Statistical Approaches to Learning and Discovery

Latent Variable Time Series Models

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Modeling time series

Sequence of observations:

$$\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, \ldots, \mathbf{y}_t$$

For example:

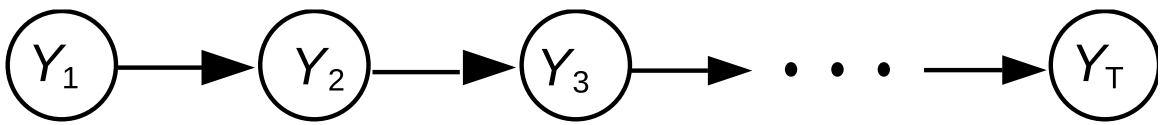
- Sequence of images
- Kinematic variables
- Speech signals
- Stock prices
- Sensor readings from an industrial process
- Amino acids, etc...

Goal: To build a model $\mathcal{M}$ of the data

Markov models

First-order Markov model:

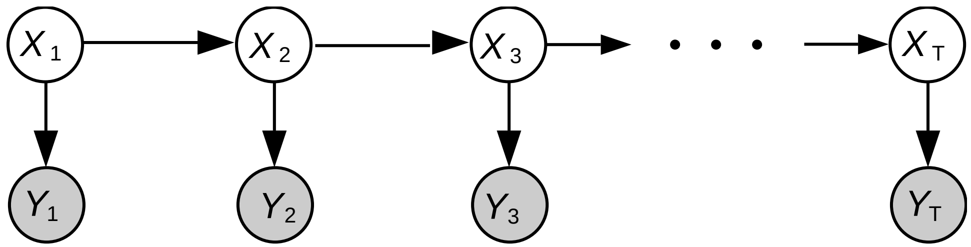
$$P(\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_t) = P(\mathbf{y}_1)P(\mathbf{y}_2|\mathbf{y}_1)\cdots P(\mathbf{y}_t|\mathbf{y}_{t-1})$$



Second-order Markov model:

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

Causal structure and "hidden variables"



Speech recognition:

- $\mathbf{x}$ - underlying phonemes or words
- $\mathbf{y}$ - acoustic waveform

Vision:

- $\mathbf{x}$ - object identities, poses, illumination
- $\mathbf{y}$ - image pixel values

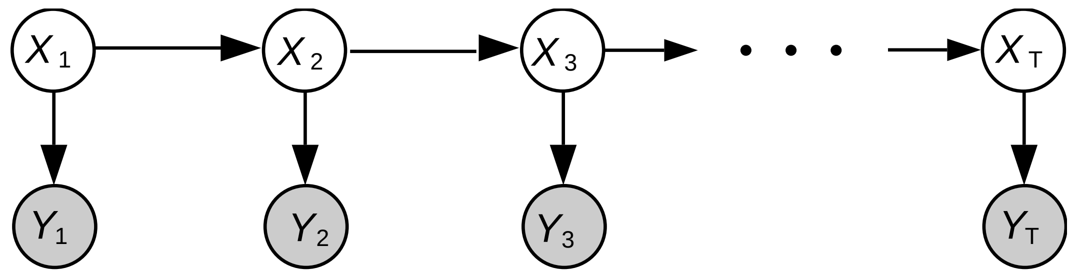
Industrial Monitoring:

- $\mathbf{x}$ - current state of molten steel in caster
- $\mathbf{y}$ - temperature and pressure sensor readings

Two frequently-used tractable models:

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

Linear-Gaussian State-space models (SSMs)



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

where $\mathbf{x}_t$ and $\mathbf{y}_t$ are both real-valued vectors

Output equation: $$y_{t,i} = \sum_j C_{ij}\, x_{t,j} + v_{t,i}$$

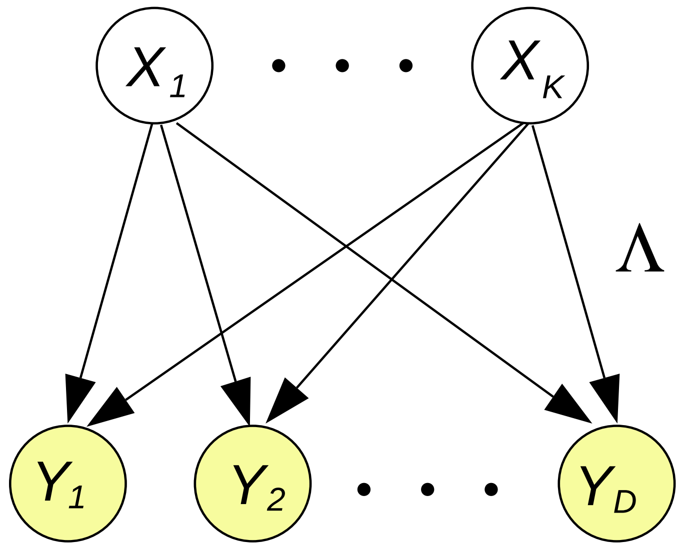
which is, in matrix form: $$\mathbf{y}_t = C\mathbf{x}_t + \mathbf{v}_t$$

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

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

These models are a.k.a. stochastic linear dynamical systems, Kalman filter models.

From Factor Analysis to State Space Models



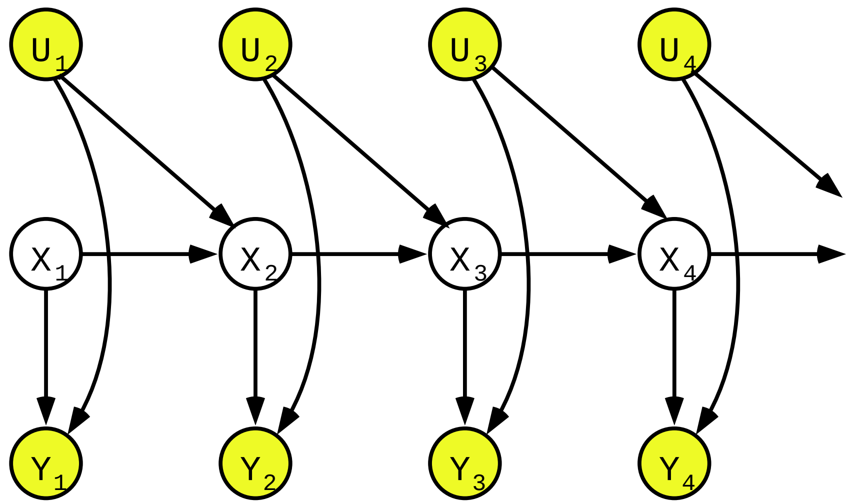
Linear generative model:

$$y_i = \sum_{j=1}^{K} C_{ij}\, x_j + v_i$$

- x_j are independent $\mathcal{N}(0, 1)$ Gaussian factors
- v_i are independent $\mathcal{N}(0, \Psi_{ii})$ Gaussian noise
- $K < D$

State-space models are a dynamical generalization of factor analysis where $x_{t,j}$ can depend linearly on $x_{t-1,\ell}$. Also, possibly $K \geq D$ and Ψ not diagonal.

State Space Models with Control Inputs



Inputs (or controls) $\mathbf{u}_t$, can also be accommodated.
State dynamics equations:

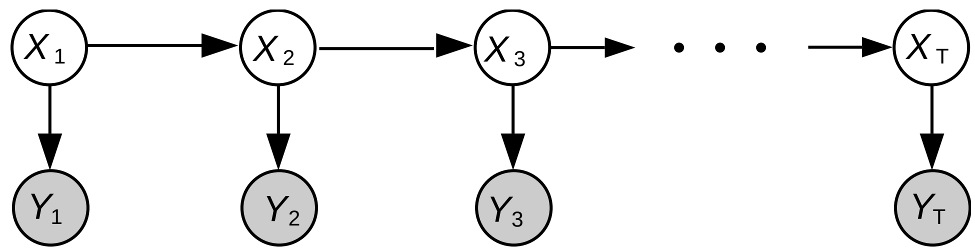
$$\mathbf{x}_t = A\mathbf{x}_{t-1} + B\mathbf{u}_{t-1} + \mathbf{w}_t.$$

Output equations:

$$\mathbf{y}_t = C\mathbf{x}_t + D\mathbf{u}_t + \mathbf{v}_t.$$

demo here...

Three Inference Problems



Filtering:

$$P(\mathbf{x}_t|\mathbf{y}_1, \ldots, \mathbf{y}_t)$$

Smoothing:

$$P(\mathbf{x}_t|\mathbf{y}_1, \ldots, \mathbf{y}_{t+\Delta t})$$

Prediction:

$$P(\mathbf{x}_t|\mathbf{y}_1, \ldots, \mathbf{y}_{t-\Delta t})$$

A very simple idea: running averages

$$\hat{\mathbf{x}}_t = \frac{1}{t}\sum_{\tau=1}^{t}\mathbf{y}_\tau$$

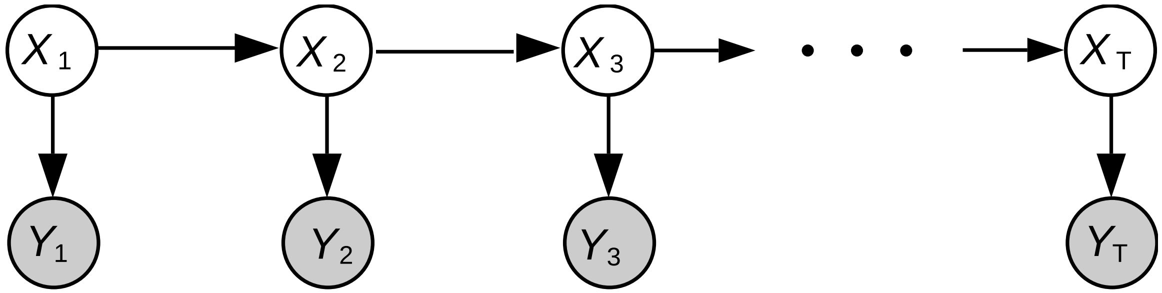
$$\hat{\mathbf{x}}_{t-1} = \frac{1}{t-1}\sum_{\tau=1}^{t-1}\mathbf{y}_\tau$$

$$\hat{\mathbf{x}}_t = \left(\frac{t-1}{t}\right)\hat{\mathbf{x}}_{t-1} + \frac{1}{t}\mathbf{y}_t$$

$$\hat{\mathbf{x}}_t = \hat{\mathbf{x}}_{t-1} + \frac{1}{t}(\mathbf{y}_t - \hat{\mathbf{x}}_{t-1})$$

we can call $K_t = \frac{1}{t}$ the "Kalman gain"

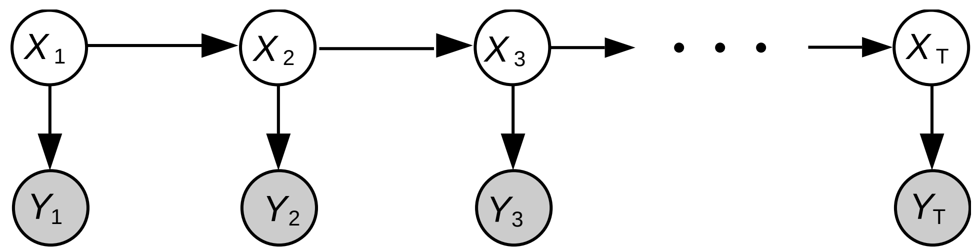
The Kalman Filter



$$
\begin{aligned}
P(\mathbf{x}_t|\mathbf{y}_{1:t}) &= \int P(\mathbf{x}_t, \mathbf{x}_{t-1}|\mathbf{y}_{1:t})\, d\mathbf{x}_{t-1} \\
&= \int \frac{P(\mathbf{x}_t, \mathbf{x}_{t-1}, \mathbf{y}_t|\mathbf{y}_{1:t-1})}{P(\mathbf{y}_t|\mathbf{y}_{1:t-1})}\, d\mathbf{x}_{t-1} \\
&\propto \int P(\mathbf{x}_{t-1}|\mathbf{y}_{1:t-1}) P(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{y}_{1:t-1}) P(\mathbf{y}_t|\mathbf{x}_t, \mathbf{x}_{t-1}, \mathbf{y}_{1:t-1})\, d\mathbf{x}_{t-1} \\
&\underset{\text{d-separation}}{=} \int P(\mathbf{x}_{t-1}|\mathbf{y}_{1:t-1}) P(\mathbf{x}_t|\mathbf{x}_{t-1}) P(\mathbf{y}_t|\mathbf{x}_t)\, d\mathbf{x}_{t-1}
\end{aligned}
$$

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

The Kalman Filter



Notation: $\mathbf{x}_t^\tau \equiv E[\mathbf{x}_t | \mathbf{y}_1, \ldots, \mathbf{y}_\tau]$

Prediction: $\mathbf{x}_t^{t-1} = A\mathbf{x}_{t-1}^{t-1}$

Correction: $\mathbf{x}_t^t = \mathbf{x}_t^{t-1} + K_t(\mathbf{y}_t - C\mathbf{x}_t^{t-1})$

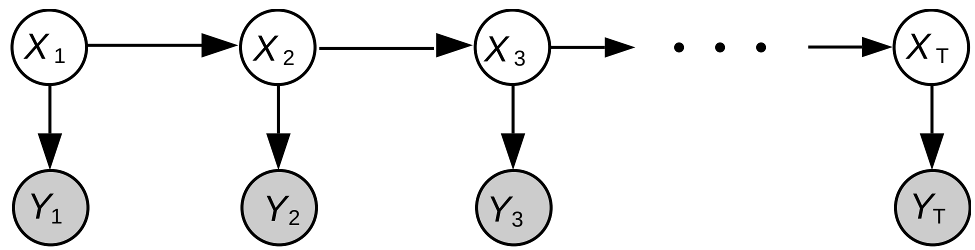
Kalman gain: $K_t = V_t^{t-1} C^\top (C V_t^{t-1} C^\top + R)^{-1}$

Prediction variance: $V_t^{t-1} = A V_{t-1}^{t-1} A^\top + Q$

Corrected variance: $V_t^t = V_t^{t-1} - K_t C V_t^{t-1}$

To get these we need the Gaussian integral: $\int \exp\left\{-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right\} dx = |2\pi\Sigma|$ and the Matrix Inversion Lemma: $(X + \mathbf{y}Z\mathbf{y}^\top)^{-1} = X^{-1} - X^{-1}\mathbf{y}(Z^{-1} + \mathbf{y}^\top X^{-1}\mathbf{y})^{-1}\mathbf{y}^\top X^{-1}$ assuming X and Z are symmetric and invertible.

The Kalman Smoother

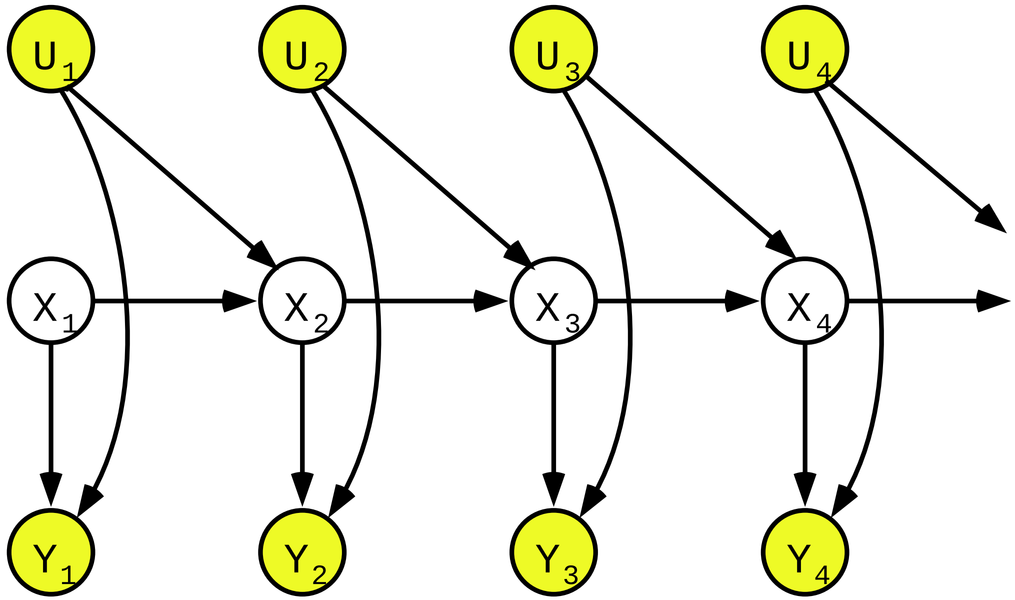


Compute $P(\mathbf{x}_t|\mathbf{y}_1, \ldots, \mathbf{y}_T)$, $T > t$.

Additional backward recursion:

$$
\begin{aligned}
J_t &= V_t^t A^\top (V_{t+1}^t)^{-1} \\
\mathbf{x}_t^T &= \mathbf{x}_t^t + J_t(\mathbf{x}_{t+1}^T - A\mathbf{x}_t^t) \\
V_t^T &= V_t^t + J_t(V_{t+1}^T - V_{t+1}^t){J_t}^\top
\end{aligned}
$$

Control Inputs and Forward Models



State equation:

$$\mathbf{x}_{t+1} = A\mathbf{x}_t + B\mathbf{u}_t + \mathbf{w}_t$$

Output equation:

$$\mathbf{y}_t = C\mathbf{x}_t + D\mathbf{u}_t + \mathbf{v}_t$$

Internal (Forward/Generative) Model:

$$\begin{aligned} \mathbf{x}_{t+1} &= \hat{A}\mathbf{x}_t + \hat{B}\mathbf{u}_t + \mathbf{w}_t \\ \mathbf{y}_t &= \hat{C}\mathbf{x}_t + \hat{D}\mathbf{u}_t + \mathbf{v}_t \end{aligned}$$

Kalman Filters: An Example from Biology/Robotics

For example:

- $\mathbf{u}_t$ motor commands sent to the arm (efference copy sent back to brain)
- $\mathbf{x}_t$ true state of the hand (pos, vel of hand)
- $\mathbf{y}_t$ proprioceptive signals (sensor readings)

A *forward model* of the dynamics of the system can be used in a Kalman filter to integrate efference copy ($\mathbf{u}$) and sensory signals ($\mathbf{y}$) to obtain an estimate of $\mathbf{x}$.

A forward model can also be used for

- prediction
- mental simulations
- learning a controller

Learning using EM

Assume a model parameterised by $\theta = \{A, B, C, D, Q, R\}$ with observable variables $\mathbf{y}$ and hidden variables $\mathbf{x}$

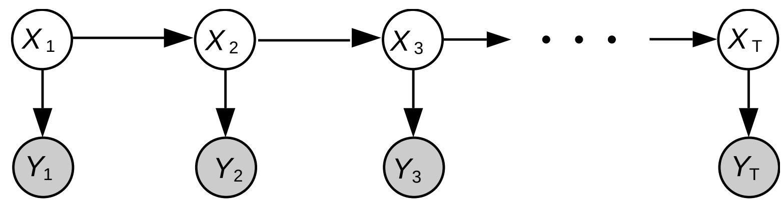
Goal: maximise log likelihood of parameters given observed data:

$$\mathcal{L}(\theta) = \ln P(\mathbf{y}|\theta) = \ln \int d\mathbf{x}\; P(\mathbf{x}, \mathbf{y}|\theta)$$

- **E-step**: infer $P(\mathbf{x}|\mathbf{y}, \theta_{\text{old}})$
- **M-step**: find θ_{new} using using "filled-in" values for the sufficient statistics of $\mathbf{x}$

The E-step requires solving the inference a.k.a. state estimation problem: finding a distribution over explanations, $\mathbf{x}$, for the data, $\mathbf{y}$, given the current model parameters, θ.

Learning SSM using batch EM



Any distribution $Q(\mathbf{x})$ over the hidden states defines a lower bound on $\ln P(\mathbf{y}|\theta)$ called $\mathcal{F}(Q,\theta)$:

$$\ln P(\mathbf{y}|\theta) \quad = \quad \ln \int d\mathbf{x} Q(\mathbf{x}) \frac{P(\mathbf{x},\mathbf{y}|\theta)}{Q(\mathbf{x})} \geq \int d\mathbf{x} Q(\mathbf{x}) \ln \frac{P(\mathbf{x},\mathbf{y}|\theta)}{Q(\mathbf{x})} = \mathcal{F}(Q,\theta)$$

E-step: Maximise $\mathcal{F}$ w.r.t. Q with θ fixed: $\qquad Q^*(\mathbf{x}) = P(\mathbf{x}|\mathbf{y},\theta)$

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

$$P(\mathbf{x},\mathbf{y}|\theta) = P(\mathbf{x}_1) \prod_{t=1}^{T} P(\mathbf{y}_t|\mathbf{x}_t) \prod_{t=1}^{T-1} P(\mathbf{x}_{t+1}|\mathbf{x}_t)$$

M-step boils down to solving a few weighted least squares problems.

Quadratics and Weighted Least Squares

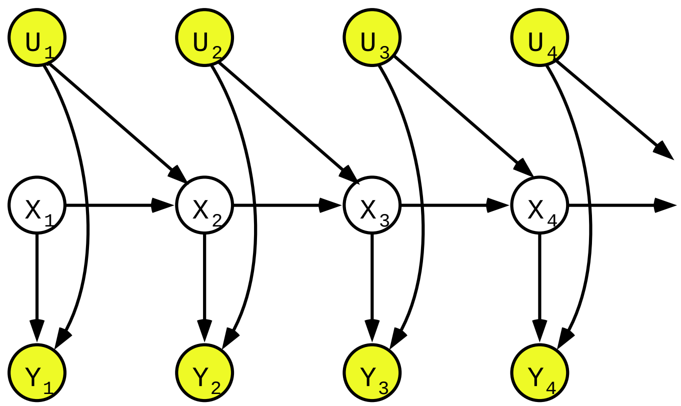
Example: M-step for C using $P(\mathbf{y}_t|\mathbf{x}_t) \propto \exp\left\{-\frac{1}{2}(\mathbf{y}_t - C\mathbf{x}_t)^\top R^{-1}(\mathbf{y}_t - C\mathbf{x}_t)\right\}$:

$$\begin{aligned}
C_{\text{new}} &= \underset{C}{\operatorname{argmax}} \left\langle \sum_t \ln P(\mathbf{y}_t|\mathbf{x}_t) \right\rangle_Q \\
&= \underset{C}{\operatorname{argmax}} \left\langle -\frac{1}{2} \sum_t (\mathbf{y}_t - C\mathbf{x}_t)^\top R^{-1}(\mathbf{y}_t - C\mathbf{x}_t) \right\rangle_Q + \text{const} \\
&= \underset{C}{\operatorname{argmin}} \left\{ \sum_t \mathbf{y}_t{}^\top R^{-1}\mathbf{y}_t - 2\mathbf{y}_t{}^\top R^{-1} C \langle \mathbf{x}_t \rangle + \langle \mathbf{x}_t{}^\top C^\top R^{-1} C \mathbf{x}_t \rangle \right\} \\
&= \underset{C}{\operatorname{argmin}} \left\{ -2\operatorname{tr}\left[C \sum_t \langle \mathbf{x}_t \rangle \mathbf{y}_t{}^\top R^{-1} \right] + \operatorname{tr}\left[C^\top R^{-1} C \left\langle \sum_t \mathbf{x}_t \mathbf{x}_t{}^\top \right\rangle \right] \right\}
\end{aligned}$$

using $\frac{\partial \operatorname{tr}[AB]}{\partial A} = B^\top$, we get: $\dfrac{\partial\{\cdot\}}{\partial C} = -2R^{-1} \sum_t \mathbf{y}_t \langle \mathbf{x}_t \rangle + 2R^{-1} C \left\langle \sum_t \mathbf{x}_t \mathbf{x}_t{}^\top \right\rangle$

Solving, we get: $C_{\text{new}} = \left(\sum_t \mathbf{y}_t \langle \mathbf{x}_t \rangle \right) \left(\sum_t \left\langle \mathbf{x}_t \mathbf{x}_t{}^\top \right\rangle \right)^{-1}$

Nonlinear Dynamical Systems



$$\begin{aligned} \mathbf{x}_{t+1} &= f(\mathbf{x}_t, \mathbf{u}_t) + \mathbf{w}_t \\ \mathbf{y}_t &= g(\mathbf{x}_t, \mathbf{u}_t) + \mathbf{v}_t \end{aligned}$$

The Extended Kalman Filter: linearise about the current estimate, i.e. $\mathbf{x}_t^t, \mathbf{u}_t$:

$$\mathbf{x}_{t+1} \approx f(\mathbf{x}_t^t, \mathbf{u}_t) + \left.\frac{\partial f}{\partial \mathbf{x}_t}\right|_{\mathbf{x}_t^t} (\mathbf{x}_t - \mathbf{x}_t^t) + \mathbf{w}_t$$

$$\mathbf{y}_t \approx g(\mathbf{x}_t^t, \mathbf{u}_t) + \left.\frac{\partial g}{\partial \mathbf{x}_t}\right|_{\mathbf{x}_t^t} (\mathbf{x}_t - \mathbf{x}_t^t) + \mathbf{v}_t$$

Run the Kalman filter (smoother) on linearised system:

- No guarantees
- Approximates non-Gaussian by a Gaussian
- Works OK in practice, for approx linear systems

EM for nonlinear dynamical systems in (Ghah. & Roweis, 1999)

Learning (Online Gradient)

We can recursively compute the log likelihood of each new data point as it arrives:

$$L = \sum_{t=1}^{T} \ln P(\mathbf{y}_t | \mathbf{y}_1, \ldots, \mathbf{y}_{t-1}) = \sum_{t=1}^{T} \ell_t$$

$$\ell_t = -\frac{p}{2} \ln 2\pi - \frac{1}{2} \ln |\Sigma| - \frac{1}{2} (\mathbf{y}_t - C\mathbf{x}_t^{t-1})^\top \Sigma^{-1} (\mathbf{y}_t - C\mathbf{x}_t^{t-1})$$

where p is dimension of $\mathbf{y}$, and:

$$\begin{aligned} \mathbf{x}_t^{t-1} &= A\mathbf{x}_{t-1}^{t-1} \\ \Sigma &= CV_t^{t-1}C^\top + R \\ V_t^{t-1} &= AV_{t-1}^{t-1}A^\top + Q \end{aligned}$$

Differentiate this to obtain gradient rules for A, C, Q, R.
Learning rate allows for modelling nonstationarity.

Learning (Online EKF)

Augment state vector to include the model parameters

$$\tilde{\mathbf{x}}_t = [\mathbf{x}_t, A, C]$$

$$\tilde{\mathbf{x}}_{t+1} = f(\tilde{\mathbf{x}}_t) + \text{noise}$$

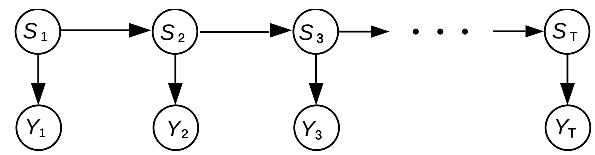
Use EKF to compute online $E[\tilde{\mathbf{x}}_t|\mathbf{y}_1, \ldots, \mathbf{y}_t]$ and $\text{Cov}[\tilde{\mathbf{x}}_t|\mathbf{y}_1, \ldots, \mathbf{y}_t]$.

- Pseudo-Bayesian approach.
- Deals with nonstationarity by controlling the noise added to A, C.
- Not clear that it works for Q and R (e.g. how does it deal with covariance constraints?).
- Faster than gradient approaches.

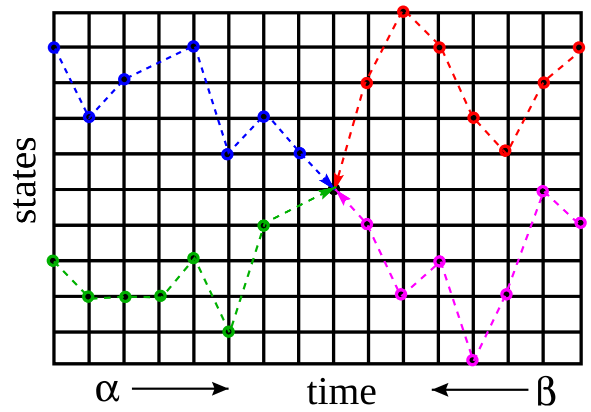
A.k.a. "joint-EKF" approaches. Also available is the "dual-EKF" approach.

HMM: Outline

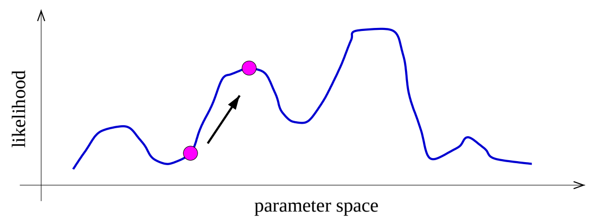
- Generative Model



- Likelihood Evaluation

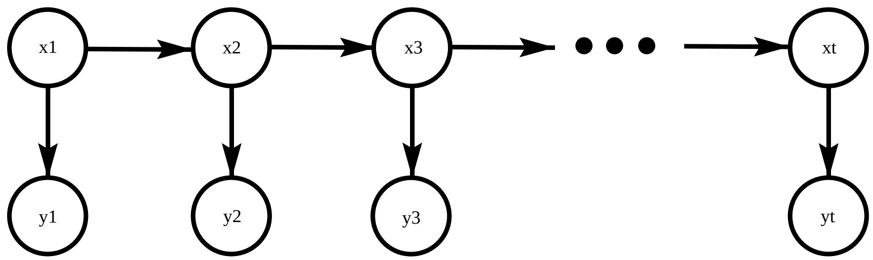


- State inference



- Parameter Estimation

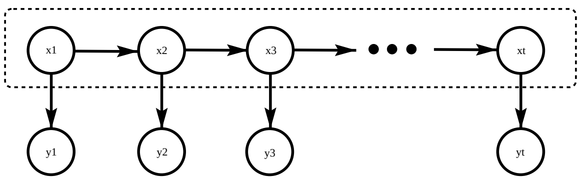
Graphical Model for HMM



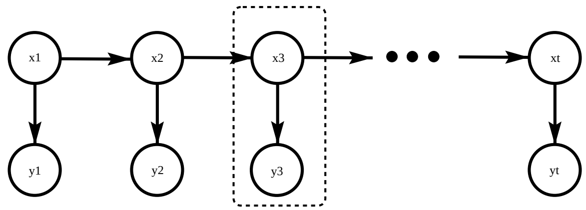
- Discrete hidden states $\mathbf{s}_t \in \{1 \ldots, K\}$, and outputs $\mathbf{y}_t$ (discrete or continuous). Joint probability factorizes:

$$\mathsf{P}(\mathbf{s}_1, \ldots, \mathbf{s}_T, \mathbf{y}_1 \ldots, \mathbf{y}_T) = \mathsf{P}(\mathbf{s}_1)\mathsf{P}(\mathbf{y}_1|\mathbf{s}_1) \prod_{t=2}^{T} \mathsf{P}(\mathbf{s}_t|\mathbf{s}_{t-1})\mathsf{P}(\mathbf{y}_t|\mathbf{s}_t)$$

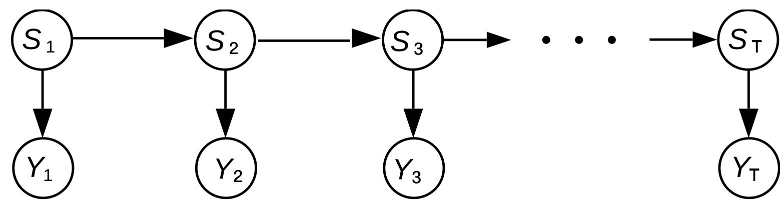
- a Markov chain with stochastic measurements:



- or a mixture model with states coupled across time:



HMM Generative Model



1. Use a 1st-order Markov chain to generate a hidden state sequence (path):

$$\mathsf{P}(s_1 = j) = \pi_j \qquad \mathsf{P}(s_{t+1} = j | s_t = i) = T_{ij}$$

2. Use a set of output prob. distributions $A_j(\cdot)$ (one per state) to convert this state path into a sequence of observable symbols or vectors

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

- Even though hidden state seq. is 1st-order Markov, the output process may not be Markov of *any* order

- Discrete state, discrete output models can approximate any continuous dynamics and observation mapping even if nonlinear; however lose ability to interpolate

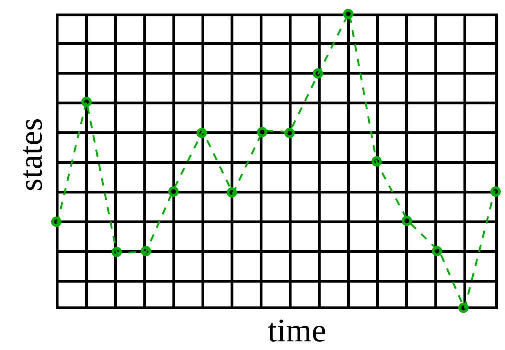
Probability of an Observed Sequence

- The probability is: $\displaystyle\sum_{\text{all paths}} \mathsf{P}(\text{ observed outputs} \,|\, \text{state path })\mathsf{P}(\text{state path})$
  which looks like an extremely hard computation because the number of possible paths grows exponentially with number of time steps τ (#paths $= N^\tau$)

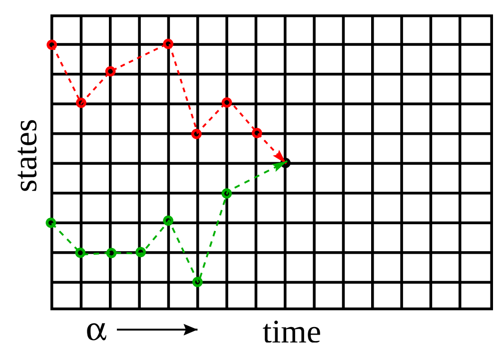
- But: there exists a forward recursion to compute the sum efficiently.
  Define $\alpha_j(t)$:
  $$\alpha_j(t) = \mathsf{P}(\, \mathbf{y}_1 \ldots \mathbf{y}_t \,,\, s_t = j \,)$$
  Now induction comes to our rescue:
  $$\alpha_j(1) = \pi_j A_j(\mathbf{y}_1) \qquad\qquad \alpha_k(t+1) = \left(\sum_j \alpha_j(t) T_{jk} \right) A_k(\mathbf{y}_{t+1})$$
  This enables us to compute the likelihood efficiently in $\mathcal{O}(\tau N^2)$
  $$L = \sum_{k=1}^{K} \alpha_k(\tau) = \mathsf{P}(\, \mathbf{y}_1 \ldots \mathbf{y}_\tau)$$

Bugs on a Grid

- Naive algorithm:
  1. start bug in each state at $t{=}1$ holding value 1
  2. move each bug forward in time: make copies of each bug to each subsequent state & multiply the value of each copy by transition prob. $\times$ output emission prob. (or use logs)
  3. go to 2 until all bugs have reached time τ
  4. sum up values on all bugs



- Clever recursion:
  adds a step between 2 and 3 above which says: at each node, replace all the bugs with a single bug carrying the sum of their values



Thanks to Sam Roweis for bugs analogy

Forward–Backward Algorithm

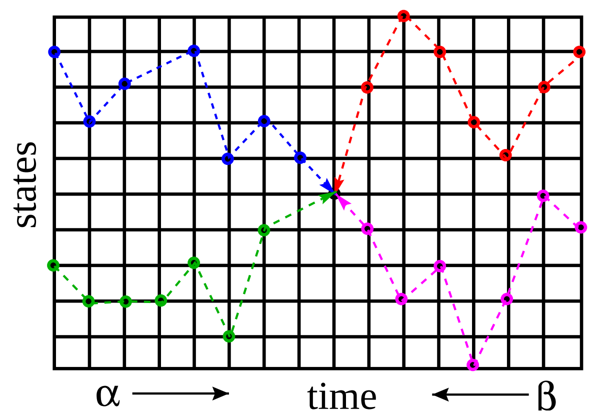
- If we knew the total prob. of all paths going through state i at time t we could compute the *conditional* prob. of being in state i at time t given the data:

$$\gamma_i(t) \equiv \mathsf{P}(s_t = i \mid \mathbf{y}_{1\ldots\tau}) = \frac{\mathsf{P}(s_t = i, \mathbf{y}_{1\ldots t})\mathsf{P}(\mathbf{y}_{t+1\ldots\tau} \mid s_t = i)}{\mathsf{P}(\mathbf{y}_{1\ldots\tau})} = \frac{\alpha_i(t)\ \beta_i(t)}{L}$$

- where there is a simple recursion for

$$\beta_j(t) \equiv \mathsf{P}(\mathbf{y}_{t+1\ldots\tau} \mid s_t = j\ ) = \sum_i T_{ij}\beta_i(t+1)A_i(\mathbf{y}_{t+1})$$

- $\alpha_i(t)$ gives total *inflow* of prob. to node (t, i);
  $\beta_i(t)$ gives total *outflow* of prob.



- Bugs again: we just let the bugs run forward from time 0 to t and backward from time τ to t.

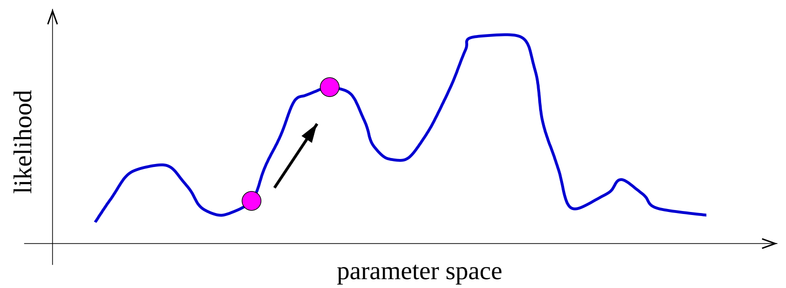
Baum-Welch Training

1. Intuition: if only we *knew* the true state path then ML parameter estimation would be trivial (count co-occurences to get π vector and T and A matrices)

2. But: we can *estimate* the state path using a trick similar to the one above.

3. What if: we estimate the states, then compute params, then re-estimate states, etc . . .

4. This works and we can *prove* that it always improves likelihood. This is the *Baum-Welch algorithm* and it is a special case of the *EM algorithm*.



However: we can also *prove* that finding the ML parameters is NP complete, so initial conditions matter a lot and convergence is hard to tell.

Viterbi Decoding

- The numbers $\gamma_j(t)$ above gave the prob. distribution over all states at any time.
- By choosing the state $\gamma_*(t)$ with the largest prob. at each time, we can make a "best" state path. This is the path with the maximum expected number of correct states.
- But it is not the single path with the highest likelihood of generating the data. In fact it may be a path of prob. zero!
- To find the single best path, we do *Viterbi decoding* which is just Bellman's dynamic programming algorithm applied to this problem.
- The recursions look the same, except with $\max$ instead of $\sum$.
- Bugs once more: same trick except at each step kill all bugs but the one with the highest value at the node.
- There is also a modified Baum-Welch training based on the Viterbi decode.

New parameters are just ratios of frequency counts

- The initial state distribution is the expected number of times in state i at $t = 1$:

$$\hat{\pi}_i = \gamma_i(1)$$

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

$$\xi_{ij}(t) \equiv \mathsf{P}(s_t = i, s_{t+1} = j | \mathbf{y}_{1\ldots\tau}) = \alpha_i(t) T_{ij} A_j(\mathbf{y}_{t+1}) \beta_j(t+1)/L$$

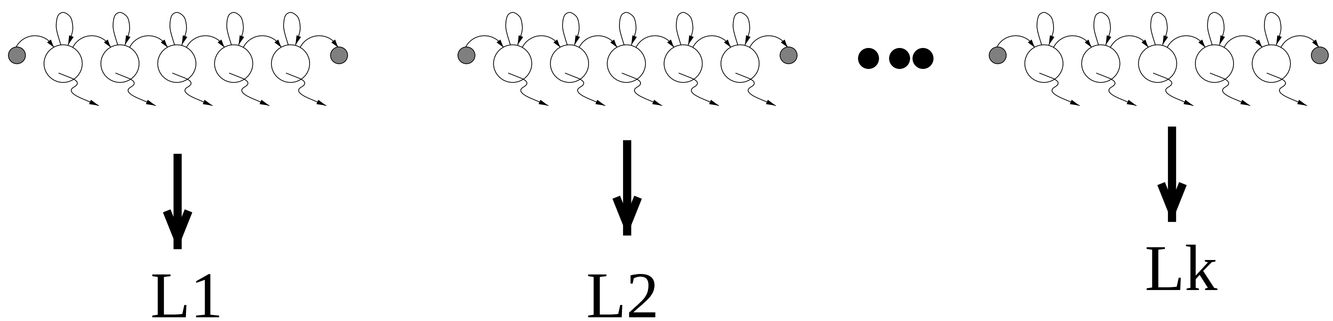
so the estimated transition probabilities are: $$\hat{T}_{ij} = \sum_{t=1}^{\tau-1} \xi_{ij}(t) \Big/ \sum_{t=1}^{\tau-1} \gamma_i(t)$$

- The output distributions are the expected number of times we observe a particular symbol in a particular state: $$\hat{A}_j(y) = \sum_{t:\mathbf{y}_t = y} \gamma_j(t) \Big/ \sum_{t=1}^{\tau} \gamma_j(t)$$

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

Using HMMs for Recognition

- Use many HMMs for recognition by:
  1. training one HMM for each class (this requires *labelled* training data)
  2. evaluating the probability of an unknown sequence under each HMM
  3. classifying the unknown sequence by the HMM which gave it the highest likelihood



- This requires the solution of two problems:
  1. Given model, evaluate prob. of a sequence. (We can do this exactly and efficiently.)
  2. Give some training sequences, estimate model parameters. (We can find a local maximum of parameter space using EM.)

HMM Practicalities

- Numerical scaling: the probability values that the bugs carry get tiny for big times and so can easily underflow. Good rescaling trick:

$$\rho_t = \mathsf{P}(\mathbf{y}_t | \mathbf{y}_{1\ldots t-1}) \qquad \alpha(t) = \tilde{\alpha}(t) \prod_{t'=1}^{t} \rho_{t'}$$

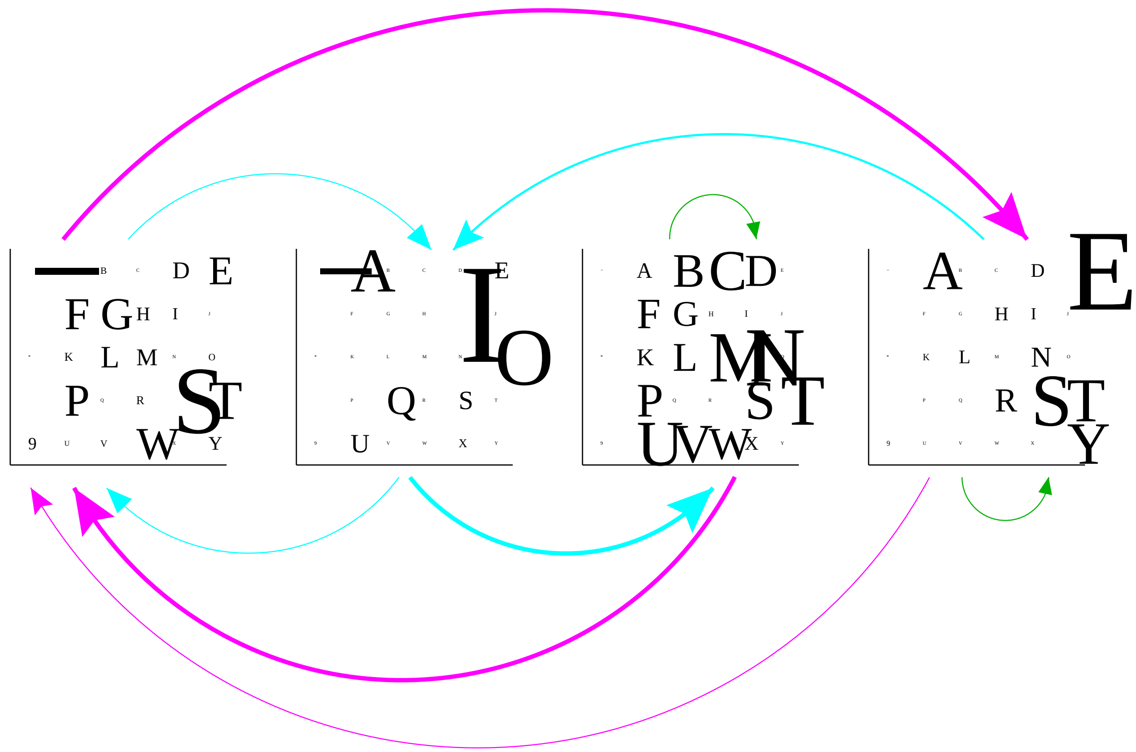
- Multiple observation sequences: can be dealt with by averaging numerators and averaging denominators in the ratios given above.

- Training data requirements: full covariance matrices in high dimensions or discrete symbol models with many symbols have *lots* of parameters.

- How do we pick the topology of the HMM? How many states?

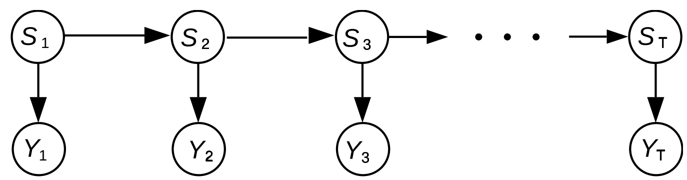
HMM Example

- Character sequences (discrete outputs)



Relationship to LDSs

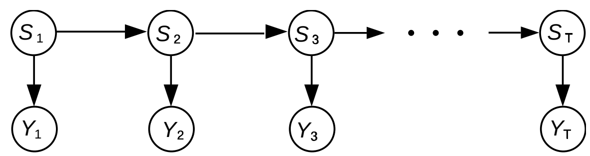
- Kalman filter models (linear dynamical systems with Gaussian noise) are exactly the continuous state analogue of Hidden Markov Models.



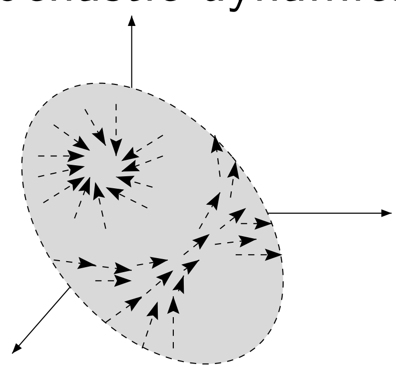
- forward algorithm $\Leftrightarrow$ Discrete Kalman Filter
  forward-backward $\Leftrightarrow$ Kalman Smoothing
  Viterbi decoding $\Leftrightarrow$ no equivalent

Strengths and Weaknesses

- Continuous vector state is very powerful.
  (For an HMM to communicate N bits of information into future, it needs 2^N states!)

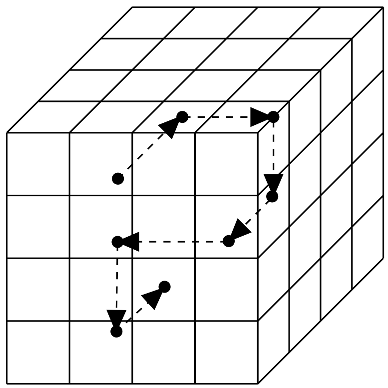


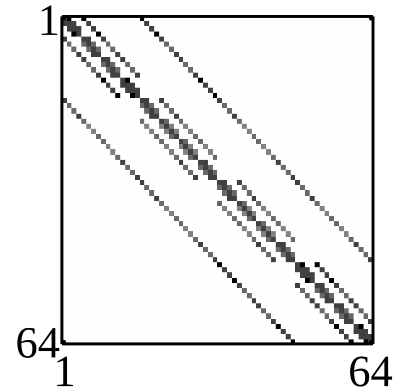
- Linear-Gaussian output/dynamics are very weak.
  (e.g. even using a mixture of Gaussians in place of single Gaussians is tricky)
  HMMs can represent arbitrary stochastic dynamics and output mappings.



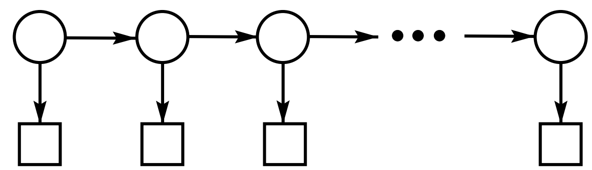
Some Extensions

- Constrained HMMs



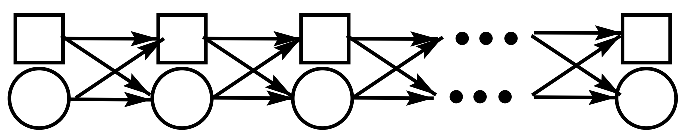


- Continuous state models with discrete outputs for time series and static data

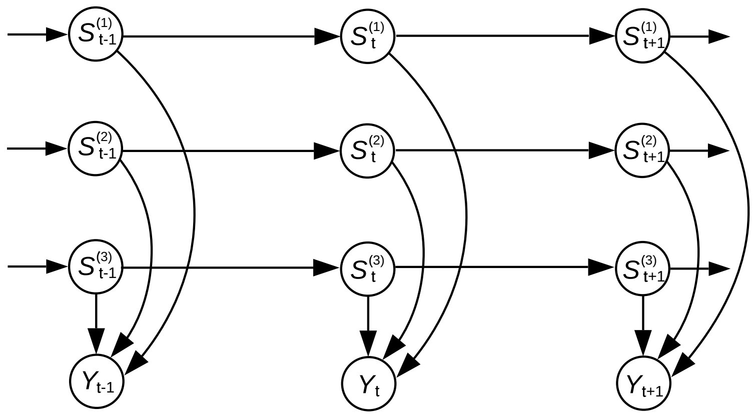


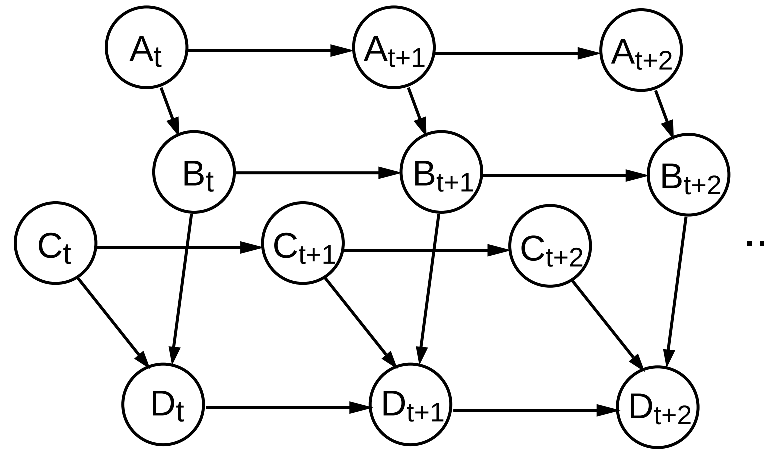
- Hierarchical HMMs

- Hybrid systems ⇔ Mixed continuous & discrete states, switching state-space models



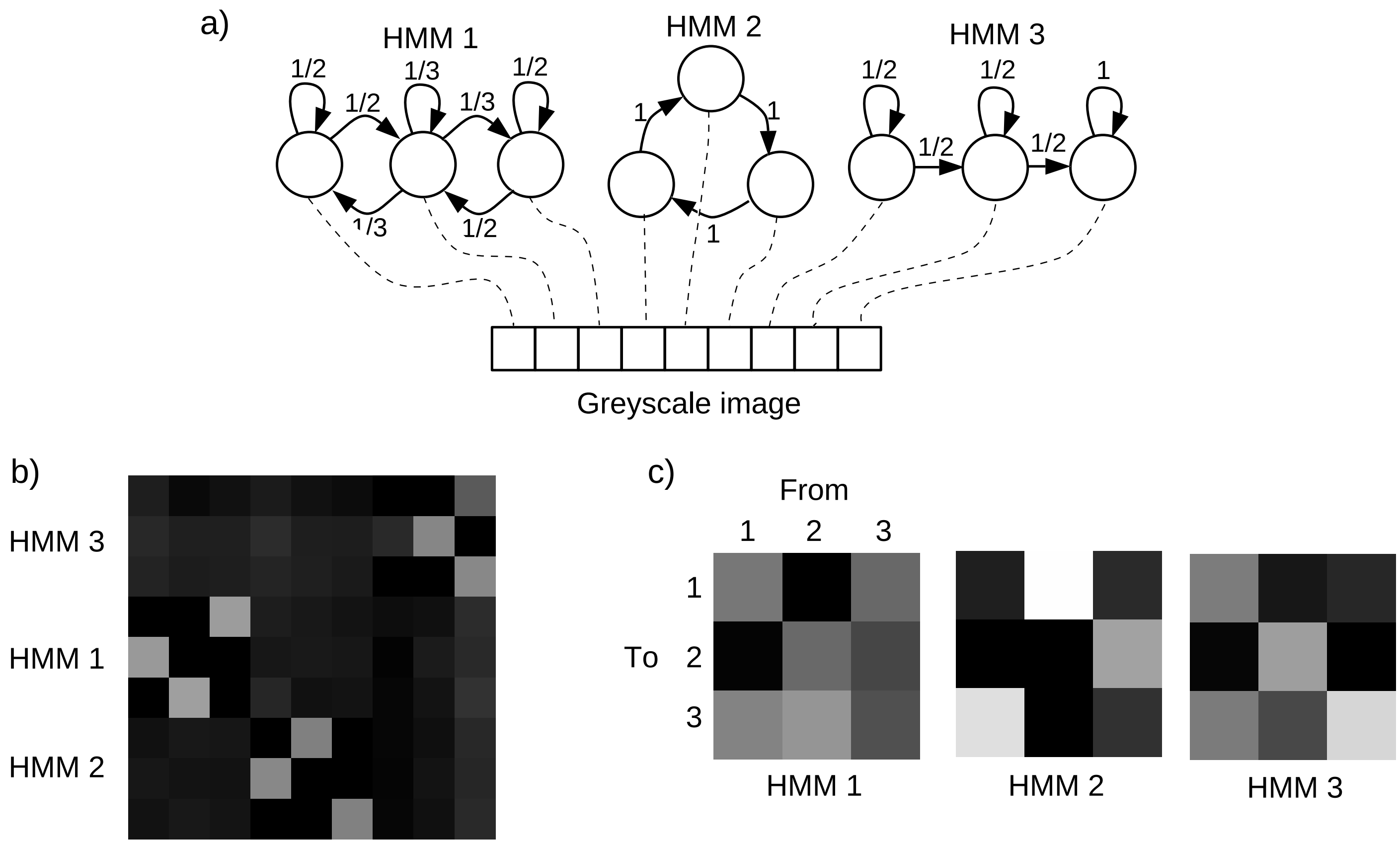
Factorial Hidden Markov Models and Dynamic Bayesian Networks





- 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).
- E step is intractable, but we can use sampling or variational methods.

Factorial Hidden Markov Models: An Toy Example



- Three parallel HMMs: (1) random walk, (2) cyclical, (3) absorbing
- Each HMM had 3 hidden states and 9 outputs
- Data set of 100 sequences of 8 observables each
- EM run for 20 iterations.

Factorial HMMs: Modeling J.S. Bach's Chorales

Discrete event sequences:

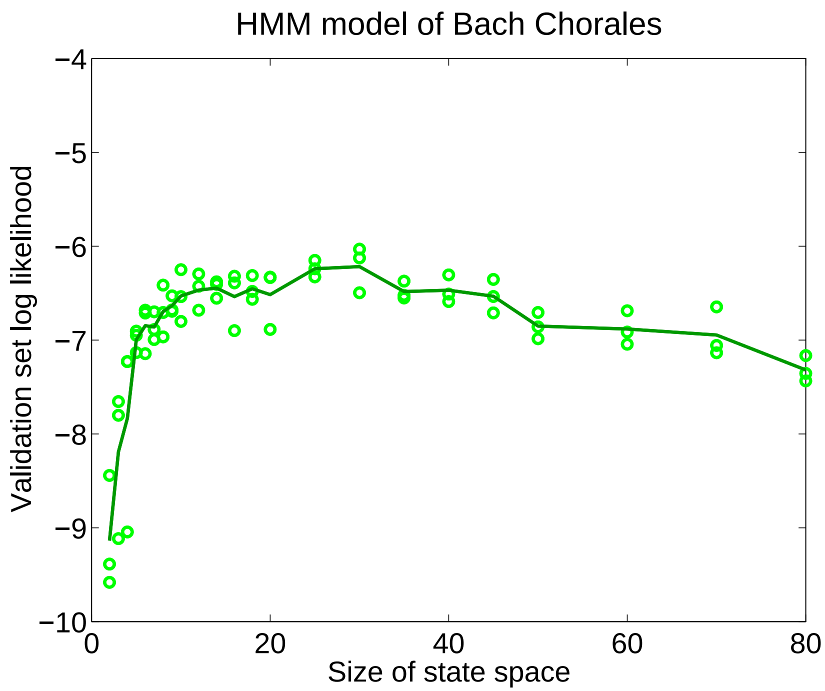
Attribute	Description	Representation
pitch	pitch of the event	int $[0, 127]$
keysig	key signature of the chorale (num of sharps and flats)	int $[-7, 7]$
timesig	time signature of the chorale	int (1/16 notes)
fermata	event under fermata?	binary
st	start time of event	int (1/16 notes)
dur	duration of event	int (1/16 notes)

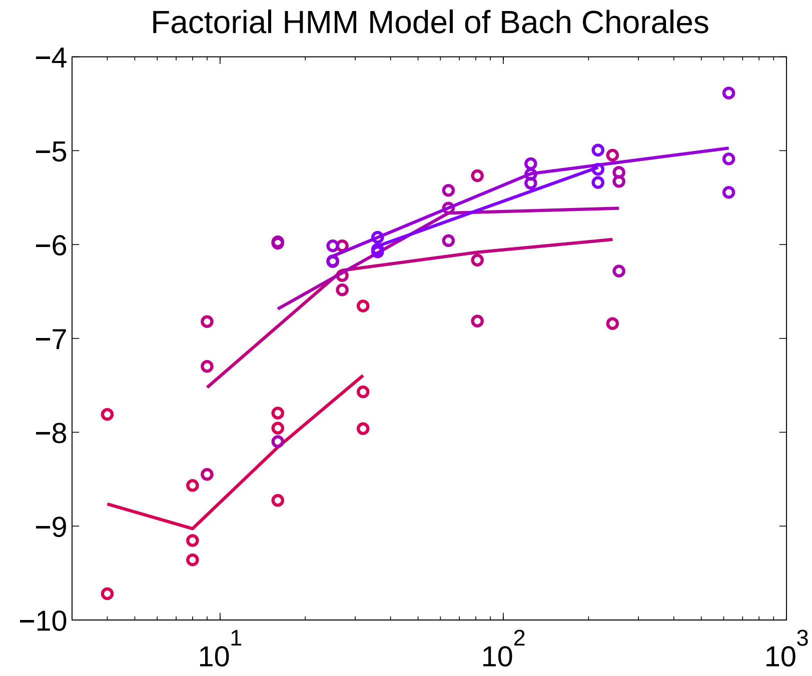
66 chorale melodies of 40 events each:

- training: 30 melodies
- validation: 18 melodies
- test: 18 melodies

See Conklin and Witten (1995) for data and a more musically informed model.

Factorial HMMs: Results on Bach Chorales





HMM Pseudocode: Inference (E step)

Forward-backward including scaling tricks

$$q_j(t) = A_j(\mathbf{y}_t)$$

$$\alpha(1) = \pi .* q(1) \qquad \rho(1) = \sum \alpha(1) \qquad \alpha(1) = \alpha(1)/\rho(1)$$

$$\alpha(t) = (T' * \alpha(t-1)) .* q(t) \qquad \rho(t) = \sum \alpha(t) \qquad \alpha(t) = \alpha(t)/\rho(t) \qquad [t = 2 : \tau]$$

$$\beta(\tau) = 1$$

$$\beta(t) = T * (\beta(t+1) .* q(t+1)/\rho(t+1) \qquad [t = (\tau - 1) : 1]$$

$$\xi = 0$$

$$\xi = \xi + T .* (\alpha(t) * (\beta(t+1) .* q(t+1))')/\rho(t+1) \qquad [t = 1 : (\tau - 1)]$$

$$\gamma = (\alpha .* \beta)$$

$$\log \mathsf{P}(\mathbf{y}_1^\tau) = \sum_t \log(\rho(t))$$

HMM Pseudocode: Parameter Re-estimation (M step)

Baum-Welch parameter updates:

For each sequence, run forward–backward to get γ and ξ, then

$$\delta_j = 0 \qquad \hat{T}_{ij} = 0 \qquad \hat{\pi} = 0 \qquad \hat{A} = 0$$

$$\hat{T} = \hat{T} + \xi \qquad\qquad \hat{\pi} = \hat{\pi} + \gamma(1) \qquad\qquad \delta = \delta + \sum_t \gamma(t)$$

$$\hat{A}_j(\mathbf{y}) = \sum_{t:\mathbf{y}_t = y} \gamma_j(t) \qquad \text{or} \qquad \hat{A} = \hat{A} + \sum_t \mathbf{y}_t \gamma(t)$$

$$\hat{T}_{ij} = \hat{T}_{ij} / \sum_k \hat{T}_{kj} \qquad \hat{\pi} = \hat{\pi} / \sum \hat{\pi} \qquad\qquad \hat{A}_j = \hat{A}_j / \delta_j$$

Some HMM History

- Markov ('13) and later Shannon ('48,'51) studied *Markov chains*.
- Baum and colleagues (BP'66, BE'67, BS'68, BPSW'70, B'72) developed much of the theory of "probabilistic functions of Markov chains".
- Viterbi ('67) (now Qualcomm) came up with an efficient optimal decoder for state inference.
- Applications to speech were pioneered independently by:
  - Baker ('75) at CMU
  - Jelinek's group ('75) at IBM (now Hopkins)
  - communications research division of IDA (Ferguson '74 unpublished)
- Dempster, Laird & Rubin ('77) recognized a general form of the Baum-Welch algorithm and called it the *EM* algorithm.

Some References for LDS

Available at: `www.cs.cmu.edu/~zoubin/papers.html`

- Ghahramani, Z. and Hinton, G.E. (1996) Parameter estimation for linear dynamical systems. University of Toronto Technical Report CRG-TR-96-2, 6 pages (short note).

- Roweis, S. and Ghahramani, Z. (1999) A Unifying Review of Linear Gaussian Models. *Neural Computation* 11(2):305–345.

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- Welling (2000) The Kalman Filter (class notes). Available at: `www.vision.caltech.edu/welling/class/KalmanFilter.ps`