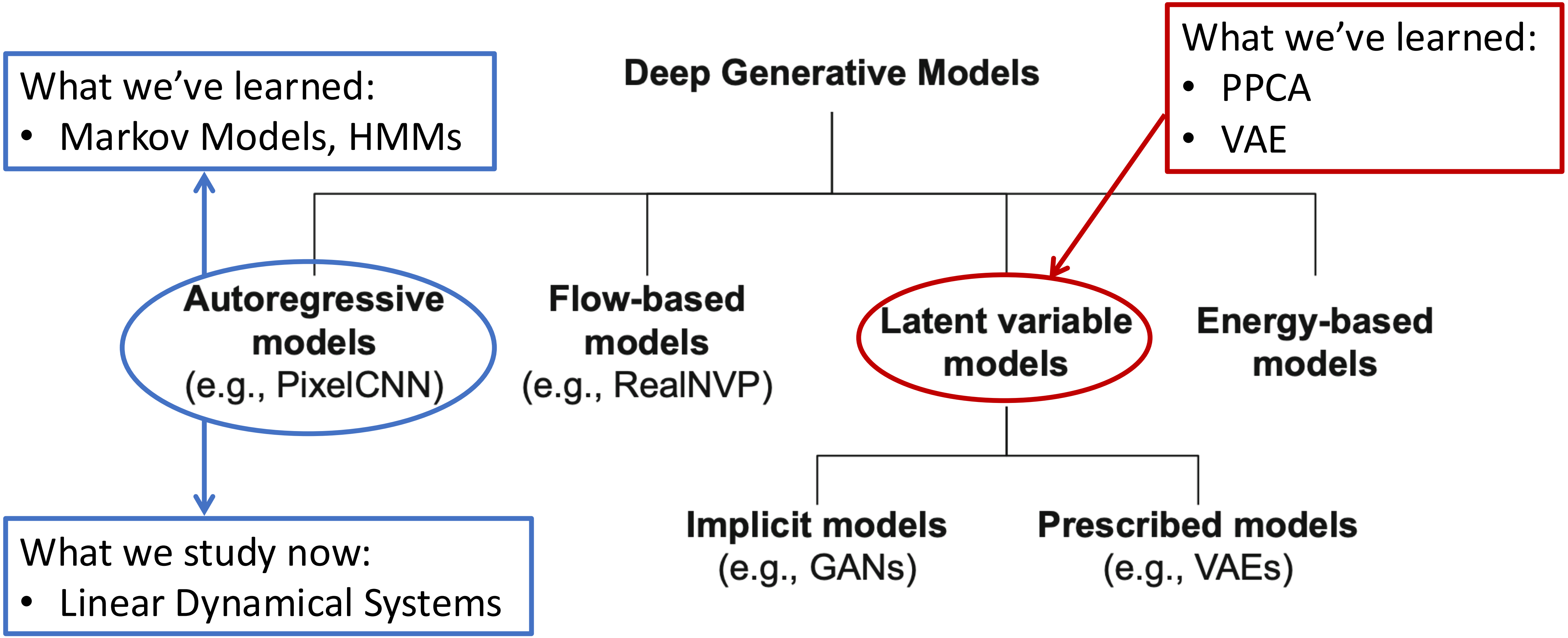
Deep Generative Models: Linear Dynamical Systems

Fall Semester 2024

René Vidal
Director of the Center for Innovation in Data Engineering and Science (IDEAS),
Rachleff University Professor, University of Pennsylvania
Amazon Scholar & Chief Scientist at NORCE

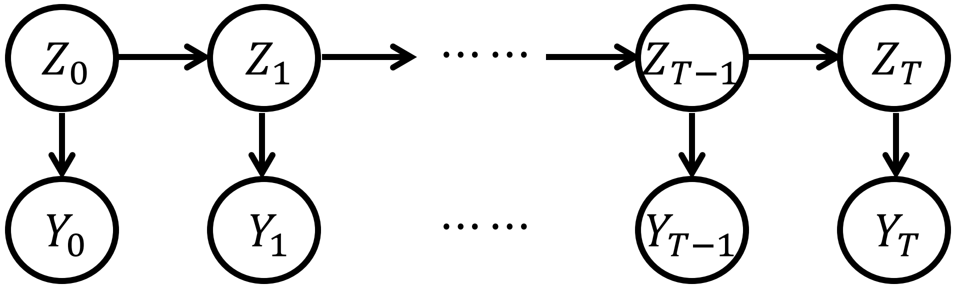
Penn
UNIVERSITY of PENNSYLVANIA

Taxonomy of Generative Models



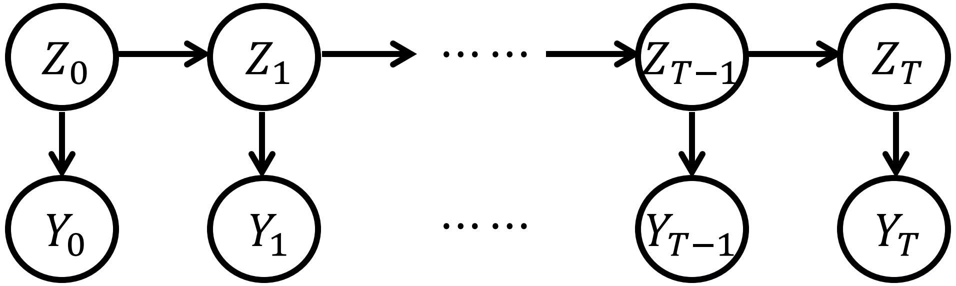
HMMs and Linear Dynamical Systems

Hidden Markov Models (HMMs)



- Hidden state Z_t and observation Y_t are discrete random scalar variables
- State transition and emission are discrete

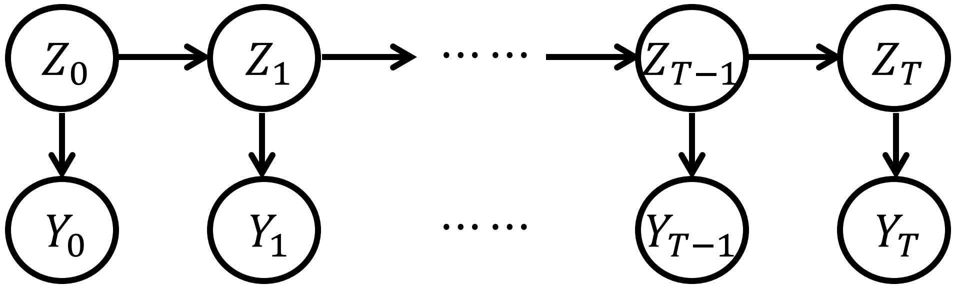
Linear Dynamical Systems (LDSs)



- Hidden state Z_t and observation Y_t are continuous (random) vectors
- State transition and emission are linear

Linear Dynamical Systems

Linear Dynamical Systems (LDSs)



- Hidden state Z_t and observation Y_t are continuous (random) vectors
- State transition and emission are linear

Model Parameters:
- $\theta := (\pi_0, \Sigma_0, A, Q, C, R)$

d: state dimension
D: output dimension

$S_0 \in \mathbb{R}^{d\times d}$
$S_0 \succ 0$

$A \in \mathbb{R}^{d\times d}$
$C \in \mathbb{R}^{D\times d}$

$Q \in \mathbb{R}^{d\times d}$
$Q \succ 0$

$R \in \mathbb{R}^{D\times D}$
$R \succ 0$

- Initial Distribution:

$$\mathbb{P}(Z_0) = \mathcal{N}(\pi_0, \Sigma_0)$$

- State Transition:

$$\mathbb{P}(Z_t | z_{t-1}) = \mathcal{N}(Az_{t-1}, Q) \xrightarrow{\text{Why}}$$

this implies "Markov Property"

- State Emission:

$$\mathbb{P}(Y_t | z_t) = \mathcal{N}(Cz_t, R) \xrightarrow{\text{Why}}$$

this implies "Output Independence"

Filtering and Smoothing

- P1: Filtering. Given θ and $(y_0, \dots, y_t)$, infer the current state z_t, that is to compute
$$p_\theta(z_t | y_0, \dots, y_t)$$
  - e.g., what is the current state of the missile given its position over some past time?
- P2: Smoothing. Given θ and $(y_0, \dots, y_T)$, infer the past state z_t, that is to compute
$$p_\theta(z_t | y_0, \dots, y_T)$$
  - e.g., where did the missile originate given we observed it over some time?
- Remark. You may find P1 and P2 familiar
  - In HMMs, we solved them via recursively updating $\alpha_j(t), \gamma_j(t)$

Background

- Before solving the filtering and smoothing problem, we will study (review) some basic properties about LDSs and Gaussian variables

Law of Total Expectation and of Total Variance

- We will heavily use the following basic results:
  - Law of Total Expectation (LoTE)

$$\mathbb{E}[x] = \mathbb{E}_y\big[\mathbb{E}_x[x|y]\big]$$

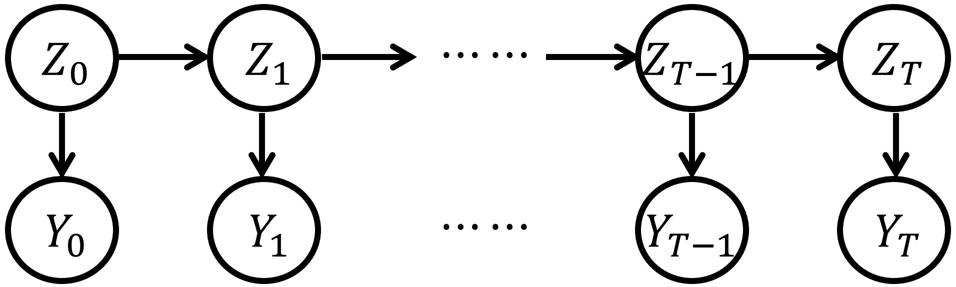
  - Law of Total Covariance (LoTC)

$$\mathrm{Cov}(x) = \mathbb{E}[\mathrm{Cov}(x|y)] + \mathrm{Cov}(\mathbb{E}[x|y])$$

$$\boxed{\begin{aligned}\mathrm{Cov}(x,y) &\coloneqq \mathbb{E}[(x-\mathbb{E}[x])(y-\mathbb{E}[y])^\top] \\ \mathrm{Cov}(x) &\coloneqq \mathrm{Cov}(x,x)\end{aligned}}$$

Basic Properties

Linear Dynamical Systems (LDSs)



- Hidden state Z_t and observation Y_t are continuous (random) vectors
- State transition and emission are linear

Model Parameters:
- $\theta \coloneqq (\pi_0, \Sigma_0, A, Q, C, R)$

d: state dimension
D: output dimension

$S_0 \in \mathbb{R}^{d \times d}$
$S_0 \succ 0$

$A \in \mathbb{R}^{d \times d}$
$C \in \mathbb{R}^{D \times d}$

$Q \in \mathbb{R}^{d \times d}$
$Q \succ 0$

$R \in \mathbb{R}^{D \times D}$
$R \succ 0$

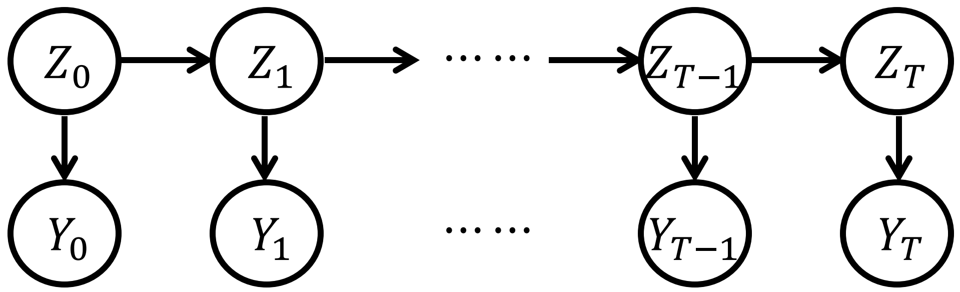
- Equivalent Descriptions:

	Probabilistic Description	Algebraic Description
State Transition	$\mathbb{P}(Z_t \mid z_{t-1}) = \mathcal{N}(Az_{t-1}, Q)$	$Z_t = Az_{t-1} + w_t$ with $w_t \sim \mathcal{N}(0, Q)$
State Emission	$\mathbb{P}(Y_t \mid z_t) = \mathcal{N}(Cz_t, R)$	$Y_t = Cz_t + v_t$ with $v_t \sim \mathcal{N}(0, R)$

- We assume w_t, v_t are independent from each other and independent from z_0

Basic Properties

Linear Dynamical Systems (LDSs)



- Hidden state Z_t and observation Y_t are continuous (random) vectors
- State transition and emission are linear

Model Parameters:

- $\theta \coloneqq (\pi_0, \Sigma_0, A, Q, C, R)$

d: state dimension
D: output dimension

$S_0 \in \mathbb{R}^{d\times d}$
$S_0 \succ 0$

$A \in \mathbb{R}^{d\times d}$
$C \in \mathbb{R}^{D\times d}$

$Q \in \mathbb{R}^{d\times d}$
$Q \succ 0$

$R \in \mathbb{R}^{D\times D}$
$R \succ 0$

- Joint distribution is Gaussian:

Gaussian

$$p_\theta(y_0, \ldots, y_T, z_0, \ldots, z_T) = \boxed{p_\theta(z_0)} \prod_{t=0}^{T} \boxed{p_\theta(y_t|z_t)} \prod_{t=1}^{T} \boxed{p_\theta(z_t|z_{t-1})}$$

- Therefore, "any conditional distribution of it" is Gaussian
  - Vague, but look at your question 1 of homework 1 (next page)

Gaussian Conditioning (Problem 1c & 1d, HW 1)

- If $\begin{bmatrix} a \\ b \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}\right)$, then the conditional distribution $p(a|b)$ is Gaussian with mean $\mu_{a|b}$ and covariance $\Sigma_{a|b}$ given by

$$\mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(b - \mu_b)$$

original mean & variance of a

correction upon observing b

$$\Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$$

Gaussian Combining (Extension of Problem 1b, HW 1)

Gaussian Combining: If $y = Cz + v$ with $z \sim \mathcal{N}(\mu_z, \Sigma_z)$ and $v \sim \mathcal{N}(0, \Sigma_v)$ then

$$\begin{bmatrix} z \\ y \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_z \\ C\mu_z \end{bmatrix}, \begin{bmatrix} \Sigma_z & \Sigma_z C^\top \\ C\Sigma_z & C\Sigma_z C^\top + R \end{bmatrix} \right)$$

- Proof: The proof is finished by computing the following quantities:
  - $\mathbb{E}[y] = \mathbb{E}_z\left[\mathbb{E}_y[y|z]\right] = \mathbb{E}_z[Cz + v] = \mathbb{E}_z[Cz] = C\mu_z$
  - $\mathrm{Cov}(z, y) = \mathbb{E}[(z - \mu_z)(y - C\mu_z)^\top] = \mathbb{E}[(z - \mu_z)(Cz + v - C\mu_z)^\top] = \Sigma_z C^\top$
  - $\mathrm{Cov}(y) = \mathbb{E}[(y - C\mu_z)(y - C\mu_z)^\top] = \mathbb{E}_z\left[\mathbb{E}_y[(y - C\mu_z)(y - C\mu_z)^\top|z]\right]$

$$= \mathbb{E}_{z,v}[(Cz + v_t - C\mu_z)(Cz + v_t - C\mu_z)^\top]$$

$$= \mathbb{E}_z[(Cz - C\mu_z)(Cz - C\mu_z)^\top] + R$$

$$= C \cdot \mathbb{E}_z[(z - \mu_z)(z - \mu_z)^\top] \cdot C^\top + R = C\Sigma_z C^\top + R$$

Remark. In the proof, LoTE is used at the colored equality

Filtering and Smoothing

- P1: Filtering. Given θ and $(y_0, \dots, y_t)$, compute
$$p_\theta(z_t | y_0, \dots, y_t)$$

- P2: Smoothing. Given θ and $(y_0, \dots, y_T)$, compute
$$p_\theta(z_t | y_0, \dots, y_T)$$

- Since $p_\theta(z_s | y_0, \dots, y_t)$ is Gaussian ($\forall s, t$), so it suffices to compute
$$\hat{z}_{s|t} := \mathbb{E}[z_s | y_0, \dots, y_t]$$
$$\hat{\Sigma}_{s|t} := \mathbb{E}\left[\left(z_s - \hat{z}_{s|t}\right)\left(z_s - \hat{z}_{s|t}\right)^\top \middle| y_0, \dots, y_t \right] = \mathrm{Cov}(z_s | y_0, \dots, y_t)$$
  - and we will do so recursively (first for filtering and then for smoothing)

Filtering: Compute $\hat{z}_{0|0}, \hat{\Sigma}_{0|0}$

$\hat{z}_{s|t} := \mathbb{E}[z_s|y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} := \mathrm{Cov}(z_s|y_0, \dots, y_t)$

- P1: Filtering. Given θ and $(y_0, \dots, y_t)$, compute
$$p_\theta(z_t|y_0, \dots, y_t)$$

- Let's begin with the simplest case:
  - What are the mean $\hat{z}_{0|0} = \mathbb{E}[z_0|y_0]$and covariance $\hat{\Sigma}_{0|0} = \mathrm{Cov}(z_0|y_0)$ of z_0 given y_0?

- High-level Idea.

1. find the mean and covariance of $\begin{bmatrix} z_0 \\ y_0 \end{bmatrix}$ via Gaussian combining

2. find the mean $\hat{z}_{0|0}$ and covariance $\hat{\Sigma}_{0|0}$ of $z_0|y_0$ via Gaussian conditioning

$$\mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(b - \mu_b),\ \Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$$

Filtering: Compute $\hat{z}_{0|0}, \hat{\Sigma}_{0|0}$

$\hat{z}_{s|t} := \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} := \mathrm{Cov}(z_s | y_0, \dots, y_t)$

$\mathbb{P}(Z_0) = \mathcal{N}(\pi_0, \Sigma_0)$
$\mathbb{P}(Y_t | z_t) = \mathcal{N}(C z_t, R)$

- Step 1: find the mean and covariance of $\begin{bmatrix} z_0 \\ y_0 \end{bmatrix}$

Gaussian Combining: If $y = Cz + v$ with $z \sim \mathcal{N}(\mu_z, \Sigma_z)$ and $v \sim \mathcal{N}(0, \Sigma_v)$ then

$$\begin{bmatrix} z \\ y \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_z \\ C\mu_z \end{bmatrix}, \begin{bmatrix} \Sigma_z & \Sigma_z C^\top \\ C\Sigma_z & C\Sigma_z C^\top + R \end{bmatrix} \right)$$

- Applying Gaussian combining yields

$$\begin{bmatrix} z_0 \\ y_0 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \pi_0 \\ C\pi_0 \end{bmatrix}, \begin{bmatrix} \Sigma_0 & \Sigma_0 C^\top \\ C\Sigma_0 & C\Sigma_0 C^\top + R \end{bmatrix} \right)$$

Filtering: Compute $\hat{z}_{0|0}$, $\hat{\Sigma}_{0|0}$

$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \dots, y_t)$

- Step 2: apply Gaussian conditioning to $\begin{bmatrix} z_0 \\ y_0 \end{bmatrix}$

$$\begin{bmatrix} z_0 \\ y_0 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \pi_0 \\ C\pi_0 \end{bmatrix}, \begin{bmatrix} \Sigma_0 & \Sigma_0 C^\top \\ C\Sigma_0 & C\Sigma_0 C^\top + R \end{bmatrix} \right)$$

$$\mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(b - \mu_b), \ \Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$$

- We have

$$\hat{z}_{0|0} = \pi_0 + \Sigma_0 C^\top (C\Sigma_0 C^\top + R)^{-1}(y_0 - C\pi_0)$$

$$\hat{\Sigma}_{0|0} = \Sigma_0 - \Sigma_0 C^\top (C\Sigma_0 C^\top + R)^{-1} C\Sigma_0$$

Filtering: From 0 to t

$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \dots, y_t)$

- P1: Filtering. Given θ and $(y_0, \dots, y_t)$, compute
$$p_\theta(z_t | y_0, \dots, y_t)$$

- We've now computed $\hat{z}_{0|0}$ and $\hat{\Sigma}_{0|0}$. This solves P1 for the case $t = 0$

- To proceed, we will update $\hat{z}_{t-1|t-1}, \hat{\Sigma}_{t-1|t-1}$ into $\hat{z}_{t|t}, \hat{\Sigma}_{t|t}$ for every t

The planned computational flow

$$\begin{tikzcd}
\hat{z}_{0|0} \arrow[dr] & \hat{z}_{0|1} & \hat{z}_{0|2} & \hat{z}_{0|3} \\
\hat{z}_{1|0} & \hat{z}_{1|1} \arrow[dr] & \hat{z}_{1|2} & \hat{z}_{1|3} \\
\hat{z}_{2|0} & \hat{z}_{2|1} & \hat{z}_{2|2} \arrow[dr] & \hat{z}_{2|3} \\
\hat{z}_{3|0} & \hat{z}_{3|1} & \hat{z}_{3|2} & \hat{z}_{3|3}
\end{tikzcd}$$

Filtering: From 0 to t

$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \dots, y_t)$

- To compute $\hat{z}_{0|0}$ and $\hat{\Sigma}_{0|0}$, we
  - (Step 0) found the mean and covariance of z_0 (already known)
  - (Step 1) found the mean and covariance of $\begin{bmatrix} z_0 \\ y_0 \end{bmatrix}$ via Gaussian combining
  - (Step 2) found the mean and covariance of $z_0 | y_0$ via Gaussian conditioning

Question: How can we generalize these steps for general t?

- To update $\hat{z}_{t-1|t-1}, \hat{\Sigma}_{t-1|t-1}$ into $\hat{z}_{t|t}, \hat{\Sigma}_{t|t}$, we will condition on $y_0, \dots, y_{t-1}$ and
  - (Step 0) find the mean and covariance of $z_t | y_0, \dots, y_{t-1}$ (using $\hat{z}_{t-1|t-1}, \hat{\Sigma}_{t-1|t-1}$)
  - (Step 1) find the mean and covariance of $\begin{bmatrix} z_t \\ y_t \end{bmatrix} | y_0, \dots, y_{t-1}$ via Gaussian combining
  - (Step 2) find the mean and covariance of $z_t | y_t, y_0, \dots, y_{t-1}$ via Gaussian conditioning

Step 0 and conditioning on $y_0, \dots, y_{t-1}$ are the only differences
- You should be able to figure out all the details without looking at the rest slides

Filtering: Compute $\hat{z}_{t|t}, \hat{\Sigma}_{t|t}$

$\hat{z}_{s|t} := \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} := \mathrm{Cov}(z_s | y_0, \dots, y_t)$

$\mathbb{P}(Z_t | z_{t-1}) = \mathcal{N}(A z_{t-1}, Q)$

- Step 0: find the mean and covariance of $z_t | y_0, \dots, y_{t-1}$
  - By definition, this is to compute $\hat{z}_{t|t-1}, \hat{\Sigma}_{t|t-1}$

- We have

$$\hat{z}_{t|t-1} = \mathbb{E}[z_t | y_0, \dots, y_{t-1}] = \mathbb{E}_{z_{t-1}}\left[\mathbb{E}_{z_t}[z_t | z_{t-1}, y_0, \dots, y_{t-1}]\right]$$
$$= \mathbb{E}[A z_{t-1} | y_0, \dots, y_{t-1}] = A \hat{z}_{t-1|t-1}$$

$$\hat{\Sigma}_{t|t-1} = \mathbb{E}\left[(z_t - \hat{z}_{t|t-1})(z_t - \hat{z}_{t|t-1})^\top \middle| y_0, \dots, y_{t-1}\right] = \cdots = A \hat{\Sigma}_{t-1|t-1} A^\top + Q$$

similar to how we computed $\mathrm{Cov}(y)$ in the proof of Gaussian combining

Filtering: Compute $\hat{z}_{t|t}, \hat{\Sigma}_{t|t}$

$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \dots, y_t)$

$\hat{z}_{t|t-1} = A\hat{z}_{t-1|t-1}$
$\hat{\Sigma}_{t|t-1} = A\hat{\Sigma}_{t-1|t-1}A^\top + Q$

$\hat{z}_{0|-1} \coloneqq \pi_0, \ \hat{\Sigma}_{0|-1} \coloneqq \Sigma_0$

- Step 1: find the mean and covariance of $\begin{bmatrix} z_t \\ y_t \end{bmatrix} | y_0, \dots, y_{t-1}$

- We applied Gaussian combining to $\begin{bmatrix} z_0 \\ y_0 \end{bmatrix}$ and obtained
  - $\begin{bmatrix} z_0 \\ y_0 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \hat{z}_{0|-1} \\ C\hat{z}_{0|-1} \end{bmatrix}, \begin{bmatrix} \hat{\Sigma}_{0|-1} & \hat{\Sigma}_{0|-1}C^\top \\ C\hat{\Sigma}_{0|-1} & C\hat{\Sigma}_{0|-1}C^\top + R \end{bmatrix} \right)$

- Similarly, now, applying Gaussian combining to $\begin{bmatrix} z_t \\ y_t \end{bmatrix} | y_0, \dots, y_{t-1}$ gives:
  - $\begin{bmatrix} z_t \\ y_t \end{bmatrix} | y_0, \dots, y_{t-1} \sim \mathcal{N}\left(\begin{bmatrix} \hat{z}_{t|t-1} \\ C\hat{z}_{t|t-1} \end{bmatrix}, \begin{bmatrix} \hat{\Sigma}_{t|t-1} & \hat{\Sigma}_{t|t-1}C^\top \\ C\hat{\Sigma}_{t|t-1} & C\hat{\Sigma}_{t|t-1}C^\top + R \end{bmatrix} \right)$

Filtering: Compute $\hat{z}_{t|t}, \hat{\Sigma}_{t|t}$

$$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \dots, y_t]$$
$$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \dots, y_t)$$

$$\hat{z}_{t|t-1} = A\hat{z}_{t-1|t-1}$$
$$\hat{\Sigma}_{t|t-1} = A\hat{\Sigma}_{t-1|t-1}A^\top + Q$$

$$\hat{z}_{0|-1} \coloneqq \pi_0, \ \hat{\Sigma}_{0|-1} \coloneqq \Sigma_0$$

- Step 2: apply Gaussian conditioning to $\begin{bmatrix} z_t \\ y_t \end{bmatrix} | y_0, \dots, y_{t-1}$

- We applied Gaussian conditioning to $\begin{bmatrix} z_0 \\ y_0 \end{bmatrix}$ and obtained:

$$\hat{z}_{0|0} = \hat{z}_{0|-1} + \hat{\Sigma}_{0|-1} C^\top \left(C\hat{\Sigma}_{0|-1}C^\top + R\right)^{-1} (y_0 - C\hat{z}_{0|-1})$$
$$\hat{\Sigma}_{0|0} = \hat{\Sigma}_{0|-1} - \hat{\Sigma}_{0|-1} C^\top \left(C\hat{\Sigma}_{0|-1}C^\top + R\right)^{-1} C\hat{\Sigma}_{0|-1}$$

- Similarly, now, applying Gaussian conditioning to $\begin{bmatrix} z_t \\ y_t \end{bmatrix} | y_0, \dots, y_{t-1}$ gives:

$$\hat{z}_{t|t} = \hat{z}_{t|t-1} + \hat{\Sigma}_{t|t-1} C^\top \left(C\hat{\Sigma}_{t|t-1}C^\top + R\right)^{-1} (y_0 - C\hat{z}_{t|t-1})$$
$$\hat{\Sigma}_{t|t} = \hat{\Sigma}_{t|t-1} - \boxed{\hat{\Sigma}_{t|t-1} C^\top \left(C\hat{\Sigma}_{t|t-1}C^\top + R\right)^{-1}} C\hat{\Sigma}_{t|t-1}$$

"Kalman gain matrix". Let us denote it by K_t

Summary: Filtering for LDSs

$$\hat{z}_{s|t} := \mathbb{E}[z_s | y_0, \dots, y_t]$$
$$\hat{\Sigma}_{s|t} := \mathrm{Cov}(z_s | y_0, \dots, y_t)$$

$$\mathbb{P}(Z_0) = \mathcal{N}(\pi_0, \Sigma_0)$$
$$\mathbb{P}(Z_t | z_{t-1}) = \mathcal{N}(A z_{t-1}, Q)$$
$$\mathbb{P}(Y_t | z_t) = \mathcal{N}(C z_t, R)$$

- Putting everything together gives Kalman Filter:

- Initialization: $\hat{z}_{0|-1} := \pi_0, \ \hat{\Sigma}_{0|-1} := \Sigma_0$
- Recursion ($\forall t = 0, \dots, T$):

“Correction”:

$$K_t = \hat{\Sigma}_{t|t-1} C^\top \left(C \hat{\Sigma}_{t|t-1} C^\top + R \right)^{-1}$$
$$\hat{z}_{t|t} = \hat{z}_{t|t-1} + K_t (y_0 - C \hat{z}_{t|t-1})$$
$$\hat{\Sigma}_{t|t} = \hat{\Sigma}_{t|t-1} - K_t C \hat{\Sigma}_{t|t-1}$$

“Prediction”:

$$\hat{z}_{t+1|t} = A \hat{z}_{t|t}$$
$$\hat{\Sigma}_{t+1|t} = A \hat{\Sigma}_{t|t} A^\top + Q$$

How To Derive Kalman Filter

$$\begin{array}{l}
p(z_{t-1} | y_0, \dots, y_{t-1}) \\
\downarrow \text{Prediction} \\
p(z_t | y_0, \dots, y_{t-1}) \\
\downarrow \text{Gaussian Combining} \\
p(z_t, y_t | y_0, \dots, y_{t-1}) \\
\downarrow \text{Gaussian Conditioning} \\
p(z_t | y_0, \dots, y_{t-1}, y_t)
\end{array}$$

Correction

Computational Trajectory of Kalman Filter

$$\begin{tikzcd}
\hat{z}_{0|0} \arrow[d] & \hat{z}_{0|1} & \hat{z}_{0|2} & \hat{z}_{0|3} \\
\hat{z}_{1|0} \arrow[r] & \hat{z}_{1|1} \arrow[d] & \hat{z}_{1|2} & \hat{z}_{1|3} \\
\hat{z}_{2|0} & \hat{z}_{2|1} \arrow[r] & \hat{z}_{2|2} \arrow[d] & \hat{z}_{2|3} \\
\hat{z}_{3|0} & \hat{z}_{3|1} & \hat{z}_{3|2} \arrow[r] & \hat{z}_{3|3}
\end{tikzcd}$$

From Filtering to Smoothing

$$\hat{z}_{s|t} := \mathbb{E}[z_s | y_0, \dots, y_t]$$
$$\hat{\Sigma}_{s|t} := \mathrm{Cov}(z_s | y_0, \dots, y_t)$$

- P1: Filtering. Given θ and $(y_0, \dots, y_t)$, compute
$$p_\theta(z_t | y_0, \dots, y_t)$$
- P2: Smoothing. Given θ and $(y_0, \dots, y_T)$, compute
$$p_\theta(z_t | y_0, \dots, y_T)$$

- Since everything is Gaussian, to solve P2 it suffices to compute $\hat{z}_{t|T}, \hat{\Sigma}_{t|T}$ for all t

What Kalman Filter gives us:

$$\begin{tikzcd}
\hat{z}_{0|0} \arrow[d] & \hat{z}_{0|1} & \hat{z}_{0|2} & \hat{z}_{0|3} \\
\hat{z}_{1|0} \arrow[r] & \hat{z}_{1|1} \arrow[d] & \hat{z}_{1|2} & \hat{z}_{1|3} \\
\hat{z}_{2|0} & \hat{z}_{2|1} \arrow[r] & \hat{z}_{2|2} \arrow[d] & \hat{z}_{2|3} \\
\hat{z}_{3|0} & \hat{z}_{3|1} & \hat{z}_{3|2} \arrow[r] & \hat{z}_{3|3}
\end{tikzcd}$$

What we will do to solve P2:

$$\begin{tikzcd}
\hat{z}_{0|0} \arrow[d] & \hat{z}_{0|1} & \hat{z}_{0|2} & \hat{z}_{0|3} \\
\hat{z}_{1|0} \arrow[r] & \hat{z}_{1|1} \arrow[d] & \hat{z}_{1|2} & \hat{z}_{1|3} \arrow[u] \\
\hat{z}_{2|0} & \hat{z}_{2|1} \arrow[r] & \hat{z}_{2|2} \arrow[d] & \hat{z}_{2|3} \arrow[u] \\
\hat{z}_{3|0} & \hat{z}_{3|1} & \hat{z}_{3|2} \arrow[r] & \hat{z}_{3|3} \arrow[u]
\end{tikzcd}$$

Goal: Given $\hat{z}_{t|t}, \hat{\Sigma}_{t|t}$ and $\hat{z}_{t|t-1}, \hat{\Sigma}_{t|t-1}$ for every t, update $\hat{z}_{t|T}, \hat{\Sigma}_{t|T}$ into $\hat{z}_{t-1|T}, \hat{\Sigma}_{t-1|T}$

Smoothing

$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \ldots, y_t]$
$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \ldots, y_t)$

Goal: Given $\hat{z}_{t|t}$, $\hat{\Sigma}_{t|t}$ and $\hat{z}_{t|t-1}$, $\hat{\Sigma}_{t|t-1}$ for every t, update $\hat{z}_{t|T}$, $\hat{\Sigma}_{t|T}$ into $\hat{z}_{t-1|T}$, $\hat{\Sigma}_{t-1|T}$

- Observation:
  - Since z_{t-1} is independent of $y_t, \ldots y_T$ given z_t, we have

$$p_\theta(z_{t-1} | z_t, y_0, \ldots, y_{t-1}) = p_\theta(z_{t-1} | z_t, y_0, \ldots, y_T)$$

- High-level Idea:
  1. Compute $p_\theta(z_{t-1} | z_t, y_0, \ldots, y_{t-1})$ via Gaussian combining and Gaussian conditioning
     - This gives us $p_\theta(z_{t-1} | z_t, y_0, \ldots, y_T)$
  2. Given $p_\theta(z_{t-1} | z_t, y_0, \ldots, y_T)$, update $\hat{z}_{t|T}$, $\hat{\Sigma}_{t|T}$ into $\hat{z}_{t-1|T}$, $\hat{\Sigma}_{t-1|T}$ via LoTE and LoTC

Smoothing

$$\mathbb{P}(Z_t|z_{t-1}) = \mathcal{N}(Az_{t-1}, Q)$$

$$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s|y_0, \dots, y_t]$$
$$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s|y_0, \dots, y_t)$$

- Step 1: Compute $p_\theta(z_{t-1}|z_t, y_0, \dots, y_{t-1})$

Gaussian Combining: If $y = Cz + v$ with $z \sim \mathcal{N}(\mu_z, \Sigma_z)$ and $v \sim \mathcal{N}(0, \Sigma_v)$ then

$$\begin{bmatrix} z \\ y \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_z \\ C\mu_z \end{bmatrix}, \begin{bmatrix} \Sigma_z & \Sigma_z C^\top \\ C\Sigma_z & C\Sigma_z C^\top + R \end{bmatrix}\right)$$

Gaussian Conditioning: $\mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(b - \mu_b),\ \Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$

- Step 1.1: Applying Gaussian combining to $\begin{bmatrix} z_{t-1} \\ z_t \end{bmatrix} |y_0, \dots, y_{t-1}$ gives:

$$\begin{bmatrix} z_{t-1} \\ z_t \end{bmatrix} |y_0, \dots, y_{t-1} \sim \mathcal{N}\left(\begin{bmatrix} \hat{z}_{t-1|t-1} \\ \hat{z}_{t|t-1} \end{bmatrix}, \begin{bmatrix} \hat{\Sigma}_{t-1|t-1} & \hat{\Sigma}_{t-1|t-1}A^\top \\ A\hat{\Sigma}_{t-1|t-1} & \hat{\Sigma}_{t|t-1} \end{bmatrix}\right)$$

$$\hat{\Sigma}_{t|t-1} = A\hat{\Sigma}_{t-1|t-1}A^\top + Q$$

- Step 1.2: From Gaussian conditioning we see $z_{t-1}|z_t, y_0, \dots, y_{t-1}$ has distribution:

$$\mathcal{N}\left(\hat{z}_{t-1|t-1} + L_{t-1}(z_t - \hat{z}_{t|t-1}), \hat{\Sigma}_{t-1|t-1} - L_{t-1}A\hat{\Sigma}_{t-1|t-1}\right)$$

$$L_{t-1} \coloneqq \hat{\Sigma}_{t-1|t-1}A^\top\hat{\Sigma}_{t|t-1}^{-1}$$

Remark. Note that $L_{t-1}A\hat{\Sigma}_{t-1|t-1} = L_{t-1}\hat{\Sigma}_{t|t-1}L_{t-1}^\top$, so the covariance $\hat{\Sigma}_{t-1|t-1} - L_{t-1}A\hat{\Sigma}_{t-1|t-1}$ is symmetric

Smoothing

$$L_{t-1} = \hat{\Sigma}_{t-1|t-1} A^\top \hat{\Sigma}_{t|t-1}^{-1}$$

$$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \dots, y_t]$$
$$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \dots, y_t)$$

- We have obtained

$$p_\theta(z_{t-1} | z_t, y_0, \dots, y_T) = \mathcal{N}\left(\hat{z}_{t-1|t-1} + L_{t-1}(z_t - \hat{z}_{t|t-1}), \hat{\Sigma}_{t-1|t-1} - L_{t-1} \hat{\Sigma}_{t|t-1} L_{t-1}^\top\right)$$

- Step 2: update $\hat{z}_{t|T}$, $\hat{\Sigma}_{t|T}$ into $\hat{z}_{t-1|T}$, $\hat{\Sigma}_{t-1|T}$ via LoTE and LoTC

$$\begin{aligned}
\hat{z}_{t-1|T} &= \mathbb{E}[z_{t-1} | y_0, \dots, y_T] = \mathbb{E}_{z_t}\left[\mathbb{E}_{z_{t-1}}[z_{t-1} | z_t, y_0, \dots, y_T]\right] \\
&= \mathbb{E}_{z_t}\left[\hat{z}_{t-1|t-1} + L_{t-1}(z_t - \hat{z}_{t|t-1}) | y_0, \dots, y_T\right] \\
&= \hat{z}_{t-1|t-1} + L_{t-1}(\hat{z}_{t|T} - \hat{z}_{t|t-1})
\end{aligned}$$

$$\begin{aligned}
\hat{\Sigma}_{t-1|T} &= \mathrm{Cov}(z_{t-1} | y_0, \dots, y_T) = \mathbb{E}[\mathrm{Cov}(z_{t-1} | z_t, y_0, \dots, y_T)] + \mathrm{Cov}(\mathbb{E}[z_{t-1} | z_t, y_0, \dots, y_T]) \\
&= \mathbb{E}\left[\hat{\Sigma}_{t-1|t-1} - L_{t-1} \hat{\Sigma}_{t|t-1} L_{t-1}^\top\right] + \mathrm{Cov}\left(\hat{z}_{t-1|t-1} + L_{t-1}(z_t - \hat{z}_{t|t-1})\right) \\
&= \hat{\Sigma}_{t-1|t-1} - L_{t-1} \hat{\Sigma}_{t|t-1} L_{t-1}^\top + \mathrm{Cov}\left(\hat{z}_{t-1|t-1} + L_{t-1}(z_t - \hat{z}_{t|t-1}) | y_0, \dots, y_T\right) \\
&= \hat{\Sigma}_{t-1|t-1} + L_{t-1}(\hat{\Sigma}_{t|T} - \hat{\Sigma}_{t|t-1}) L_{t-1}^\top
\end{aligned}$$

Summary: Smoothing for LDS

$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \dots, y_t)$

- **Goal**. Given θ and $(y_0, \dots, y_T)$, compute

$$p_\theta(z_t | y_0, \dots, y_T)$$

- **Algorithm** (known as "Rauch-Tung-Striebel smoother").
  1. (Forward Pass) Run Kalman filtering to compute $\hat{z}_{t|t}, \hat{\Sigma}_{t|t}$ and $\hat{z}_{t+1|t}, \hat{\Sigma}_{t+1|t}$ for all t
  2. (Backward Pass) For $t = T, \dots, 1$, compute the following:
     - $L_{t-1} = \hat{\Sigma}_{t-1|t-1} A^\top \hat{\Sigma}_{t|t-1}^{-1}$
     - $\hat{z}_{t-1|T} = \hat{z}_{t-1|t-1} + L_{t-1}\left(\hat{z}_{t|T} - \hat{z}_{t|t-1}\right)$
     - $\hat{\Sigma}_{t-1|T} = \hat{\Sigma}_{t-1|t-1} + L_{t-1}(\hat{\Sigma}_{t|T} - \hat{\Sigma}_{t|t-1}) L_{t-1}^\top$

Remark: L_{t-1} might also be computed in the forward pass

Computational Trajectory of Smoothing:

$$\begin{tikzcd}
\hat{z}_{0|0} \arrow[d] & \hat{z}_{0|1} & \hat{z}_{0|2} & \hat{z}_{0|3} \\
\hat{z}_{1|0} \arrow[r] & \hat{z}_{1|1} \arrow[d] & \hat{z}_{1|2} & \hat{z}_{1|3} \arrow[u] \\
\hat{z}_{2|0} & \hat{z}_{2|1} \arrow[r] & \hat{z}_{2|2} \arrow[d] & \hat{z}_{2|3} \arrow[u] \\
\hat{z}_{3|0} & \hat{z}_{3|1} & \hat{z}_{3|2} \arrow[r] & \hat{z}_{3|3} \arrow[u]
\end{tikzcd}$$

State Estimation and Learning

- Now that we've studied algorithms for filtering and smoothing, we are prepared to perform more complicated tasks

- State Estimation ("Decoding"). Given θ and $(y_0, \dots, y_T)$, solve:

$$\underset{z_0,\dots,z_T}{\operatorname{argmax}}\, p_\theta(z_0, \dots, z_T | y_0, \dots, y_T)$$

- Learning. Given N observations $\{\boldsymbol{y}^{(n)}\}_{n=1}^N$, find best θ:

$$\max_\theta \prod_{n=1}^N p_\theta(\boldsymbol{y}^{(n)})$$

State Estimation

$$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s|y_0, \dots, y_t]$$
$$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s|y_0, \dots, y_t)$$

- State Estimation. Given θ and $(y_0, \dots, y_T)$, solve:

$$\operatorname*{argmax}_{z_0, \dots, z_T} p_\theta(z_0, \dots, z_T | y_0, \dots, y_T)$$

- Solution:
  - Since $p_\theta(z_0, \dots, z_T | y_0, \dots, y_T)$ is Gaussian, the optimal solution to state estimation is

$$\mathbb{E}\left[\begin{bmatrix} z_0 \\ z_1 \\ \vdots \\ z_T \end{bmatrix} \middle| y_0, \dots, y_T \right] = \begin{bmatrix} \mathbb{E}[z_0|y_0, \dots, y_T] \\ \mathbb{E}[z_1|y_0, \dots, y_T] \\ \vdots \\ \mathbb{E}[z_T|y_0, \dots, y_T] \end{bmatrix} = \begin{bmatrix} \hat{z}_{0|T} \\ \hat{z}_{1|T} \\ \vdots \\ \hat{z}_{T|T} \end{bmatrix}$$

  - And then what?

Learning

Model Parameters:
- $\theta := (\pi_0, \Sigma_0, A, Q, C, R)$

- Learning. Given N observations $\{\boldsymbol{y}^{(n)}\}_{n=1}^{N}$, find best θ:

$$\max_{\theta} \prod_{n=1}^{N} p_\theta(\boldsymbol{y}^{(n)})$$

- We are going to apply the EM algorithm (iteration: k):

E-step:

$$q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)}) = p_{\theta^k}(\boldsymbol{z}\,|\boldsymbol{y}^{(n)})$$

M-step:

$$\theta^{k+1} = \mathrm{argmax}_\theta \sum_{n=1}^{N} \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}\left[\log p_\theta(\boldsymbol{y}^{(n)}, \boldsymbol{z})\right]$$

EM (iteration: k)

Model Parameters:
- $\theta := (\pi_0, \Sigma_0, A, Q, C, R)$

E-step:

$$q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)}) = p_{\theta^k}(\boldsymbol{z}\,|\boldsymbol{y}^{(n)})$$

M-step:

$$\theta^{k+1} = \mathrm{argmax}_\theta \sum_{n=1}^{N} \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}\left[\log p_\theta\left(\boldsymbol{y}^{(n)}, \boldsymbol{z}\right)\right]$$

- In deriving the EM algorithm, we will encounter problems of the form:

$$\min_{\Sigma} M \cdot \log\det\Sigma - \sum_{m=1}^{M} \mathrm{tr}(S_m \Sigma^{-1})$$

- In lecture 2 (MLE for Gaussians), we showed that the optimal Σ is $\sum_{m=1}^{M} S_m/M$.

- This fact will be referred to as:

$M \cdot \log\det\Sigma - \sum_{m=1}^{M} \mathrm{tr}(S_m\Sigma^{-1})$ *is minimized at* $\Sigma = \sum_{m=1}^{M} S_m/M$

EM (iteration: k)

$\hat{z}_{s|t} := \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} := \mathrm{Cov}(z_s | y_0, \dots, y_t)$

E-step:
$$q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)}) = p_{\theta^k}(\boldsymbol{z}\,|\boldsymbol{y}^{(n)})$$

M-step:
$$\theta^{k+1} = \mathrm{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}\left[\log p_\theta\left(\boldsymbol{y}^{(n)}, \boldsymbol{z}\right)\right]$$

- In M-step, we will need to compute the expectation $\mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[\cdot]$.
- *"It turns out that"* …… we only needs to compute the following expectations:

$$\mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t]$$
$$\mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_t^\top]$$
$$\mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_{t-1}^\top]$$

- They are respectively equal to:

$$\mathbb{E}_k^{(n)}[z_t] := \mathbb{E}_{\theta^k}\left[z_t | \boldsymbol{y}^{(n)}\right]$$
$$\mathbb{E}_k^{(n)}[z_t z_t^\top] := \mathbb{E}_{\theta^k}\left[z_t z_t^\top | \boldsymbol{y}^{(n)}\right]$$
$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] := \mathbb{E}_{\theta^k}\left[z_t z_{t-1}^\top | \boldsymbol{y}^{(n)}\right]$$

EM (iteration: k)

$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s|y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s|y_0, \dots, y_t)$

E-step:
$$q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)}) = p_{\theta^k}(\boldsymbol{z}\,|\boldsymbol{y}^{(n)})$$

M-step:
$$\theta^{k+1} = \mathrm{argmax}_\theta \textstyle\sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}\left[\log p_\theta(\boldsymbol{y}^{(n)}, \boldsymbol{z})\right]$$

$$\mathbb{E}_k^{(n)}[z_t] \coloneqq \mathbb{E}_{\theta^k}[z_t|\boldsymbol{y}^{(n)}] = \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t]$$
$$\mathbb{E}_k^{(n)}[z_t z_t^\top] \coloneqq \mathbb{E}_{\theta^k}[z_t z_t^\top|\boldsymbol{y}^{(n)}] = \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_t^\top]$$
$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] \coloneqq \mathbb{E}_{\theta^k}[z_t z_{t-1}^\top|\boldsymbol{y}^{(n)}] = \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_{t-1}^\top]$$

- These expectations can all be computed via smoothing using θ^k and $\boldsymbol{y}^{(n)}$.
  - To see this, dropping indices k, n for clarity, we have

$$\mathbb{E}_\theta[z_t|\boldsymbol{y}] = \mathbb{E}_\theta[z_t|y_0, \dots, y_T] = \hat{z}_{t|T}$$
$$\mathbb{E}_\theta[z_t z_t^\top|\boldsymbol{y}] = \mathrm{Cov}(z_t|y_0, \dots, y_T) + \mathbb{E}_\theta[z_t|y_0, \dots, y_T]\mathbb{E}_\theta[z_t^\top|y_0, \dots, y_T]$$
$$= \hat{\Sigma}_{t|T} + \hat{z}_{t|T}\hat{z}_{t|T}^\top$$

- **Your homework is to prove**:

$$\mathbb{E}_\theta[z_t z_{t-1}^\top|\boldsymbol{y}] = L_{t-1}\hat{\Sigma}_{t|T} + \hat{z}_{t|T}\hat{z}_{t-1|T}^\top$$

$L_{t-1} = \hat{\Sigma}_{t-1|t-1}A^\top\hat{\Sigma}_{t|t-1}^{-1}$

E-step (iteration: k)

$L_{t-1} = \hat{\Sigma}_{t-1|t-1} A^\top \hat{\Sigma}_{t|t-1}^{-1}$

$\hat{z}_{s|t} \coloneqq \mathbb{E}[z_s | y_0, \dots, y_t]$
$\hat{\Sigma}_{s|t} \coloneqq \mathrm{Cov}(z_s | y_0, \dots, y_t)$

E-step:
$$q^k(\boldsymbol{z} | \boldsymbol{y}^{(n)}) = p_{\theta^k}(\boldsymbol{z} \,| \boldsymbol{y}^{(n)})$$

M-step:
$$\theta^{k+1} = \mathrm{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z} \sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})} \left[\log p_\theta(\boldsymbol{y}^{(n)}, \boldsymbol{z})\right]$$

- We've just shown that, at iteration k, in the E-step, we can compute the following terms via smoothing for every n:

$$\mathbb{E}_k^{(n)}[z_t] \coloneqq \mathbb{E}_{\theta^k}\left[z_t | \boldsymbol{y}^{(n)}\right] = \mathbb{E}_{\boldsymbol{z} \sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t]$$
$$\mathbb{E}_k^{(n)}[z_t z_t^\top] \coloneqq \mathbb{E}_{\theta^k}\left[z_t z_t^\top | \boldsymbol{y}^{(n)}\right] = \mathbb{E}_{\boldsymbol{z} \sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_t^\top]$$
$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] \coloneqq \mathbb{E}_{\theta^k}\left[z_t z_{t-1}^\top | \boldsymbol{y}^{(n)}\right] = \mathbb{E}_{\boldsymbol{z} \sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_{t-1}^\top]$$

M-step (iteration: k)

$$\mathbb{P}(Z_0) = \mathcal{N}(\pi_0, \Sigma_0)$$
$$\mathbb{P}(Z_t|z_{t-1}) = \mathcal{N}(Az_{t-1}, Q)$$
$$\mathbb{P}(Y_t|z_t) = \mathcal{N}(Cz_t, R)$$

Model Parameters:

- $\theta := (\pi_0, \Sigma_0, A, Q, C, R)$

$$\mathbb{E}_k^{(n)}[z_t] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t]$$
$$\mathbb{E}_k^{(n)}[z_t z_t^\top] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_t^\top]$$
$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_{t-1}^\top]$$

$$\theta^{k+1} = \operatorname{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}\left[\log p_\theta\left(\boldsymbol{y}^{(n)}, \boldsymbol{z}\right)\right]$$

- Observation. In the joint log-likelihood

$$p_\theta(y_0, \dots, y_T, z_0, \dots, z_T) = p_\theta(z_0) \prod_{t=0}^T p_\theta(y_t|z_t) \prod_{t=1}^T p_\theta(z_t|z_{t-1}),$$

  - π_0, Σ_0 only appear in $p_\theta(z_0)$
  - A, Q only appear in $\prod_{t=1}^T p_\theta(z_t|z_{t-1})$
  - C, R only appear in $\prod_{t=0}^T p_\theta(y_t|z_t)$

  - So the objective of the M-step is separable (as in HMMs), this gives … (next page)

M-step (iteration: k)

$$\mathbb{P}(Z_0) = \mathcal{N}(\pi_0, \Sigma_0)$$
$$\mathbb{P}(Z_t|z_{t-1}) = \mathcal{N}(Az_{t-1}, Q)$$
$$\mathbb{P}(Y_t|z_t) = \mathcal{N}(Cz_t, R)$$

Model Parameters:

- $\theta := (\pi_0, \Sigma_0, A, Q, C, R)$

$$\mathbb{E}_k^{(n)}[z_t] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t]$$
$$\mathbb{E}_k^{(n)}[z_t z_t^\top] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_t^\top]$$
$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_{t-1}^\top]$$

$$\theta^{k+1} = \operatorname{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}\left[\log p_\theta\left(\boldsymbol{y}^{(n)}, \boldsymbol{z}\right)\right]$$

- We can therefore decompose M-step into 3 optimization problems (as in HMMs):

M-step (π_0, Σ_0):

$$(\pi_0^{k+1}, \Sigma_0^{k+1}) = \operatorname{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[\log p_\theta(z_0)]$$

M-step (C, R):

$$(C^{k+1}, R^{k+1}) = \operatorname{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}\left[\sum_{t=0}^T \log p_\theta\left(y_t^{(n)} \middle| z_t\right)\right]$$

M-step (A, Q):

$$(A^{k+1}, A^{k+1}) = \operatorname{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}\left[\sum_{t=1}^T \log p_\theta(z_t|z_{t-1})\right]$$

- We will address them one by one next

M-step (π_0, Σ_0)

$$\mathbb{P}(Z_0) = \mathcal{N}(\pi_0, \Sigma_0)$$

$$\mathbb{E}_k^{(n)}[z_t] \coloneqq \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t]$$
$$\mathbb{E}_k^{(n)}[z_t z_t^\top] \coloneqq \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_t^\top]$$
$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] \coloneqq \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_{t-1}^\top]$$

$$(\pi_0^{k+1}, \Sigma_0^{k+1}) = \mathrm{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[\log p_\theta(z_0)]$$

- Since $p_\theta(z_0)$ is Gaussian, we have:

$$\log p_\theta(z_0) \propto -\log\det\Sigma_0 - (z_0 - \pi_0)^\top \Sigma_0^{-1}(z_0 - \pi_0)$$

- And now we get this:

$$(\pi_0^{k+1}, \Sigma_0^{k+1}) = \mathrm{argmin}_\theta\, N\log\det\Sigma_0 + \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[(z_0 - \pi_0)^\top \Sigma_0^{-1}(z_0 - \pi_0)]$$

- This should remind you of the ML estimator for PPCA (Lecture 2)
  - But here we get a weird $\boldsymbol{z} \sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})$, so we will show how to solve it in detail

M-step (π_0, Σ_0)

$$\mathbb{E}_k^{(n)}[z_t] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t]$$
$$\mathbb{E}_k^{(n)}[z_t z_t^\top] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_t^\top]$$
$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] := \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[z_t z_{t-1}^\top]$$

$$(\pi_0^{k+1}, \Sigma_0^{k+1}) = \operatorname{argmin}_\theta N \log\det\Sigma_0 + \sum_{n=1}^N \mathbb{E}_{\boldsymbol{z}\sim q^k(\boldsymbol{z}|\boldsymbol{y}^{(n)})}[(z_0 - \pi_0)^\top \Sigma_0^{-1}(z_0 - \pi_0)]$$

use the definitions of $\mathbb{E}_k^{(n)}[z_0]$ and $\mathbb{E}_k^{(n)}[z_0 z_0^\top]$

$$(\pi_0^{k+1}, \Sigma_0^{k+1}) = \operatorname{argmin}_\theta N \log\det\Sigma_0 + N\pi_0^\top \Sigma_0^{-1}\pi_0 + \sum_{n=1}^N \operatorname{tr}\left(\mathbb{E}_k^{(n)}[z_0 z_0^\top]\Sigma_0^{-1}\right) - 2\sum_{n=1}^N \pi_0^\top \Sigma_0^{-1}\mathbb{E}_k^{(n)}[z_0]$$

- Setting the derivative with respect to π_0 to 0 yields $\pi_0^{k+1} = \dfrac{\sum_{n=1}^N \mathbb{E}_k^{(n)}[z_0]}{N}$
- Substitute this back to the objective and we get:

$$\Sigma_0^{k+1} = \operatorname{argmin}_\theta N \cdot \log\det\Sigma_0 + \sum_{n=1}^N \operatorname{tr}\left(\mathbb{E}_k^{(n)}[z_0 z_0^\top]\Sigma_0^{-1}\right) - N \cdot \operatorname{tr}\left(\pi_0^{k+1}\left(\pi_0^{k+1}\right)^\top \Sigma_0^{-1}\right)$$

$M \cdot \log\det\Sigma - \sum_{m=1}^M \operatorname{tr}(S_m \Sigma^{-1})$ *is minimized at* $\Sigma = \sum_{m=1}^M S_m / M$

$$\Sigma_0^{k+1} = \pi_0^{k+1}\left(\pi_0^{k+1}\right)^\top - \sum_{n=1}^N \frac{\mathbb{E}_k^{(n)}[z_0 z_0^\top]}{N}$$

M-step (C, R)

$$\mathbb{P}(Y_t|z_t) = \mathcal{N}(Cz_t, R)$$

$$\mathbb{E}_k^{(n)}[z_t] \coloneqq \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}[z_t]$$

$$\mathbb{E}_k^{(n)}[z_t z_t^\top] \coloneqq \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}[z_t z_t^\top]$$

$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] \coloneqq \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}[z_t z_{t-1}^\top]$$

$$(C^{k+1}, R^{k+1}) = \operatorname{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}\left[\sum_{t=0}^T \log p_\theta\left(y_t^{(n)}\middle|z_t\right)\right]$$

$p_\theta\left(y_t^{(n)}\middle|z_t\right)$ is Gaussian

$$(C^{k+1}, R^{k+1}) = \operatorname{argmin}_\theta N(T+1)\log\det R + \sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_{z_t\sim q^k(z_t|\mathbf{y}^{(n)})}\left[\left(y_t^{(n)} - Cz_t\right)^\top R^{-1}\left(y_t^{(n)} - Cz_t\right)\right]$$

use the definitions of $\mathbb{E}_k^{(n)}[z_t]$ and $\mathbb{E}_k^{(n)}[z_t z_t^\top]$

$$\min_\theta N(T+1)\log\det R + \sum_{n=1}^N \sum_{t=0}^T \left\{\operatorname{tr}\left(\left(C\mathbb{E}_k^{(n)}[z_t z_t^\top]C^\top + y_t^{(n)}\left(y_t^{(n)}\right)^\top\right)R^{-1} - 2y_t^{(n)}\mathbb{E}_k^{(n)}[z_t]^\top C^\top R^{-1}\right)\right\}$$

- Setting the derivative with respect to C to 0 yields

$$C^{k+1} = \left(\sum_{n=1}^N \sum_{t=0}^T y_t^{(n)}\,\mathbb{E}_k^{(n)}[z_t]^\top\right)\left(\sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_k^{(n)}[z_t z_t^\top]\right)^{-1}$$

Use C^{k+1}

$$\min_\theta N(T+1)\log\det R + \sum_{n=1}^N \sum_{t=0}^T \left\{\operatorname{tr}\left(y_t^{(n)}\left(y_t^{(n)}\right)^\top R^{-1} - y_t^{(n)}\mathbb{E}_k^{(n)}[z_t]^\top (C^{k+1})^\top R^{-1}\right)\right\}$$

$M\cdot\log\det\Sigma - \sum_{m=1}^M \operatorname{tr}(S_m\Sigma^{-1})$ is minimized at $\Sigma = \sum_{m=1}^M S_m/M$

$$R^{k+1} = \frac{\sum_{n=1}^N \sum_{t=0}^T y_t^{(n)}\left(y_t^{(n)}\right)^\top - C^{k+1}\sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_k^{(n)}[z_t]\left(y_t^{(n)}\right)^\top}{N(T+1)}$$

M-step (A, Q)

$$\mathbb{P}(Z_t|z_{t-1}) = \mathcal{N}(Az_{t-1}, Q)$$

$$\mathbb{E}_k^{(n)}[z_t] := \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}[z_t]$$
$$\mathbb{E}_k^{(n)}[z_t z_t^\top] := \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}[z_t z_t^\top]$$
$$\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] := \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}[z_t z_{t-1}^\top]$$

$$(A^{k+1}, Q^{k+1}) = \mathrm{argmax}_\theta \sum_{n=1}^N \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}\left[\sum_{t=1}^T \log p_\theta(z_t|z_{t-1})\right]$$

$p_\theta(z_t|z_{t-1})$ is Gaussian

$$(A^{k+1}, Q^{k+1}) = \mathrm{argmin}_\theta\, NT \log\det Q + \sum_{n=1}^N \sum_{t=1}^T \mathbb{E}_{\mathbf{z}\sim q^k(\mathbf{z}|\mathbf{y}^{(n)})}\left[(z_t - Az_{t-1})^\top Q^{-1}(z_t - Az_{t-1})\right]$$

use the definitions of $\mathbb{E}_k^{(n)}[z_t z_t^\top]$ and $\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top]$

$$\min_\theta NT \log\det Q + \sum_{n=1}^N \sum_{t=1}^T \left\{\mathrm{tr}\left(\left(A\left(\mathbb{E}_k^{(n)}[z_{t-1} z_{t-1}^\top]\right)A^\top + \mathbb{E}_k^{(n)}[z_t z_t^\top]\right)Q^{-1} - 2\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top]A^\top Q^{-1}\right)\right\}$$

- Setting the derivative with respect to A to 0 yields

$$A^{k+1} = \left(\sum_{n=1}^N \sum_{t=1}^T \mathbb{E}_k^{(n)}[z_t z_{t-1}^\top]\right)\left(\sum_{n=1}^N \sum_{t=1}^T \mathbb{E}_k^{(n)}[z_{t-1} z_{t-1}^\top]\right)^{-1}$$

Use A^{k+1}

$$\min_\theta NT \log\det Q + \sum_{n=1}^N \sum_{t=1}^T \left\{\mathrm{tr}\left(\mathbb{E}_k^{(n)}[z_t z_t^\top]Q^{-1} - \mathbb{E}_k^{(n)}[z_t z_{t-1}^\top](A^{k+1})^\top Q^{-1}\right)\right\}$$

$M \cdot \log\det\Sigma - \sum_{m=1}^M \mathrm{tr}(S_m \Sigma^{-1})$ *is minimized at* $\Sigma = \sum_{m=1}^M S_m / M$

$$Q^{k+1} = \frac{\sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_k^{(n)}[z_t z_t^\top] - A^{k+1} \sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_k^{(n)}[z_{t-1} z_t^\top]}{NT}$$

Summary: EM for LDSs (iteration: k)

- $\hat{z}_{s|t} := \mathbb{E}[z_s | y_0, \dots, y_t]$
- $\hat{\Sigma}_{s|t} := \mathrm{Cov}(z_s | y_0, \dots, y_t)$
- $L_{t-1} := \hat{\Sigma}_{t-1|t-1} A^\top \hat{\Sigma}_{t|t-1}^{-1}$

E-step

Given θ^k, for each $\boldsymbol{y}^{(n)}$, use Kalman Filter & Smoothing to compute:

- $\mathbb{E}_k^{(n)}[z_t] := \mathbb{E}_{\theta^k}\left[z_t | \boldsymbol{y}^{(n)}\right]$
- $\mathbb{E}_k^{(n)}[z_t z_t^\top] := \mathbb{E}_{\theta^k}\left[z_t z_t^\top | \boldsymbol{y}^{(n)}\right]$
- $\mathbb{E}_k^{(n)}[z_t z_{t-1}^\top] := \mathbb{E}_{\theta^k}\left[z_t z_{t-1}^\top | \boldsymbol{y}^{(n)}\right]$

add indices n, k

Kalman Filter & Smoothing can compute

- $\mathbb{E}_\theta[z_t | \boldsymbol{y}] = \hat{z}_{t|T}$
- $\mathbb{E}_\theta[z_t z_t^\top | \boldsymbol{y}] = \hat{\Sigma}_{t|T} + \hat{z}_{t|T} \hat{z}_{t|T}^\top$
- $\mathbb{E}_\theta[z_t z_{t-1}^\top | \boldsymbol{y}] = L_{t-1} \hat{\Sigma}_{t|T} + \hat{z}_{t|T} \hat{z}_{t-1|T}^\top$

via forward & backward passes

$$
\begin{tikzcd}
\hat{z}_{0|0} \arrow[d] & \hat{z}_{0|1} & \hat{z}_{0|2} & \hat{z}_{0|3} \\
\hat{z}_{1|0} \arrow[r] & \hat{z}_{1|1} \arrow[d] & \hat{z}_{1|2} & \hat{z}_{1|3} \arrow[u] \\
\hat{z}_{2|1} & \hat{z}_{2|1} \arrow[r] & \hat{z}_{2|2} \arrow[d] & \hat{z}_{2|3} \arrow[u] \\
\hat{z}_{1|2} & \hat{z}_{3|1} & \hat{z}_{3|2} \arrow[r] & \hat{z}_{3|3} \arrow[u]
\end{tikzcd}
$$

M-step

Update parameters:

- $\pi_0^{k+1} = \dfrac{\sum_{n=1}^N \mathbb{E}_k^{(n)}[z_0]}{N}$
- $\Sigma_0^{k+1} = \pi_0^{k+1}\left(\pi_0^{k+1}\right)^\top - \sum_{n=1}^N \dfrac{\mathbb{E}_k^{(n)}[z_0 z_0^\top]}{N}$
- $C^{k+1} = \left(\sum_{n=1}^N \sum_{t=0}^T y_t^{(n)} \, \mathbb{E}_k^{(n)}[z_t]^\top\right)\left(\sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_k^{(n)}[z_t z_t^\top]\right)^{-1}$
- $R^{k+1} = \dfrac{\sum_{n=1}^N \sum_{t=0}^T y_t^{(n)} \left(y_t^{(n)}\right)^\top - C^{k+1} \sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_k^{(n)}[z_t] \left(y_t^{(n)}\right)^\top}{N(T+1)}$
- $A^{k+1} = \left(\sum_{n=1}^N \sum_{t=1}^T \mathbb{E}_k^{(n)}[z_t z_{t-1}^\top]\right)\left(\sum_{n=1}^N \sum_{t=1}^T \mathbb{E}_k^{(n)}[z_{t-1} z_{t-1}^\top]\right)^{-1}$
- $Q^{k+1} = \dfrac{\sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_k^{(n)}[z_t z_t^\top] - A^{k+1} \sum_{n=1}^N \sum_{t=0}^T \mathbb{E}_k^{(n)}[z_{t-1} z_t^\top]}{NT}$

Model Parameters:

- $\theta := (\pi_0, \Sigma_0, A, Q, C, R)$

$$\mathbb{P}(Z_0) = \mathcal{N}(\pi_0, \Sigma_0)$$
$$\mathbb{P}(Z_t | z_{t-1}) = \mathcal{N}(A z_{t-1}, Q)$$
$$\mathbb{P}(Y_t | z_t) = \mathcal{N}(C z_t, R)$$