

Probabilistic & Unsupervised Learning

Latent Variable Models for Time Series

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Modeling time series

Thus far, our data have been (marginally) iid. Now consider a sequence of observations:

$$\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \dots, \mathbf{x}_t$$

that are *not* independent.

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- ▶ Kinematic variables in a robot
- ▶ Sensor readings from an industrial process
- ▶ Amino acids, DNA, etc. . .

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- ▶ Predict $p(\mathbf{x}_t | \mathbf{x}_1, \dots, \mathbf{x}_{t-1})$
- ▶ Detect abnormal/changed behaviour (if $p(\mathbf{x}_t, \mathbf{x}_{t+1}, \dots | \mathbf{x}_1, \dots, \mathbf{x}_{t-1})$ small)

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- ▶ Recover underlying/latent/hidden causes linking entire sequence

Markov models

In general:

$$P(\mathbf{x}_1, \dots, \mathbf{x}_t) = P(\mathbf{x}_1)P(\mathbf{x}_2|\mathbf{x}_1)P(\mathbf{x}_3|\mathbf{x}_1, \mathbf{x}_2) \cdots P(\mathbf{x}_t|\mathbf{x}_1, \mathbf{x}_2 \dots \mathbf{x}_{t-1})$$

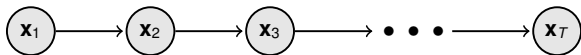
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First-order Markov model:

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The term *Markov* refers to a conditional independence relationship. In this case, the Markov property is that, given the present observation (\mathbf{x}_t), the future (\mathbf{x}_{t+1}, \dots) is independent of the past ($\mathbf{x}_1, \dots, \mathbf{x}_{t-1}$).

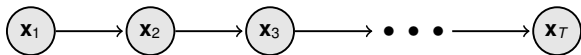
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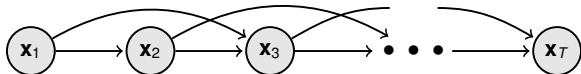
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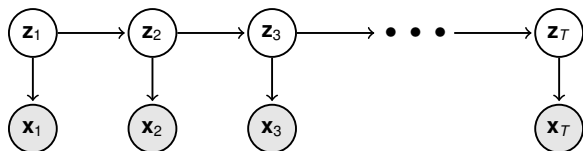
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Second-order Markov model:

$$P(\mathbf{x}_1, \dots, \mathbf{x}_t) = P(\mathbf{x}_1)P(\mathbf{x}_2|\mathbf{x}_1) \cdots P(\mathbf{x}_{t-1}|\mathbf{x}_{t-3}, \mathbf{x}_{t-2})P(\mathbf{x}_t|\mathbf{x}_{t-2}, \mathbf{x}_{t-1})$$



Causal structure and latent variables



Temporal dependence captured by latents, with observations conditionally independent.

Speech recognition:

- ▶ z - underlying phonemes or words
- ▶ x - acoustic waveform

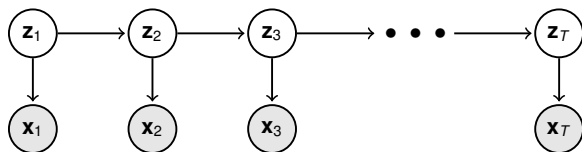
Vision:

- ▶ z - object identities, poses, illumination
- ▶ x - image pixel values

Industrial Monitoring:

- ▶ z - current state of molten steel in caster
- ▶ x - temperature and pressure sensor readings

Latent-Chain models



Joint probability factorizes:

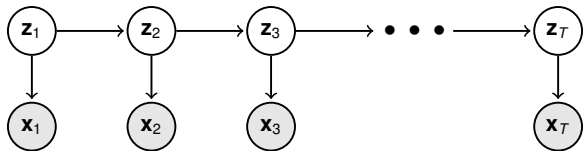
$$P(\mathbf{z}_{1:T}, \mathbf{x}_{1:T}) = P(\mathbf{z}_1) P(\mathbf{x}_1 | \mathbf{z}_1) \prod_{t=2}^T P(\mathbf{z}_t | \mathbf{z}_{t-1}) P(\mathbf{x}_t | \mathbf{z}_t)$$

where \mathbf{z}_t and \mathbf{x}_t are both real-valued vectors, and $\square_{1:T} \equiv \square_1, \dots, \square_T$.

Two frequently-used tractable models:

- ▶ Linear-Gaussian state-space models
- ▶ Hidden Markov models

Linear-Gaussian state-space models (SSMs)



In a **linear Gaussian SSM** all conditional distributions are linear and Gaussian:

Output equation: $\mathbf{x}_t = \mathbf{C}\mathbf{z}_t + \mathbf{v}_t$

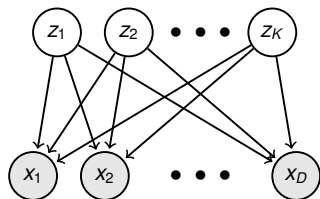
State dynamics equation: $\mathbf{z}_t = \mathbf{A}\mathbf{z}_{t-1} + \mathbf{w}_t$

where \mathbf{v}_t and \mathbf{w}_t are uncorrelated zero-mean multivariate Gaussian noise vectors.

Also assume \mathbf{z}_1 is multivariate Gaussian. The joint distribution over all variables $\mathbf{x}_{1:T}, \mathbf{z}_{1:T}$ is (one big) multivariate Gaussian.

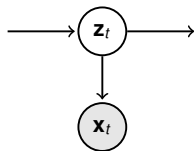
These models are also known as stochastic **linear dynamical systems**, **Kalman filter models**.

From factor analysis to state space models



Factor analysis:
$$x_i = \sum_{j=1}^K \Lambda_{ij} z_j + \epsilon_i$$

\Leftrightarrow

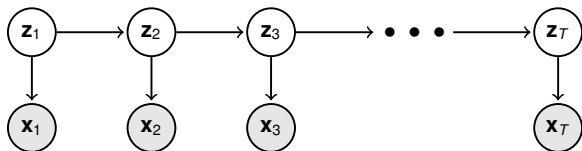


SSM output:
$$x_{t,i} = \sum_{j=1}^K C_{ij} z_{t,j} + v_{t,i}.$$

Interpretation 1:

- ▶ Observations confined near low-dimensional subspace (as in FA/PCA).
- ▶ Successive observations are generated from correlated points in the latent space.
- ▶ However:
 - ▶ FA requires $K < D$ and Ψ diagonal; SSMs may have $K \geq D$ and arbitrary output noise. **Why?**
 - ▶ Thus ML estimates of subspace by FA and SSM may differ.

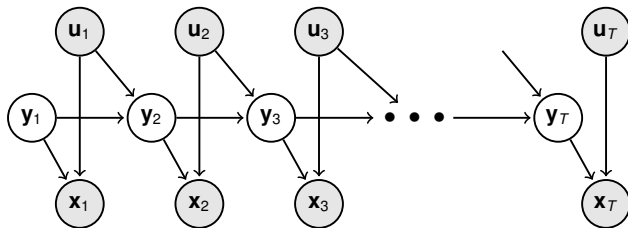
Linear dynamical systems



Interpretation 2:

- ▶ Markov chain with **linear dynamics** $\mathbf{z}_t = \mathbf{A}\mathbf{z}_{t-1} \dots$
- ▶ \dots perturbed by Gaussian **innovations** noise – may describe stochasticity, unknown control, or model mismatch.
- ▶ Observations are a linear projection of the dynamical state, with additive iid Gaussian noise.
- ▶ Note:
 - ▶ Dynamical process (\mathbf{z}_t) may be higher dimensional than the observations (\mathbf{x}_t).
 - ▶ Observations **do not** form a Markov chain – longer-scale dependence reflects/reveals latent dynamics.

State Space Models with Control Inputs



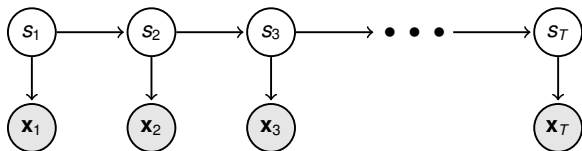
State space models can be used to model the input–output behaviour of controlled systems. The observed variables are divided into **inputs** (u_t) and **outputs** (x_t).

State dynamics equation: $z_t = Az_{t-1} + Bu_{t-1} + w_t$.

Output equation: $x_t = Cz_t + Du_t + v_t$.

Note that we can have many variants, e.g. $z_t = Az_{t-1} + Bu_t + w_t$ or even $z_t = Az_{t-1} + Bx_{t-1} + w_t$.

Hidden Markov models



Discrete hidden states $s_t \in \{1 \dots, K\}$; outputs \mathbf{x}_t can be discrete or continuous.

Joint probability factorizes:

$$P(s_{1:T}, \mathbf{x}_{1:T}) = P(s_1)P(\mathbf{x}_1|s_1) \prod_{t=2}^T P(s_t|s_{t-1})P(\mathbf{x}_t|s_t)$$

Generative process:

- ▶ A first-order Markov chain generates the hidden state sequence (path):

initial state probs: $\pi_j = P(s_1 = j)$

transition matrix: $\Phi_{ij} = P(s_{t+1} = j | s_t = i)$

- ▶ A set of emission (output) distributions $A_j(\cdot)$ (one per state) converts state path to a sequence of observations \mathbf{x}_t .

$$A_j(\mathbf{x}) = P(\mathbf{x}_t = \mathbf{x} | s_t = j)$$

(for continuous \mathbf{x}_t)

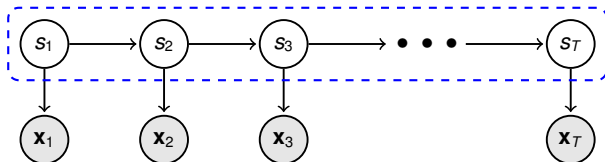
$$A_{jk} = P(\mathbf{x}_t = k | s_t = j)$$

(for discrete \mathbf{x}_t)

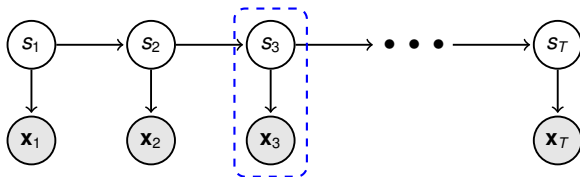
Hidden Markov models

Two interpretations:

- ▶ a Markov chain with stochastic measurements:



- ▶ or a mixture model with states coupled across time:

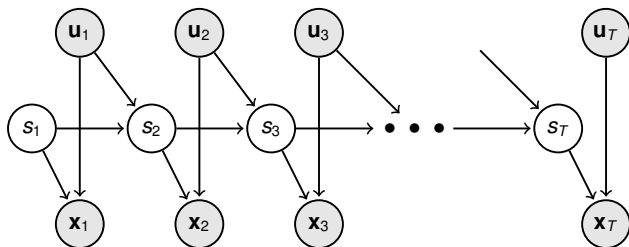


Even though hidden state sequence is first-order Markov, the output process may not be Markov of **any** order (for example: 11111211111311121111131 ...).

Discrete state, discrete output models can approximate any continuous dynamics and observation mapping even if nonlinear; however this is usually not practical.

HMMs are related to [stochastic finite state machines/automata](#).

Input-output hidden Markov models



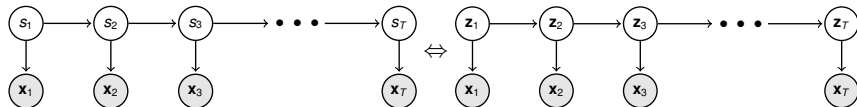
Hidden Markov models can also be used to model sequential input-output behaviour:

$$P(s_{1:T}, \mathbf{x}_{1:T} | u_{1:T}) = P(s_1 | u_1) P(\mathbf{x}_1 | s_1, u_1) \prod_{t=2}^T P(s_t | s_{t-1}, u_{t-1}) P(\mathbf{x}_t | s_t, u_t)$$

IOHMMs can capture arbitrarily complex input-output relationships, however the number of states required is often impractical.

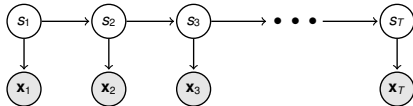
HMMs and SSMs

(Linear Gaussian) State space models are the **continuous state analogue** of hidden Markov models.



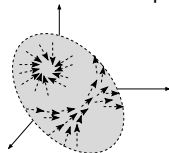
- ▶ A continuous vector state is a very powerful representation.

For an HMM to communicate N bits of information about the past, it needs 2^N states! But a real-valued state vector can store an arbitrary number of bits in principle.

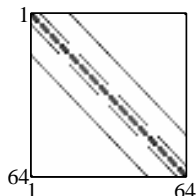
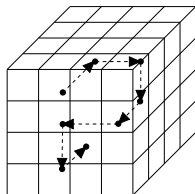


- ▶ Linear-Gaussian output/dynamics are very weak.

The types of dynamics linear SSMs can capture is very limited. HMMs can in principle represent arbitrary stochastic dynamics and output mappings.

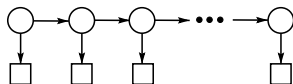


Many Extensions



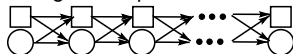
- ▶ Constrained HMMs

- ▶ Continuous state models with discrete outputs for time series and static data

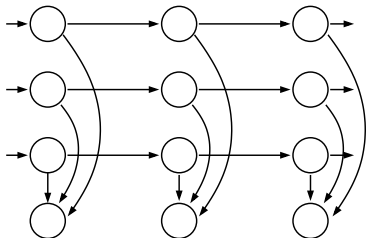


- ▶ Hierarchical models

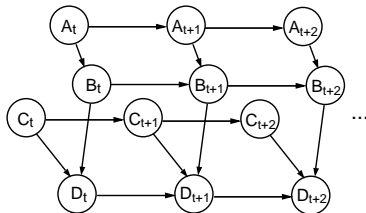
- ▶ Hybrid systems \Leftrightarrow Mixed continuous & discrete states, switching state-space models



Richer state representations



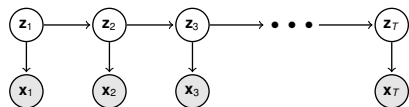
Factorial HMMs



Dynamic Bayesian Networks

- ▶ These are hidden Markov models with many state variables (i.e. a distributed representation of the state).
- ▶ The state can capture many more bits of information about the sequence (linear in the number of state variables).

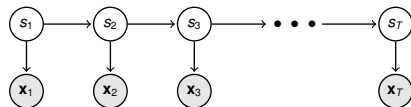
Chain models: ML Learning with EM



$$z_1 \sim \mathcal{N}(\mu_0, Q_0)$$

$$z_t | z_{t-1} \sim \mathcal{N}(Az_{t-1}, Q)$$

$$x_t | z_t \sim \mathcal{N}(Cz_t, R)$$



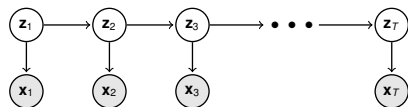
$$s_1 \sim \pi$$

$$s_t | s_{t-1} \sim \Phi_{s_{t-1}, \cdot}$$

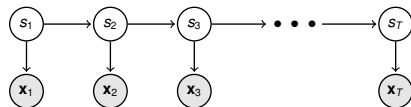
$$x_t | s_t \sim A_{s_t}$$

The structure of learning and inference for both models is dictated by the factored structure.

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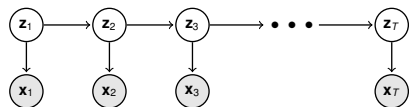


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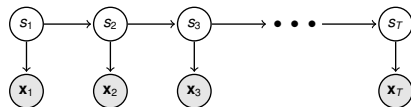
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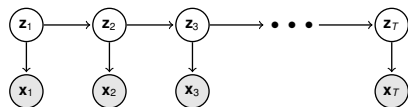
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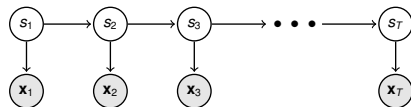
Learning (M-step):

$$\begin{aligned}\operatorname{argmax} \langle \log P(\mathbf{x}_1, \dots, \mathbf{x}_T, \mathbf{z}_1, \dots, \mathbf{z}_T) \rangle_{q(\mathbf{z}_1, \dots, \mathbf{z}_T)} = \\ \operatorname{argmax} \left[\langle \log P(\mathbf{z}_1) \rangle_{q(\mathbf{z}_1)} + \sum_{t=2}^T \langle \log P(\mathbf{z}_t | \mathbf{z}_{t-1}) \rangle_{q(\mathbf{z}_t, \mathbf{z}_{t-1})} + \sum_{t=1}^T \langle \log P(\mathbf{x}_t | \mathbf{z}_t) \rangle_{q(\mathbf{z}_t)} \right]\end{aligned}$$

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So the expectations needed (in E-step) are derived from singleton and pairwise marginals.

Chain models: Inference

Three general inference problems:

Filtering: $P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_t)$

Smoothing: $P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_T)$ (also $P(\mathbf{z}_t, \mathbf{z}_{t-1} | \mathbf{x}_1, \dots, \mathbf{x}_T)$ for learning)

Prediction: $P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_{t-\Delta t})$

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Prediction: $P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_{t-\Delta t})$

Naively, these marginal posteriors seem to require very large integrals (or sums)

$$P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_t) = \int \cdots \int d\mathbf{z}_1 \dots d\mathbf{z}_{t-1} P(\mathbf{z}_1, \dots, \mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_t)$$

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Three general inference problems:

Filtering: $P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_t)$

Smoothing: $P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_T)$ (also $P(\mathbf{z}_t, \mathbf{z}_{t-1} | \mathbf{x}_1, \dots, \mathbf{x}_T)$ for learning)

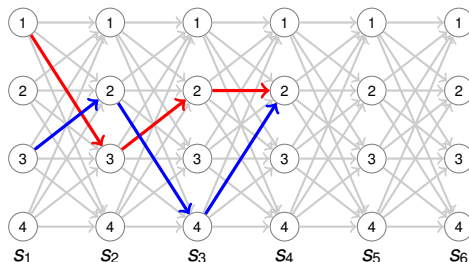
Prediction: $P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_{t-\Delta t})$

Naively, these marginal posteriors seem to require very large integrals (or sums)

$$P(\mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_t) = \int \cdots \int d\mathbf{z}_1 \dots d\mathbf{z}_{t-1} P(\mathbf{z}_1, \dots, \mathbf{z}_t | \mathbf{x}_1, \dots, \mathbf{x}_t)$$

but again the factored structure of the distributions will help us. The algorithms rely on a form of [temporal updating](#) or [message passing](#).

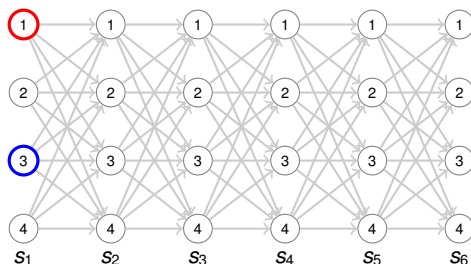
Crawling the HMM state-lattice



Consider an HMM, where we want to find $P(s_t=k|\mathbf{x}_1 \dots \mathbf{x}_t) =$

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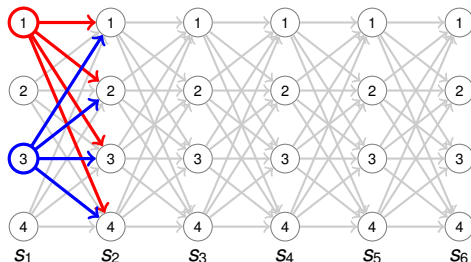
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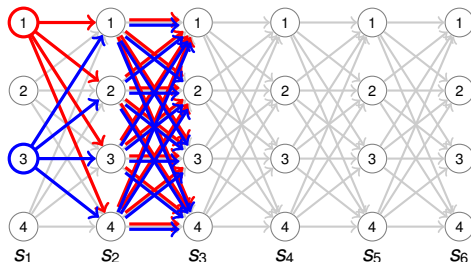
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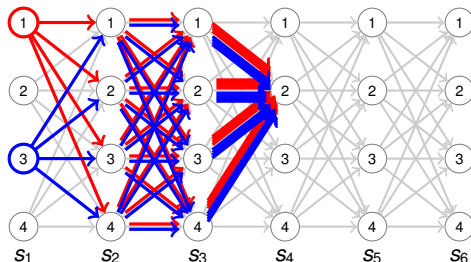
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- ▶ repeat

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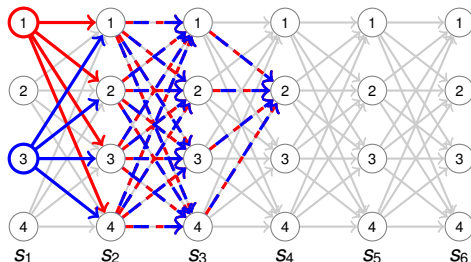
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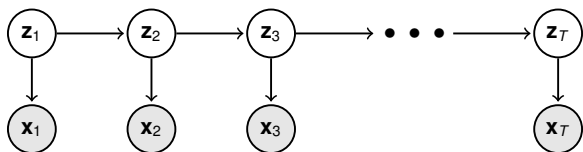
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Clever recursion:

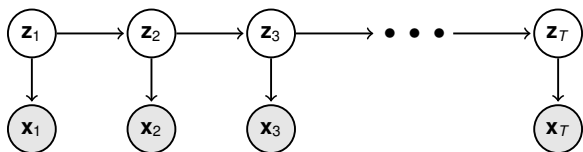
- ▶ at every step, replace bugs at each node with a single bug carrying sum of values

Probability updating: “Bayesian filtering”



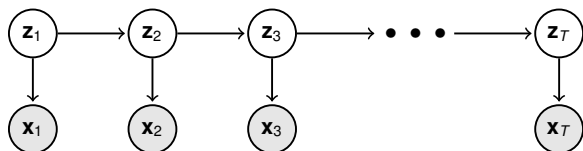
$$P(\mathbf{z}_t | \mathbf{x}_{1:t}) = \int P(\mathbf{z}_t, \mathbf{z}_{t-1} | \mathbf{x}_{1:t}) d\mathbf{z}_{t-1}$$

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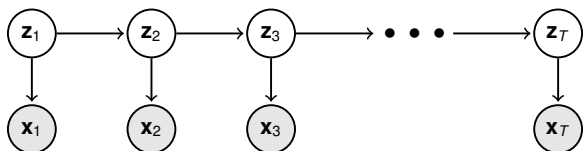
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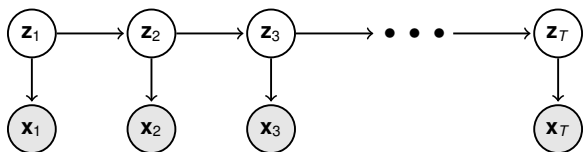
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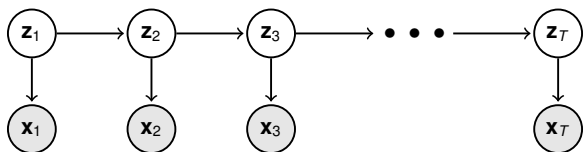
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Markov property

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Markov property

This is a **forward recursion** based on Bayes rule.

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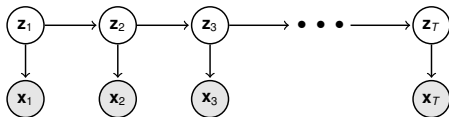
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This form enables us to compute the likelihood for $\theta = \{A, \Phi, \pi\}$ efficiently in $\mathcal{O}(TK^2)$ time:

$$P(\mathbf{x}_1 \dots \mathbf{x}_T | \theta) = \sum_{s_1, \dots, s_T} P(\mathbf{x}_1, \dots, \mathbf{x}_T, s_1, \dots, s_T, \theta) = \sum_{k=1}^K \alpha_T(k)$$

avoiding the exponential number of paths in the naïve sum (**number of paths = K^T**).

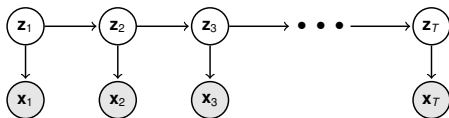
The LGSSM: Kalman Filtering



$$\begin{aligned} \mathbf{z}_1 &\sim \mathcal{N}(\boldsymbol{\mu}_0, \mathbf{Q}_0) \\ \mathbf{z}_t | \mathbf{z}_{t-1} &\sim \mathcal{N}(\mathbf{A}\mathbf{z}_{t-1}, \mathbf{Q}) \\ \mathbf{x}_t | \mathbf{z}_t &\sim \mathcal{N}(\mathbf{C}\mathbf{z}_t, \mathbf{R}) \end{aligned}$$

For the SSM, the sums become integrals.

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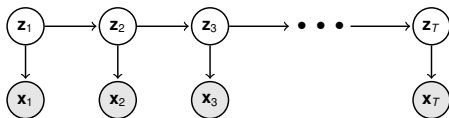


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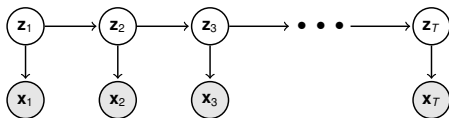


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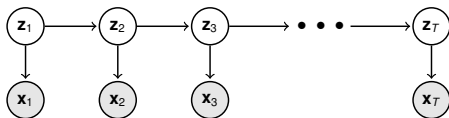


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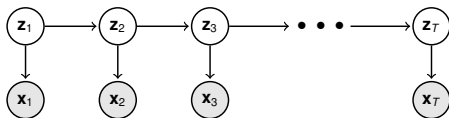
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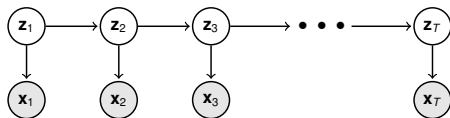
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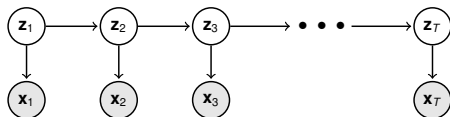
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The LGSSM: Kalman Filtering



$$\begin{aligned} \mathbf{z}_1 &\sim \mathcal{N}(\boldsymbol{\mu}_0, \mathbf{Q}_0) \\ \mathbf{z}_t | \mathbf{z}_{t-1} &\sim \mathcal{N}(\mathbf{A}\mathbf{z}_{t-1}, \mathbf{Q}) \\ \mathbf{x}_t | \mathbf{z}_t &\sim \mathcal{N}(\mathbf{C}\mathbf{z}_t, \mathbf{R}) \end{aligned}$$

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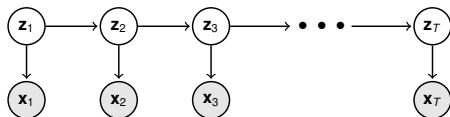
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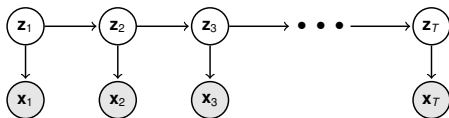
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Kalman gain

The LGSSM: Kalman Filtering



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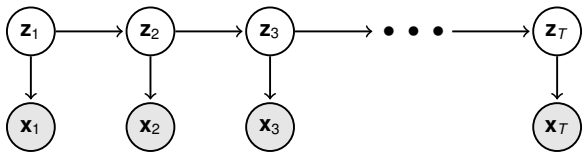
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Kalman gain

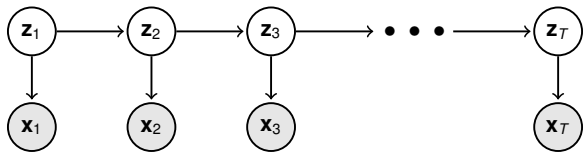
$$\text{FA: } \boldsymbol{\beta} = (\mathbf{I} + \boldsymbol{\Lambda}^\top \boldsymbol{\Psi}^{-1} \boldsymbol{\Lambda})^{-1} \boldsymbol{\Lambda}^\top \boldsymbol{\Psi}^{-1} \stackrel{\text{mat. inv. lem.}}{=} \boldsymbol{\Lambda}^\top (\boldsymbol{\Lambda} \boldsymbol{\Lambda}^\top + \boldsymbol{\Psi})^{-1}; \quad \boldsymbol{\mu} = \boldsymbol{\beta} \mathbf{x}_n; \quad \boldsymbol{\Sigma} = \mathbf{I} - \boldsymbol{\beta} \boldsymbol{\Lambda}.$$

The marginal posterior: “Bayesian smoothing”



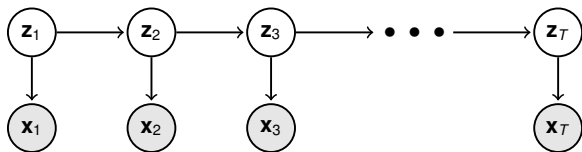
$$P(\mathbf{z}_t | \mathbf{x}_{1:T})$$

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$$P(\mathbf{z}_t | \mathbf{x}_{1:T}) = \frac{P(\mathbf{z}_t, \mathbf{x}_{t+1:T} | \mathbf{x}_{1:t})}{P(\mathbf{x}_{t+1:T} | \mathbf{x}_{1:t})}$$

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The marginal combines a **backward message** with the **forward message** found by filtering.

The HMM: Forward–Backward Algorithm

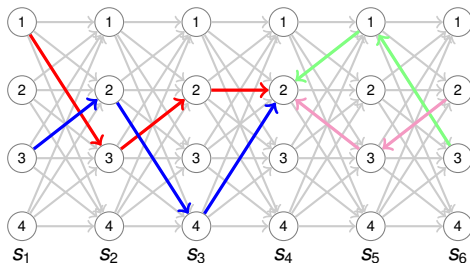
State estimation: compute marginal posterior distribution over state at time t :

$$\gamma_t(i) \equiv P(s_t=i|\mathbf{x}_{1:T}) = \frac{P(s_t=i, \mathbf{x}_{1:t})P(\mathbf{x}_{t+1:T}|s_t=i)}{P(\mathbf{x}_{1:T})} = \frac{\alpha_t(i)\beta_t(i)}{\sum_j \alpha_t(j)\beta_t(j)}$$

where there is a simple **backward recursion** for

$$\begin{aligned}\beta_t(i) &\equiv P(\mathbf{x}_{t+1:T}|s_t=i) = \sum_{j=1}^K P(s_{t+1}=j, \mathbf{x}_{t+1}, \mathbf{x}_{t+2:T}|s_t=i) \\ &= \sum_{j=1}^K P(s_{t+1}=j|s_t=i)P(\mathbf{x}_{t+1}|s_{t+1}=j)P(\mathbf{x}_{t+2:T}|s_{t+1}=j) = \sum_{j=1}^K \Phi_{ij}A_j(\mathbf{x}_{t+1})\beta_{t+1}(j)\end{aligned}$$

$\alpha_t(i)$ gives total *inflow* of probabilities to node (t, i) ; $\beta_t(i)$ gives total *outflow* of probabilities.



Bugs again: the bugs run forward from time 0 to t and backward from time T to t .

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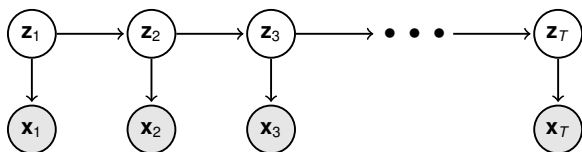
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- ▶ There is also a modified EM training based on the Viterbi decoder (assignment).

The LGSSM: Kalman smoothing



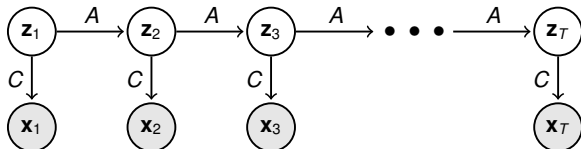
We use a slightly different decomposition:

$$\begin{aligned} P(\mathbf{z}_t | \mathbf{x}_{1:T}) &= \int P(\mathbf{z}_t, \mathbf{z}_{t+1} | \mathbf{x}_{1:T}) d\mathbf{z}_{t+1} \\ &= \int P(\mathbf{z}_t | \mathbf{z}_{t+1}, \mathbf{x}_{1:T}) P(\mathbf{z}_{t+1} | \mathbf{x}_{1:T}) d\mathbf{z}_{t+1} \\ &\stackrel{\text{Markov property}}{=} \int P(\mathbf{z}_t | \mathbf{z}_{t+1}, \mathbf{x}_{1:t}) P(\mathbf{z}_{t+1} | \mathbf{x}_{1:T}) d\mathbf{z}_{t+1} \end{aligned}$$

This gives the additional **backward recursion**:

$$\begin{aligned} J_t &= \hat{V}_t^t A^T (\hat{V}_{t+1}^t)^{-1} \\ \hat{\mathbf{z}}_t^T &= \hat{\mathbf{z}}_t^t + J_t (\hat{\mathbf{z}}_{t+1}^T - A \hat{\mathbf{z}}_t^t) \\ \hat{V}_t^T &= \hat{V}_t^t + J_t (\hat{V}_{t+1}^T - \hat{V}_{t+1}^t) J_t^T \end{aligned}$$

ML Learning for SSMs using batch EM



Parameters: $\theta = \{\mu_0, Q_0, A, Q, C, R\}$

Free energy:

$$\mathcal{F}(q, \theta) = \int d\mathbf{z}_{1:T} q(\mathbf{z}_{1:T}) (\log P(\mathbf{x}_{1:T}, \mathbf{z}_{1:T} | \theta) - \log q(\mathbf{z}_{1:T}))$$

E-step: Maximise \mathcal{F} w.r.t. q with θ fixed:

$$q^*(\mathbf{z}) = p(\mathbf{z} | \mathbf{x}, \theta)$$

This can be achieved with a two-state extension of the Kalman smoother.

M-step: Maximize \mathcal{F} w.r.t. θ with q fixed.

This boils down to solving a few weighted least squares problems, since all the variables in:

$$p(\mathbf{z}, \mathbf{x} | \theta) = p(\mathbf{z}_1) p(\mathbf{x}_1 | \mathbf{z}_1) \prod_{t=2}^T p(\mathbf{z}_t | \mathbf{z}_{t-1}) p(\mathbf{x}_t | \mathbf{z}_t)$$

form a multivariate Gaussian.

The M step for C

$$p(\mathbf{x}_t | \mathbf{z}_t) \propto \exp \left[-\frac{1}{2} (\mathbf{x}_t - C\mathbf{z}_t)^\top R^{-1} (\mathbf{x}_t - C\mathbf{z}_t) \right] \Rightarrow$$

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$$C_{\text{new}} = \operatorname{argmax}_C \left\langle \sum_t \ln p(\mathbf{x}_t | \mathbf{z}_t) \right\rangle_q$$

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using $\frac{\partial \operatorname{Tr}[AB]}{\partial A} = B^T$, we have $\frac{\partial \{\cdot\}}{\partial C} = R^{-1} \sum_t \mathbf{x}_t \langle \mathbf{z}_t \rangle^T - R^{-1} C \left\langle \sum_t \mathbf{z}_t \mathbf{z}_t^T \right\rangle$

The M step for C

$$p(\mathbf{x}_t | \mathbf{z}_t) \propto \exp \left[-\frac{1}{2} (\mathbf{x}_t - C\mathbf{z}_t)^T R^{-1} (\mathbf{x}_t - C\mathbf{z}_t) \right] \Rightarrow$$

$$\begin{aligned} C_{\text{new}} &= \operatorname{argmax}_C \left\langle \sum_t \ln p(\mathbf{x}_t | \mathbf{z}_t) \right\rangle_q \\ &= \operatorname{argmax}_C \left\langle -\frac{1}{2} \sum_t (\mathbf{x}_t - C\mathbf{z}_t)^T R^{-1} (\mathbf{x}_t - C\mathbf{z}_t) \right\rangle_q + \text{const} \\ &= \operatorname{argmax}_C \left\{ -\frac{1}{2} \sum_t \mathbf{x}_t^T R^{-1} \mathbf{x}_t - 2 \sum_t \mathbf{x}_t^T R^{-1} C \langle \mathbf{z}_t \rangle + \sum_t \langle \mathbf{z}_t^T C^T R^{-1} C \mathbf{z}_t \rangle \right\} \\ &= \operatorname{argmax}_C \left\{ \operatorname{Tr} \left[C \sum_t \langle \mathbf{z}_t \rangle \mathbf{x}_t^T R^{-1} \right] - \frac{1}{2} \operatorname{Tr} \left[C^T R^{-1} C \left\langle \sum_t \mathbf{z}_t \mathbf{z}_t^T \right\rangle \right] \right\} \end{aligned}$$

using $\frac{\partial \operatorname{Tr}[AB]}{\partial A} = B^T$, we have $\frac{\partial \{\cdot\}}{\partial C} = R^{-1} \sum_t \mathbf{x}_t \langle \mathbf{z}_t \rangle^T - R^{-1} C \left\langle \sum_t \mathbf{z}_t \mathbf{z}_t^T \right\rangle$

$$\Rightarrow C_{\text{new}} = \left(\sum_t \mathbf{x}_t \langle \mathbf{z}_t \rangle^T \right) \left(\sum_t \langle \mathbf{z}_t \mathbf{z}_t^T \rangle \right)^{-1}$$

Note the connection to linear regression (and factor analysis).

The M step for A

$$p(\mathbf{z}_{t+1}|\mathbf{z}_t) \propto \exp \left\{ -\frac{1}{2}(\mathbf{z}_{t+1} - A\mathbf{z}_t)^\top Q^{-1}(\mathbf{z}_{t+1} - A\mathbf{z}_t) \right\} \Rightarrow$$

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$$A_{\text{new}} = \operatorname{argmax}_A \left\langle \sum_t \ln p(\mathbf{z}_{t+1}|\mathbf{z}_t) \right\rangle_q$$

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using $\frac{\partial \operatorname{Tr}[AB]}{\partial A} = B^\top$, we have $\frac{\partial \{\cdot\}}{\partial A} = Q^{-1} \sum_t \langle \mathbf{z}_{t+1} \mathbf{z}_t^\top \rangle - Q^{-1} A \sum_t \langle \mathbf{z}_t \mathbf{z}_t^\top \rangle$

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This is still analogous to factor analysis and linear regression, with an extra expectation.

Learning (online gradient)

Time series data must often be processed in real-time, and we may want to update parameters **online** as observations arrive. We can do so by updating a **local** version of the likelihood based on the Kalman filter estimates.

Consider the log likelihood contributed by each data point (ℓ_t):

$$\ell = \sum_{t=1}^T \ln p(\mathbf{x}_t | \mathbf{x}_1, \dots, \mathbf{x}_{t-1}) = \sum_{t=1}^T \ell_t$$

Then,

$$\ell_t = -\frac{D}{2} \ln 2\pi - \frac{1}{2} \ln |\Sigma| - \frac{1}{2} (\mathbf{x}_t - C\hat{\mathbf{z}}_t^{t-1})^T \Sigma^{-1} (\mathbf{x}_t - C\hat{\mathbf{z}}_t^{t-1})$$

where D is dimension of \mathbf{x} , and:

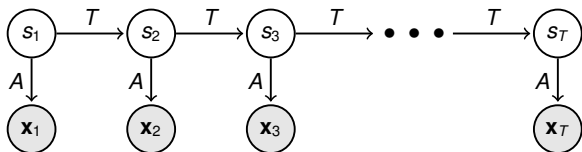
$$\hat{\mathbf{z}}_t^{t-1} = A\hat{\mathbf{z}}_{t-1}^{t-1}$$

$$\Sigma = C\hat{V}_t^{t-1}C^T + R$$

$$\hat{V}_t^{t-1} = A\hat{V}_{t-1}^{t-1}A^T + Q$$

We differentiate ℓ_t to obtain gradient rules for A , C , Q , R . The size of the gradient step (learning rate) reflects our expectation about **nonstationarity**.

Learning HMMs using EM



Parameters: $\theta = \{\pi, \Phi, A\}$

Free energy:

$$\mathcal{F}(q, \theta) = \sum_{s_{1:T}} q(s_{1:T}) (\log P(x_{1:T}, s_{1:T} | \theta) - \log q(s_{1:T}))$$

E-step: Maximise \mathcal{F} w.r.t. q with θ fixed: $q^*(s_{1:T}) = P(s_{1:T} | \mathbf{x}_{1:T}, \theta)$

We will only need the marginal probabilities $q(s_t, s_{t+1})$, which can also be obtained from the [forward-backward algorithm](#).

M-step: Maximize \mathcal{F} w.r.t. θ with q fixed.

We can re-estimate the parameters by computing the expected number of times the HMM was in state i , emitted symbol k and transitioned to state j .

This is the [Baum-Welch algorithm](#) and it predates the (more general) EM algorithm.

M step: Parameter updates are given by ratios of expected counts

We can derive the following updates by taking derivatives of \mathcal{F} w.r.t. θ .

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- ▶ The expected number of transitions from state i to j which begin at time t is:

$$\xi_t(i \rightarrow j) \equiv P(s_t = i, s_{t+1} = j | \mathbf{x}_{1:T}) = \alpha_t(i) \Phi_{ij} A_j(\mathbf{x}_{t+1}) \beta_{t+1}(j) / P(\mathbf{x}_{1:T})$$

so the estimated transition probabilities are:

$$\hat{\Phi}_{ij} = \frac{\sum_{t=1}^{T-1} \xi_t(i \rightarrow j)}{\sum_{t=1}^{T-1} \gamma_t(i)}$$

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- ▶ The output distributions are the expected number of times we observe a particular symbol in a particular state:

$$\hat{A}_{jk} = \sum_{t: \mathbf{x}_t = k} \gamma_t(i) / \sum_{t=1}^T \gamma_t(i)$$

(or the state-probability-weighted mean and variance for a Gaussian output model).

HMM practicalities

- **Numerical scaling**: the conventional message definition is in terms of a large joint:

$\alpha_t(i) = P(\mathbf{x}_{1:t}, s_t=i) \rightarrow 0$ as t grows, and so can easily underflow.

Rescale:

$$\bar{\alpha}_t(i) = A_i(\mathbf{x}_t) \sum_j \tilde{\alpha}_{t-1}(j) \Phi_{ji} \quad \rho_t = \sum_{i=1}^K \bar{\alpha}_t(i) \quad \tilde{\alpha}_t(i) = \bar{\alpha}_t(i) / \rho_t$$

Exercise: show that:

$$\rho_t = P(\mathbf{x}_t | \mathbf{x}_{1:t-1}, \theta) \quad \prod_{t=1}^T \rho_t = P(\mathbf{x}_{1:T} | \theta)$$

What does this make $\tilde{\alpha}_t(i)$?

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- ▶ **Multiple observed sequences**: average numerators and denominators in the ratios of updates.
- ▶ Local optima (random restarts, annealing; see discussion later).

HMM pseudocode: inference (E step)

Forward-backward including scaling tricks.

[\circ is the element-by-element (Hadamard/Schur) product: `.*` in matlab.]

$$\text{for } t = 1:T, i = 1:K \quad \rho_t(i) = A_i(\mathbf{x}_t)$$

$$\alpha_1 = \boldsymbol{\pi} \circ \boldsymbol{\rho}_1 \quad \rho_1 = \sum_{i=1}^K \alpha_1(i) \quad \alpha_1 = \alpha_1 / \rho_1$$

$$\text{for } t = 2:T \quad \alpha_t = (\boldsymbol{\Phi}^T * \alpha_{t-1}) \circ \boldsymbol{\rho}_t \quad \rho_t = \sum_{i=1}^K \alpha_t(i) \quad \alpha_t = \alpha_t / \rho_t$$

$$\beta_T = 1$$

$$\text{for } t = T-1:1 \quad \beta_t = \boldsymbol{\Phi} * (\beta_{t+1} \circ \boldsymbol{\rho}_{t+1}) / \rho_{t+1}$$

$$\log P(\mathbf{x}_{1:T}) = \sum_{t=1}^T \log(\rho_t)$$

$$\text{for } t = 1:T \quad \gamma_t = \alpha_t \circ \beta_t$$

$$\text{for } t = 1:T-1 \quad \xi_t = \boldsymbol{\Phi} \circ (\alpha_t * (\beta_{t+1} \circ \boldsymbol{\rho}_{t+1})^T) / \rho_{t+1}$$

HMM pseudocode: parameter re-estimation (M step)

Baum-Welch parameter updates:

For each sequence $l = 1 : L$, run forward–backward to get $\gamma^{(l)}$ and $\xi^{(l)}$, then

$$\pi_i = \frac{1}{L} \sum_{l=1}^L \gamma_1^{(l)}(i)$$

$$\Phi_{ij} = \frac{\sum_{l=1}^L \sum_{t=1}^{T^{(l)}-1} \xi_t^{(l)}(ij)}{\sum_{l=1}^L \sum_{t=1}^{T^{(l)}-1} \gamma_t^{(l)}(i)}$$

$$A_{ik} = \frac{\sum_{l=1}^L \sum_{t=1}^{T^{(l)}} \delta(\mathbf{x}_t = k) \gamma_t^{(l)}(i)}{\sum_{l=1}^L \sum_{t=1}^{T^{(l)}} \gamma_t^{(l)}(i)}$$

Degeneracies

Recall that the FA likelihood is conserved with respect to **orthogonal** transformations of \mathbf{z} :

$$P(\mathbf{z}) = \mathcal{N}(\mathbf{0}, I)$$

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The LGSSM likelihood is conserved with respect to **any invertible** transform of the latent:

$$\begin{array}{l} P(\mathbf{z}_{t+1}|\mathbf{z}_t) = \mathcal{N}(A\mathbf{z}_t, Q) \\ P(\mathbf{x}_t|\mathbf{z}_t) = \mathcal{N}(C\mathbf{z}_t, R) \end{array}$$

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$$\begin{aligned} P(\mathbf{z}_{t+1}|\mathbf{z}_t) = \mathcal{N}(A\mathbf{z}_t, Q) & \quad \& \quad \tilde{\mathbf{z}} = G\mathbf{z} & \quad \tilde{A} = GAG^{-1} \\ P(\mathbf{x}_t|\mathbf{z}_t) = \mathcal{N}(C\mathbf{z}_t, R) & \quad \& \quad \tilde{Q} = GQG^T & \quad \tilde{C} = CG^{-1} \\ & \quad \Rightarrow & \quad P(\tilde{\mathbf{z}}_{t+1}|\tilde{\mathbf{z}}_t) = \mathcal{N}(GAG^{-1}G\mathbf{z}_t, GQG^T) = \mathcal{N}(\tilde{A}\tilde{\mathbf{z}}_t, \tilde{Q}) \\ & \quad \Rightarrow & \quad P(\mathbf{x}_t|\tilde{\mathbf{z}}_t) = \mathcal{N}(CG^{-1}G\mathbf{z}_t, R) = \mathcal{N}(\tilde{C}\tilde{\mathbf{z}}_t, R) \end{aligned}$$

and the HMM is invariant to permutations (and to relaxations into something called an **observable operator model**).

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Besides the degenerate solutions, both LGSSMs and HMMs likelihood functions tend to have multiple **local maxima**. This complicates any ML-based approach to learning (including EM and gradient methods).

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W can be found by solving the [generalised eigenvalue problem](#)

$$WA = \Omega WB \quad \text{where } A = \sum_t (\mathbf{x}_t - \mathbf{x}_{t-1})(\mathbf{x}_t - \mathbf{x}_{t-1})^T \text{ and } B = \sum_t \mathbf{x}_t \mathbf{x}_t^T.$$

See <http://www.gatsby.ucl.ac.uk/~maneesh/papers/turner-sahani-2007-sfa.pdf>.

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and as you found, if $P \in \text{ExpFam}$ with sufficient statistic T then

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That is, we find estimate θ^* with

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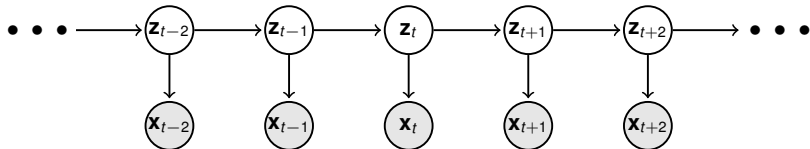
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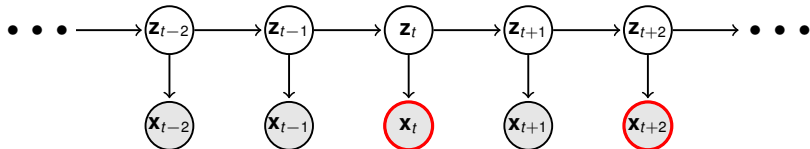
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Judicious choice of T and metric \mathcal{C} might make solution unique (no local optima) and consistent (correct given infinite within-model data).

Ho-Kalman SSID for LGSSMs

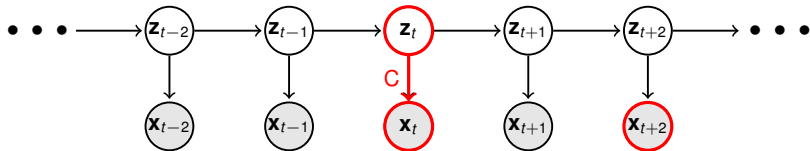


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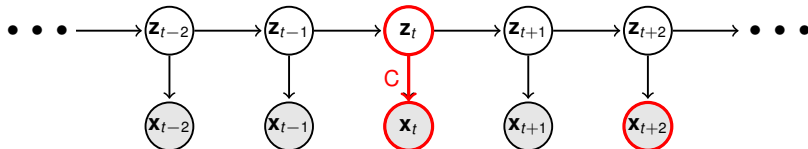
$$M_\tau \equiv \langle \mathbf{x}_{t+\tau} \mathbf{x}_t^\top \rangle$$

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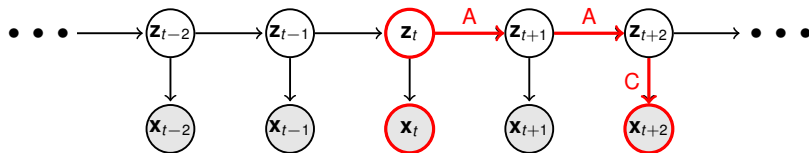
$$M_\tau \equiv \langle \mathbf{x}_{t+\tau} \mathbf{x}_t^\top \rangle = \langle \mathbf{x}_{t+\tau} (C\mathbf{z}_t + \boldsymbol{\eta})^\top \rangle$$

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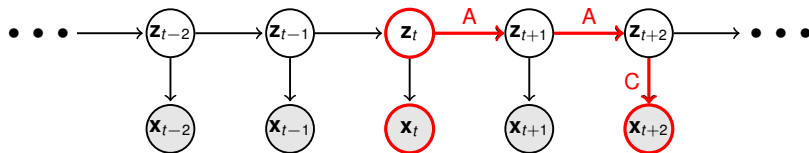
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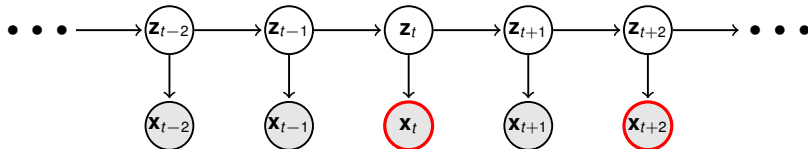
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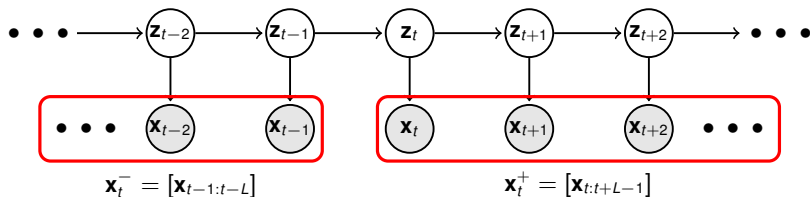
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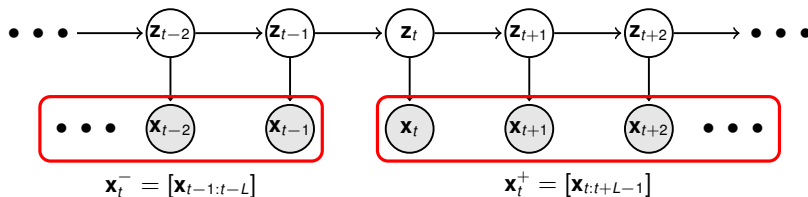
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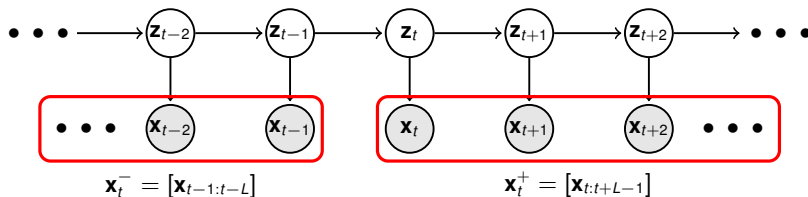
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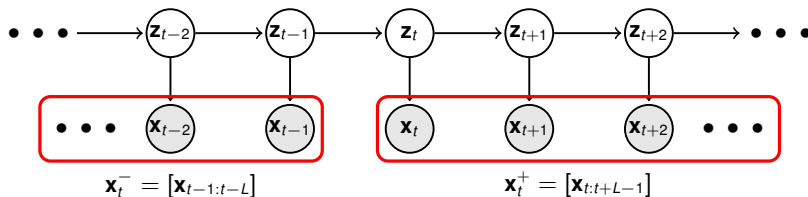


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$LD \times LD$
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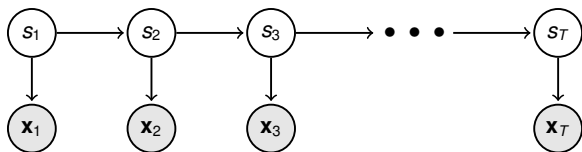
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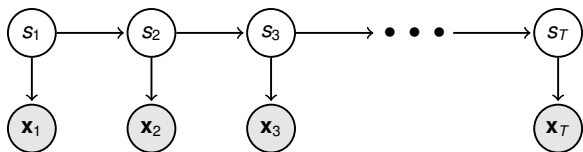
Off-diagonal correlation unaffected by noise. $SVD(\frac{1}{\tau} \sum \mathbf{x}_t^+ \mathbf{x}_t^{-\top})$ yields least-squares estimates of Ξ and Υ . Regression between blocks of Ξ yields $\hat{\mathbf{A}}$ and $\hat{\mathbf{C}}$.

HMMs \rightarrow OOMs



Now consider an HMM with discrete output symbols.

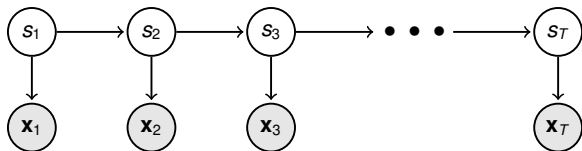
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$$P(x_{1:T} | \pi, \Phi, A) = \sum_i \pi_i A_i(x_1) \sum_j \Phi_{ji} A_j(x_2) \sum_k \Phi_{kj} A_k(x_3) \dots$$

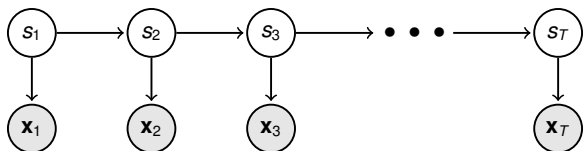
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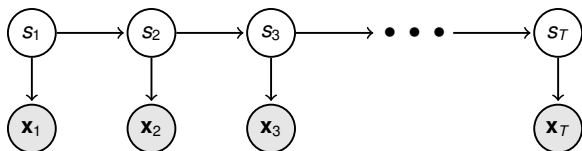


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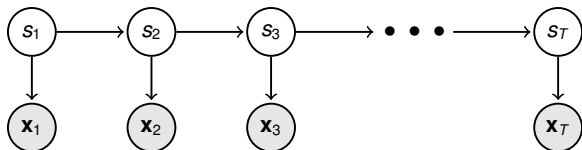
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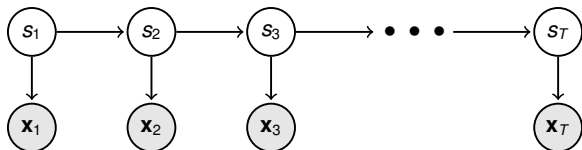
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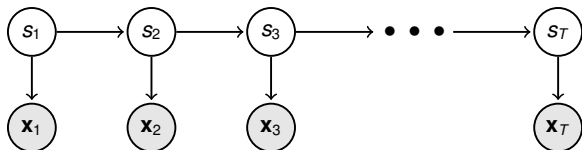
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Observable operator model (OOM) representation.

- ▶ OOMs with arbitrary O matrices describe a larger class of distributions than HMMs.
- ▶ Not easy to normalise or even guarantee all assigned “probabilities” are positive.

HMMs \rightarrow OOMs



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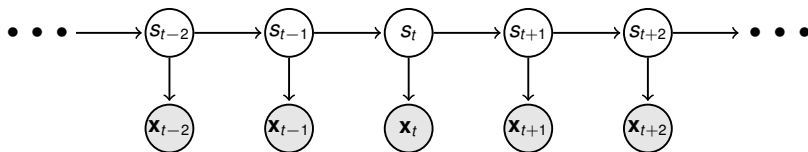
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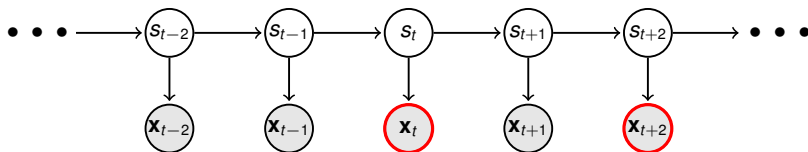
- ▶ OOMs with arbitrary O matrices describe a larger class of distributions than HMMs.
- ▶ Not easy to normalise or even guarantee all assigned “probabilities” are positive.
- ▶ Degenerate with respect to similarity transform $\tilde{O} = GOG^{-1}$.

Spectral learning for HMMs



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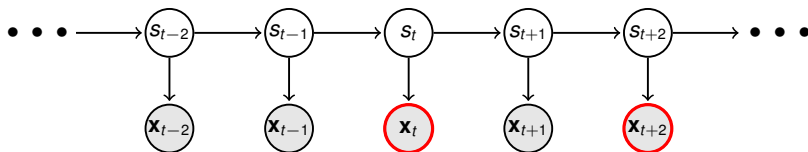
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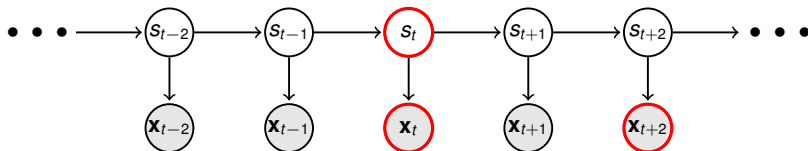
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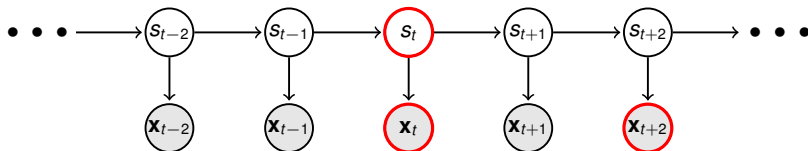
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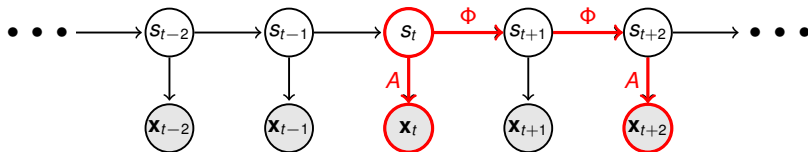
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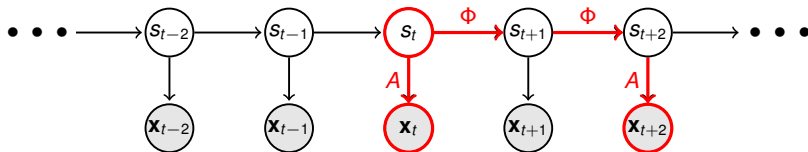
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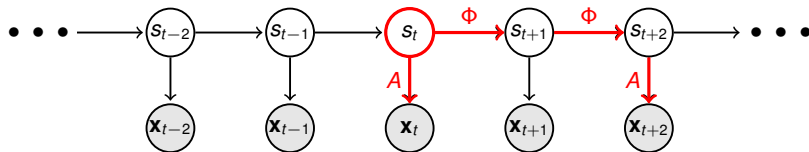
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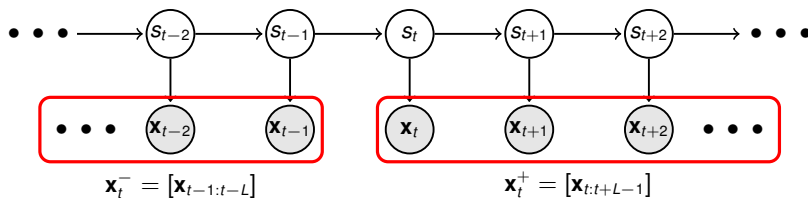
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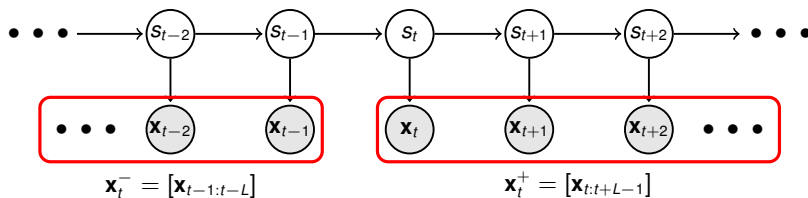
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(The conventional algorithm is written slightly differently, but follows similar logic).

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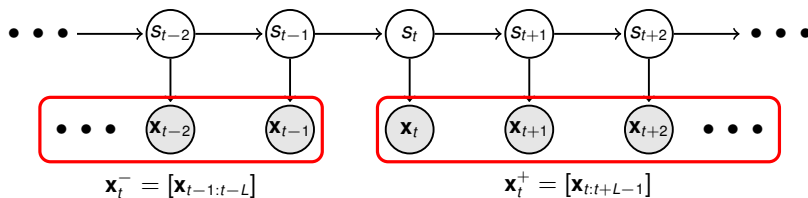
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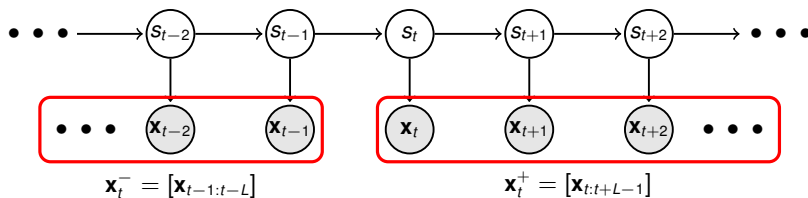
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'Projection' to HMM space possible, but amplifies estimation errors.

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Spectral learning:

Maximum likelihood learning:

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- ▶ Efficient closed-form solution.

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- ▶ Requires iterative maximisation.

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- ▶ Often valuable as initialisation for ML methods.

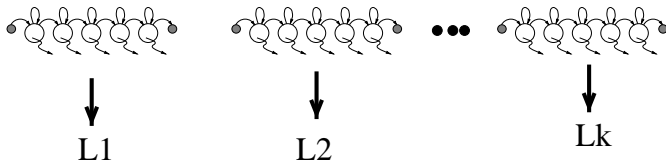
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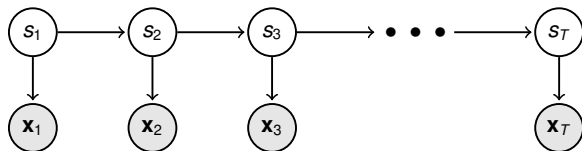
Recognition (classification) with HMMs

Multiple HMM models:

1. train one HMM for each class (requires each sequence to be labelled by the class)
2. evaluate the probability of an unknown sequence under each HMM
3. classify the unknown sequence by the HMM which gave it the highest likelihood



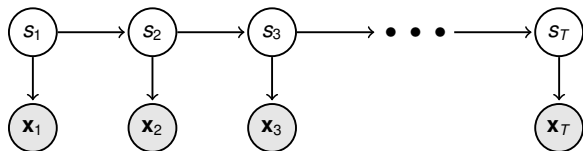
Recognition (labelling) with HMMs



Use a single HMM to label sequences:

1. train a single HMM on sequences of data $\mathbf{x}_1, \dots, \mathbf{x}_T$ and corresponding labels s_1, \dots, s_T .
2. On an unlabelled test sequence, compute the posterior distribution over label sequences $P(s_1, \dots, s_T | \mathbf{x}_1, \dots, \mathbf{x}_T)$.
3. Return the label sequence either with highest expected number of correct states, or highest probability under the posterior (Viterbi).

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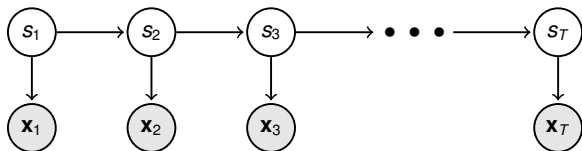
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- ▶ May be more accurate and more efficient use of data to model $P(s_{1:T} | \mathbf{x}_{1:T})$ directly.
- ▶ This leads to a model called a **Conditional Random Field**.

Conditional distribution in a HMM

Conditional distribution over label sequences of a HMM:

$$\begin{aligned} P(\mathbf{s}_{1:T} | \mathbf{x}_{1:T}, \theta) &= \frac{P(\mathbf{s}_{1:T}, \mathbf{x}_{1:T} | \theta)}{\sum_{\mathbf{s}_{1:T}} P(\mathbf{s}_{1:T}, \mathbf{x}_{1:T} | \theta)} \\ &\propto P(\mathbf{s}_1 | \pi) \prod_{t=1}^{T-1} P(\mathbf{s}_{t+1} | \mathbf{s}_t, \Phi) \prod_{t=1}^T P(\mathbf{x}_t | \mathbf{s}_t, A) \\ &= \exp \left(\sum_i \delta(\mathbf{s}_1=i) \log \pi_i + \sum_{t=1}^{T-1} \sum_{ij} \delta(\mathbf{s}_t=i, \mathbf{s}_{t+1}=j) \log \Phi_{ij} \right. \\ &\quad \left. + \sum_{t=1}^T \sum_{ik} \delta(\mathbf{s}_t=i, \mathbf{x}_t=k) \log A_{ik} \right). \end{aligned}$$

This functional form gives a well-defined conditional distribution, even if we do not enforce the constraints

$$\Phi_{ij} \geq 0 \quad \sum_j \Phi_{ij} = 1$$

or the similar ones for π and A (cf. OOMs). The forward-backward algorithm can still be applied to compute the conditional distribution.

This is an example of a [conditional random field](#).

Conditional random fields

Define two sets of functions: single label and label-pair functions.

Single label functions:

$$f_i(s_t, \mathbf{x}_t) \quad \text{for } i = 1, \dots, I$$

Label-pair functions:

$$g_j(s_t, s_{t+1}, \mathbf{x}_t, \mathbf{x}_{t+1}) \quad \text{for } j = 1, \dots, J$$

Each function is associated with a real-valued parameter: λ_i, κ_j .

A **conditional random field** defines a conditional distribution over $s_{1:T}$ given $\mathbf{x}_{1:T}$ as follows:

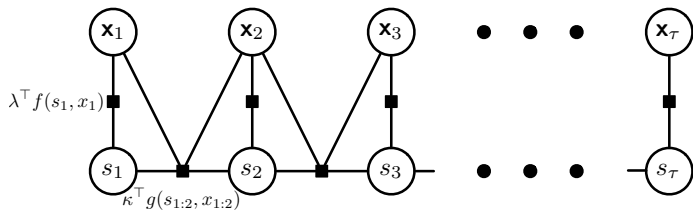
$$P(s_{1:T} | \mathbf{x}_{1:T}, \boldsymbol{\lambda}, \boldsymbol{\kappa}) \propto \exp \left(\sum_{t=1}^T \sum_i \lambda_i f_i(s_t, \mathbf{x}_t) + \sum_{t=1}^{T-1} \sum_j \kappa_j g_j(s_t, s_{t+1}, \mathbf{x}_t, \mathbf{x}_{t+1}) \right)$$

The forward-backward algorithm can be used to compute:

$$P(s_t | \mathbf{x}_{1:T}, \boldsymbol{\lambda}, \boldsymbol{\kappa}) \quad P(s_t, s_{t+1} | \mathbf{x}_{1:T}, \boldsymbol{\lambda}, \boldsymbol{\kappa}) \quad \operatorname{argmax}_{s_{1:T}} P(s_{1:T} | \mathbf{x}_{1:T}, \boldsymbol{\lambda}, \boldsymbol{\kappa})$$

Factor graph notation for CRFs

$$P(s_{1:T} | \mathbf{x}_{1:T}, \boldsymbol{\lambda}, \boldsymbol{\kappa}) \propto \exp \left(\sum_{t=1}^T \sum_i \lambda_i f_i(s_t, \mathbf{x}_t) + \sum_{t=1}^{T-1} \sum_j \kappa_j g_j(s_t, s_{t+1}, \mathbf{x}_t, \mathbf{x}_{t+1}) \right)$$



Discriminative vs generative modelling

Labelled training data comes from a **true underlying distribution** $\tilde{P}(s_{1:T}, \mathbf{x}_{1:T})$.

Generative modelling: train a HMM by maximizing likelihood:

$$\theta_{\text{Joint}} = \underset{\theta}{\operatorname{argmax}} E_{\tilde{P}}[\log P(s_{1:T}, \mathbf{x}_{1:T}|\theta)]$$

(note do not need EM here, since no latent variables)

Discriminative modelling: train another HMM by maximizing conditional likelihood:

$$\theta_{\text{Cond}} = \underset{\theta}{\operatorname{argmax}} E_{\tilde{P}}[\log P(s_{1:T}|\mathbf{x}_{1:T}, \theta)]$$

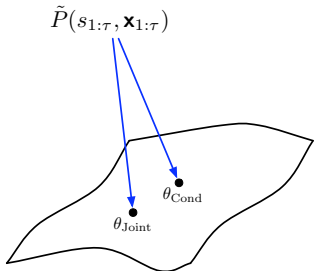
By construction:

$$E_{\tilde{P}}[\log P(s_{1:T}|\mathbf{x}_{1:T}, \theta_{\text{Cond}})] \geq E_{\tilde{P}}[\log P(s_{1:T}|\mathbf{x}_{1:T}, \theta_{\text{Joint}})]$$

If \tilde{P} belongs to model class, $P(\cdot|\theta_{\text{Joint}}) = \tilde{P}$ and equality holds.

Caveats:

- ▶ Underlying distribution \tilde{P} not usually in model class.
- ▶ training set differs from \tilde{P} .
- ▶ Overfitting easier in discriminative setting.
- ▶ Generative modelling often much simpler (fits each conditional probability separately, not iterative).



Major point of debate in machine learning.

Structured generalized linear models

$$P(s_{1:T} | \mathbf{x}_{1:T}, \boldsymbol{\lambda}, \boldsymbol{\kappa}) \propto \exp \left(\sum_{t=1}^T \sum_i \lambda_i f_i(s_t, \mathbf{x}_t) + \sum_{t=1}^{T-1} \sum_j \kappa_j g_j(s_t, s_{t+1}, \mathbf{x}_t, \mathbf{x}_{t+1}) \right)$$

The conditional distribution over $s_{1:T}$ forms an exponential family parameterized by $\boldsymbol{\lambda}, \boldsymbol{\kappa}$ and dependent on $\mathbf{x}_{1:T}$.

CRFs are a multivariate generalization of [generalized linear models \(GLMs\)](#).

The labels s_t in a CRF are not independently predicted, but they have a Markov property: $s_{1:t-1}$ is independent of $s_{t+1:T}$ given s_t and $\mathbf{x}_{1:T}$.

This allows efficient inference using the forward-backward algorithm.

CRFs are models for [structured prediction](#) (another major machine learning frontier).

CRFs are very flexible.

CRFs have found wide spread applications across a number of fields: natural language processing (part-of-speech tagging, named-entity recognition, coreference resolution), information retrieval (information extraction), computer vision (image segmentation, object recognition, depth perception), bioinformatics (protein structure prediction, gene finding)...

Learning CRFs

$$P(s_{1:T} | \mathbf{x}_{1:T}, \boldsymbol{\lambda}, \boldsymbol{\kappa}) \propto \exp \left(\sum_{t=1}^T \sum_i \lambda_i f_i(s_t, \mathbf{x}_t) + \sum_{t=1}^{T-1} \sum_j \kappa_j g_j(s_t, s_{t+1}, \mathbf{x}_t, \mathbf{x}_{t+1}) \right)$$

Given labelled data $\{s_{1:T}^{(c)}, \mathbf{x}_{1:T}^{(c)}\}_{c=1}^N$, we train CRFs by maximum likelihood:

$$\frac{\partial \sum_c \log P(s_{1:T}^{(c)} | \mathbf{x}_{1:T}^{(c)}, \boldsymbol{\lambda}, \boldsymbol{\kappa})}{\partial \lambda_i} = \sum_{c=1}^N \sum_{t=1}^T f_i(s_t^{(c)}, \mathbf{x}_t^{(c)}) - E_{P(s_{1:T} | \mathbf{x}_{1:T}^{(c)})} [f_i(s_t^{(c)}, \mathbf{x}_t^{(c)})]$$

$$\frac{\partial \sum_c \log P(s_{1:T}^{(c)} | \mathbf{x}_{1:T}^{(c)}, \boldsymbol{\lambda}, \boldsymbol{\kappa})}{\partial \kappa_j} = \sum_{c=1}^N \sum_{t=1}^{T-1} g_j(s_{t:t+1}^{(c)}, \mathbf{x}_{t:t+1}^{(c)}) - E_{P(s_{1:T} | \mathbf{x}_{1:T}^{(c)})} [g_j(s_{t:t+1}^{(c)}, \mathbf{x}_{t:t+1}^{(c)})]$$

There is no closed-form solution for the parameters, so we use gradient ascent instead.

Note: expectations are computed using the forward-backward algorithm.

The log likelihood is concave, so unlike EM we will get to [global optimum](#) (another major frontier in machine learning).

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