Computer Science

CSC535: Probabilistic Graphical Models

Dynamical Systems

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(Some material from Prof. Kobus Barnard)

Outline

- Sequence Models / Hidden Markov Models
- Linear Dynamical Systems
- LDS Extensions

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- Sequence Models
- Linear Dynamical Systems
- LDS Extensions

Sequential data

Sequential data has order, and the order matters.

What has happened, informs what will happen.

Sequential data is everywhere.

Examples:

- spoken language (word production)
- written language (sentence level statistics)
- weather
- human movement
- stock market data
- genomes

Sequential data

Graphical models for such data?

The complexity of the representation seems to increase with time.

Observations over time tend to depend on the past.

We can simply life by assuming that the distant past does not matter.

If we assume that history does not matter other than the immediate previous entity, we have a first order Markov model.

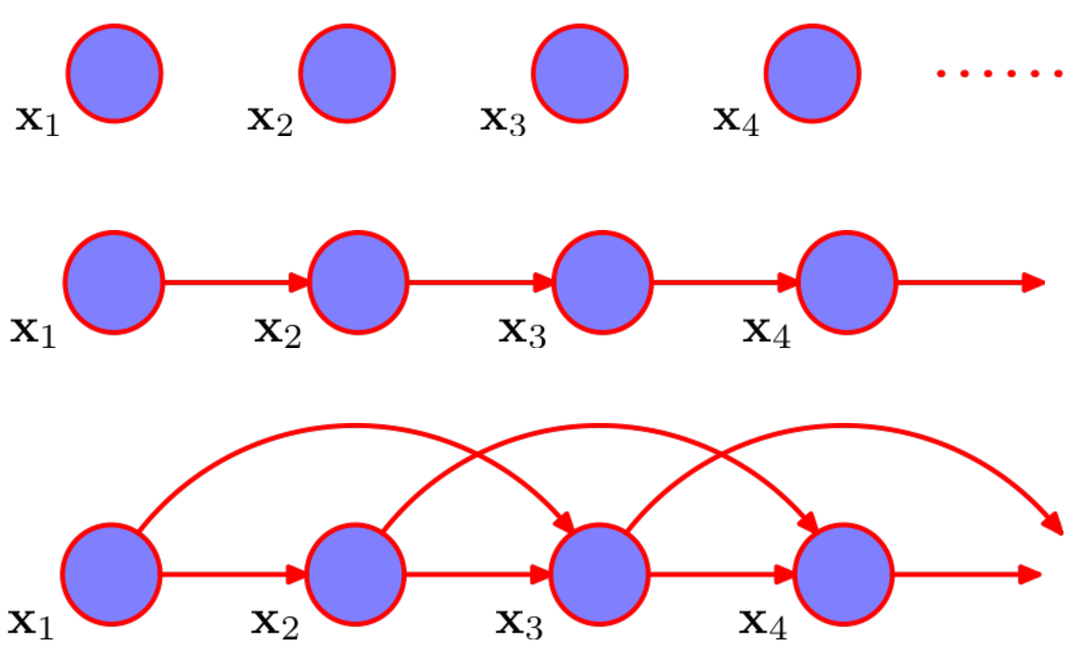
If what happens now depends on two previous entities, we have a second order Markov model.

Markov chains

Zeroth order

First order

Second order

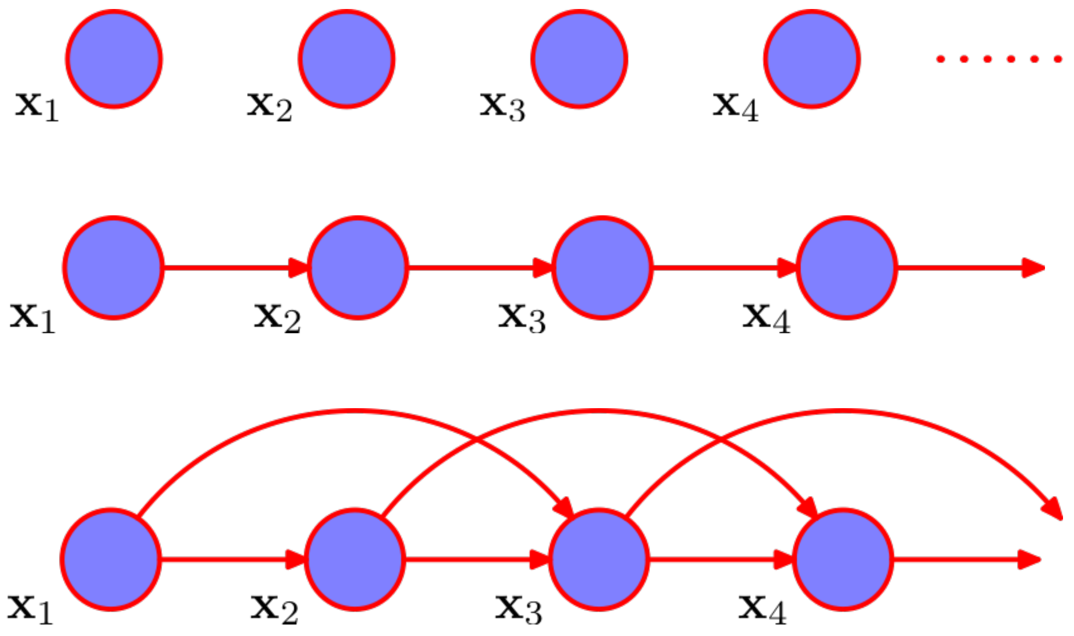


Markov chains

Zeroth order

First order

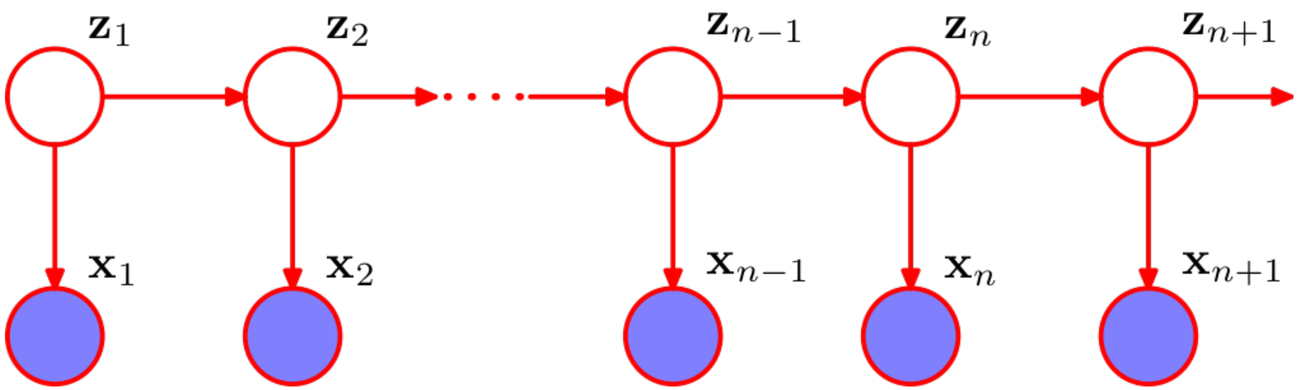
Second order



Notice that this plan has arrows **from** data-this complicates model specification

Hidden Markov Model (HMM)

Introducing latent state simplifies modeling data likelihood…



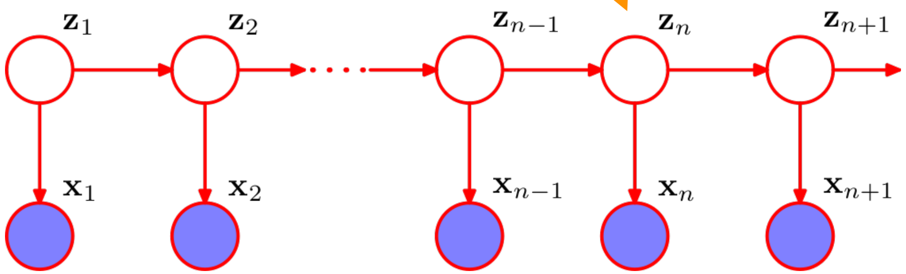
Intuition Temporal extension of mixture model

- Data clusters into hidden "states" Z at each time
- Hidden state encodes important part of history
- Markov chain models transitions among clusters

Markovian assumptions

The basic HMM is like a mixture model, with the mixture component being used for the current observations depends on the last previous component.

$$z_{n+1} \perp z_{n-1} \mid z_n$$

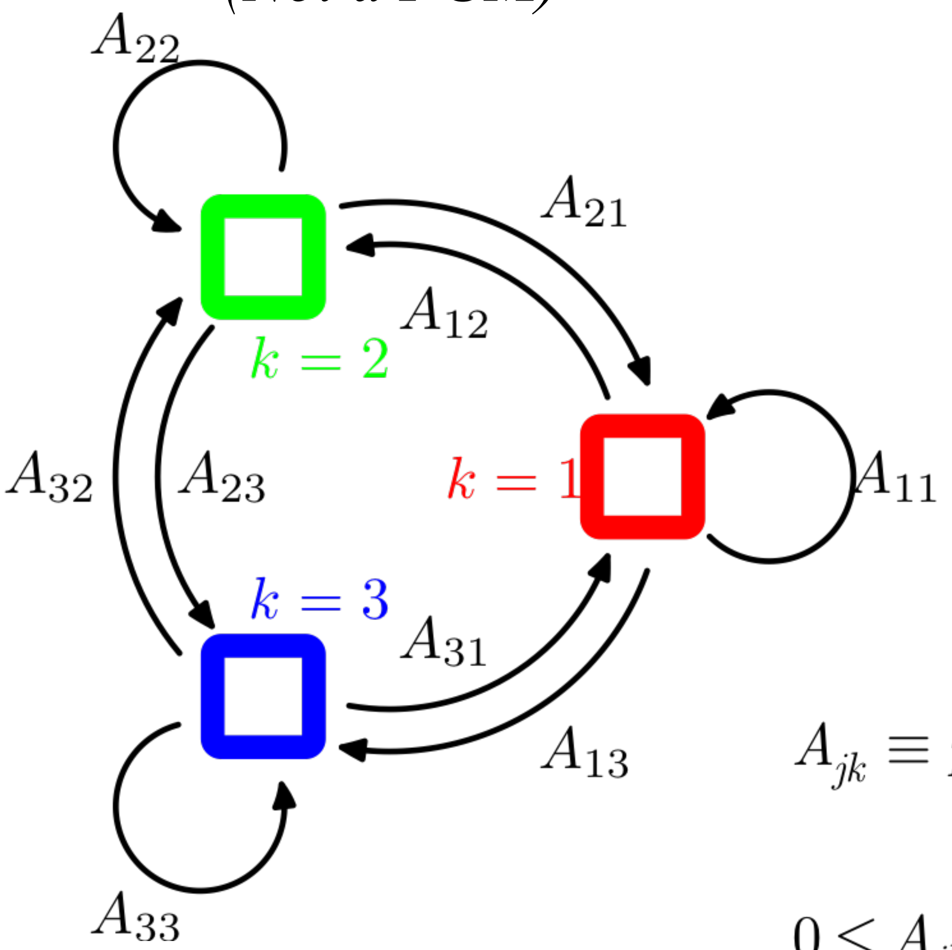


Observation likelihood $p(x_n \mid z_n)$ models how data from a component are generated (things are *easy* if you know the cluster)

Transition Dynamics

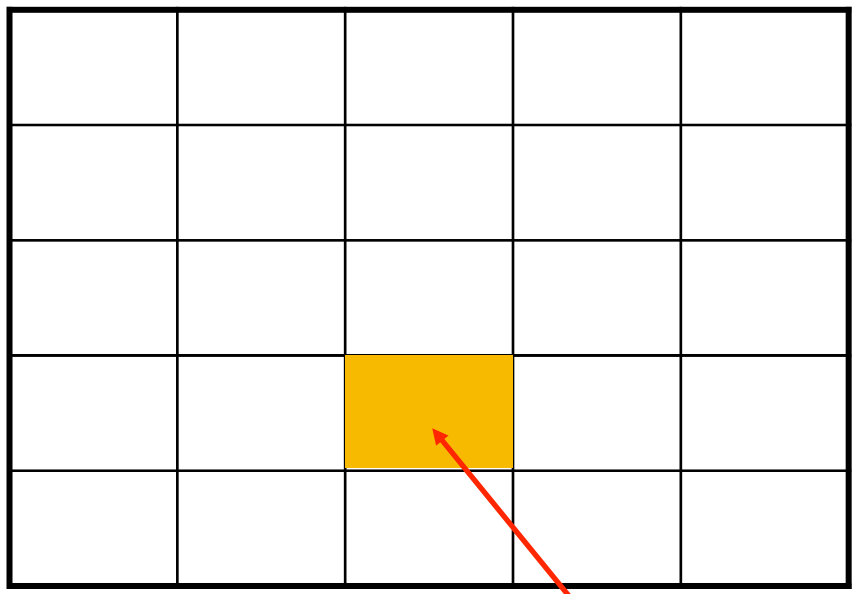
State Transition Diagram

(Not a PGM)



<—next state —>

current state



$$A_{jk} \equiv p\left(z_{nk} = 1 \middle| z_{n-1,j} = 1\right)$$

A_{jk} : Probability of going from state j=4 to state k=3

$$0 \leq A_{jk} \leq 1 \quad \text{and} \quad \sum_k A_{jk} = 1$$

Starting state

Our HMM will be a pure* generative model, so we need to know how to start.

$$\pi_k \equiv p\left(z_{1k} = 1\right)$$

$$\text{with } 0 \le \pi_k \le 1 \quad \text{and} \quad \sum_k \pi_k = 1$$

*By pure, I mean that we can do ancestral sampling, i.e., a Bayes net.

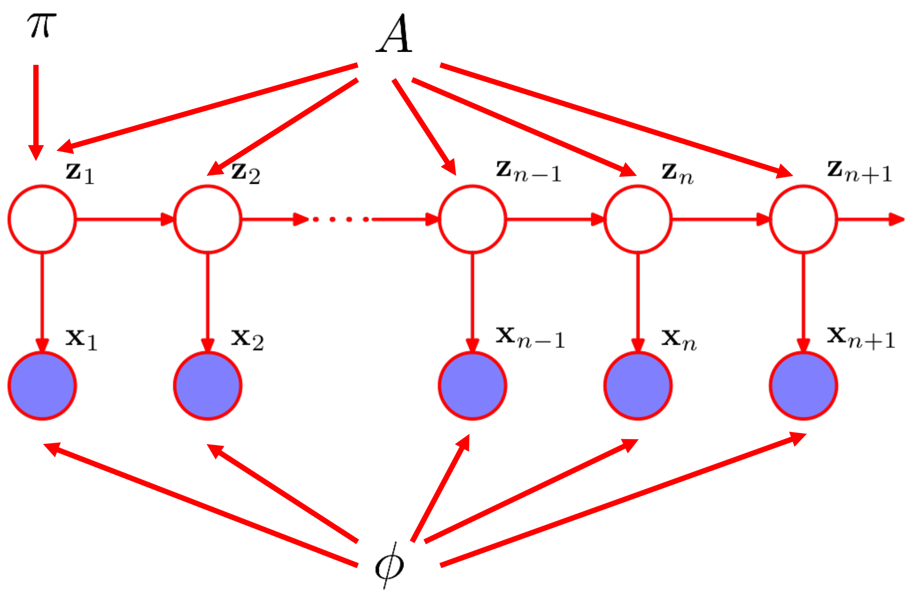
HMM parameter summary

$\Theta = \{\pi, A, \phi\}$

π is probability over initial states

A is transition matrix

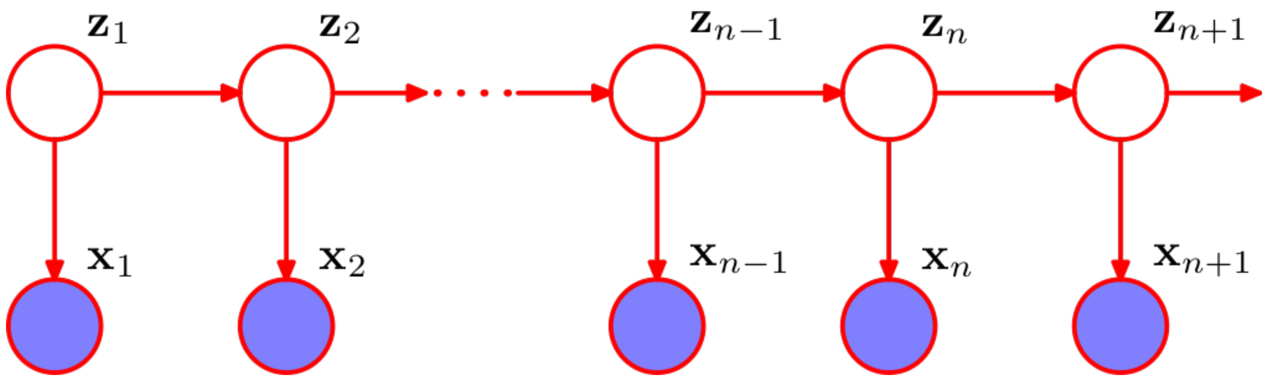
ϕ are the parameters for the data emmission probabilities (i.e., for $p(\mathbf{x}_n | z_n)$, e.g., means of Gaussians)



Data distribution from an HMM

Let $X = \{\mathbf{x}_n\}$ be the observed sequence

$$p(X|\theta) \quad = ? \qquad .$$



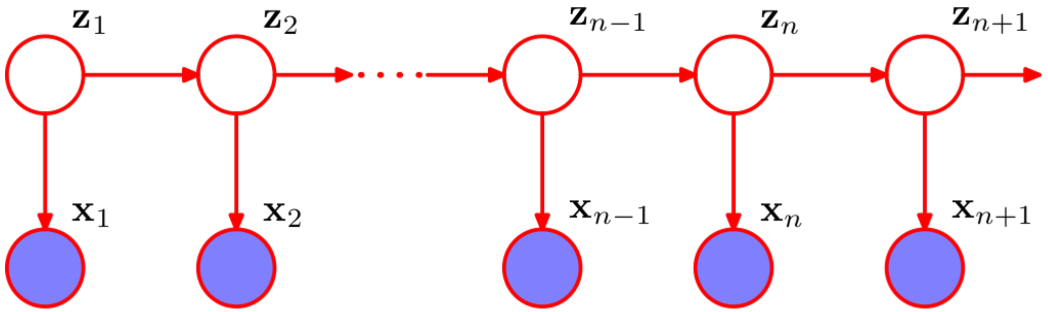
Data distribution from an HMM

Let $X = \{\mathbf{x}_n\}$ be the observed sequence

$p(X|\theta)$ is a marginalization over Z.

$p(X, Z|\theta) = ?$

Data distribution from an HMM



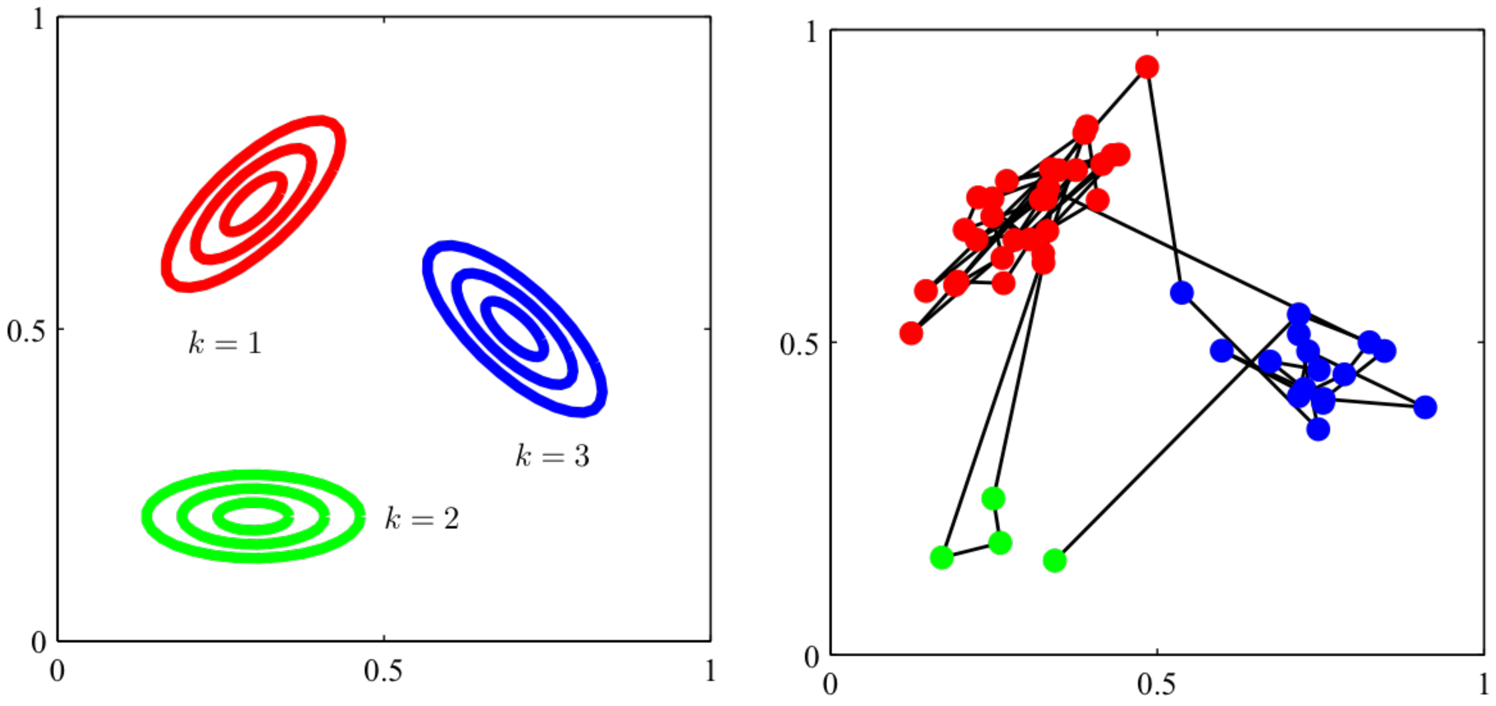
An HMM is specified by: $\theta = \{\pi, A, \phi\}$

$$p(X,Z|\theta) = p(z_1|\pi)\left[\prod_{n=2}^{N} p(z_n|z_{n-1}, A)\right]\prod_{n=1}^{N} p(\mathbf{x}_n|z_n, \phi)$$

(complete data, i.e., we can generate from this).

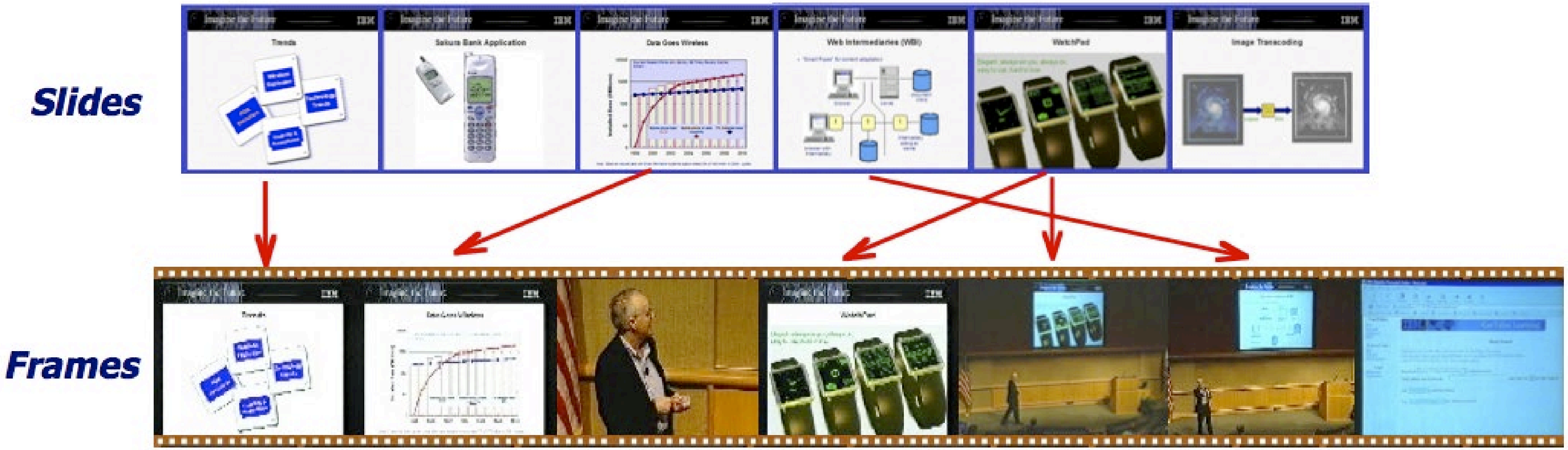
Data distribution from an HMM

Gaussian likelihood model $p(x_n|z_n)$

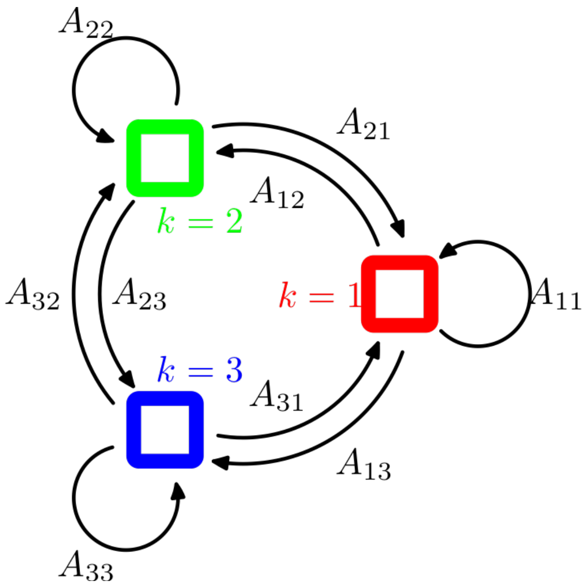


Transition probability to another state is 5% (from Bishop—the short visits in green seem a bit anomalous).

Example: Matching slides to video frames



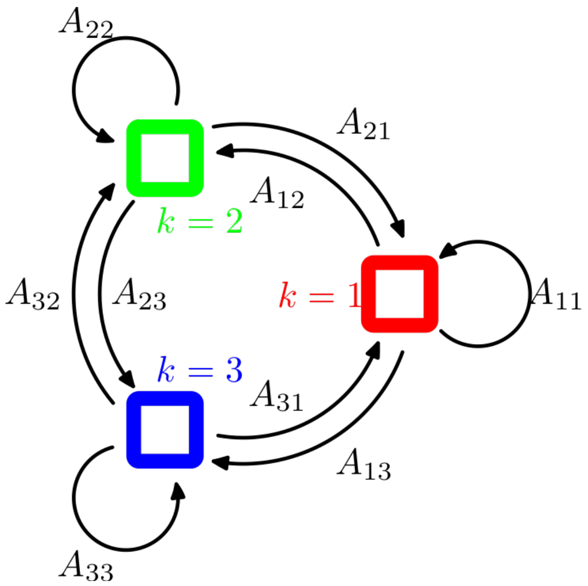
Matching slides to video frames



Our state sequence corresponds to what slide is being shown.

We assume that only the jump matters. IE, going from slide 6 to 8 has the same chance of going from 10 to 12.

Matching slides to video frames



Our state sequence corresponds to what slide is being shown.

$$p(X,Z|\theta) = p(z_1|\pi)\left[\prod_{n=2}^{N} p(z_n|z_{n-1}, A)\right]\boxed{\prod_{m=1}^{N} p(x_m|z_m, \phi)}$$

Image matching likelihood

Classic HMM computational problems

1. Given unlabeled* data, what is the HMM (**parameter learning**).
2. Given an HMM and observed data, what is the **probability distribution of states** for each time point (z_n in our notation).
3. Given an HMM and observed data, what is the most probable **state sequence**?

*We could have data with labels (annotated) which means this step becomes trivial, much like training naive Bayes versus fitting a GMM using EM. This is what we did in the matching slides to video project.

Classic HMM computational problems

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#2 and #3 seem similar, but to understand the difference consider a three state system about doing HW problems A, B, and C in order, with B being very easy. So you will spend most of your time in state A and C. State B may be the least likely state for every time point. But the most likely state sequence must include it.

Classic HMM computational problems

1. Given unlabeled data, what is the HMM (**learning**).

    This is a missing value problem, which we can tackle using EM, but we will need to solve #2 as sub-problem.

2. Given an HMM and data, what is the **probability distribution of states** for each time point (z_n in our notation).

    These are marginals in a Bayes net, and so we use the sum-product algorithm (in HMM often called alpha-beta or forwards backwards).

3. Given an HMM and data, what is the most likely **state sequence**?

    This is a maximal configuration of a Bayes net, and so we use max-sum (in HMM this is Viterbi).

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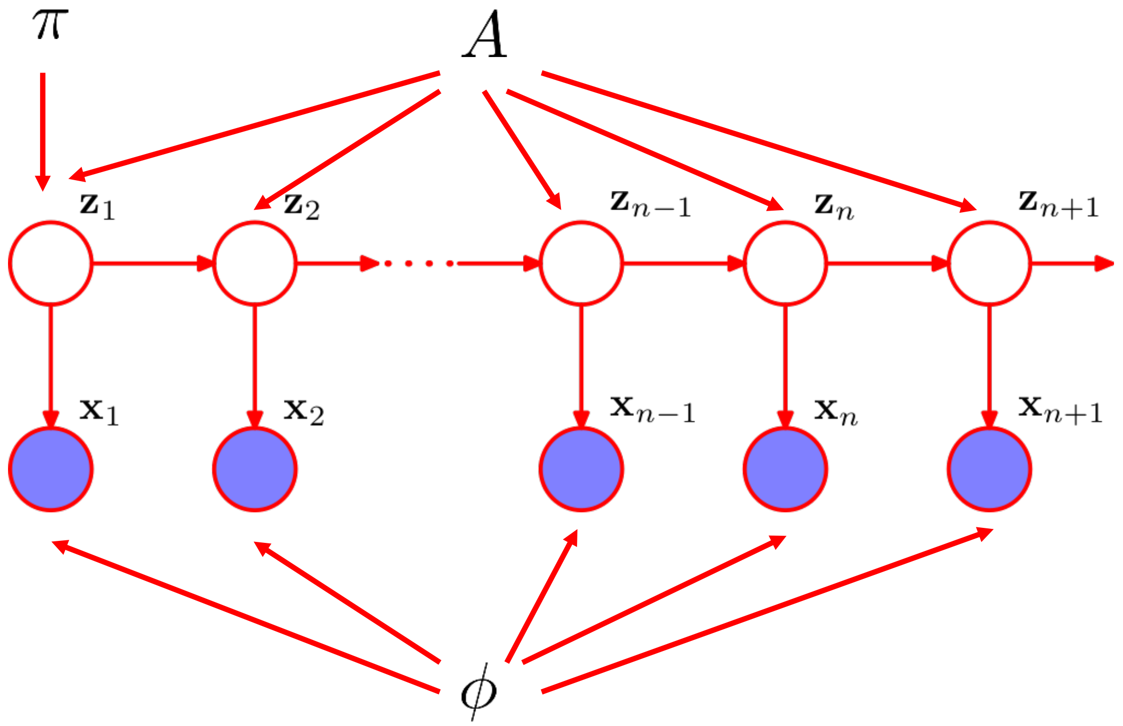
Learning HMM Parameters

Learn These E.g. via maximum likelihood:

$$\theta = \{\pi, A, \phi\}$$

Problem Don't know latent states

Observations e.g. training data



Need to compute *marginal likelihood*:

$$\max_{\theta} \mathcal{L}(\theta) = \int p(\mathbf{z})p(\mathbf{x} \mid \mathbf{z})\, dz$$

Natural approach is to use Expectation Maximization

Learning the HMM with EM (sketch)

If we know the state distributions, and the successive state pair distributions (needed for the transition matrix, A), for each training sequence, we can compute the parameters.

If we know the parameters, we can compute the state distributions, for each training sequence (this is HMM computation problem #2, which we need to solve as a subproblem if we use EM).

Blue text highlights differences from the mixture model for one sequence.

Green text reminds us that we need a bit of book-keeping when we train on multiple sequences.

Recall the General EM algorithm

1. Choose initial values for $\theta^{(s=1)}$

2. E step: Evalute $p\left(Z \middle| X, \theta^{(s)}\right)$

3. M step: Evalute $\theta^{(s+1)} = \underset{\theta}{\arg\max}\left\{Q\left(\theta^{(s+1)}, \theta^{(s)}\right)\right\}$

   where $Q\left(\theta^{(s+1)}, \theta^{(s)}\right) = \sum_{Z} p\left(Z \middle| X, \theta^{(s)}\right) \log\left(p\left(X, Z \middle| \theta^{(s+1)}\right)\right)$

4. Check for convergence; If not done, goto 2.

★ At each step, our objective function increases unless it is at a local maximum. It is important to check this is happening for debugging!

HMM complete data likelihood (one sequence)

$$p(X,Z|\theta) = p(z_1|\boldsymbol{\pi})\left[\prod_{n=2}^{N} p(z_n|z_{n-1}, A)\right]\prod_{n=1}^{N} p(x_n|z_n, \phi)$$

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$$= \prod_{k=1}^{K} \pi_k^{z_{1,k}} \left[\prod_{n=2}^{N}\prod_{j=1}^{K}\prod_{k=1}^{K} A_{j,k}^{z_{n-1,j} \bullet z_{n,k}}\right] \prod_{n=1}^{N}\prod_{k=1}^{K} \left(p(x_n|\phi_k)\right)^{z_{n,k}}$$

Remember our "indicator variable" notation. *Z* is a particular assignment of the missing values (i.e., which cluster the HMM was in at each time. For each time point, *n*, one of the values of z_n is one, and the others are zero. So, it "selects" the factor for the particular state at that time.

HMM complete data likelihood (one sequence)

$$p(X,Z|\theta) = p(z_1|\boldsymbol{\pi})\left[\prod_{n=2}^{N} p(z_n|z_{n-1}, A)\right]\prod_{n=1}^{N} p(x_n|z_n, \phi)$$

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$$\log\left(p(X,Z|\theta)\right) = \sum_{k=1}^{K} z_{1k}\log(\pi_k) + \sum_{n=2}^{N}\sum_{j=1}^{K}\sum_{k=1}^{K} z_{n-1,j}z_{n,k}\log(A_{j,k}) + \sum_{n=1}^{N}\sum_{k}^{K} z_{n,k}\log\left(p(x_n|\phi_k)\right)$$

(complete data log-likelihood)

HMM complete data likelihood (E training sequences)

$$p(X,Z|\theta)=\prod_{e=1}^{E}p(z_{e,1}|\boldsymbol{\pi})\left[\prod_{e=1}^{E}\prod_{n=2}^{N_e}p(z_{e,n}|z_{e,n-1},A)\right]\prod_{e=1}^{E}\prod_{n=1}^{N_e}p(x_{e,n}|z_{e,n},\phi)$$

$$=\prod_{e=1}^{E}\prod_{k=1}^{K}\pi_k^{z_{s,1,k}}\left[\prod_{e=1}^{E}\prod_{n=2}^{N_e}\prod_{j=1}^{K}\prod_{k=1}^{K}A_{j,k}^{z_{n-1,j}\bullet z_{n,k}}\right]\prod_{e=1}^{E}\prod_{n=1}^{N_e}\prod_{k=1}^{K}\left(p(x_{e,n}|\phi_k)\right)^{z_{e,n,k}}$$

$$\log(p(X,Z|\theta))=\sum_{e=1}^{E}\sum_{k=1}^{K}z_{s,1k}\log(\pi_k)+\sum_{e=1}^{E}\sum_{n=2}^{N_e}\sum_{j=1}^{K}\sum_{k=1}^{K}z_{e,n-1,j}z_{e,n,k}\log(A_{j,k})+\sum_{e=1}^{E}\sum_{n=1}^{N_e}\sum_{k}^{K}z_{e,n,k}\log(p(x_{e,n}|\phi_k))$$

(complete data log likelihood)

Learning the HMM with EM (sketch)

In the simple clustering case (e.g., GMM), the E step was simple. For HMM it is a bit more involved.

The M step works a lot like the GMM, except we need to deal with successive states. Consider the M step first.

E-Step for HMM

Provides two distributions (responsibilities)…

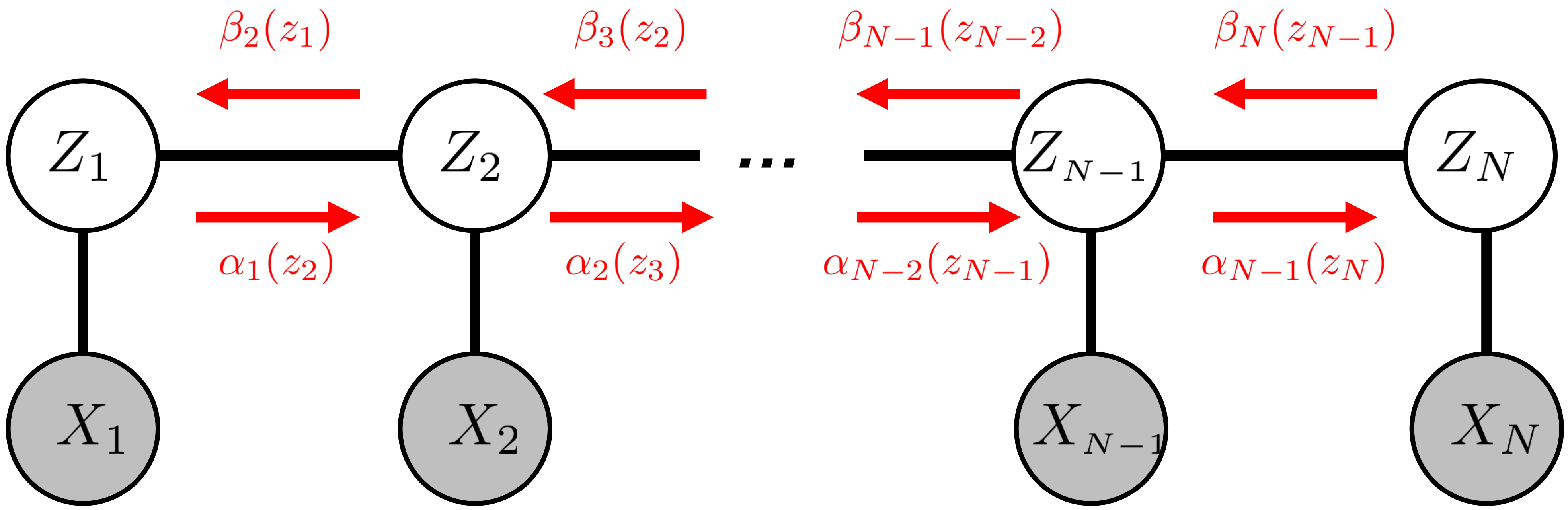
The degree each state explains each data point (analogous to GMM responsibilities). $\gamma\left(z_{e,n,k}\right) = p\left(z_{e,n,k} \middle| X_e, \theta^{(s)}\right)$

The degree that the combination of a state, and a previous one explain two data points.

$$\xi\left(e, \boldsymbol{z}_{n-1,j}, \boldsymbol{z}_{n,k}\right) = p\left(\boldsymbol{z}_{e,n-1,j}, \boldsymbol{z}_{e,n,k} \middle| X_e, \theta^{(s)}\right)$$

Q: How can we compute one / two stage-marginals in HMM?

Forward-Backward Algorithm



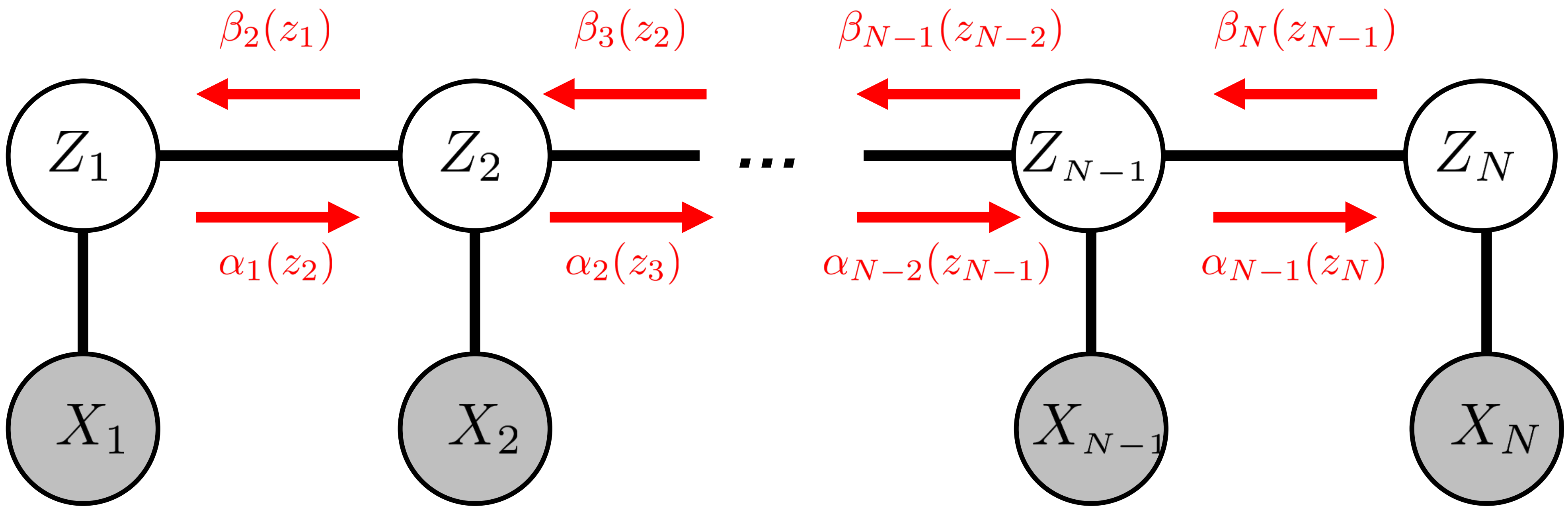
Forward message:

$$\alpha_{n-1}(z_n) = \psi(z_n, x_n) \sum_{z_{n-1}} \alpha_{n-2}(z_{n-1}) \psi(z_{n-1}, z_n)$$

Forward message:

$$\beta_{n+1}(z_n) = \sum_{z_{n+1}} \beta_{n+2}(z_{n+1}) \psi(z_n, z_{n+1}) \psi(z_{n+1}, x_{n+1})$$

Forward-Backward Algorithm



Node Responsibility (a.k.a. marginal):

$$\gamma(z_n) = p(z_n \mid \mathcal{X}) \propto \alpha_n(z_n)\beta_n(z_n)$$

Two-Node Responsibility (a.k.a. pairwise marginal):

$$\xi(z_n, z_{n+1}) = p(z_n, z_{n+1} \mid \mathcal{X}) \propto \alpha_n(z_n)\psi(z_n, z_{n+1})\beta_{n+1}(z_{n+1})$$

M-Step for HMM

Recall the complete data log-likelihood:

$$\log(p(X,Z|\theta)) = \sum_{e=1}^{E}\sum_{k=1}^{K} z_{e,1k} \log(\pi_k) + \sum_{e=1}^{E}\sum_{n=2}^{N_e}\sum_{j=1}^{K}\sum_{k=1}^{K} z_{e,n-1,j} z_{e,n,k} \log(A_{j,k}) + \sum_{e=1}^{E}\sum_{n=1}^{N_e}\sum_{k}^{K} z_{e,n,k} \log(p(x_{e,n}|\phi_k))$$

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Expected complete data log-likelihood:

$$\begin{aligned}Q\left(\theta^{(s+1)},\theta^{(s)}\right)&=\sum_{z}p\left(Z\middle|\theta^{(s)}\right)\log\left(p\left(X,Z\middle|\theta^{(s+1)}\right)\right)\\&=\sum_{e=1}^{E}\sum_{k=1}^{K}\gamma\left(z_{e,1,k}\right)\log\left(\pi_k\right)+\sum_{e=1}^{E}\sum_{n=2}^{N_e}\sum_{j=1}^{K}\sum_{k=1}^{K}\xi\left(e,z_{n-1,j}z_{n,k}\right)\log\left(A_{j,k}\right)+\sum_{e=1}^{E}\sum_{n=1}^{N_e}\sum_{k}^{K}\gamma\left(z_{e,n,k}\right)\log\left(p\left(x_{e.n}\middle|z_{e,n},\phi\right)\right)\end{aligned}$$

M-Step for HMM

Doing the maximization using Lagrange multipliers (or intuition) gives us

$$\pi_k = \frac{\sum_{e=1}^{E} \gamma\left(z_{e,1,k}\right)}{\sum_{e=1}^{E} \sum_{k'} \gamma\left(z_{e,1,k'}\right)}$$

$$A_{jk} = \frac{\sum_{e=1}^{E} \sum_{n=2} \zeta\left(e, z_{n-1,j}, z_{n,k}\right)}{\sum_{e=1}^{E} \sum_{k'} \sum_{n=2} \zeta\left(z_{n-1,j}, z_{n,k'}\right)}$$

Much like the GMM. Taking the partial derivative for π_k kills second and third terms.

M-Step for HMM

The maximization of $p\left(\mathbf{x}_{e,n}\middle|\phi\right)$ is exactly the same as the mixture model.

For example, if we have Gaussian emmisions, then

$$\boldsymbol{\mu}_k = \frac{\sum_{e=1}^{E}\sum_{n}\mathbf{x}_{e,n}\,\gamma\left(z_{e,n,k}\right)}{\sum_{e=1}^{E}\sum_{n}\gamma\left(z_{e,n,k}\right)}$$

Classic HMM computational problems

Given data, what is the HMM (**learning**).

Given an HMM, what is the **distribution over the state** variables. Also, **how likely** are the observations, given the model.

Given an HMM, what is the most probable **state sequence** for some data?

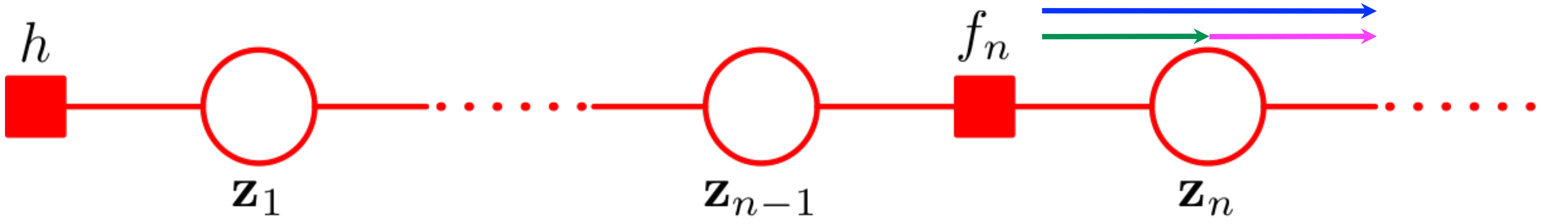
Viterbi algorithm (special case of max-sum)

Recall max-sum

Forward direction is like sum-product, except
- Factor nodes take the max over logs instead of sum
- Variable nodes use sum of logs instead of product
- We remember incoming variable values* that give max

Backwards direction is simply backtracking on (*).

Recall sum-product for HMM

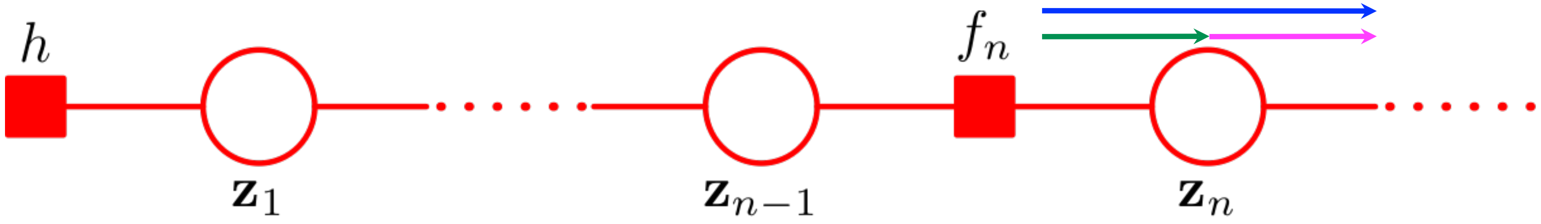


If we identify $\mu_{f_n \to f_{n+1}}(z_n) = \alpha(z_n)$

$$\alpha(z_1) = p(z_1)p(x_1|z_1)$$

$$\begin{aligned}\alpha(z_n) &= \sum_{z_{n-1}} f_n(z_{n-1}, z_n)\alpha(z_{n-1}) \\ &= \sum_{z_{n-1}} p(z_n|z_{n-1})p(x_n|z_n)\alpha(z_{n-1}) \\ &= p(x_n|z_n)\sum_{z_{n-1}} p(z_n|z_{n-1})\alpha(z_{n-1})\end{aligned}$$

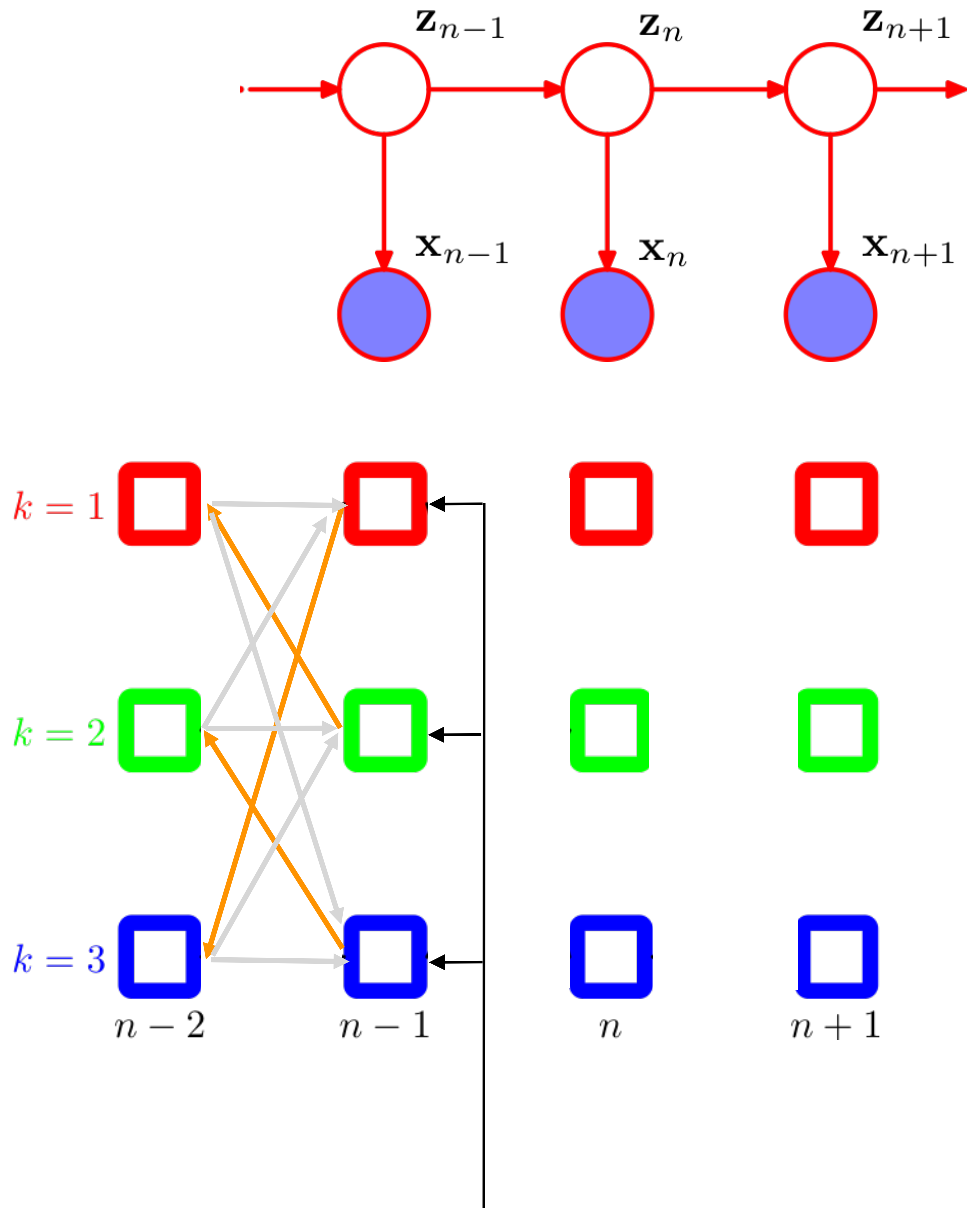
By analogy we get max sum



Left to right messages for max-sum

$$\omega(z_n) = \log(p(x_n|z_n)) + \max_{z_{n-1}}\{\log(p(z_n|z_{n-1})) + \omega(z_{n-1})\}$$

$$\omega(z_1) = \log(p(z_1)) + \log(p(x_1|z_1))$$



Store $\omega_{n-1,k}$ and $k' = \arg\max(\bullet)$ for k

Squares represent being in each of the three states at a given time.

We store the log of the probability of the maximal likely way to get there.

And the particular previous state that gave the max (orange)

Story for the preceding picture

Consider all possible paths **to each** of the *K* states for time *n*.

The message encodes the probabilities for the maximum probability path for each of the *K* states.

I.E., for a given time, for each state *k*, it records is the probability of being there by via the maximal probably sequence.

That value is (recursively defined by)

$$\omega\left(z_n\right) = \log\left(p\left(x_n \middle| z_n\right)\right) + \max_{z_{n-1}}\left\{\log\left(p\left(z_n \middle| z_{n-1}\right)\right) + \omega\left(z_{n-1}\right)\right\}$$

Story (continued)

The incoming message is the vector of probabilities for the maximum probability path for each of the K states at the previous time.

$$\omega(z_n) = \log\left(p\left(x_n \middle| z_n\right)\right) + \max_{z_{n-1}} \underbrace{\left\{\log\left(p\left(z_n \middle| z_{n-1}\right)\right) + \omega\left(z_{n-1}\right)\right\}}_{\text{Consider getting there from each previous state k'}}$$

For each state k

This gives the maximal probability way to be in each of K states, k, at time n.

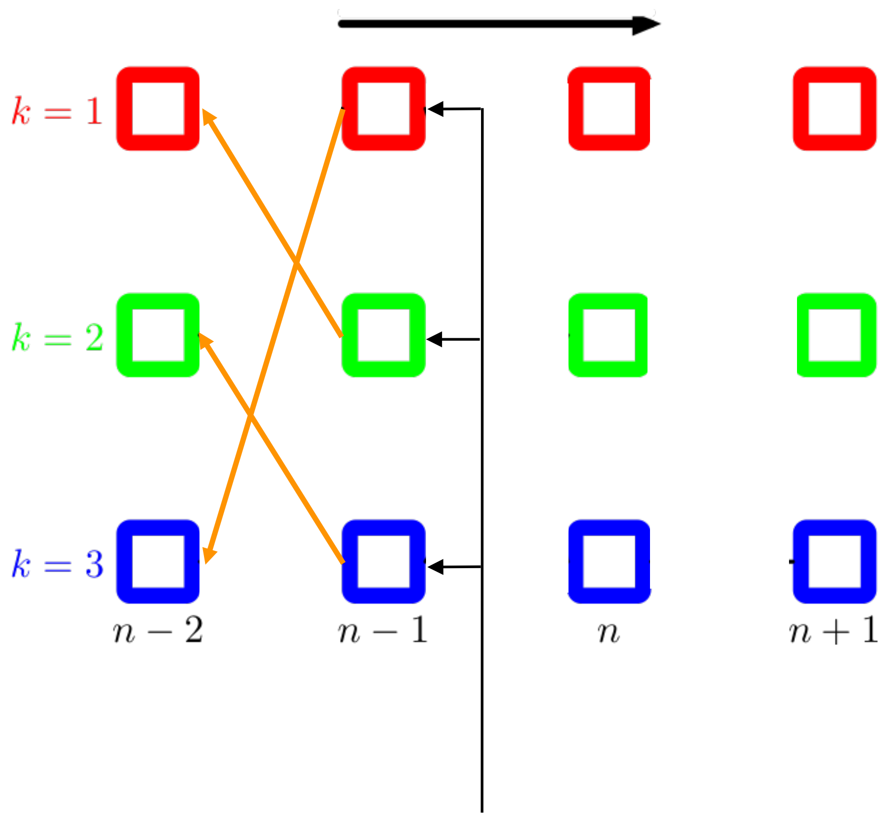
Story (continued)

For Viterbi, we remember the previous state, *k'*, leading to the max for each *k*. (This is simpler than the general case because no branches).

Once we know the end state of the maximal probability path, we can find the maximal probability path by back-tracking.

You might also recognize this as dynamic programming (think minimum cost path).

Intuitive understanding



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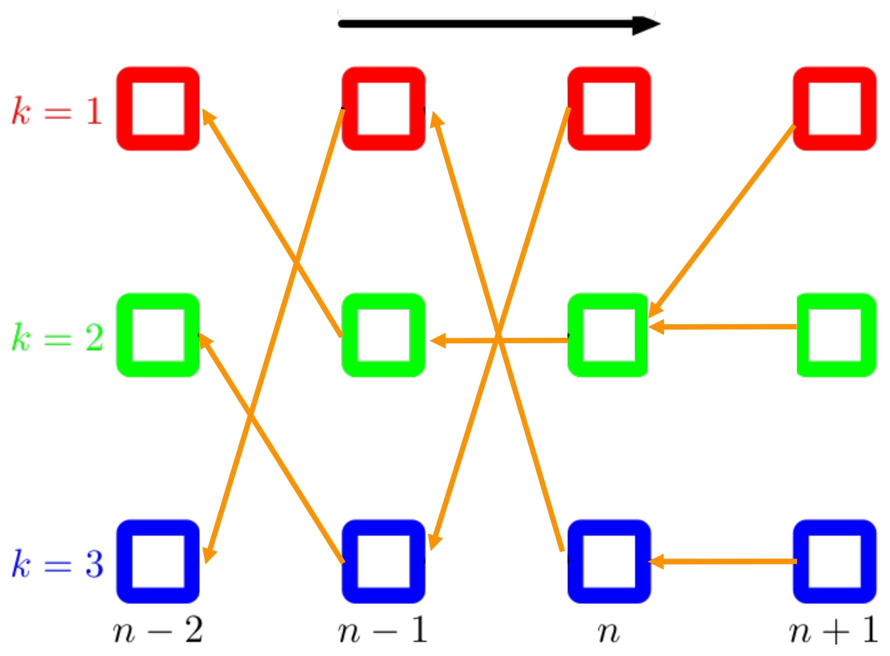
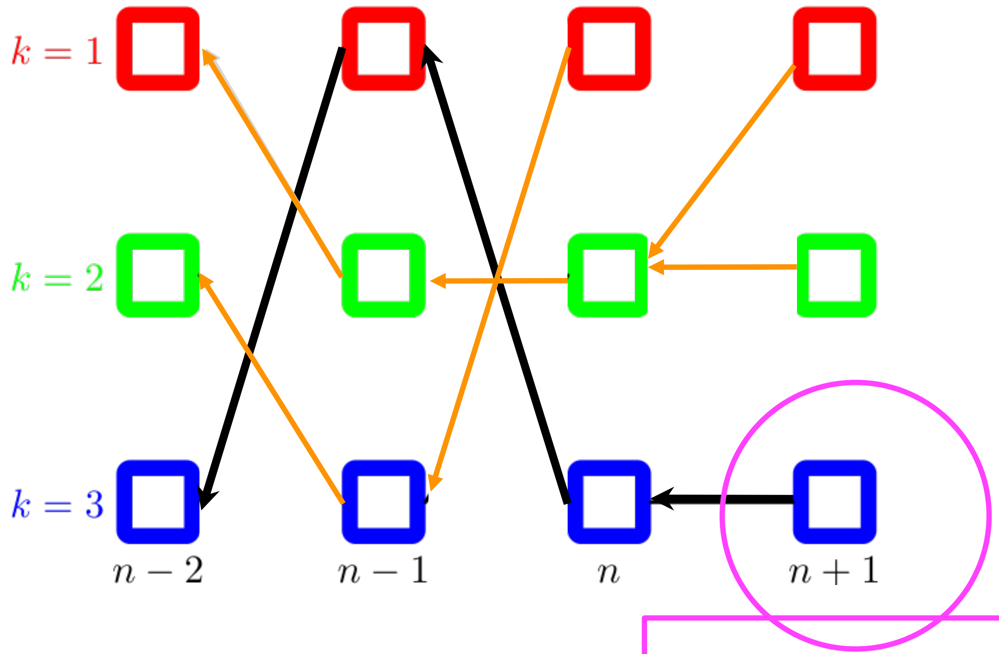
Intuitive understanding



If this is the end, we now know the max, and what the ending state is.

Intuitive understanding



Suppose the max is attained at *k=3*.

The max path is dark (but we only know it when we get to the end).

To find the path, we need to chase the back pointers.

Classic HMM computational problems

Given data, what is the HMM (**learning**). ✓

Given an HMM, what is the **distribution over the state** variables. Also, **how likely** are the observations, given the model. ✓

Given an HMM, what is the most probable **state sequence** for some data? ✓

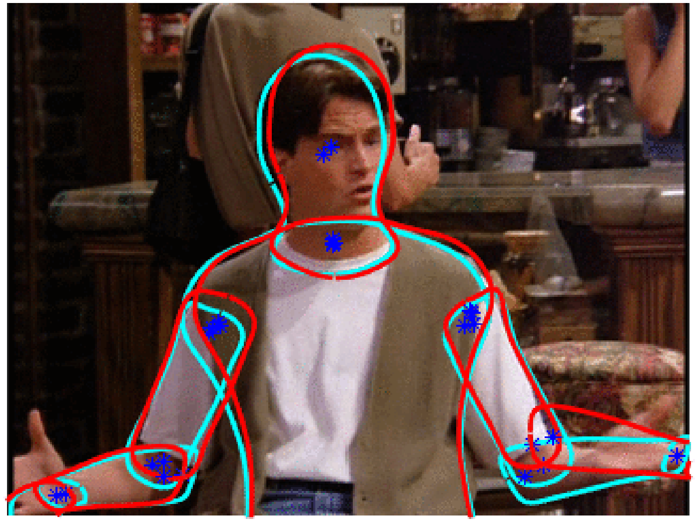
Outline

- Sequence Models
- Linear Dynamical Systems
- LDS Extensions

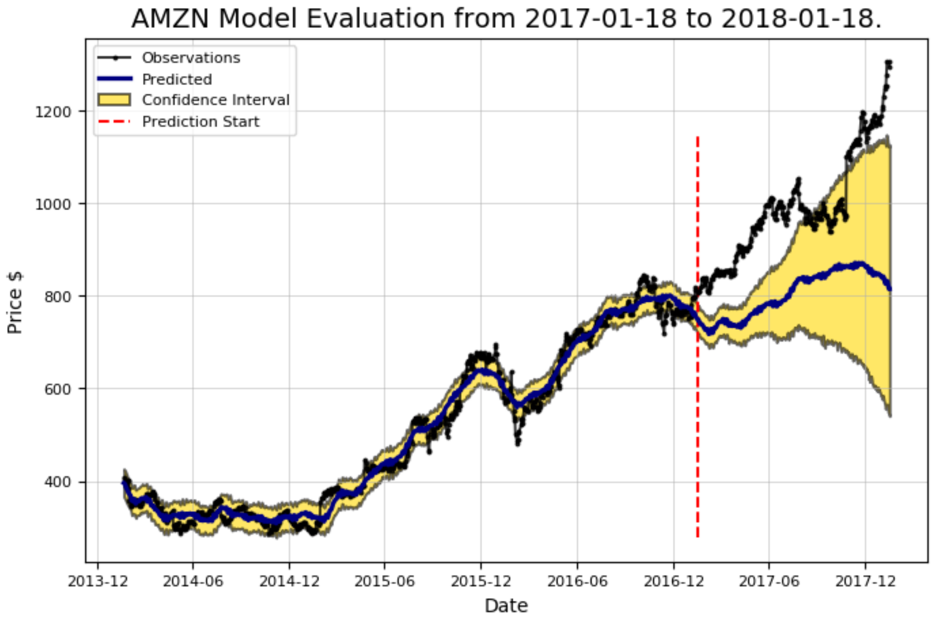
Dynamical System

Models of latent states evolving over time/space

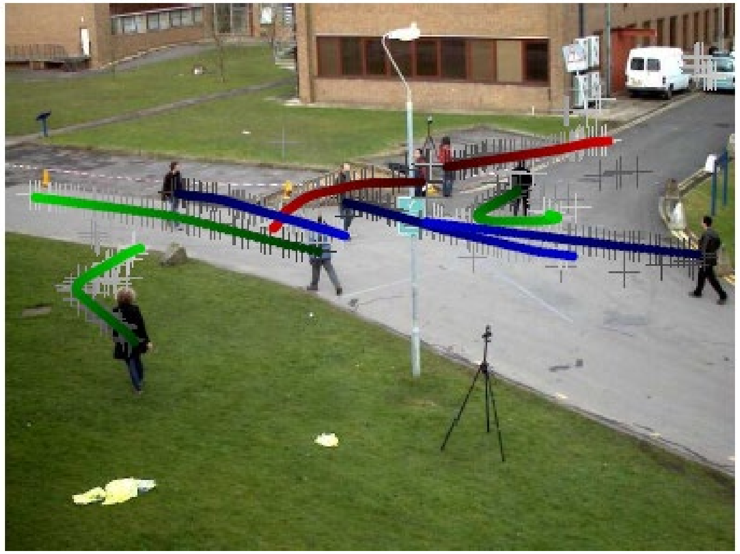
Human Pose Tracking



Stock Market Prediction

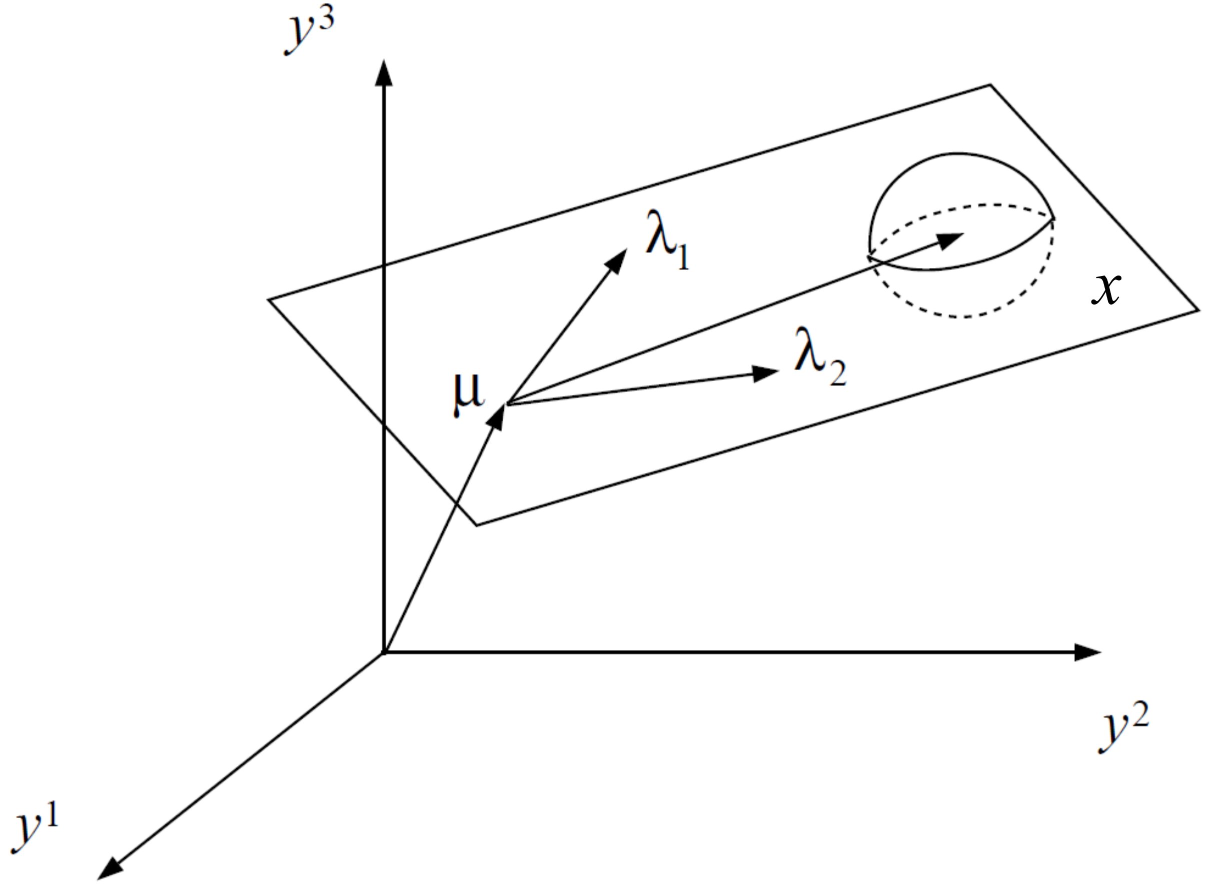


Visual Object Tracking



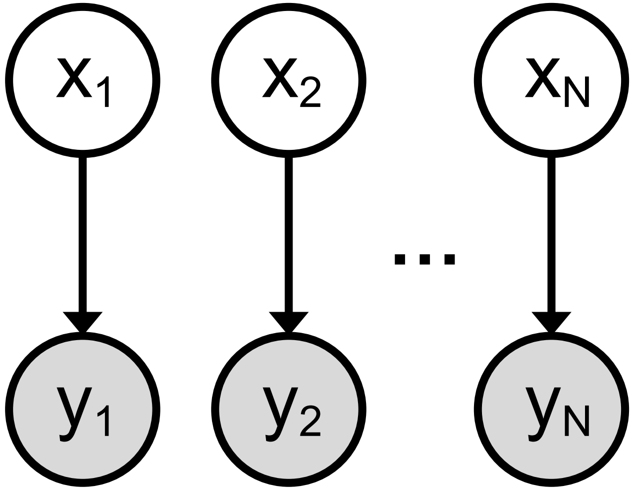
Move away from discrete HMM states to continuous ones…

Probabilistic Principal Component Analysis (PPCA)



Latent: $x \in \mathbb{R}^p$ Data: $y \in \mathbb{R}^q$

Typically p<q for dimension reduction



$$x \sim \mathcal{N}(0, I)$$

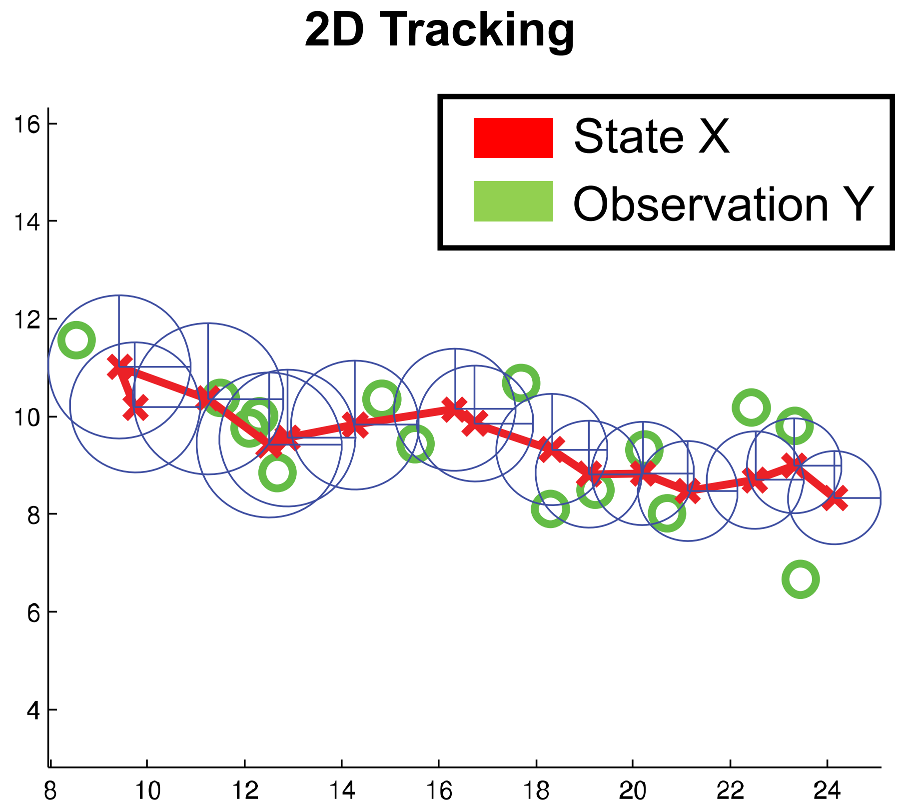
$$y \mid x \sim \mathcal{N}(\Lambda x + \mu, \sigma^2 I)$$

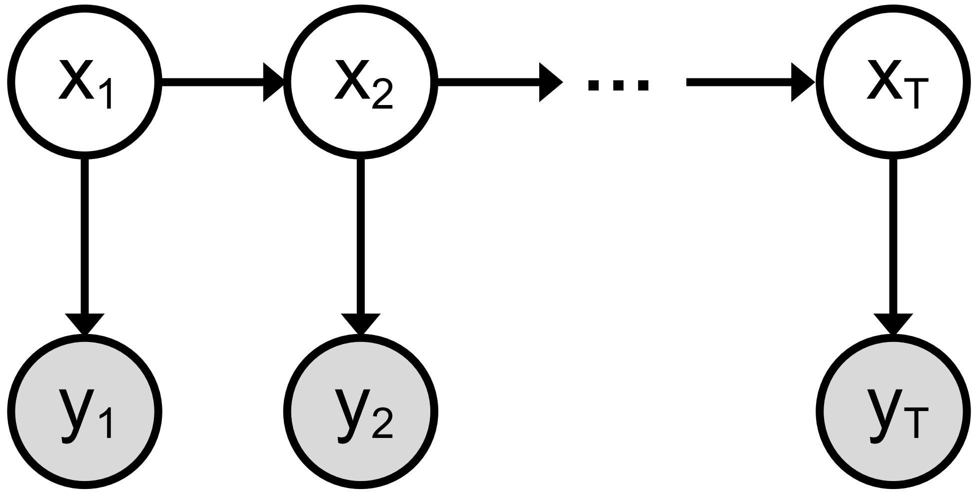
Data are exchangeable linear Gaussian projections of latent quantities

[Source: M. I. Jordan]

Gaussian Linear Dynamical System (LDS)

Temporal extension of probabilistic PCA…





$$x_0 \sim \mathcal{N}(0, I)$$

$$x_t \mid x_{t-1} \sim \mathcal{N}(F x_{t-1}, \Sigma)$$

$$y_t \mid x_t \sim \mathcal{N}(H x_t, R)$$

Data are time-dependent and non-exchangeable

Linear State-Space Model

Consider the state vector:

$$x_t = \begin{pmatrix} x(t) \\ \dot{x}(t) \end{pmatrix}$$ where $x(t)$: Position $\quad \dot{x}(t) \triangleq \frac{d}{dt}x(t)$: Velocity

Differential equations for constant velocity dynamics:

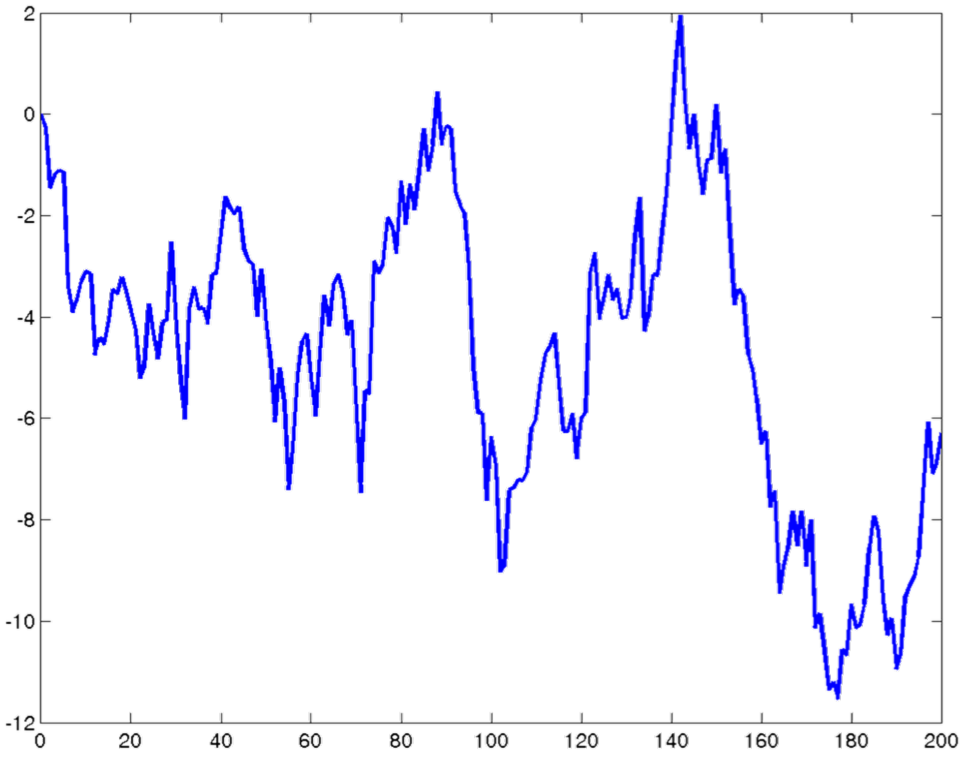
$$x(t) = x(t-1) + \dot{x}(t-1) \qquad \dot{x}(t) = \dot{x}(t-1)$$

Linear Gaussian state-space model

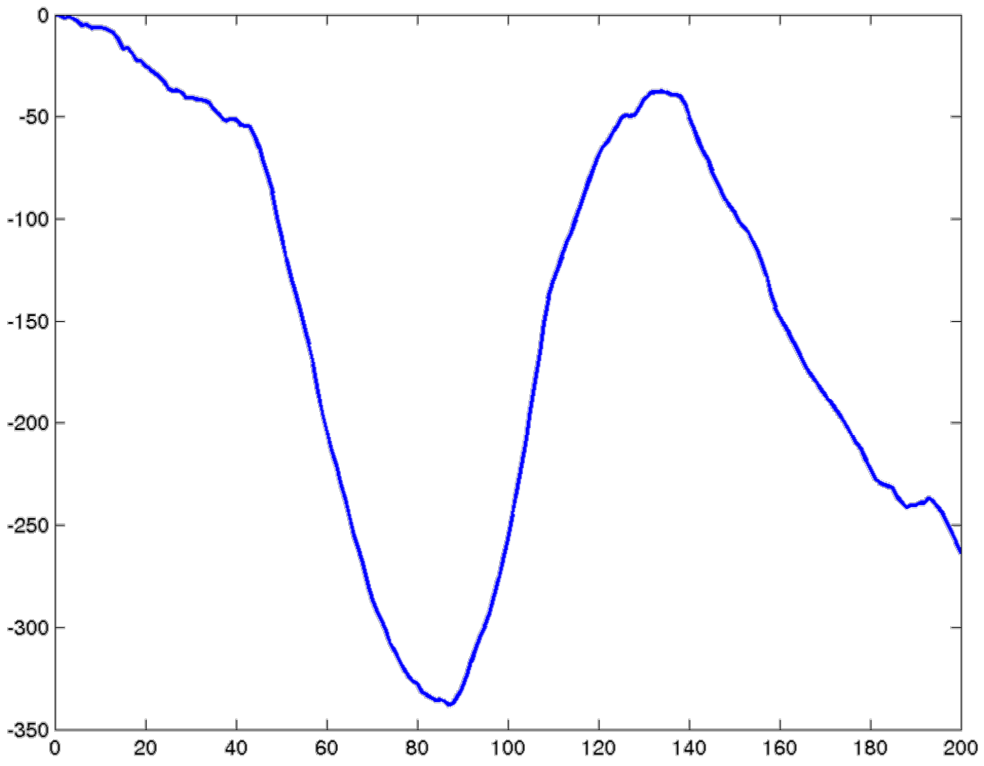
$$\underbrace{x_t = F x_{t-1} + \epsilon}_{\substack{\text{State-space notation} \\ \text{Linear regression model}}}$$ where $F = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ and $\epsilon \sim \mathcal{N}(0, \Sigma)$

Simple Linear Gaussian Dynamics

Random Walk
(Brownian Motion)



Constant Velocity
(a.k.a. zero acceleration)

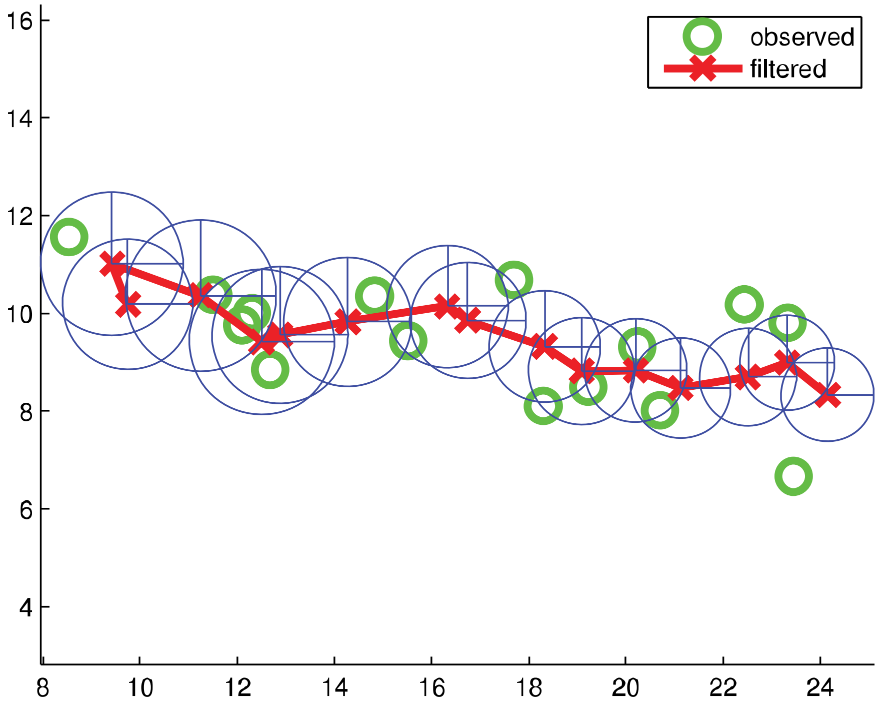


Acceleration can be included in higher-order models as well

Dynamical System Inference

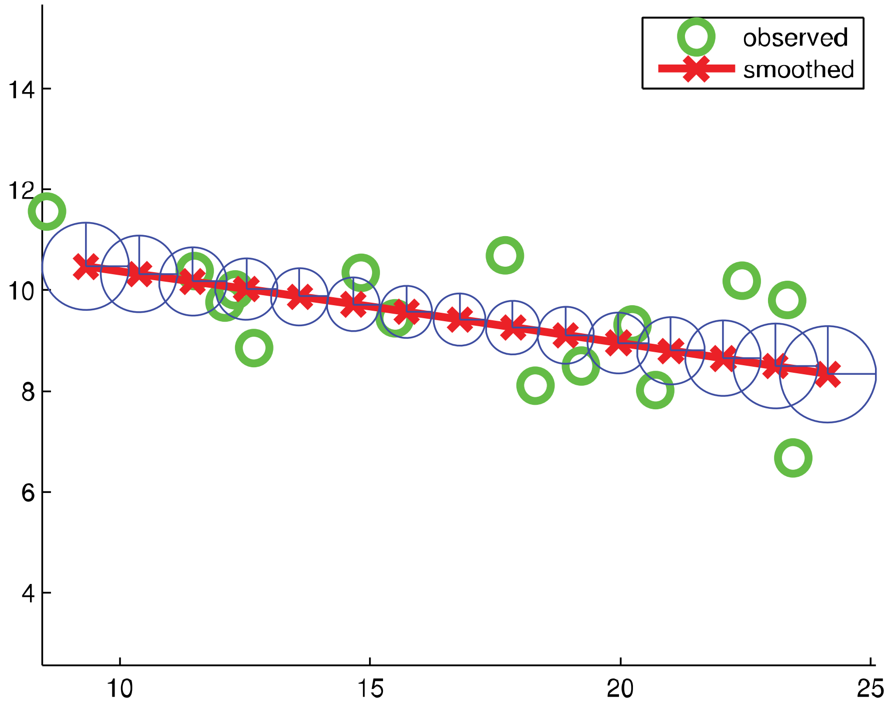
Define shorthand notation: $y_1^{t-1} \triangleq \{y_1, \ldots, y_{t-1}\}$

Filtering



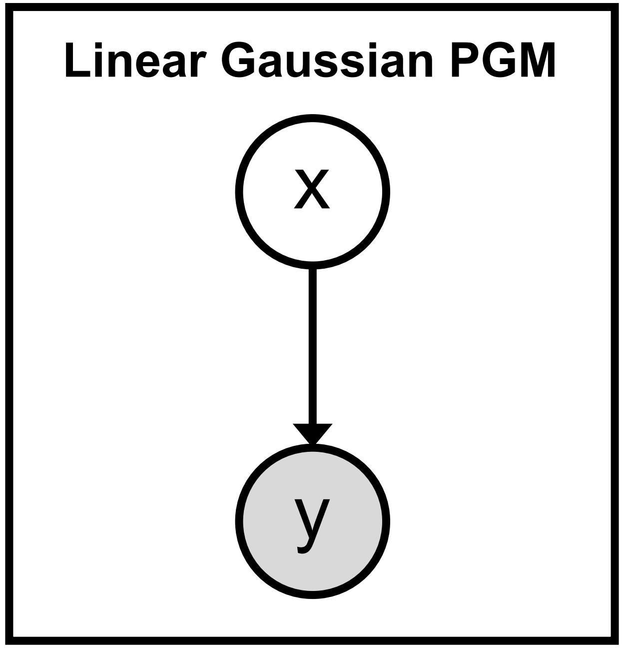
Compute $p(x_t \mid y_1^t)$ at each time t

Smoothing



Compute full posterior marginal $p(x_t \mid y_1^T)$ at each time t

Linear Gaussian Inference



Suppose we have jointly Gaussian model,

$$x \sim \mathcal{N}(\mu, \Sigma) \qquad y \mid x \sim \mathcal{N}(Ax + b, R)$$

Key quantities of inference:

- Marginal: $p(y)$
- Posterior: $p(x \mid y)$

Both are Gaussian distributions!

Gaussians closed under marginalization / conditioning

Marginal $p(y) = \mathcal{N}(A\mu + b, R + A\Sigma A^T)$

Posterior $p(x \mid y) = \mathcal{N}(\mu_{x|y}, \Sigma_{x|y})$

Where, $\Sigma_{x|y}^{-1} = \Sigma^{-1} + A^T R^{-1} A$ and $\mu_{x|y} = \Sigma_{x|y} \left[A^T R^{-1}(y - b) + \Sigma^{-1}\mu \right]$

Linear Gaussian Inference

Deriving marginal and posterior Gaussian is straightforward

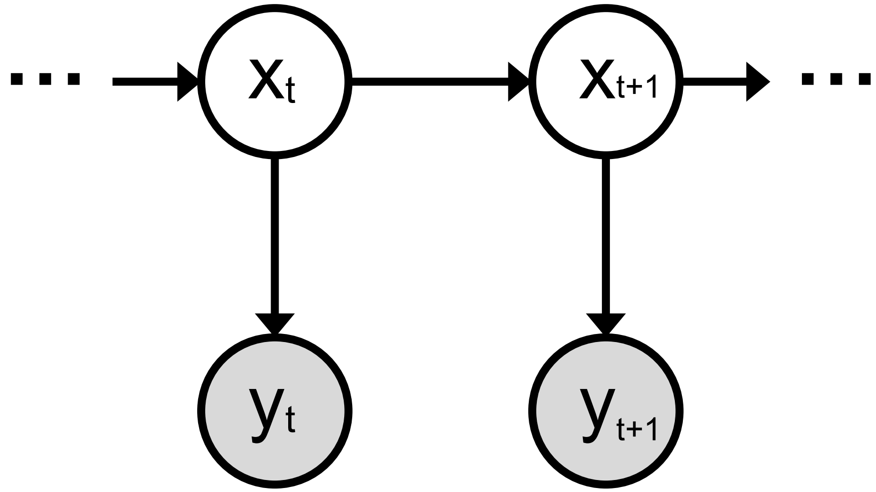
- …but takes too long in lecture… (See Murphy Sec. 4.3)
- Those who did HW2 Extra Credit have seen this already!

Basic Approach

- Marginal and Posterior are closed-form Gaussians
- Use final formulas as **building blocks** for linear dynamical systems

Gaussian Linear Dynamical System (LDS) Inference

Gaussian LDS



$$x_{t+1} \mid x_t \sim \mathcal{N}(Fx_t, \Sigma)$$
$$y_t \mid x_t \sim \mathcal{N}(Hx_t, R)$$

At time t assume we have posterior,

$$p(x_t \mid y_1, \ldots, y_t) = p(x_t \mid y_1^t)$$ **shorthand**

Key inference steps

1) *Predict* state at next time

$$p(x_{t+1} \mid y_1^t)$$ **Data only up to previous time**

2) Update posterior with measurement

$$p(x_{t+1} \mid y_1^{t+1})$$ **Data at time t+1**

All distributions remain Gaussian because of closure properties

Gaussian LDS Prediction

Suppose we have a Gaussian posterior at time t-1:

$$p(x_{t-1} \mid y_1^{t-1}) = \mathcal{N}(\mu_{t-1}, \Sigma_{t-1}) \qquad \text{where} \qquad y_1^{t-1} \triangleq \{y_1, \ldots, y_{t-1}\}$$

Forward prediction at time t:

$$\begin{aligned}
p(x_t \mid y_1^{t-1}) &= \int p(x_t \mid x_{t-1}) p(x_{t-1} \mid y_1^{t-1}) \, dx_{t-1} \\
&= \int \mathcal{N}(x_t \mid F x_{t-1}, \Sigma) \mathcal{N}(x_{t-1} \mid \mu_{t-1}, \Sigma_{t-1}) \, dx_{t-1} \\
&= \mathcal{N}(x_t \mid F\mu_{t-1}, \Sigma + F\Sigma_{t-1}F^T) \boxed{\int \mathcal{N}(x_{t-1} \mid \cdot, \cdot) \, dx_{t-1}}
\end{aligned}$$

Integrates to 1

Same form as marginal likelihood on previous slide

Gaussian LDS Filtering

- Forward prediction at time t: $p(x_t \mid y_1^{t-1}) = \mathcal{N}(x_t \mid \mu_{t|t-1}, \Sigma_{t|t-1})$

where $\mu_{t|t-1} \triangleq F\mu_{t-1}$ and $\Sigma_{t|t-1} = \Sigma + F\Sigma_{t-1}F^T$

State Prediction — Predicted Covariance

- Posterior at time t is also Gaussian:

$$p(x_t \mid y_1^t) \propto p(x_t \mid y_1^{t-1})p(y_t \mid x_t)$$

$$= \mathcal{N}(x_t \mid \mu_{t|t-1}, \Sigma_{t|t-1})\mathcal{N}(y_t \mid Hx_t, R) \propto \mathcal{N}(x_t \mid \mu_{t|t}, \Sigma_{t|t})$$

Gain Matrix: $K_t = \Sigma_{t|t-1}H^T(H\Sigma_{t|t-1}H^T + R)^{-1}$

Filter Covariance: $\Sigma_{t|t} = \Sigma_{t|t-1} - K_tH\Sigma_{t|t-1}$

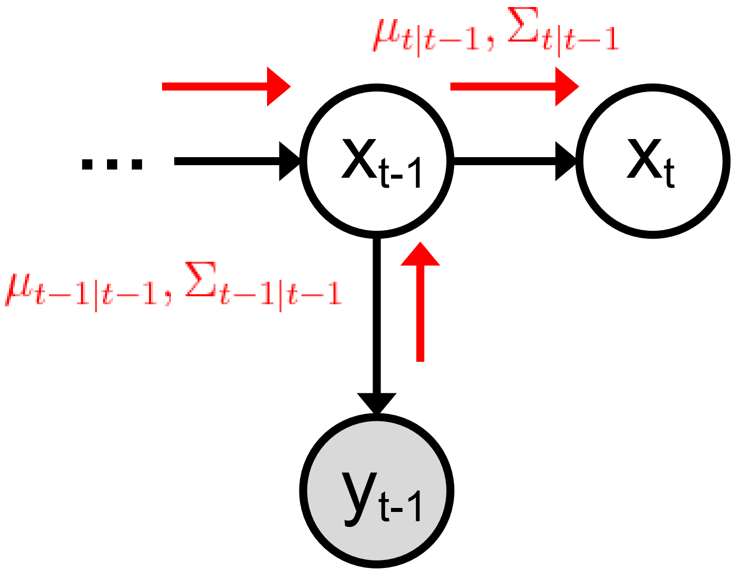
Filter Mean: $\mu_{t|t} = \mu_{t|t-1} + K_t(y_t - H\mu_{t|t-1})$

Can be derived from Gaussian conditional formulas and Woodbury matrix identity

Kalman Filter

Prediction Step:

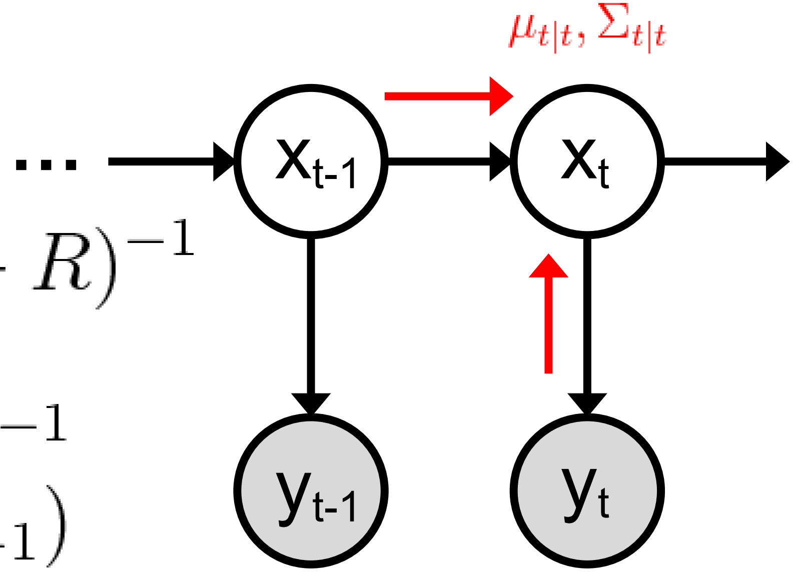
State Prediction: $\mu_{t|t-1} = F\mu_{t-1|t-1}$



Covariance Prediction:

$$\Sigma_{t|t-1} = \Sigma + F\Sigma_{t-1|t-1}F^T$$

Measurement Update Step:



Gain Matrix: $K_t = \Sigma_{t|t-1}H^T(H\Sigma_{t|t-1}H^T + R)^{-1}$

Filter Covariance: $\Sigma_{t|t} = \Sigma_{t|t-1} - K_tH\Sigma_{t|t-1}$

Filter Mean: $\mu_{t|t} = \mu_{t|t-1} + K_t(y_t - H\mu_{t|t-1})$

Kalman Filter

Prediction Step:

State Prediction: $\mu_{t|t-1} = F\mu_{t-1|t-1}$

Covariance Prediction:

$$\Sigma_{t|t-1} = \Sigma + F\Sigma_{t-1|t-1}F^T$$

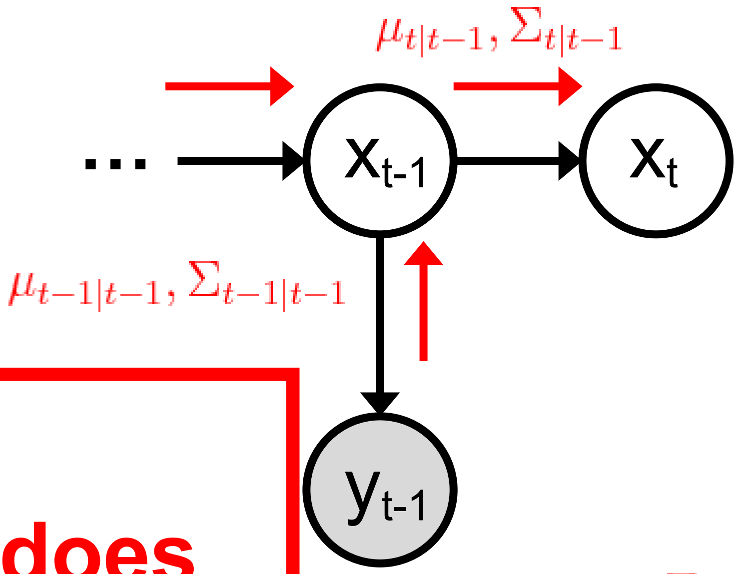
What algorithm does this look like?

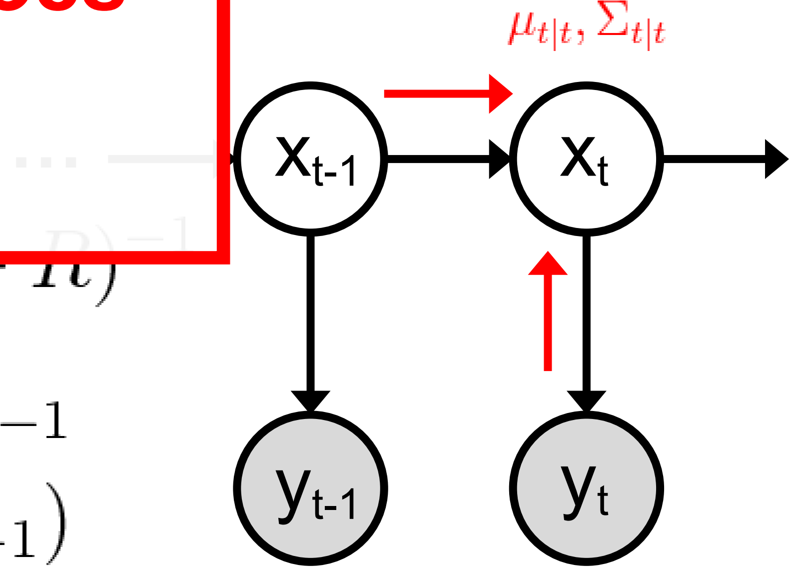
Measurement Update Step:

Gain Matrix: $K_t = \Sigma_{t|t-1}H^T(H\Sigma_{t|t-1}H^T + R)^{-1}$

Filter Covariance: $\Sigma_{t|t} = \Sigma_{t|t-1} - K_tH\Sigma_{t|t-1}$

Filter Mean: $\mu_{t|t} = \mu_{t|t-1} + K_t(y_t - H\mu_{t|t-1})$





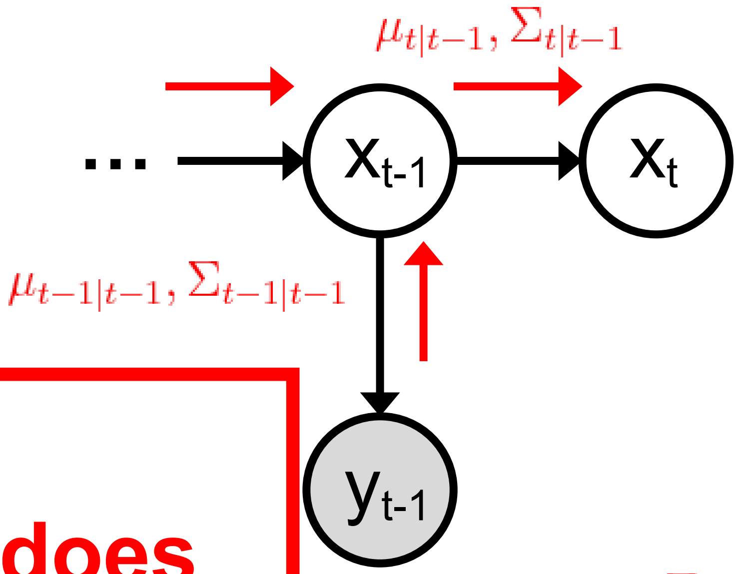
Kalman Filter

Prediction Step:

State Prediction: $\mu_{t|t-1} = F\mu_{t-1|t-1}$

Covariance Prediction:

$$\Sigma_{t|t-1} = \Sigma_x + F\Sigma_{t-1|t-1}F^T$$



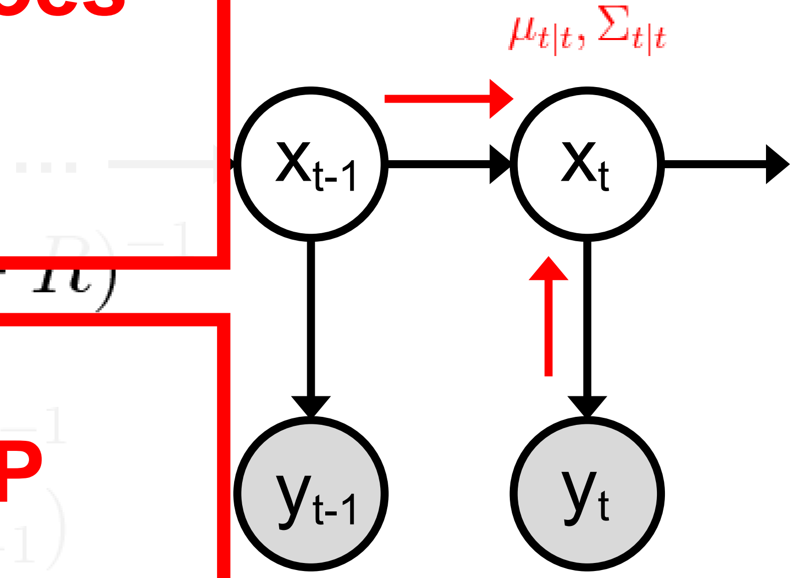
What algorithm does this look like?

Measurement Update Step:

Gain Matrix: $K_t = \Sigma_{t|t-1}H^T(H\Sigma_{t|t-1}H^T + R)^{-1}$

Filter Covariance: $\Sigma_{t|t} = \Sigma_{t|t-1} - K_t H \Sigma_{t|t-1}$

Filter Mean: $\mu_{t|t} = \mu_{t|t-1} + K_t(y_t - H\mu_{t|t-1})$



Sum-Product BP

Gaussian Parameterization

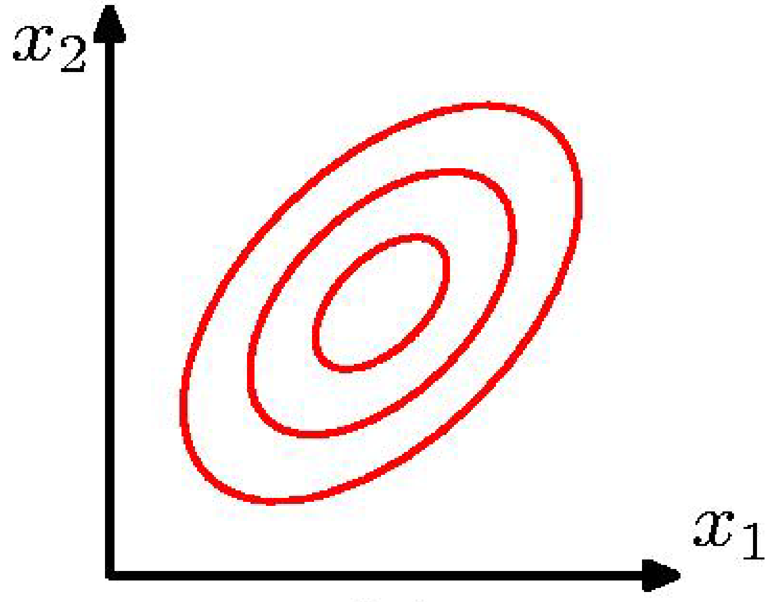
Mean Parameterization:

$$\mathcal{N}(x \mid \mu, \Sigma) = \frac{1}{(2\pi)^{N/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)\right\}$$

Canonical Parameterization

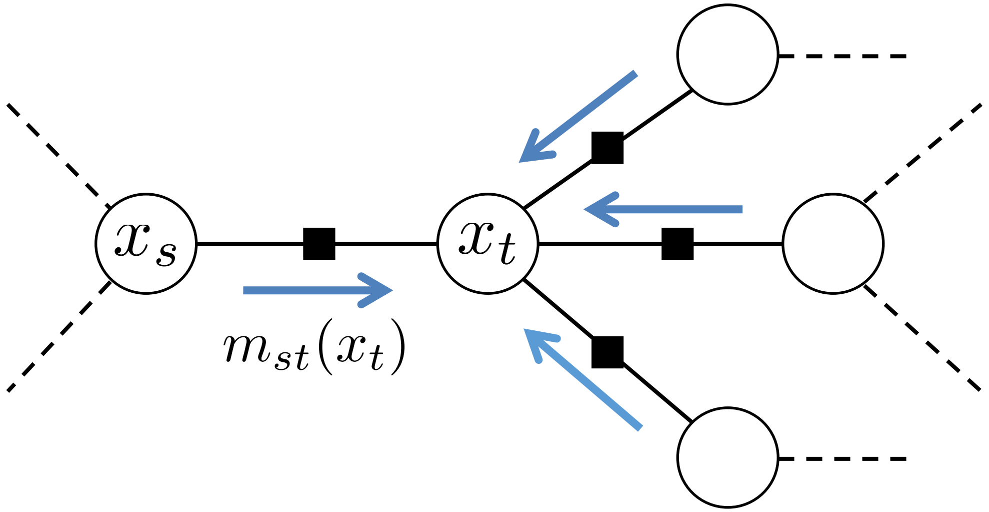
$$\mathcal{N}^{-1}(x \mid \vartheta, \Lambda) \propto \exp\left\{-\frac{1}{2} x^T \Lambda x + \vartheta^T x\right\}$$

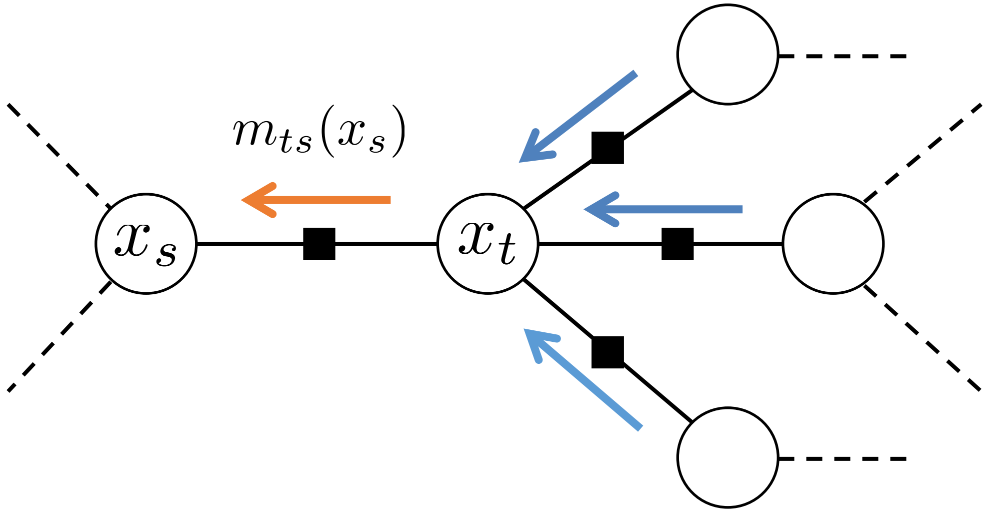
where $\Lambda = \Sigma^{-1} \quad \vartheta = \Sigma^{-1}\mu$



Also called <u>natural</u> parameters and <u>information</u> parameters in some texts…

Gaussian Belief Propagation





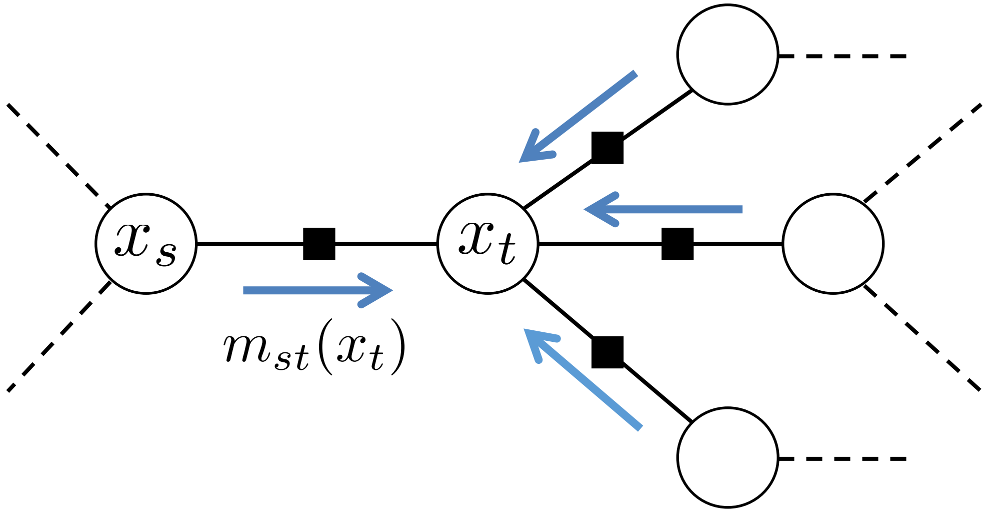
$$p_t(x_t) \propto \prod_{s \in \Gamma(t)} m_{st}(x_t) \qquad m_{ts}(x_s) = \int_{\mathcal{X}_t} \psi_{st}(x_s, x_t) \prod_{u \in \Gamma(t) \setminus s} m_{ut}(x_t)\, dx_t$$

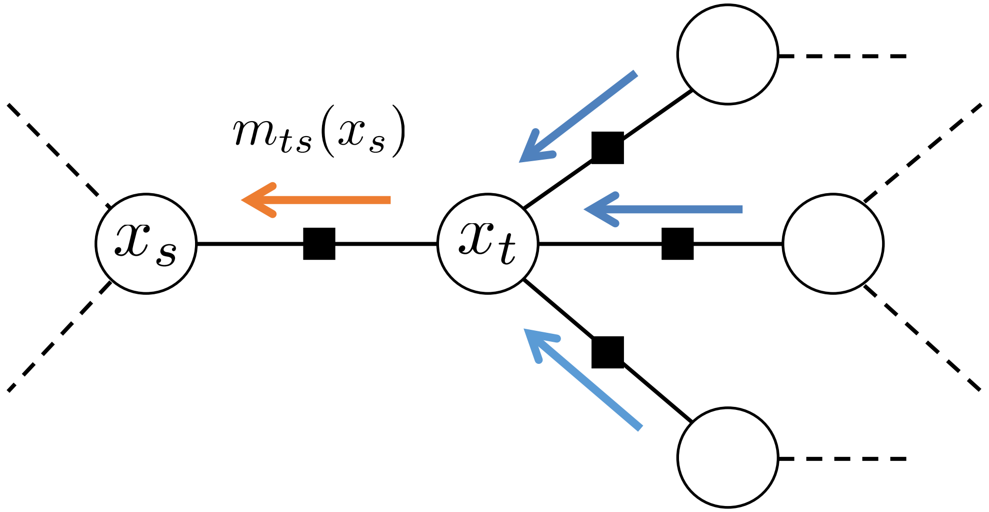
$$p_t(x_t) = \mathcal{N}^{-1}(x_t \mid \vartheta_t, \Lambda_t) \qquad m_{ts}(x_s) \propto \mathcal{N}^{-1}(x_s \mid \vartheta_{ts}, \Lambda_{ts})$$

Computing *marginal mean and covariance* from messages:

$$\Lambda_t = \sum_{s \in \Gamma(t)} \Lambda_{st} \qquad \vartheta_t = \sum_{s \in \Gamma(t)} \vartheta_{st}$$

Gaussian Belief Propagation



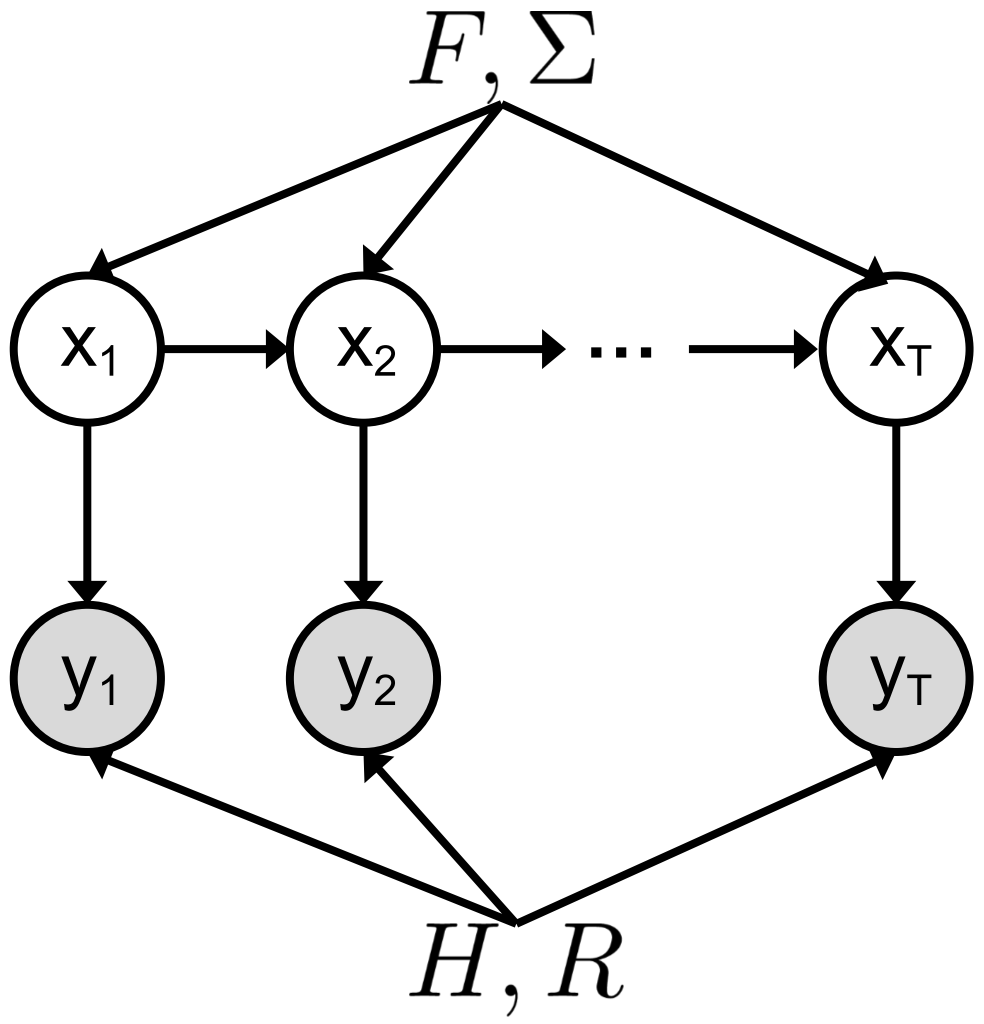


- Compute message mean & covar as algebraic function of incoming message mean & covar (generalizes Kalman)
- For tree of *N* nodes of dimension *d*, cost is *O(Nd³)*

Computing *marginal mean and covariance* from messages:

$$\Lambda_t = \sum_{s\in\Gamma(t)} \Lambda_{st} \qquad \vartheta_t = \sum_{s\in\Gamma(t)} \vartheta_{st}$$

Learning : Gaussian LDS



Probability Model

$$x_t \mid x_{t-1} \sim \mathcal{N}(F x_{t-1}, \Sigma)$$

$$y_t \mid x_t \sim \mathcal{N}(H x_t, R)$$

Learning Model Parameters

Given observations $\{y_1, y_2, \ldots, y_T\}$ across all timesteps, maximize log-marginal likelihood:

$$\max_{F,H,\Sigma,R} \log p(y_1, \ldots, y_T \mid F, H, \Sigma, R)$$

Problem We do not know the latent states $\{x_1, x_2, \ldots, x_T\}$. How to find maximum likelihood estimates?

Kalman Filter

Learning : Gaussian LDS

The Kalman filter *exactly* marginalizes latent state, e.g. at time t=1:

(Law of total Probability) $$p(y_1) = \int p(x_1)p(y_1 \mid x_1)\, dx_1$$

(LDS Model) $$= \int \mathcal{N}(x_1 \mid \mu_0, P_0)\mathcal{N}(y_1 \mid Hx_1, R)\, dx_1$$

(Gaussian Marginal) $$= \mathcal{N}(y_1 \mid H\mu_0, R + HP_0H^T)$$

For 2 timesteps we have:

(Probability Chain Rule) $$p(y_1, y_2) = p(y_1)p(y_2 \mid y_1)$$

Just did this

Let's compute this

Learning : Gaussian LDS

Conditional likelihood at time t=2:

$$p(y_2 \mid y_1) = \int_{\mathcal{X}_2}\int_{\mathcal{X}_1} p(x_1, x_2 \mid y_1) p(y_2 \mid x_2)\, dx_1 dx_2$$

(Chain rule and $x_2 \perp y_1 \mid x_1$) $$= \int_{\mathcal{X}_2}\int_{\mathcal{X}_1} p(x_1 \mid y_1) p(x_2 \mid x_1) p(y_2 \mid x_2)\, dx_1 dx_2$$

(LDS Model) $$= \int_{\mathcal{X}_2}\int_{\mathcal{X}_1} p(x_1 \mid y_1) \mathcal{N}(x_2 \mid F x_1, \Sigma) \mathcal{N}(y_2 \mid H x_2, R)\, dx_1 dx_2$$

Kalman filter distribution at time t=1 (Gaussian)

We can compute these integrals using Gaussian formulas

Surprise, $p(y_2 \mid y_1)$ is Gaussian

Learning : Gaussian LDS

Using probability chain rule we can write log-marginal likelihood as,

$$\max_{\theta} \log p(y_1^T \mid \theta) = \max_{\theta} \log p(y_1 \mid \theta) + \sum_{t=1}^{T} \log p(y_t \mid y_1^{t-1}, \theta)$$

Where $\theta = \{F, H, \Sigma, R\}$ and $y_1^T = \{y_1, \dots, y_T\}$

- Every term is Gaussian
- We can compute every term in closed-form using Kalman updates
- Directly maximizing above w.r.t. parameters is cumbersome in this form

Using Expectation Maximization turns is much easier

Expectation Maximization : Gaussian LDS

Recall the EM lower bound of the log-marginal likelihood:

$$\max_{\theta} \log p(y_1^T \mid \theta) \geq \max_{q,\theta} \mathbf{E}_q \left[\log \frac{p(x_1^T, y_1^T \mid \theta)}{q(x_1^T)} \right] \equiv \mathcal{L}(q, \theta)$$

Initialize Parameters: $\theta^{(0)}$

At iteration t do:

E-Step: $q^{(t)}(z) = p(z \mid y, \theta^{(t-1)})$

M-Step: $\theta^{(t)} = \arg\max_{\theta} \mathcal{L}(q^{(t)}, \theta)$

Until convergence

EM : Gaussian LDS

E-Step Compute *expected complete data log-likelihood,*

$$\mathbf{E}\left[\log p(x_1^T, y_1^T \mid \theta)\right] =$$

Expectation taken w.r.t. posterior $p(x_1^T \mid y_1^T, \theta^{\text{old}})$

$$= \mathbf{E}\left[\log p(x_1) + p(y_1 \mid x_1, \theta) + \sum_{t=2}^{T} \log p(x_t \mid x_{t-1}, \theta) + \log p(y_t \mid x_t, \theta)\right]$$

$$= \mathbf{E}\Big[\log \mathcal{N}(x_1 \mid \mu_0, \Sigma_0) + \log \mathcal{N}(y_1 \mid Hx_1, R) +$$

$$\sum_{t=2}^{T} \log \mathcal{N}(x_t \mid Fx_{t-1}, \Sigma) + \log \mathcal{N}(y_t \mid Hx_t, R)\Big]$$

$$= \ldots \text{ Algebra left for exercise } \ldots$$

EM : Gaussian LDS

M-Step Update estimate of the parameters,

$$\theta^{\text{new}} = \arg\max_{\theta} \; \mathbf{E}\left[\log p(x_1^T, y_1^T \mid \theta)\right]$$

- E-step + algebra = expected complete data log-like likelihood
- Solve for zero-gradient conditions of parameters,

$$\theta^{\text{new}} = \{F^{\text{new}}, H^{\text{new}}, \Sigma^{\text{new}}, R^{\text{new}}\}$$

- We won’t go through calculations here (they are somewhat tedious)

LDS Summary

Linear dynamical system,

$$x_t \mid x_{t-1} \sim \mathcal{N}(Fx_{t-1}, \Sigma) \qquad\qquad y_t \mid x_t \sim \mathcal{N}(Hx_t, R)$$

Linear Gaussian Dynamics | **Linear Gaussian Observation**

State-space representation same as linear regression,

$$x_t = Fx_{t-1} + \epsilon \quad \text{where} \quad \epsilon \sim \mathcal{N}(0, \Sigma)$$

Exact posterior inference via Kalman filter

- Recursively pass marginal moments
- Two steps: prediction, measurement update
- Forward pass filtering, backward pass smoothing

Kalman is special case of Gaussian sum-product BP

Outline

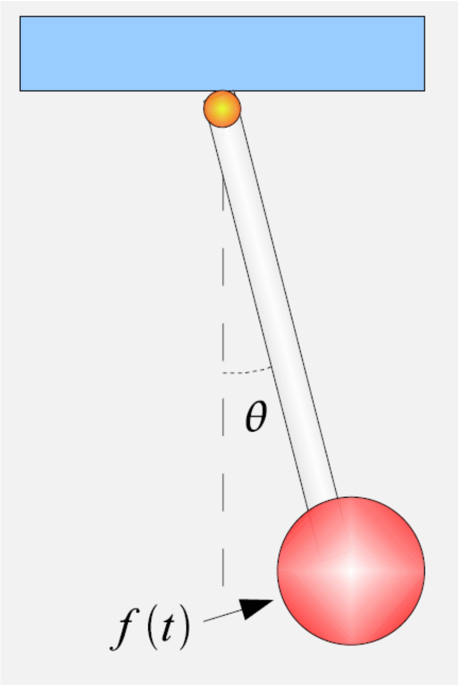
- Sequence Models
- Linear Dynamical Systems
- LDS Extensions

Nonlinear Dynamical System

Pendulum with mass m=1,pole length L=1:

$$x_t = \begin{pmatrix} \theta_t \\ \dot{\theta}_t \end{pmatrix} = \underbrace{\begin{pmatrix} \theta_{t-1} + \dot{\theta}_{t-1} \\ \dot{\theta}_{t-1} - g\sin(\theta_{t-1}) \end{pmatrix}}_{f(x_{t-1})} + \epsilon$$

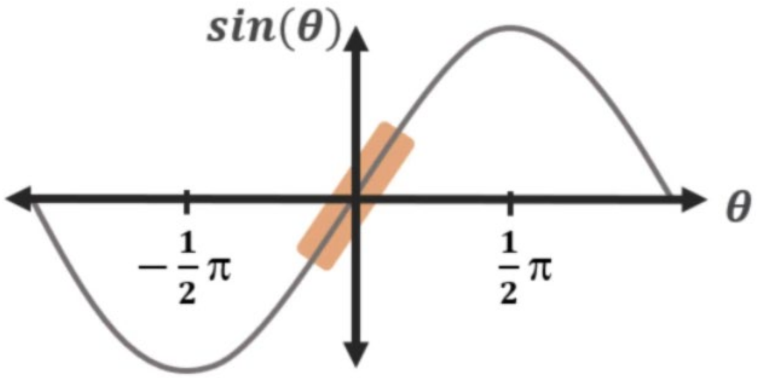
$$y_t = \underbrace{\sin(\theta_t)}_{h(x_t)} + \omega$$



Nonlinear dynamics / measurement:

$$x_t = f(x_{t-1}) + \epsilon \sim \mathcal{N}(0, \Sigma)$$

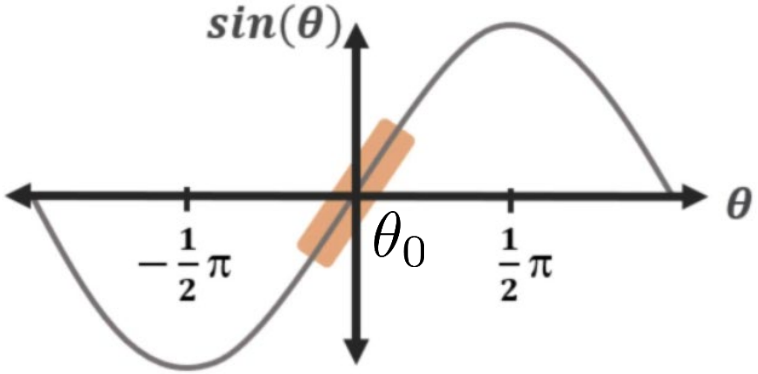
$$y_t = h(x_t) + \omega \sim \mathcal{N}(0, R)$$



Linearizing a Nonlinear Function

Suppose that we have a nonlinear function:

$$h(\theta) = \sin(\theta)$$



Taylor series representation

- Choose any evaluation point θ_0
- Represent via successive derivatives, evaluated at θ_0

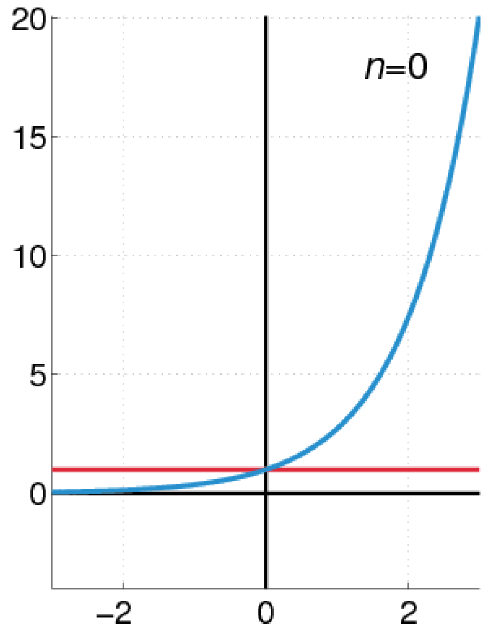
Approximation error grows with distance from θ_0

$$h(\theta) = h(\theta_0) + \frac{h^{'}(\theta_0)}{1!}(\theta - \theta_0) + \frac{h^{''}(\theta_0)}{2!}(\theta - \theta_0)^2 + \frac{h^{'''}(\theta_0)}{3!}(\theta - \theta_0)^3 + \ldots$$

Infinite series holds with equality

Linear approximation discards higher-order derivatives:

$$h(\theta) \approx h(\theta_0) + \frac{h^{'}(\theta_0)}{1!}(\theta - \theta_0)$$



Linearizing Vector-Valued Functions

- Let $f : \mathbb{R}^N \rightarrow \mathbb{R}^M$ be vector-valued function
- Linear approximation about a is given by:

$$f(x) \approx f(a) + \mathbf{J}(a)(x - a)$$

- $\mathbf{J}(a)$ is the *Jacobian* matrix of partial derivatives (evaluated at a)

$$\mathbf{J} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_N} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_M}{\partial x_1} & \frac{\partial f_M}{\partial x_2} & \cdots & \frac{\partial f_M}{\partial x_N} \end{pmatrix}$$

- Partial derivatives of each output dim w.r.t each input dim
- First dim. Matches function output, second dim. Input

$$\mathbf{J} \in \mathbb{R}^{N \times M}$$

- All partials will be evaluated at chosen point a
- Thus function is approximation *about the point* a

Nonlinear Dynamical System

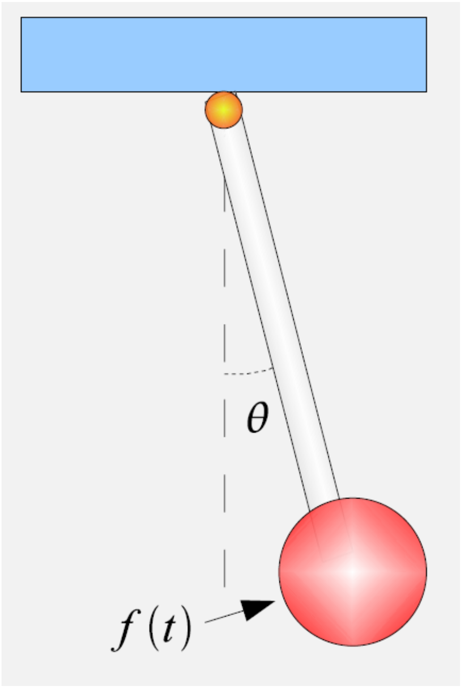
Filter equations lack a closed-form:

Prediction:

$$p(x_t \mid y_1^{t-1}) = \int \mathcal{N}(x_t \mid f(x_{t-1}), \Sigma) p(x_{t-1} \mid y_1^{t-1})\, dx_{t-1}$$

Measurement Update:

$$p(x_t \mid y_1^t) \propto \mathcal{N}(y_t \mid h(x_t), R) p(x_t \mid y_1^{t-1})$$



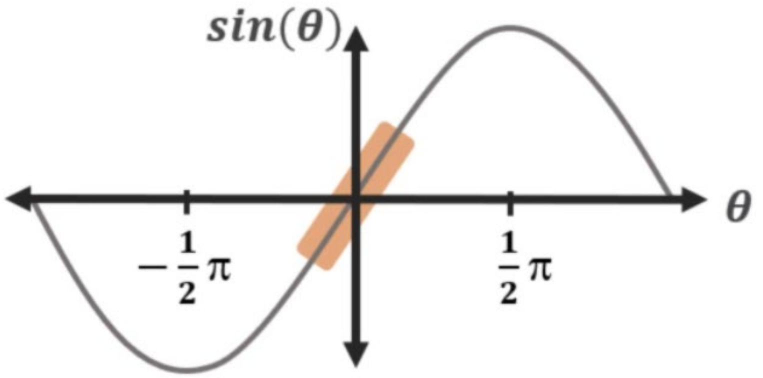
Idea *Linearize* f(.) and h(.) about a point m:

$$f(x) \approx f(m) + \mathbf{J}_f(m)(x - m)$$

$$h(x) \approx h(m) + \mathbf{J}_h(m)(x - m)$$

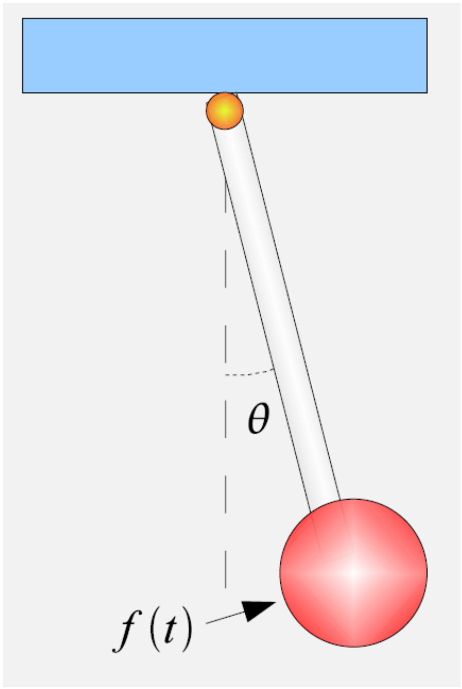
1st Order Taylor expansion

where $\mathbf{J}_f = \left(\frac{\partial f_i}{\partial x_j} \right)$ is Jacobian matrix of partials



Extended Kalman Filter

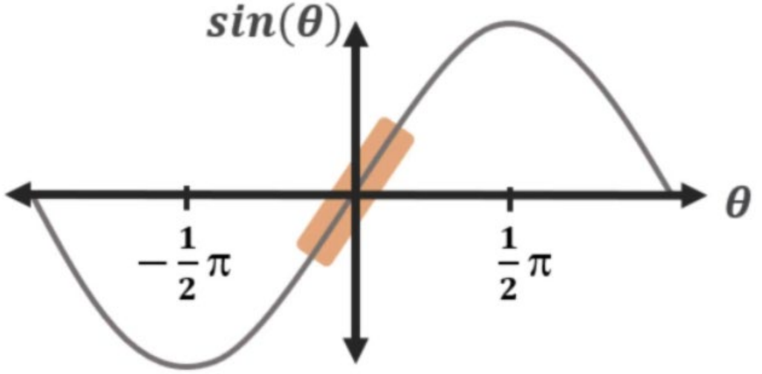
1. Linearize f(.) and h(.) about filter mean
2. Assume linear Gaussian model
3. Do standard Kalman updates



Example Linearization of pendulum model

$$x_t = \begin{pmatrix} \theta_t \\ \dot{\theta}_t \end{pmatrix} = \underbrace{\begin{pmatrix} \theta_{t-1} + \dot{\theta}_{t-1} \\ \dot{\theta}_{t-1} - g\sin(\theta_{t-1}) \end{pmatrix}}_{f(x_{t-1})} + \epsilon \qquad y_t = \underbrace{\sin(\theta_t)}_{h(x_t)} + \omega$$

$$\mathbf{J}_f(x) = \begin{pmatrix} 1 & 1 \\ -g\cos(x^1) & 1 \end{pmatrix} \qquad \mathbf{J}_h(x) = (\cos(x^1), 0)$$



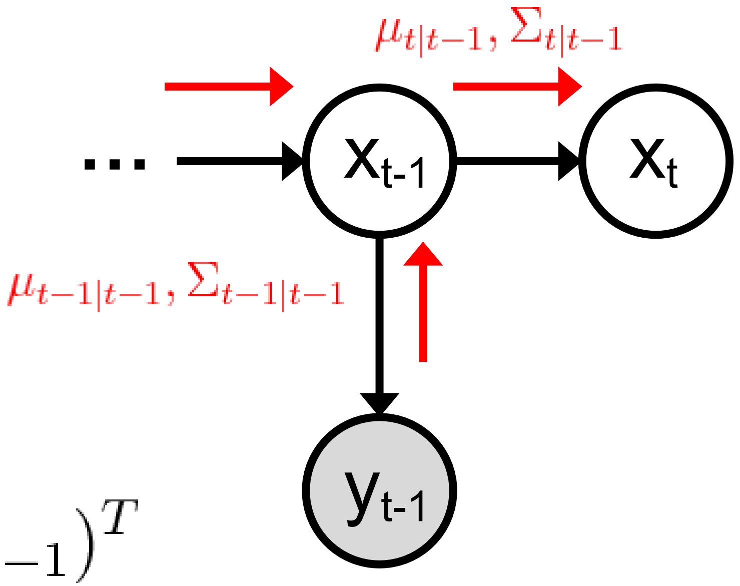
EKF Update Equations

Prediction Step:

State Prediction: $\mu_{t|t-1} = f(\mu_{t-1|t-1})$

Covariance Prediction:

$$\Sigma_{t|t-1} = \Sigma + \mathbf{J}_f(\mu_{t-1|t-1})\Sigma_{t-1|t-1}\mathbf{J}_f(\mu_{t-1|t-1})^T$$

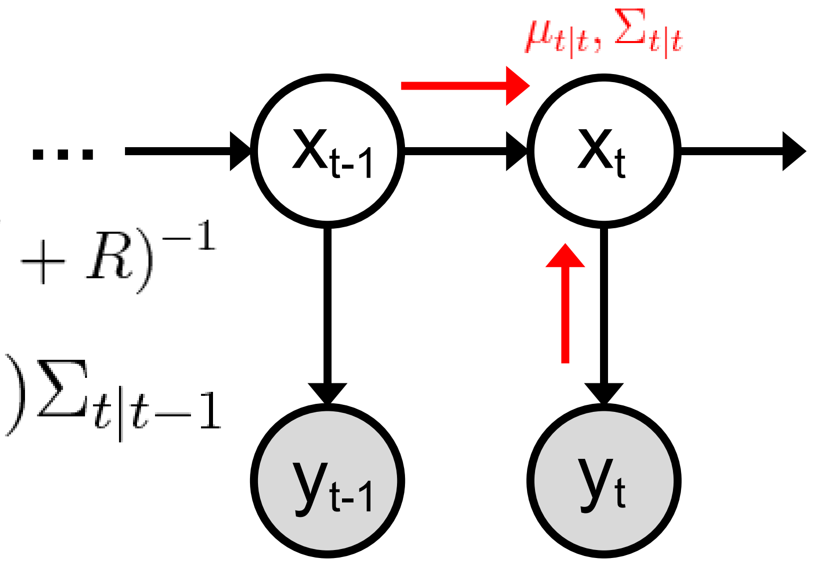


Measurement Update Step:

Gain: $K_t = \Sigma_{t|t-1}\mathbf{J}_h(\mu_{t|t-1})^T(\mathbf{J}_h(\mu_{t|t-1})\Sigma_{t|t-1}\mathbf{J}_h(\mu_{t|t-1})^T + R)^{-1}$

Filter Covariance: $\Sigma_{t|t} = \Sigma_{t|t-1} - K_t\mathbf{J}_h(\mu_{t|t-1})\Sigma_{t|t-1}$

Filter Mean: $\mu_{t|t} = \mu_{t|t-1} + K_t(y_t - h(\mu_{t|t-1}))$



Extended Kalman Filter

PROS:

- Easy to implement – updates analogous to standard Kalman
- Computationally efficient
- Known theoretical stability results

CONS:

- Linearity assumption poor for highly nonlinear models
- Requires model differentiability
- Jacobian matrices can be hard to calculate & implement

Unscented Kalman filter (UKF) typically more accurate in practice

Other Nonlinear Filtering Options

Key issue is approximating integrals:

$$p(x_t \mid y_1^{t-1}) = \int p(x_t \mid x_{t-1}) p(x_{t-1} \mid y_1^{t-1}) \, dx_{t-1}$$

Dynamics Filter at t-1

$$= \int \mathcal{N}(x_t \mid f(x_{t-1}), Q) p(x_{t-1} \mid y_1^{t-1}) \, dx_{t-1}$$

Option 1 : Use Gaussian quadrature → *Unscented Kalman Filter* (UKF)

- Approximates integral using deterministic control points
- Tends to be more accurate than EKF

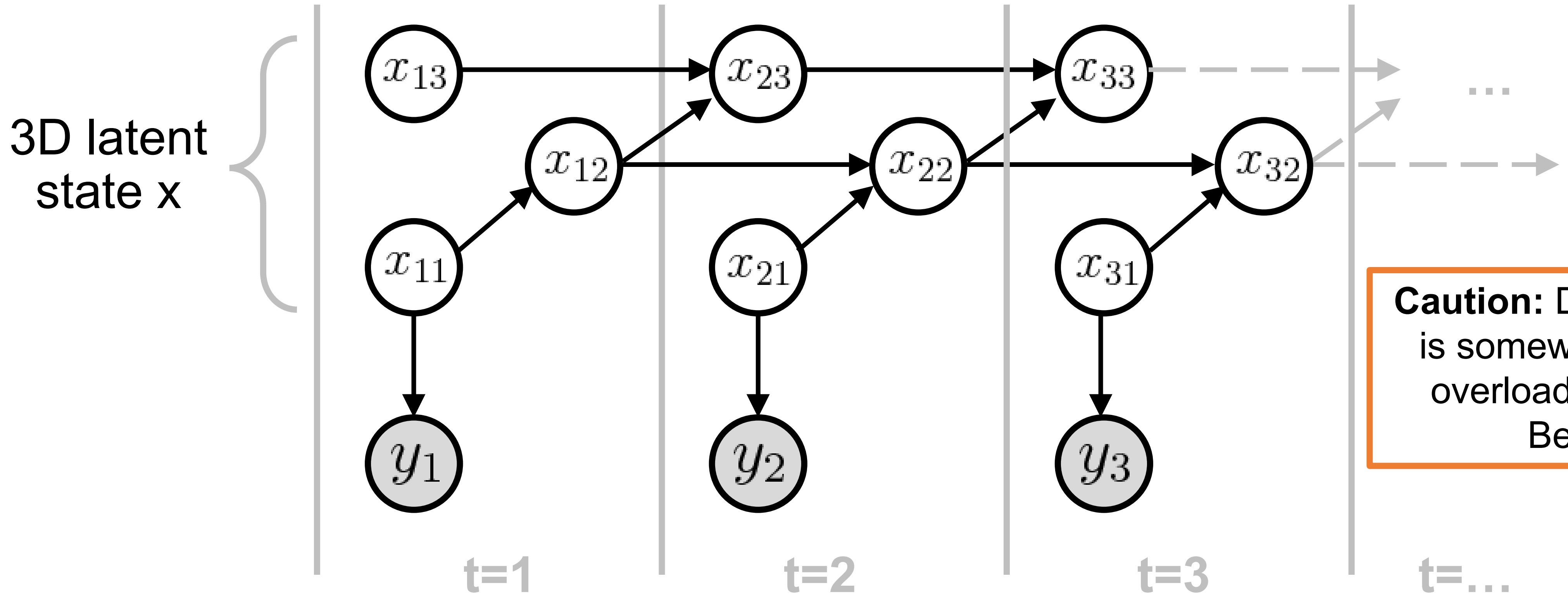
Option 2 : Sample-based approximation → *Particle Filter* (PF)

- Draw samples from filter $\{x_{t-1}^{(i)}\}_{i=1}^M \sim p(x_{t-1} \mid y_1^{t-1})$
- Monte Carlo approximation of integral using samples,

$$p(x_t \mid y_1^{t-1}) \approx \mathbb{E}_{\{x_{t-1}^{(i)}\}} [\mathcal{N}(x_t \mid f(x_{t-1}), Q)]$$

We will cover this…

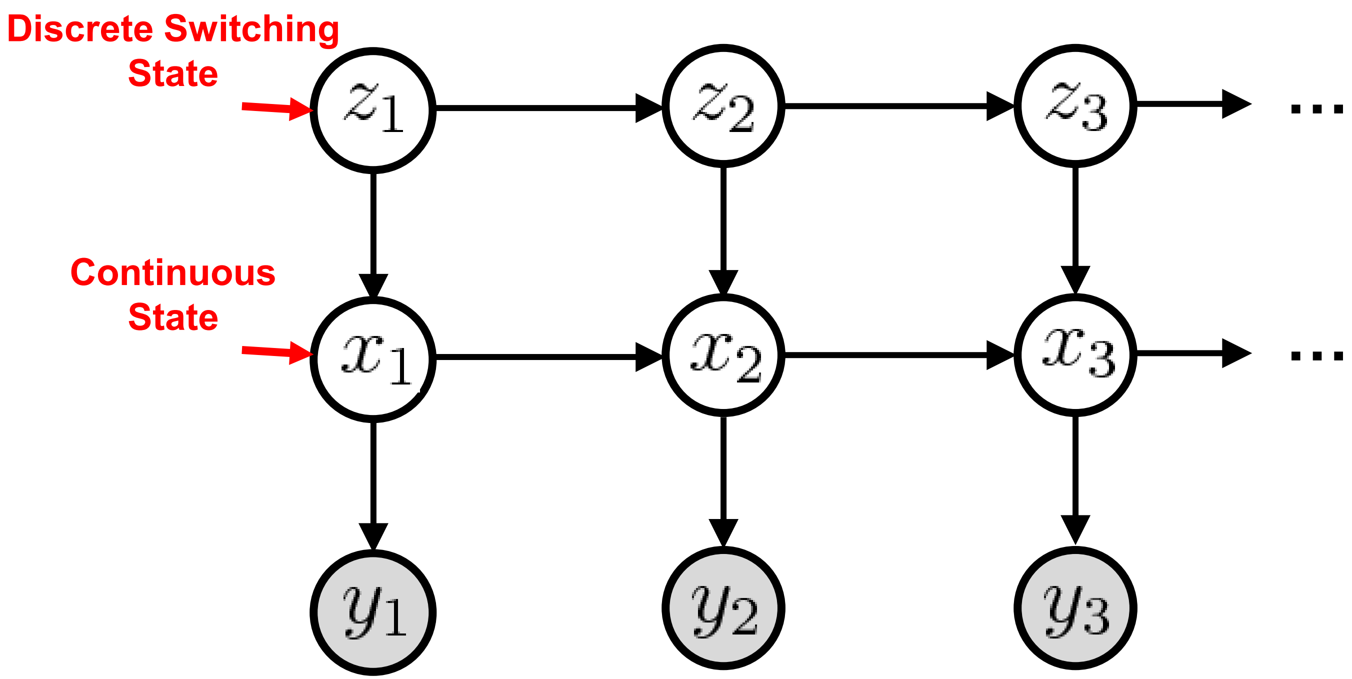
Dynamic Bayesian Networks

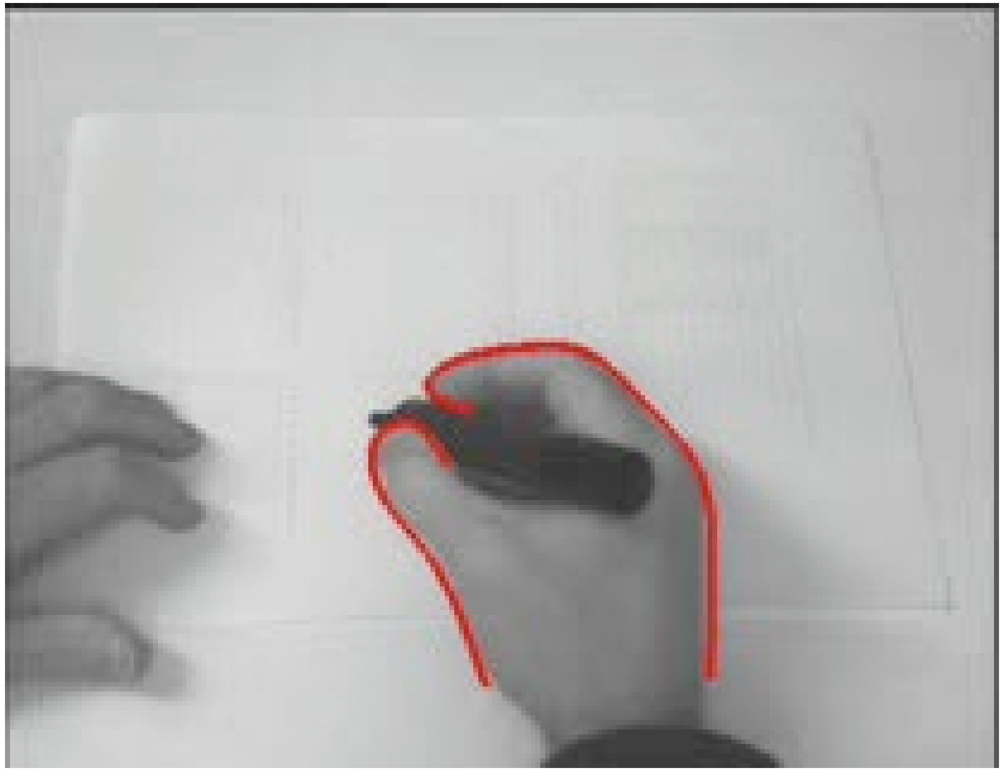


Caution: DBN terminology is somewhat vague and overloaded (e.g. Deep Belief Net)

- Multivariate latent state (e.g. $x \in \mathbb{R}^3$)
- Dynamics for each component within and across time
- Sometimes used as catch-all term for dynamical systems

Switching Linear Dynamical System





Colors indicate 3 writing modes

[Video: Isard & Blake, ICCV 1998.]

Discrete switching state:

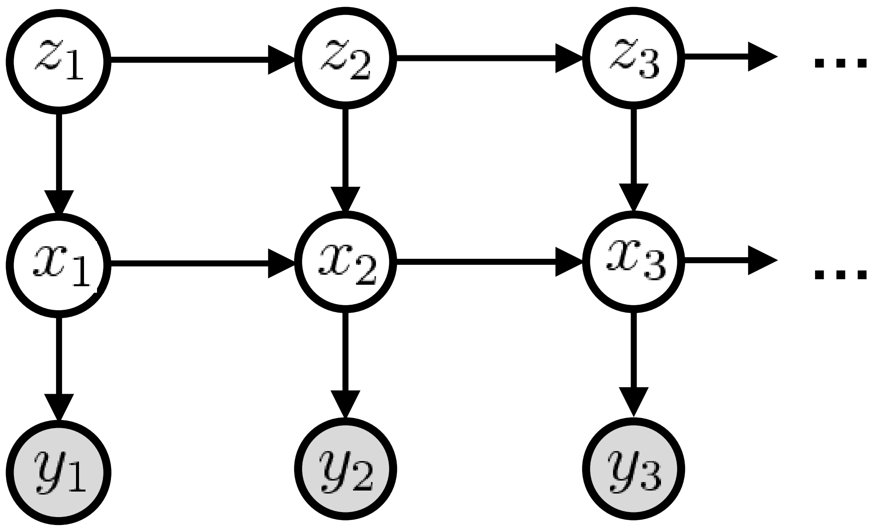
$$z_t \mid z_{t-1} \sim \mathrm{Cat}(\pi(z_{t-1}))$$ With stochastic transition matrix π

Switching state selects linear dynamics:

$$x_t \mid x_{t-1} \sim \mathcal{N}(A_{z_t} x_{t-1}, \Sigma_{z_t})$$ (e.g. Linear Gaussian)

Switching Linear Dynamical System

We can do sum-product for HMM and LDS, so maybe we can do it for SLDS…



Forward message,

$$m_{t-1,t}(z_t, x_t) \propto \int \sum_{z_{t-1}} m_{t-2,t-1}(z_{t-1}, x_{t-1}) p(y_{t-1} \mid x_{t-1}) \\ p(z_t \mid z_{t-1}) p(x_t \mid x_{t-1}, z_t) dx_{t-1}$$

Integrates to Gaussian for each possible state z_{t-1}

$$= \int \sum_{z_{t-1}} m_{t-2,t-1}(z_{t-1}, x_{t-1}) \mathcal{N}(y_{t-1} \mid H x_{t-1}, R) \mathrm{Cat}(z_t \mid \pi(z_{t-1})) \mathcal{N}(x_t \mid A_{z_t} x_{t-1}, \Sigma_{z_t}) dx_{t-1}$$

- Message is Gaussian mixture over K states (for some K)
- But incoming message is also a Gaussian mixture
- Number of components (K) grows exponentially with time t

One way is to use sample-based methods (Particle Filter)

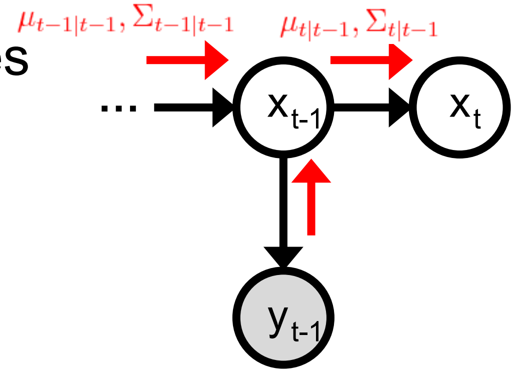
Summary

- Linear dynamical system is time-extension of PCA,

$$x_t \mid x_{t-1} \sim \mathcal{N}(Fx_{t-1}, \Sigma) \qquad\qquad y_t \mid x_t \sim \mathcal{N}(Hx_t, R)$$

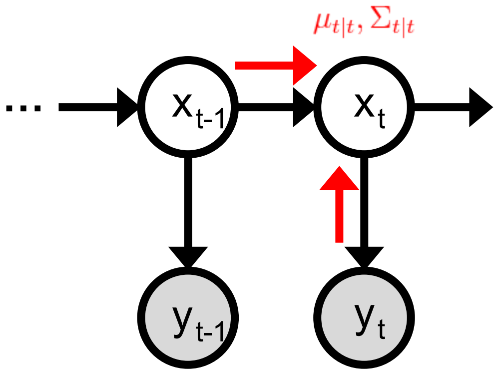
- Exact inference via Kalman filtering,

Prediction step updates moments of predictive distribution $p(x_t \mid y_1^{t-1})$

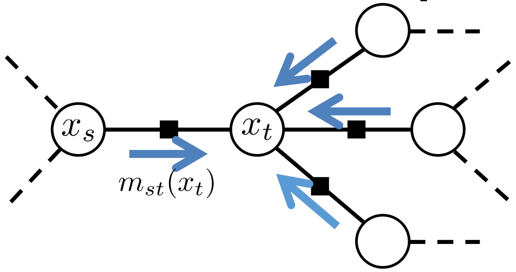


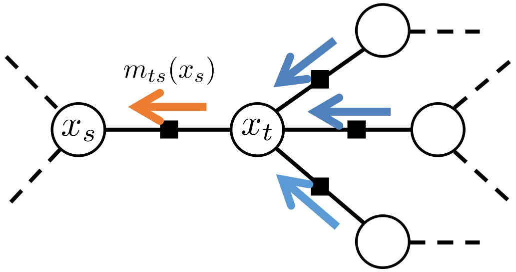
Measurement step updates filter distribution with newest measumrent

$$p(x_t \mid y_1^t)$$



- Kalman filter is special case of Gaussian belief propagation





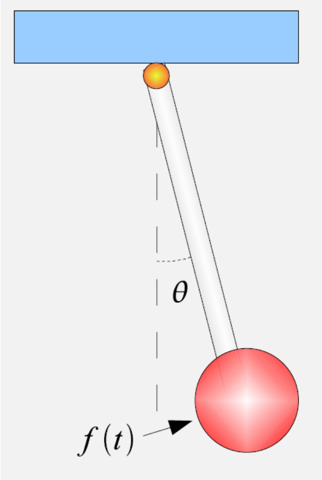
Messages represented as Gaussian **natural parameters**

Summary

- Nonlinear state-space models allow more complex dynamics,

$$x_t = \begin{pmatrix} \theta_t \\ \dot{\theta}_t \end{pmatrix} = \underbrace{\begin{pmatrix} \theta_{t-1} + \dot{\theta}_{t-1} \\ \dot{\theta}_{t-1} - g\sin(\theta_{t-1}) \end{pmatrix}}_{f(x_{t-1})} + \epsilon$$

$$y_t = \underbrace{\sin(\theta_t)}_{h(x_t)} + \omega$$



Approximate Kalman filter inference via linearization (Extended Kalman Filter) or Gaussian quadrature (Unscented Kalman Filter)

- Switching state-space model represents discrete & continuous states,

Exact inference intractable due to exponential growth in message parameters

Both nonlinear and SSMs can be addressed using sample-based methods (e.g. Particle Filtering) as we will see