# CPSC 440: Advanced Machine Learning Hidden Markov Models

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## Last Time: Chapman-Kolmogorov Equations

- Chapman-Kolmogorov (CK) equations:
  - Recursive formula for computing  $p(x_j = s)$  for all j and s in a Markov chain.

$$p(x_j) = \sum_{x_{j-1}=1}^k p(x_j \mid x_{j-1}) p(x_{j-1}),$$

- Allows us to compute all these marginal probabilities p(x<sub>j</sub> = s) in O(dk<sup>2</sup>).
   For a length-d chain with k states.
- We also discussed stationary distributions of homogeneous Markov chains.

$$\pi(c) = \sum_{c'} p(x_j = c \mid x_{j-1} = c') \pi(c'),$$

which are sets of marginal probabilities  $\pi$  that don't change over time.

- You can think of this as the "long-run average probability of being in each state".
- Stationary distribution exists and is unique if all transitions are positive.

## Application: Voice Photoshop

#### • Adobe VoCo uses decoding in a Markov chain as part of synthesizing voices:



Fig. 7. Dynamic triphone preselection. For each query triphone (top) we find a candidate set of good potential matches (columns below). Good paths through this set minimize differences from the query, number and severity of breaks, and contextual mismatches between neighboring triphones.

http://gfx.cs.princeton.edu/pubs/Jin\_2017\_VTI/Jin2017-VoCo-paper.pdf

#### https://www.youtube.com/watch?v=I314XLZ59iw

# Decoding: Maximizing Joint Probability

• Decoding in density models: finding x with highest joint probability:

 $\underset{x_1, x_2, \dots, x_d}{\operatorname{argmax}} p(x_1, x_2, \dots, x_d).$ 

- For CS grad student (d = 60) the decoding is "industry" for all years.
  - The decoding often doesn't look like a typical sample.
  - The decoding can change if you increase d.
- Decoding is easy for independent models:
  - Here,  $p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2)p(x_3)p(x_4)$ .
  - You can optimize  $p(x_1, x_2, x_3, x_4)$  by optimizing each  $p(x_j)$  independently.
- Can we also maximize the marginals to decode a Markov chain?

## Example of Decoding vs. Maximizing Marginals

• Consider the "plane of doom" 2-variable Markov chain:

$$X = \begin{bmatrix} ``land'' ``alive'' \\ ``land'' ``alive'' \\ ``crash'' ``dead'' \\ ``explode'' ``dead'' \\ ``crash'' ``dead'' \\ ``land'' ``alive'' \\ \vdots & \vdots \end{bmatrix}.$$

- $\bullet~40\%$  of the time the plane lands and you live.
- $\bullet~30\%$  of the time the plane crashes and you die.
- 30% of the time the explodes and you die.

#### Example of Decoding vs. Maximizing Marginals

• Initial probabilities are given by

 $p(x_1 = \text{``land''}) = 0.4, \quad p(x_1 = \text{``crash''}) = 0.35, \quad p(x_1 = \text{``explode''}) = 0.25,$ 

and transition probabilities are:

$$\begin{split} p(x_2 = \text{``alive''} \mid x_1 = \text{``land''}) = 1, \quad p(x_2 = \text{``alive''} \mid x_1 = \text{``crash''}) = 0, \\ p(x_2 = \text{``alive''} \mid x_1 = \text{``explode''}) = 0. \end{split}$$

• If we apply the CK equations we get

$$p(x_2 = \text{``alive''}) = 0.4, \quad p(x_2 = \text{``dead''}) = 0.6,$$

so maximizing the marginals  $p(x_j)$  independently gives ("land", "dead").

- This actually has probability 0, since  $p(\text{"dead}'' \mid \text{"land}'') = 1$ .
- Decoding considers the joint assignment to x<sub>1</sub> and x<sub>2</sub> maximizing probability.
  In this case it's ("land", "alive"), which has probability 0.4.

# Decoding with Dynamic Programming

- Note that decoding can't be done forward in time as in CK equations.
  - Even if  $p(x_1 = 1) = 0.99$ , the most likely sequence could have  $x_1 = 2$ .
  - So we need to optimize over all  $k^d$  assignments to all variables.
- Fortunately, we can solve this problem using dynamic programming.
- Ingredients of dynamic programming:
  - Optimal sub-structure.
    - We can divide the problem into sub-problems that can individual be solved.
  - Overlapping sub-problems.
    - The same sub-problems are reused several times.

# Decoding with Dynamic Programming

• For decoding in Markov chains, we will use the following sub-problem:

- Compute the highest probability sequence of length j ending in state s.
- We'll use  $M_j(s)$  as the probability of this sequence.

$$M_j(s) = \max_{x_1, x_2, \dots, x_{j-1}} p(x_1, x_2, \dots, x_j = s).$$

#### • Optimal sub-structure:

- We can find the decoding by finding the s maximizing  $M_d(s)$  (then "backtracking").
- We can compute other  $M_j(s)$  recursively (derivation of this coming up),

$$M_j(s) = \max_{x_{j-1}} \underbrace{p(x_j = s \mid x_{j-1})}_{\text{given}} \underbrace{M_{j-1}(x_{j-1})}_{\text{recurse}},$$

with a base case of  $M_1(s) = p(x_1 = s)$  (which is given by the initial probability).

- Overlapping sub-problems:
  - The same k values of  $M_{j-1}(s)$  are used to compute the k values of  $M_j(s)$ .

#### Digression: Recursive Joint Maximization

• To derive the  $M_j$  formula, it will be helpful to re-write joint maximizations as

$$\max_{x_1, x_2} f(x_1, x_2) = \max_{x_1} f_1(x_1),$$

where  $f_1(x_1) = \max_{x_2} f(x_1, x_2)$  (this  $f_1$  "maximizes out" over  $x_2$ ). • This is similar to the marginalization rule in probability.

• Plugging in the definition of  $f_1(x_1)$  we obtain:

$$\max_{x_1, x_2} f(x_1, x_2) = \max_{x_1} \underbrace{\max_{x_2} f(x_1, x_2)}_{f_1(x_1)}.$$

• You can do this trick repeatedly and/or with any number of variables.

# Decoding with Dynamic Programming

• Derivation of recursive calculation  $M_j(x_j)$  for decoding Markov chains:

$$\begin{split} M_{j}(x_{j}) &= \max_{x_{1}, x_{2}, \dots, x_{j-1}} p(x_{1}, x_{2}, \dots, x_{j}) & (\text{definition of } M_{j}(x_{j})) \\ &= \max_{x_{1}, x_{2}, \dots, x_{j-1}} p(x_{j} \mid x_{1}, x_{2}, \dots, x_{j-1}) p(x_{1}, x_{2}, \dots, x_{j-1}) & (\text{product rule}) \\ &= \max_{x_{1}, x_{2}, \dots, x_{j-1}} p(x_{j} \mid x_{j-1}) p(x_{1}, x_{2}, \dots, x_{j-1}) & (\text{Markov property}) \\ &= \max_{x_{j-1}} \left\{ \max_{x_{1}, x_{2}, \dots, x_{j-2}} p(x_{j} \mid x_{j-1}) p(x_{1}, x_{2}, x_{j-1}) \right\} & (\max_{a, b} f(a, b) = \max_{a} \{\max_{b} f(a, b)\}) \\ &= \max_{x_{j-1}} \left\{ p(x_{j} \mid x_{j-1}) \max_{x_{1}, x_{2}, \dots, x_{j-2}} p(x_{1}, x_{2}, x_{j-1}) \right\} & (\max_{i} \alpha a_{i} = \alpha \max_{i} a_{i} \text{ for } \alpha \ge 0) \\ &= \max_{x_{j-1}} \underbrace{p(x_{j} \mid x_{j-1}) \underbrace{M_{j-1}(x_{j-1})}_{\text{recurse}} p(x_{1}, x_{2}, x_{j-1})}_{\text{recurse}} \end{split}$$

- For each (j, s) we also store the maximizing value of  $x_{j-1}$ .
  - Once we have  $M_j(x_j = s)$  for all j and s values, backtrack using these values to solve problem.

## Example: Decoding the Plane of Doom

• We have  $M_1(x_1) = p(x_1)$  so in "plane of doom" we have

 $M_1(\text{``land''}) = 0.4, \quad M_1(\text{``crash''}) = 0.3, \quad M_1(\text{``explode''}) = 0.3.$ 

• We have  $M_2(x_2) = \max_{x_1} p(x_2 \mid x_1) M_1(x_1)$  so we get

$$M_2(\text{``alive''}) = 0.4, \quad M_2(\text{``dead''}) = 0.3.$$

M<sub>2</sub>(2) ≠ p(x<sub>2</sub> = 2) because we needed to choose either "crash" or "explode".
And notice that ∑<sup>k</sup><sub>c=1</sub> M<sub>2</sub>(x<sub>j</sub> = c) ≠ 1 (this is not a distribution over x<sub>2</sub>).

We maximize M<sub>2</sub>(x<sub>2</sub>) to find that the optimal decoding ends with "alive".
We now need to backtrack to find the state that lead to "alive", giving "land".

#### Viterbi Decoding

# Viterbi Decoding

- The Viterbi decoding dynamic programming algorithm:
  - **1** Set  $M_1(x_1) = p(x_1)$  for all  $x_1$ .

2 Compute  $M_2(x_2)$  for all  $x_2$ , store value of  $x_1$  leading to the best value of each  $x_2$ .

- Sompute  $M_3(x_3)$  for all  $x_3$ , store value of  $x_2$  leading to the best value of each  $x_3$ .
- 4 ...
- **(5)** Maximize  $M_d(x_d)$  to find value of  $x_d$  in a decoding.
- **(**) Bactrack to find the value of  $x_{d-1}$  that lead to this  $x_d$ .
- **O** Backtrack to find the value of  $x_{d-2}$  that lead to this  $x_{d-1}$ .
- 8 . . .
- **(9)** Backtrack to find the value of  $x_1$  that lead to this  $x_2$ .
- For a fixed j, computing all  $M_j(x_j)$  given all  $M_{j-1}(x_{j-1})$  costs  $O(k^2)$ .
  - Total cost is only  $O(dk^2)$  to search over all  $k^d$  paths.
  - Has numerous applications like decoding digital TV.

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## Decoding with Dynamic Programming

• What Viterbi decoding data structures might look like (d = 4, k = 3):

$$M = \begin{bmatrix} 0.25 & 0.25 & 0.50 \\ 0.35 & 0.15 & 0.05 \\ 0.10 & 0.05 & 0.05 \\ 0.02 & 0.03 & 0.05 \end{bmatrix}, \quad B = \begin{bmatrix} \emptyset & \emptyset & \emptyset \\ 1 & 1 & 3 \\ 2 & 1 & 1 \\ 2 & 2 & 1 \end{bmatrix}$$

- The  $d \times k$  matrix M stores the values  $M_i(s)$ , while B stores the argmax values.
- From the last row of M and the bactracking matrix B, the decoding is  $x_1 = 1, x_2 = 2, x_3 = 1, x_4 = 3$ .

Viterbi Decoding

Hidden Markov Models

## Outline

#### Viterbi Decoding

2 Hidden Markov Models

#### Back to the Rain Data

• We previously considered the "Vancouver Rain" data:



• We used homogeneous Markov chains to model between-day dependence.

## Back to the Rain Data

- But doesn't it rain less in the summer?
- There are hidden clusters in the data not captured by the Markov chain.
  - But mixture of independent models are inefficient at representing direct dependency.
- Mixture of Markov chains could capture direct dependence and clusters,

$$p(x_1, x_2, \dots, x_d) = \sum_{c=1}^k p(z=c) \underbrace{p(x_1 \mid z=c) p(x_2 \mid x_1, z=c) \cdots p(x_d \mid x_{d-1}, z=c)}_{\text{Markov chain } c}.$$

- Cluster z chooses which homogeneous Markov chain parameters to use.
  - We could learn that we're more likely to have rain in winter.
  - Can modify CK equations to take into account z, and then apply EM.

# Comparison of Models on Rain Data

- Independent (homogeneous) Bernoulli:
  - Average NLL: 18.97 (1 parameter).
- Independent Bernoullis:
  - Average NLL: 18.95, (28 parmaeters).
- Mixture of Bernoullis (k = 10, five random restarts of EM):
  - Average NLL: 17.06  $(10 + 10 \times 28 = 290 \text{ parameters})$
- Homogeneous Markov chain:
  - Average NLL: 16.81 (3 parameters)
- Mixture of Markov chains (k = 10, five random restarts of EM):
  - Average NLL: 16.53 ( $10 + 10 \times 3 = 40$  parameters).
  - Included what I call a "summer" cluster:

$$\begin{array}{l} p(z=5)=0.14\\ p(x_1=\text{``rain''}\mid z=5)=0.22\\ p(x_j=\text{``rain''}\mid x_{j-1}=\text{``rain''}, z=5)=0.49\\ p(x_j=\text{``rain''}\mid x_{j-1}=\text{``not rain''}, z=5)=0.11 \end{array} (instead of usual 35\%) \end{array}$$

#### Viterbi Decoding

#### Back to the Rain Data

- The rain data is artificially divideded into months.
- We previously discussed viewing rain data as one very long sequence (n = 1).
- We could apply homogeneous Markov chains due to parameter tieing.
- But a mixture doesn't make sense when n = 1.
- What we want: different "parts" of the sequence come from different clusters.
  We transition from "summer" cluster to "fall" cluster at some time *j*.
- One way to address this is with a "hidden" Markov model (HMM):
  - Instead of months being assigned to clusters, days are assigned to clusters.
  - Have a Markov dependency between cluster values of adjacent days.

# Hidden Markov Models (MEMORIZE)

• Hidden Markov models have each  $x_j$  depend on hidden Markov chain.



- We're going to learn clusters  $z_j$  and the hidden dynamics.
  - Hidden cluster  $z_j$  could be "summer" or "winter" (we're learning the clusters).
  - Transition probability  $p(z_j \mid z_{j-1})$  is probability of staying in "summer".
    - Initial probability  $p(z_1)$  is probability of starting chain in "summer".
  - Emission probability  $p(x_j \mid z_j)$  is probability of "rain" during "summer".

#### Hidden Markov Models

• Hidden Markov models have each  $x_i$  depend on hidden Markov chain.



• You observe the  $x_j$  values but do not see the  $z_j$  values.

• There is a "hidden" Markov chain, whose state determines the cluster at each time.

• Note that the  $x_j$  can be continuous even with discrete clusters  $z_j$ .

• Data could come from a mixture of Gaussians, with cluster changing in time.

#### Hidden Markov Models

• Hidden Markov models have each  $x_j$  depend on hidden Markov chain.



- If the  $z_j$  are continuous it's often called a state-space model.
  - If everything is Gaussian, it leads to Kalman filtering.
  - Keywords for non-Gaussian: unscented Kalman filter and particle filter.
- Variants of HMMs are probably the most-used time-series model...

# Applications of HMMs and Kalman Filters

#### Applications [edit]

HMMs can be applied in many fields where the goal is to recover a data sequence that is not immediately observable (but other data that depend on the sequence are). Applications include:

- . Single Molecule Kinetic analysis<sup>[16]</sup>
- . Cryptanalysis
- . Speech recognition
- . Speech synthesis
- . Part-of-speech tagging
- . Document Separation in scanning solutions
- . Machine translation
- . Partial discharge
- . Gene prediction
- . Alignment of bio-sequences
- . Time Series Analysis
- . Activity recognition
- Protein folding<sup>[17]</sup>
- . Metamorphic Virus Detection<sup>[18]</sup>
- . DNA Motif Discovery<sup>[19]</sup>

#### Applications [edit]

- . Attitude and Heading Reference Systems
- . Autopilot
- . Battery state of charge (SoC) estimation<sup>[39][40]</sup>
- . Brain-computer interface
- . Chaotic signals
- . Tracking and Vertex Fitting of charged particles in Particle Detectors<sup>[41]</sup>
- . Tracking of objects in computer vision
- . Dynamic positioning

- Economics, in particular macroeconomics, time series analysis, and econometrics<sup>[42]</sup>
- . Inertial guidance system
- . Orbit Determination
- . Power system state estimation
- . Radar tracker
- . Satellite navigation systems
- Seismology<sup>[43]</sup>
- . Sensorless control of AC motor variable-frequency
- drives

- . Simultaneous localization and mapping
- . Speech enhancement
- . Visual odometry
- . Weather forecasting
- . Navigation system
- . 3D modeling
- . Structural health monitoring
- . Human sensorimotor processing[44]

## Example: Modeling DNA Sequences

• Markov model for elements of sequence (dependence on previous symbol):



# Example: Modeling DNA Sequences

• Hidden Markov model (HMM) for elements of sequence (two hidden clusters):



- This is a (hidden) state transition diagram.
  - Can reflect that probabilities are different in different regions.
  - The actual regions are not given, but instead are nuissance variables handled by EM.
- A better model might use a hidden and visible Markov chain.
  - With 2 hidden clusters, you would have 8 "probability wheels" (4 per cluster).
  - Would have "treewidth 2", which we'll show later means it's tractable to use.

# Summary

- Decoding is task of finding most probable x.
- Viterbi decoding allow efficient decoding with Markov chains.
  - A special case of dynamic programming.
- Hidden Markov models model time-series with hidden per-time cluster.
  - Tons of applications, typically more realistic than Markov models.
- Next time: measuring defence in the NBA.