Sequential Data

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Bishop PRML Ch. 13
Russell and Norvig, AIMA

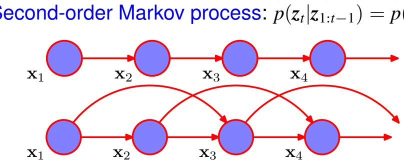
Outline

Temporal Models

- The world changes over time
  - Explicitly model this change using Bayesian networks
  - Undirected models also exist (will not cover)
- Basic idea: copy state and evidence variables for each time step
- e.g. Diabetes management
- z_t is set of unobservable state variables at time t
  - $bloodSugar_t$, $stomachContents_t$, ...
- $\boldsymbol{x}_t$ is set of observable evidence variables at time t
  - $measuredBloodSugar_t$, $foodEaten_t$, ...
- Assume discrete time step, fixed
- Notation: $\boldsymbol{x}_{a:b} = \boldsymbol{x}_a, \boldsymbol{x}_{a+1}, \dots, \boldsymbol{x}_{b-1}, \boldsymbol{x}_b$

Markov Chain

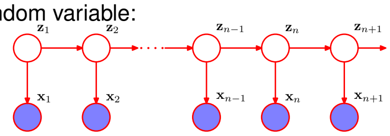
- Construct Bayesian network from these variables
  - parents? distributions? for state variables z_t:
- Markov assumption: z_t depends on bounded subset of $z_{1:t-1}$
  - First-order Markov process: $p(z_t|z_{1:t-1}) = p(z_t|z_{t-1})$
  - Second-order Markov process: $p(z_t|z_{1:t-1}) = p(z_t|z_{t-2}, z_{t-1})$



- Stationary process: $p(z_t|z_{t-1})$ fixed for all t

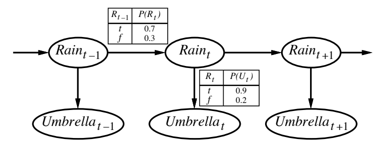
Hidden Markov Model (HMM)

- Sensor Markov assumption: $p(\boldsymbol{x}_t|z_{1:t}, \boldsymbol{x}_{1:t-1}) = p(\boldsymbol{x}_t|z_t)$
- Stationary process: transition model $p(z_t|z_{t-1})$ and sensor model $p(\boldsymbol{x}_t|z_t)$ fixed for all t (separate $p(z_1)$)
- HMM special type of Bayesian network, z_t is a single discrete random variable:



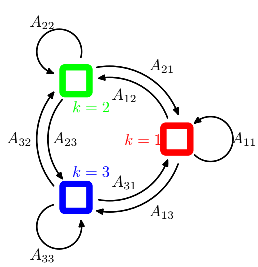
- Joint distribution:
$p(z_{1:t}, x_{1:t}) = p(z_1) \prod_{i=2:t} p(z_i|z_{i-1}) \prod_{i=1:t} p(x_i|z_i)$

HMM Example



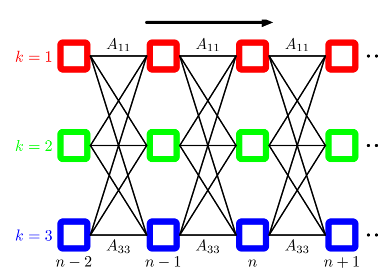
- First-order Markov assumption not true in real world
- Possible fixes:
  - Increase order of Markov process
  - Augment state, add $temp_t$, $pressure_t$

Transition Diagram



- z_n takes one of 3 values
- Using one-of-K coding scheme, $z_{nk} = 1$ if in state k at time n
- Transition matrix $\boldsymbol{A}$ where $p(z_{nk} = 1|z_{n-1,j} = 1) = \boldsymbol{A}_{jk}$

Lattice / Trellis Representation



- The lattice or trellis representation shows possible paths through the latent state variables z_n

Inference Tasks

- Filtering: $p(z_t|x_{1:t})$
  - Estimate current unobservable state given all observations to date
- Prediction: $p(z_n|x_{1:t})$ for $n > t$
  - Similar to filtering, without evidence
- Smoothing: $p(z_n|x_{1:t})$ for $n < t$
  - Better estimate of past states
- Most likely explanation: $\arg\max_{z_{1:t}} p(z_{1:t}|x_{1:t})$
  - e.g. speech recognition, decoding noisy input sequence

Filtering

- Aim: devise a recursive state estimation algorithm:

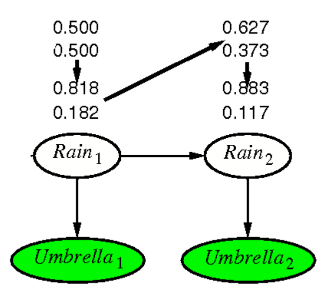
$$p(z_{t+1}|x_{1:t+1}) = f(x_{t+1}, p(z_t|x_{1:t}))$$

$$\begin{aligned} p(z_{t+1}|x_{1:t+1}) &= p(z_{t+1}|x_{1:t}, x_{t+1}) \\ &= \alpha p(x_{t+1}|x_{1:t}, z_{t+1}) p(z_{t+1}|x_{1:t}) \\ &= \alpha p(x_{t+1}|z_{t+1}) p(z_{t+1}|x_{1:t}) \end{aligned}$$

- I.e. prediction + estimation. Prediction by summing out z_t:

$$\begin{aligned} p(z_{t+1}|x_{1:t+1}) &= \alpha p(x_{t+1}|z_{t+1}) \sum_{z_t} p(z_{t+1}, z_t|x_{1:t}) \\ &= \alpha p(x_{t+1}|z_{t+1}) \sum_{z_t} p(z_{t+1}|z_t, x_{1:t}) p(z_t|x_{1:t}) \\ &= \alpha p(x_{t+1}|z_{t+1}) \sum_{z_t} p(z_{t+1}|z_t) p(z_t|x_{1:t}) \end{aligned}$$

Filtering Example



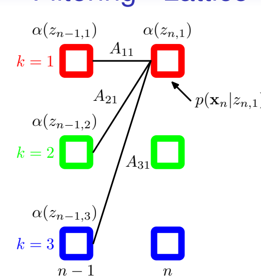
R_{t-1}	$P(R_t)$
t	0.7
f	0.3

R_t	$P(U_t)$
t	0.9
f	0.2

$p(rain_1 = true) = 0.5$

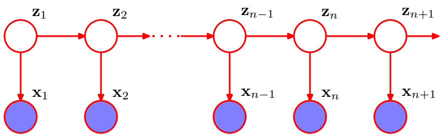
$p(z_{t+1}|x_{1:t+1}) = \alpha p(x_{t+1}|z_{t+1}) \sum_{z_t} p(z_{t+1}|z_t) p(z_t|x_{1:t})$

Filtering - Lattice



- Using notation in PRML, forward message is $\alpha(z_n)$
- Compute $\alpha(z_{n,i})$ using sum over k of $\alpha(z_{n-1,k})$ multiplied by A_{ki}, then multiplying in evidence $p(x_t|z_{ni})$
- Each step, computing $\alpha(z_n)$ takes $O(K^2)$ time, with K values for z_n

Smoothing

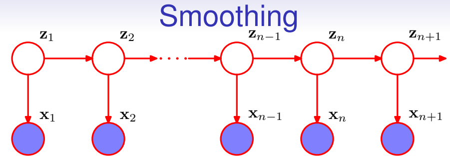


- Divide evidence $x_{1:t}$ into $x_{1:n}$, $x_{n+1:t}$

$$\begin{aligned} p(z_n|x_{1:t}) &= p(z_n|x_{1:n}, x_{n+1:t}) \\ &= \alpha p(z_n|x_{1:n})p(x_{n+1:t}|z_n, x_{1:n}) \\ &= \alpha p(z_n|x_{1:n})p(x_{n+1:t}|z_n) \\ &= \alpha\alpha(z_n)\beta(z_n) \end{aligned}$$

- Backwards message $\beta(z_n)$ another recursion:

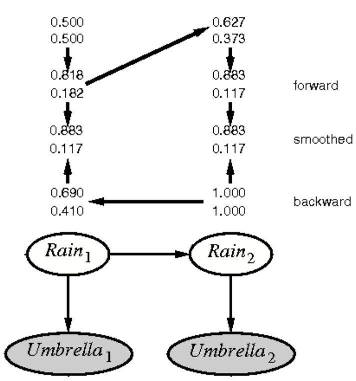
Smoothing



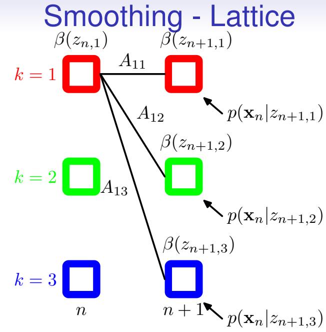
- Divide evidence $x_{1:t}$ into $x_{1:n}$, $x_{n+1:t}$, $p(z_n|x_{1:t}) = \alpha\alpha(z_n)\beta(z_n)$
- Backwards message another recursion:

$$\begin{aligned} p(x_{n+1:t}|z_n) &= \sum_{z_{n+1}} p(x_{n+1:t}, z_{n+1}|z_n) \\ &= \sum_{z_{n+1}} p(x_{n+1:t}|z_{n+1}, z_n)p(z_{n+1}|z_n) \\ &= \sum_{z_{n+1}} p(x_{n+1:t}|z_{n+1})p(z_{n+1}|z_n) \\ &= \sum_{z_{n+1}} p(x_{n+1}|z_{n+1})p(x_{n+2:t}|z_{n+1})p(z_{n+1}|z_n) \end{aligned}$$

Smoothing Example

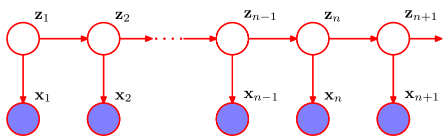


Smoothing - Lattice



- Using notation in PRML, backward message is $\beta(z_n)$
- Compute $\beta(z_{n,i})$ using sum over k of $\beta(z_{n+1,k})$ multiplied by A_{ik} and evidence $p(x_{n+1}|z_{n+1,k})$
- Each step, computing $\beta(z_n)$ takes $O(K^2)$ time, with K values for z_n

Forward-Backward Algorithm



- Filter from time 1 to N, and cache forward messages $\alpha(z_n)$
- Smooth from time N to 1, and cache backward messages $\beta(z_n)$
- Can now compute $p(z_n|x_1, x_2, \ldots, x_N)$ for all n
- Total complexity $O(NK^2)$
- a.k.a Baum-Welch algorithm

HMM Parameters

- The parameters of an HMM are:
  - Transition matrix $\boldsymbol{A}$ where $p(z_{nk} = 1|z_{n-1,j} = 1) = \boldsymbol{A}_{jk}$
  - Sensor model ϕ_k parameters to each $p(\boldsymbol{x}_n|z_{nk} = 1, \phi_k)$ (e.g. ϕ_k could be mean and variance of Gaussian)
  - Prior for initial state z_1, model as multinomial $p(z_{1k} = 1) = \pi_k$, parameters $\boldsymbol{\pi}$
- Call these parameters $\boldsymbol{\theta} = (\boldsymbol{A}, \boldsymbol{\pi}, \boldsymbol{\phi})$
- Learning problem: given one sequence $\boldsymbol{x}$, find best $\boldsymbol{\theta}$
  - Extension to multiple sequences straight-forward (assume independent, log of product is sum)

Maximum Likelihood for HMMs

- We can use maximum likelihood to choose the best parameters:
$$\boldsymbol{\theta}_{ML} = \arg\max p(\boldsymbol{x}|\boldsymbol{\theta})$$
- Unfortunately this is hard to do: we can get $p(\boldsymbol{x}|\boldsymbol{\theta})$ by summing out from the joint distribution:
$$\begin{aligned} p(\boldsymbol{x}|\boldsymbol{\theta}) &= \sum_{z_1}\sum_{z_2}\cdots\sum_{z_N} p(\boldsymbol{x}, z_1, z_2, \ldots, z_N|\boldsymbol{\theta}) \\ &\equiv \sum_{z} p(\boldsymbol{x}, z|\boldsymbol{\theta}) \end{aligned}$$
  - But this sum has K^N terms in it
  - And, as in the mixture distribution case, no simple closed-form solution
- Instead, use expectation-maximization (EM)

EM for HMMs

- Start with initial guess for parameters $\boldsymbol{\theta}^{old} = (\boldsymbol{A}, \boldsymbol{\pi}, \boldsymbol{\phi})$
- **E-step**: Calculate posterior on latent variables $p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old})$
- **M-step**: Maximize $Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{old}) = \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \ln p(\boldsymbol{x}, z|\boldsymbol{\theta})$ wrt $\boldsymbol{\theta}$
- Let's look at the M-step, and see how the HMM structure helps us

HMM M-step

- **M-step**: Maximize $Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{old}) = \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \ln p(\boldsymbol{x}, z|\boldsymbol{\theta})$ wrt $\boldsymbol{\theta}$:
- The complete data log-likelihood factors nicely:

$$\begin{aligned}\ln p(\boldsymbol{x}, z|\boldsymbol{\theta}) &= \ln \left\{ p(z_1|\boldsymbol{\pi}) \prod_{i=2:N} p(z_i|z_{i-1}, \boldsymbol{A}) \prod_{i=1:N} p(x_i|z_i, \boldsymbol{\phi}) \right\} \\ &= \ln p(z_1|\boldsymbol{\pi}) + \sum_{i=2:N} \ln p(z_i|z_{i-1}, \boldsymbol{A}) + \sum_{i=1:N} \ln p(x_i|z_i, \boldsymbol{\phi})\end{aligned}$$

- To maximize Q we now have 3 separate problems, one for each parameter
  - Let's consider each in turn

Prior $\boldsymbol{\pi}$

- Maximize Q wrt prior on initial state $\boldsymbol{\pi}$:

$$\begin{aligned}Q(\boldsymbol{\pi}, \boldsymbol{\theta}^{old}) &= \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \ln p(z_1|\boldsymbol{\pi}) \\ = \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \ln \prod_{k=1}^{K} \pi_k^{z_{1k}} &= \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \sum_{k=1}^{K} z_{1k} \ln \pi_k \\ &= \sum_{k=1}^{K} \ln \pi_k \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) z_{1k} \\ &= \sum_{k=1}^{K} p(z_{1k} = 1|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \ln \pi_k\end{aligned}$$

- I.e. smoothed value for z_1 being in state k

$$Q(\boldsymbol{\pi}, \boldsymbol{\theta}^{old}) = \sum_{k=1}^{K} p(z_{1k} = 1|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \ln \pi_k$$

- Can solve for best $\boldsymbol{\pi}$
- Use Lagrange multiplier to enforce constraint $\sum_k \pi_k = 1$

$$\pi_k = \frac{p(z_{1k} = 1|\boldsymbol{x}, \boldsymbol{\theta}^{old})}{\sum_{j=1}^{K} p(z_{1j} = 1|\boldsymbol{x}, \boldsymbol{\theta}^{old})}$$

- Intuitively sensible result: new π_k is smoothed probability of being in state k at time 1 using old parameters
- E-step needs to calculate smoothed $p(z_{1k} = 1|\boldsymbol{x}, \boldsymbol{\theta}^{old})$ – this is fast $O(NK^2)$

Transition Matrix $\boldsymbol{A}$

- Maximize Q wrt transition matrix $\boldsymbol{A}$:

$$\begin{aligned}Q(\boldsymbol{A}, \boldsymbol{\theta}^{old}) &= \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \sum_{i=2:N} \ln p(z_i|z_{i-1}, \boldsymbol{A}) \\ &= \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \sum_{i=2:N} \ln \prod_{k=1:K} \prod_{j=1:K} \boldsymbol{A}_{jk}^{z_{i-1,j} z_{i,k}} \\ &= \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) \sum_{i=2:N} \sum_{k=1:K} \sum_{j=1:K} z_{i-1,j} z_{i,k} \ln \boldsymbol{A}_{jk} \\ &= \sum_{k=1:K} \sum_{j=1:K} \ln \boldsymbol{A}_{jk} \sum_{i=2:N} \sum_z p(z|\boldsymbol{x}, \boldsymbol{\theta}^{old}) z_{i-1,j} z_{i,k} \\ &= \sum_{k=1:K} \sum_{j=1:K} \ln \boldsymbol{A}_{jk} \sum_{i=2:N} p(z_{i-1} = j, z_i = k|\boldsymbol{x}, \boldsymbol{\theta}^{old})\end{aligned}$$

- E-step needs to calculate $p(z_{i-1} = j, z_i = k|\boldsymbol{x}, \boldsymbol{\theta}^{old})$ – can be done quickly using forward and backward messages

$$Q(\boldsymbol{A}, \boldsymbol{\theta}^{old}) = \sum_{k=1:K} \sum_{j=1:K} \ln \boldsymbol{A}_{jk} \sum_{i=2:N} p(z_{n-1} = j, z_n = k | \boldsymbol{x}, \boldsymbol{\theta}^{old})$$

- Can solve for best $\boldsymbol{A}$
- Again use Lagrange multipliers to enforce constraint $\sum_k \boldsymbol{A}_{jk} = 1$

$$\boldsymbol{A}_{jk} = \frac{\sum_{n=2:N} p(z_{n-1} = j, z_n = k | \boldsymbol{x}, \boldsymbol{\theta}^{old})}{\sum_{l=1:K} \sum_{n=2:N} p(z_{n-1} = j, z_n = l | \boldsymbol{x}, \boldsymbol{\theta}^{old})}$$

- Again sensible result: $\boldsymbol{A}_{jk}$ set to expected number of times we transition from state j to k using the smoothed results from old parameters

Sensor Model

- Similar derivation for sensor model parameters ϕ
- Again end up with weighted parameter estimated based on expected values of states given smoothed estimates

HMM EM Summary

- Start with initial guess for parameters $\boldsymbol{\theta}^{old} = (\boldsymbol{A}, \boldsymbol{\pi}, \phi)$
- Run forward-backward algorithm to get all messages $\alpha(z_n)$, $\beta(z_n)$ (E-step)
  - $O(NK^2)$ time complexity
  - Can use these to compute any smoothed posterior $p(z_{nk} = 1 | \boldsymbol{x}, \boldsymbol{\theta}^{old})$
  - Also can compute any $p(z_{n-1,j} = 1, z_{n,k} = 1 | \boldsymbol{x}, \boldsymbol{\theta}^{old})$
- Using these, update values for parameters (M-step)
  - π_k is smoothed probability of being in in state k at time 1
  - $\boldsymbol{A}_{jk}$ is smoothed probability of transitioning from state j to k averaged over all time steps
  - ϕ is weighted sensor parameters using smoothed probabilities (e.g. similar to mixture of Gaussians)
- Repeat until convergence

Conclusion

- Readings: Ch. 13.2, 13.2.1, 13.2.2
- HMM - Probabilistic model of temporal data
  - Discrete hidden (unobserved, latent) state variable at each time
    - Continuous (next)
  - Observation (can be discrete / continuous) at each time
  - Conditional independence assumptions (Markov)
  - Assumptions on distributions (stationary)
- Inference
  - Filtering
  - Smoothing
  - Most likely sequence (next)
- Maximum likelihood learning
  - EM – efficient computation $O(NK^2)$ time using forward-backward smoothing