10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Hidden Markov Models

+

Midterm Exam 2 Review

Matt Gormley
Lecture 19
Mar. 27, 2020

Reminders

- Homework 6: Learning Theory / Generative Models
  - Out: Fri, Mar 20
  - Due: Fri, Mar 27 at 11:59pm
- Practice Problems for Exam 2
  - Out: Fri, Mar 20
- Midterm Exam 2
  - Thu, Apr 2 – evening exam, details announced on Piazza

- Today's In-Class Poll
  - http://poll.mlcourse.org

MIDTERM EXAM LOGISTICS

Midterm Exam

- **Time / Location**
  - **Time:** Evening Exam
    Thu, Apr. 2 at 6:00pm – 9:00pm
  - **Location:** We will contact you with additional details about how to join the appropriate Zoom meeting.
  - **Seats:** There will be **assigned Zoom rooms**. Please arrive online early.
  - Please watch Piazza carefully for announcements.
- **Logistics**
  - Covered material: Lecture 9 – Lecture 18 (95%), Lecture 1 – 8 (5%)
  - Format of questions:
    - Multiple choice
    - True / False (with justification)
    - Derivations
    - Short answers
    - Interpreting figures
    - Implementing algorithms on paper
  - No electronic devices
  - You are allowed to **bring** one 8½ x 11 sheet of notes (front and back)

Midterm Exam

- **How to Prepare**
  - Attend the midterm review lecture (right now!)
  - Review prior year's exam and solutions (we'll post them)
  - Review this year's homework problems
  - Consider whether you have achieved the "learning objectives" for each lecture / section

Midterm Exam

- **Advice (for during the exam)**
  - Solve the easy problems first
    (e.g. multiple choice before derivations)
    - if a problem seems extremely complicated you're likely missing something
  - Don't leave any answer blank!
  - If you make an assumption, write it down
  - If you look at a question and don't know the answer:
    - we probably haven't told you the answer
    - but we've told you enough to work it out
    - imagine arguing for some answer and see if you like it

Topics for Midterm 1

- Foundations
  - Probability, Linear Algebra, Geometry, Calculus
  - Optimization
- Important Concepts
  - Overfitting
  - Experimental Design
- Classification
  - Decision Tree
  - KNN
  - Perceptron
- Regression
  - Linear Regression

Topics for Midterm 2

- Classification
  - Binary Logistic Regression
  - Multinomial Logistic Regression
- Important Concepts
  - Stochastic Gradient Descent
  - Regularization
  - Feature Engineering
- Feature Learning
  - Neural Networks
  - Basic NN Architectures
  - Backpropagation
- Learning Theory
  - PAC Learning
- Generative Models
  - Generative vs. Discriminative
  - MLE / MAP
  - Naïve Bayes

SAMPLE QUESTIONS

Sample Questions

3.2 Logistic regression

Given a training set $\{(x_i, y_i), i = 1, \ldots, n\}$ where $x_i \in \mathbb{R}^d$ is a feature vector and $y_i \in \{0, 1\}$ is a binary label, we want to find the parameters $\hat{w}$ that maximize the likelihood for the training set, assuming a parametric model of the form

$$p(y = 1|x; w) = \frac{1}{1 + \exp(-w^T x)}.$$

The conditional log likelihood of the training set is

$$\ell(w) = \sum_{i=1}^{n} y_i \log p(y_i, |x_i; w) + (1 - y_i) \log(1 - p(y_i, |x_i; w)),$$

and the gradient is

$$\nabla \ell(w) = \sum_{i=1}^{n} (y_i - p(y_i|x_i; w)) x_i.$$

(b) [5 pts.] What is the form of the classifier output by logistic regression?

(c) [2 pts.] **Extra Credit:** Consider the case with binary features, i.e, $x \in \{0, 1\}^d \subset \mathbb{R}^d$, where feature x_1 is rare and happens to appear in the training set with only label 1. What is $\hat{w}_1$? Is the gradient ever zero for any finite w? Why is it important to include a regularization term to control the norm of $\hat{w}$?

Samples Questions

2.1 Train and test errors

In this problem, we will see how you can debug a classifier by looking at its train and test errors. Consider a classifier trained till convergence on some training data $\mathcal{D}^{\text{train}}$, and tested on a separate test set $\mathcal{D}^{\text{test}}$. You look at the test error, and find that it is very high. You then compute the training error and find that it is close to 0.

1. **[4 pts]** Which of the following is expected to help? Select all that apply.

   (a) Increase the training data size.

   (b) Decrease the training data size.

   (c) Increase model complexity (For example, if your classifier is an SVM, use a more complex kernel. Or if it is a decision tree, increase the depth).

   (d) Decrease model complexity.

   (e) Train on a combination of $\mathcal{D}^{\text{train}}$ and $\mathcal{D}^{\text{test}}$ and test on $\mathcal{D}^{\text{test}}$

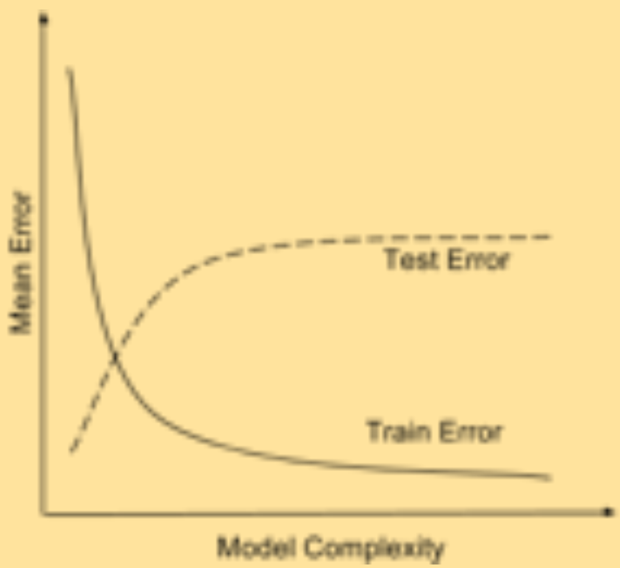
   (f) Conclude that Machine Learning does not work.

Samples Questions

2.1 Train and test errors

In this problem, we will see how you can debug a classifier by looking at its train and test errors. Consider a classifier trained till convergence on some training data $\mathcal{D}^{\text{train}}$, and tested on a separate test set $\mathcal{D}^{\text{test}}$. You look at the test error, and find that it is very high. You then compute the training error and find that it is close to 0.

4. **[1 pts]** Say you plot the train and test errors as a function of the model complexity. Which of the following two plots is your plot expected to look like?



(a)

(b)

Sample Questions

5 Learning Theory [20 pts.]

(a) [3 pts.] **T or F**: It is possible to label 4 points in $\mathbb{R}^2$ in all possible 2^4 ways via linear separators in $\mathbb{R}^2$.

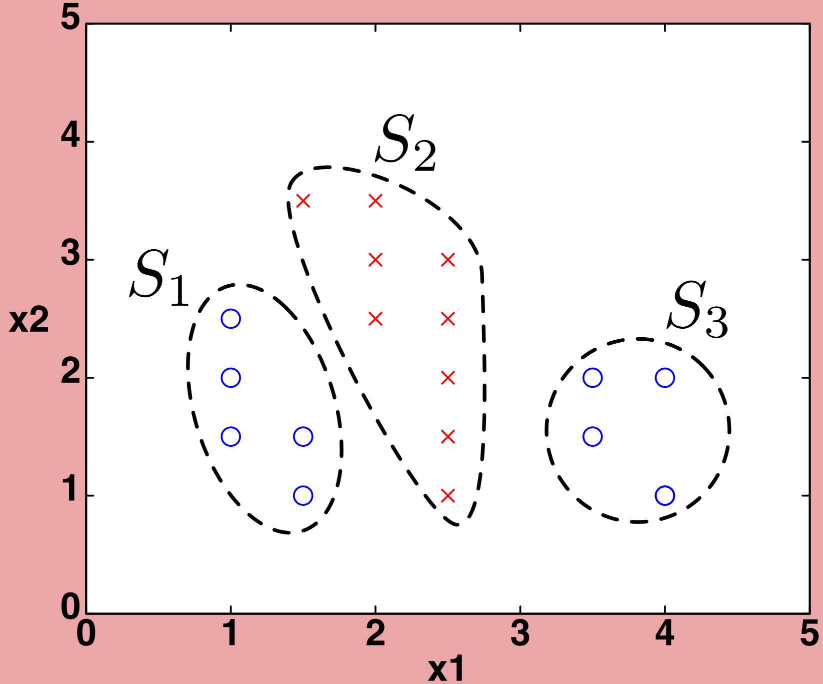
(d) [3 pts.] **T or F**: The VC dimension of a concept class with infinite size is also infinite.

(f) [3 pts.] **T or F**: Given a realizable concept class and a set of training instances, a consistent learner will output a concept that achieves 0 error on the training instances.

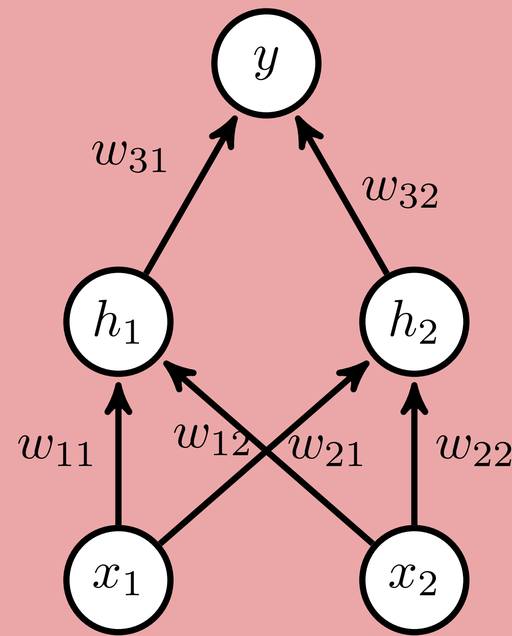
Sample Questions

Neural Networks

Can the neural network in Figure (b) correctly classify the dataset given in Figure (a)?



(a) The dataset with groups S_1, S_2, and S_3.

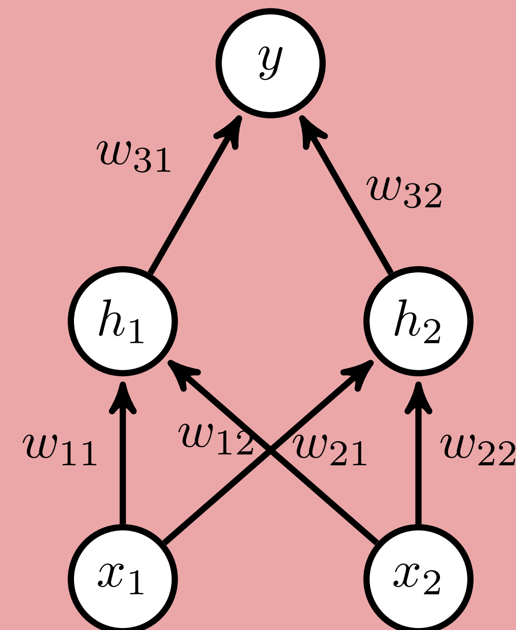


(b) The neural network architecture

Sample Questions

Neural Networks

Apply the backpropagation algorithm to obtain the partial derivative of the mean-squared error of y with the true value y^* with respect to the weight w_{22} assuming a sigmoid nonlinear activation function for the hidden layer.



(b) The neural network architecture

Sample Questions

1.2 Maximum Likelihood Estimation (MLE)

Assume we have a random sample that is Bernoulli distributed $X_1, \ldots, X_n \sim \text{Bernoulli}(\theta)$. We are going to derive the MLE for θ. Recall that a Bernoulli random variable X takes values in $\{0, 1\}$ and has probability mass function given by

$$P(X; \theta) = \theta^X (1 - \theta)^{1-X}.$$

(a) [2 pts.] Derive the likelihood, $L(\theta; X_1, \ldots, X_n)$.

(c) **Extra Credit:** [2 pts.] Derive the following formula for the MLE: $\hat{\theta} = \frac{1}{n} \left(\sum_{i=1}^{n} X_i\right)$.

Sample Questions

1.3 MAP vs MLE

Answer each question with **T** or **F** and **provide a one sentence explanation of your answer**:

(a) [2 pts.] **T or F:** In the limit, as n (the number of samples) increases, the MAP and MLE estimates become the same.

Sample Questions

1.1 Naive Bayes

You are given a data set of 10,000 students with their sex, height, and hair color. You are trying to build a classifier to predict the sex of a student, so you randomly split the data into a training set and a testing set. Here are the specifications of the data set:

- sex $\in$ {male,female}
- height $\in$ [0,300] centimeters
- hair $\in$ {brown, black, blond, red, green}
- 3240 men in the data set
- 6760 women in the data set

Under the assumptions necessary for Naive Bayes (not the distributional assumptions you might naturally or intuitively make about the dataset) answer each question with **T** or **F** and **provide a one sentence explanation of your answer**:

(a) [2 pts.] **T or F:** As height is a continuous valued variable, Naive Bayes is not appropriate since it cannot handle continuous valued variables.

(c) [2 pts.] **T or F:** $P(\texttt{height}|\texttt{sex}, \texttt{hair}) = P(\texttt{height}|\texttt{sex})$.

HIDDEN MARKOV MODEL (HMM)

HMM Outline

- **Motivation**
  - Time Series Data
- **Hidden Markov Model (HMM)**
  - Example: Squirrel Hill Tunnel Closures [courtesy of Roni Rosenfeld]
  - Background: Markov Models
  - From Mixture Model to HMM
  - History of HMMs
  - Higher-order HMMs
- **Training HMMs**
  - (Supervised) Likelihood for HMM
  - Maximum Likelihood Estimation (MLE) for HMM
  - EM for HMM (aka. Baum-Welch algorithm)
- **Forward-Backward Algorithm**
  - Three Inference Problems for HMM
  - Great Ideas in ML: Message Passing
  - Example: Forward-Backward on 3-word Sentence
  - Derivation of Forward Algorithm
  - Forward-Backward Algorithm
  - Viterbi algorithm

Markov Models

Whiteboard

- Example: Tunnel Closures
  [courtesy of Roni Rosenfeld]
- First-order Markov assumption
- Conditional independence assumptions


SQUIRREL HILL SOUTH
Taylor Allderdice High School
Map data ©2018 Google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Murray Ave
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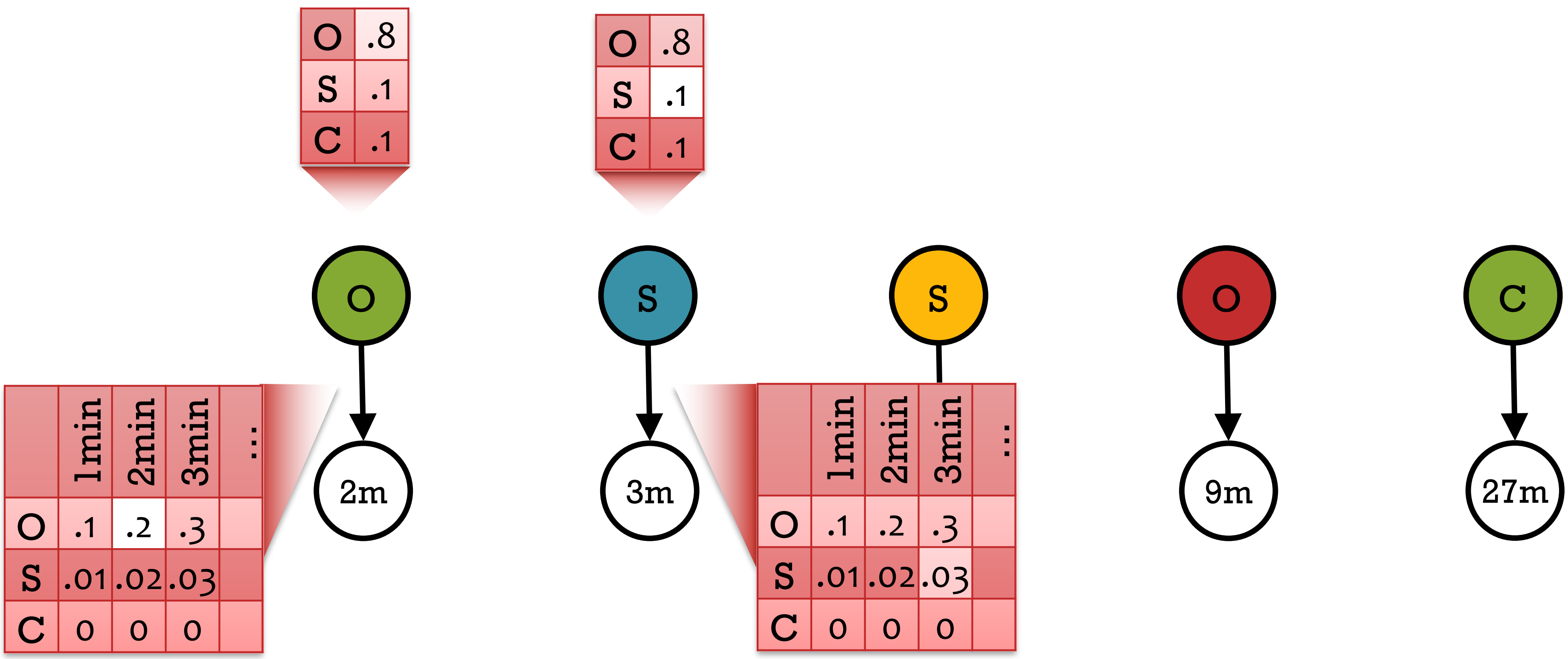
Mixture Model for Time Series Data

We could treat each (tunnel state, travel time) pair as independent. This corresponds to a Naïve Bayes model with a single feature (travel time).

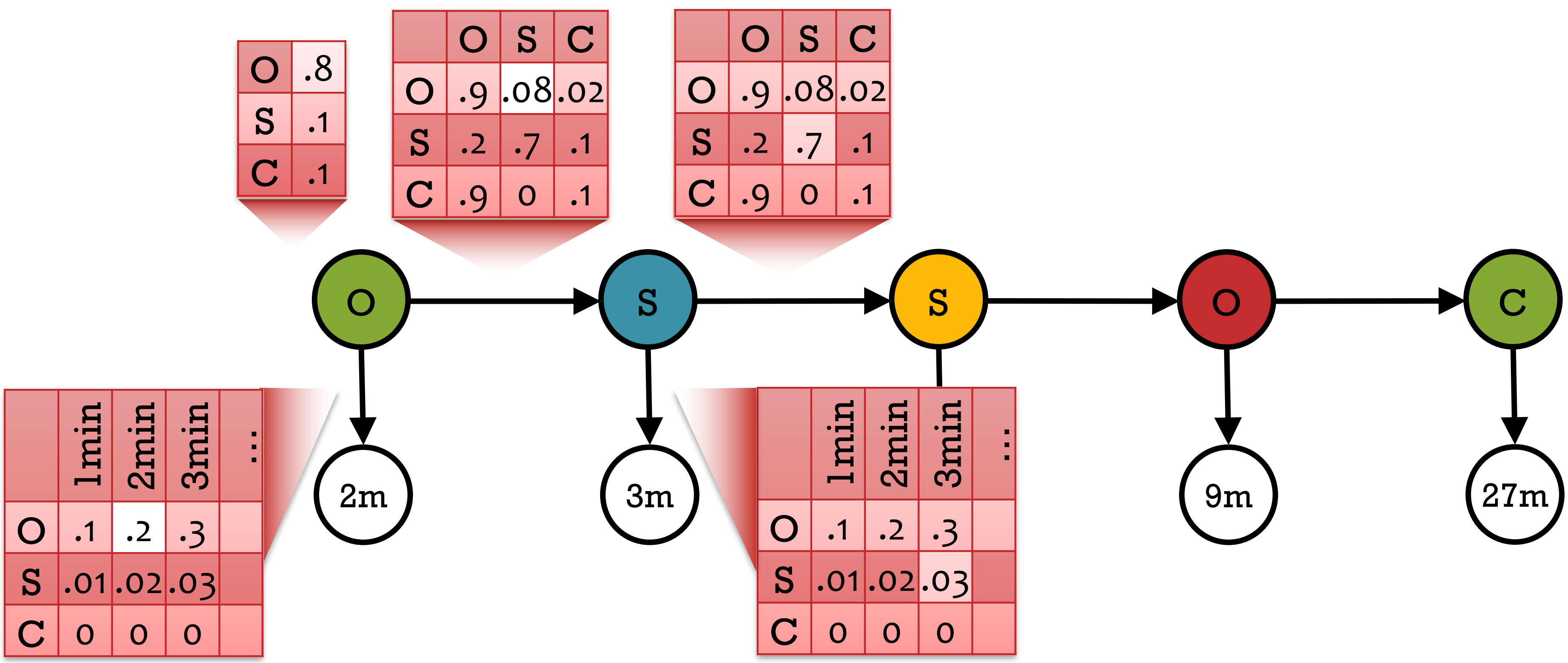
$$p(\text{O, S, S, O, C, 2m, 3m, 18m, 9m, 27m}) = (.8 * .2 * .1 * .03 * \ldots)$$



Hidden Markov Model

A Hidden Markov Model (HMM) provides a joint distribution over the the tunnel states / travel times with an assumption of dependence between adjacent tunnel states.

$$p(\text{O}, \text{S}, \text{S}, \text{O}, \text{C}, 2\text{m}, 3\text{m}, 18\text{m}, 9\text{m}, 27\text{m}) = (.8 * .08 * .2 * .7 * .03 * \ldots)$$



O	.8
S	.1
C	.1

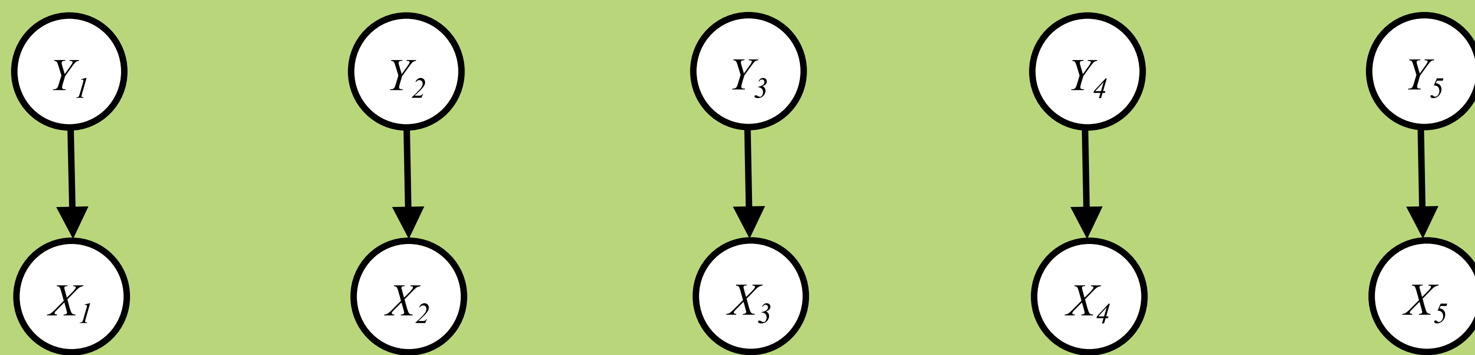
	O	S	C
O	.9	.08	.02
S	.2	.7	.1
C	.9	0	.1

	O	S	C
O	.9	.08	.02
S	.2	.7	.1
C	.9	0	.1

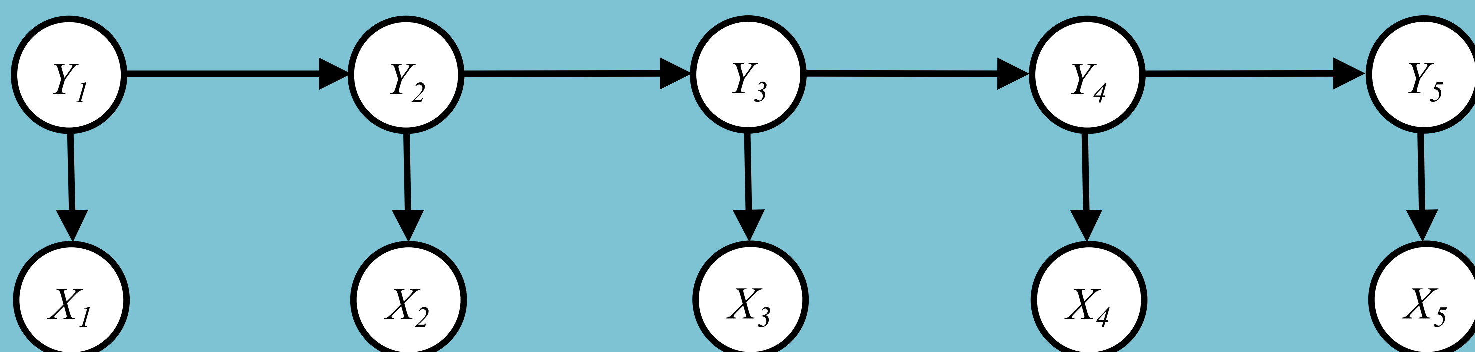
	1min	2min	3min	…
O	.1	.2	.3	
S	.01	.02	.03	
C	0	0	0	

	1min	2min	3min	…
O	.1	.2	.3	
S	.01	.02	.03	
C	0	0	0	

From Mixture Model to HMM

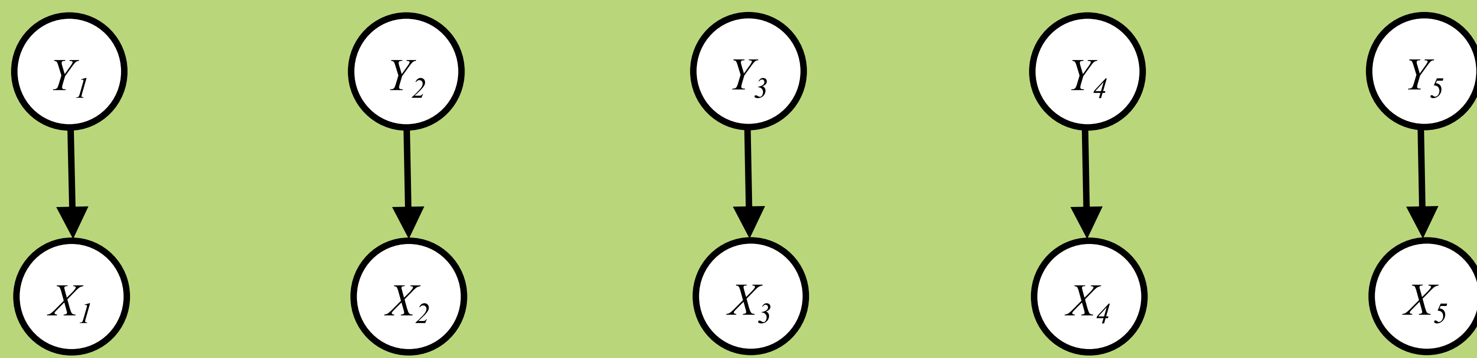


"Naïve Bayes": $$P(\mathbf{X}, \mathbf{Y}) = \prod_{t=1}^{T} P(X_t|Y_t)p(Y_t)$$

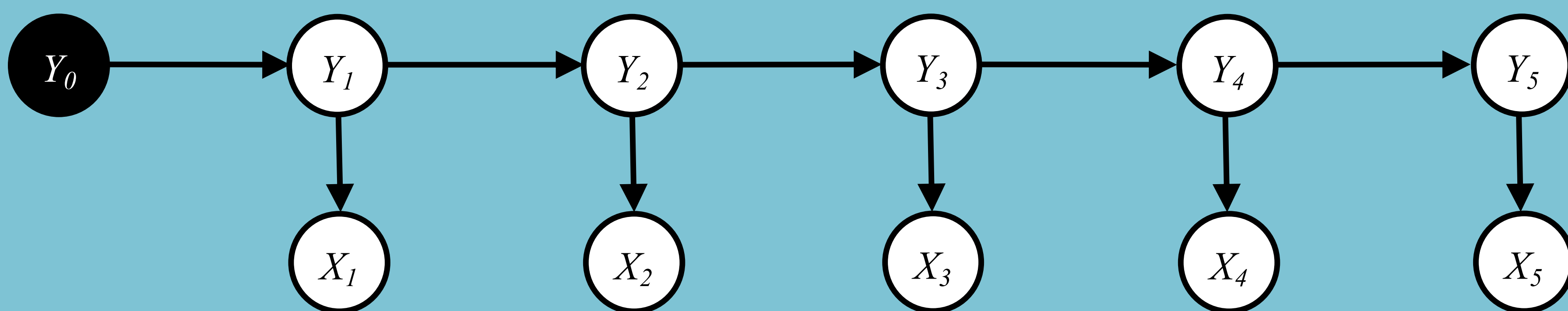


HMM: $$P(\mathbf{X}, \mathbf{Y}) = P(Y_1)\left(\prod_{t=1}^{T} P(X_t|Y_t)\right)\left(\prod_{t=2}^{T} p(Y_t|Y_{t-1})\right)$$

From Mixture Model to HMM



"Naïve Bayes": $$P(\mathbf{X}, \mathbf{Y}) = \prod_{t=1}^{T} P(X_t|Y_t)p(Y_t)$$



$$P(\mathbf{X}, \mathbf{Y}|Y_0) = \prod_{t=1}^{T} P(X_t|Y_t)p(Y_t|Y_{t-1})$$

HMM:

SUPERVISED LEARNING FOR HMMS

Recipe for Closed-form MLE

1. Assume data was generated i.i.d. from some model (i.e. write the generative story)

   $x^{(i)} \sim p(x|\boldsymbol{\theta})$

2. Write log-likelihood

   $\ell(\boldsymbol{\theta}) = \log p(x^{(1)}|\boldsymbol{\theta}) + \ldots + \log p(x^{(N)}|\boldsymbol{\theta})$

3. Compute partial derivatives (i.e. gradient)

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_1 = \ldots$

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_2 = \ldots$

   …

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_M = \ldots$

4. Set derivatives to zero and solve for $\boldsymbol{\theta}$

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_m = 0$ for all $m \in \{1, \ldots, M\}$

   $\boldsymbol{\theta}^{MLE}$ = solution to system of M equations and M variables

5. Compute the second derivative and check that $\ell(\boldsymbol{\theta})$ is concave down at $\boldsymbol{\theta}^{MLE}$

MLE of Categorical Distribution

1. Suppose we have a **dataset** obtained by repeatedly rolling a M-sided (weighted) die N times. That is, we have data

$$\mathcal{D} = \{x^{(i)}\}_{i=1}^{N}$$

where $x^{(i)} \in \{1, \ldots, M\}$ and $x^{(i)} \sim \text{Categorical}(\phi)$.

2. A random variable is **Categorical** written $X \sim \text{Categorical}(\phi)$ iff

$$P(X = x) = p(x; \phi) = \phi_x$$

where $x \in \{1, \ldots, M\}$ and $\sum_{m=1}^{M} \phi_m = 1$. The **log-likelihood** of the data becomes:

$$\ell(\phi) = \sum_{i=1}^{N} \log \phi_{x^{(i)}} \text{ s.t. } \sum_{m=1}^{M} \phi_m = 1$$

3. Solving this constrained optimization problem yields the **maximum likelihood estimator** (MLE):

$$\phi_m^{MLE} = \frac{N_{x=m}}{N} = \frac{\sum_{i=1}^{N} \mathbb{I}(x^{(i)} = m)}{N}$$

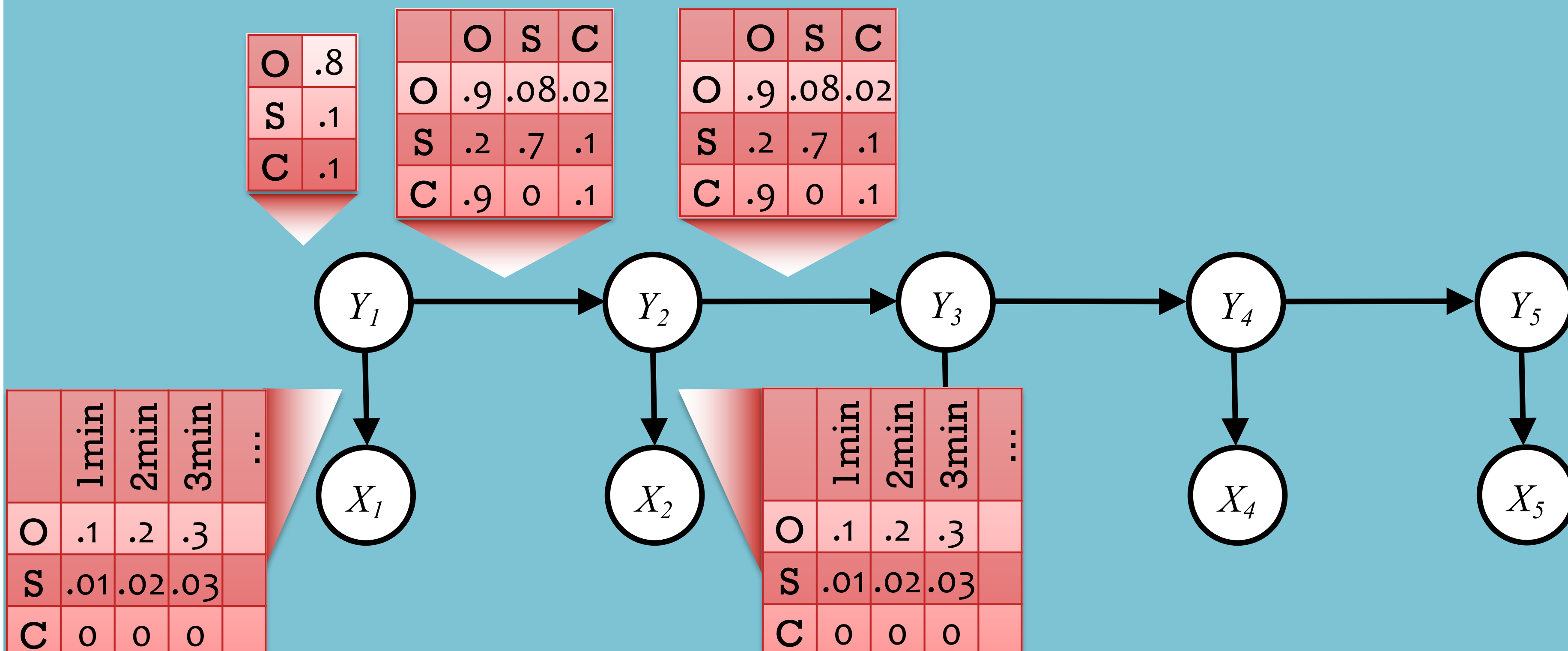
Hidden Markov Model

HMM Parameters:

Emission matrix, $\mathbf{A}$, where $P(X_t = k | Y_t = j) = A_{j,k}, \forall t, k$

Transition matrix, $\mathbf{B}$, where $P(Y_t = k | Y_{t-1} = j) = B_{j,k}, \forall t, k$

Initial probs, $\mathbf{C}$, where $P(Y_1 = k) = C_k, \forall k$



O	.8
S	.1
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	O	S	C
O	.9	.08	.02
S	.2	.7	.1
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	O	S	C
O	.9	.08	.02
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	1min	2min	3min	…
O	.1	.2	.3	
S	.01	.02	.03	
C	0	0	0	

	1min	2min	3min	…
O	.1	.2	.3	
S	.01	.02	.03	
C	0	0	0	

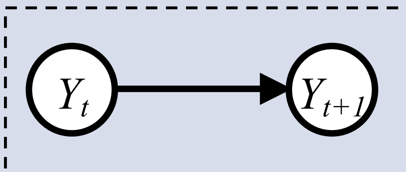
Training HMMs

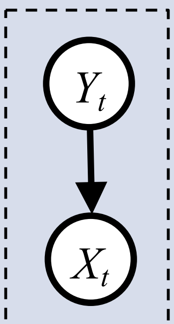
Whiteboard

- (Supervised) Likelihood for an HMM
- Maximum Likelihood Estimation (MLE) for HMM

Supervised Learning for HMMs

Learning an HMM decomposes into solving two (independent) Mixture Models





Data: $\mathcal{D} = \{(\vec{x}^{(i)}, \vec{y}^{(i)})\}_{i=1}^{N}$ $\quad \vec{x} = [x_1, \ldots, x_T]^T$, $\vec{y} = [y_1, \ldots, y_T]^T$

Likelihood:

$$\ell(A,B,C) = \sum_{i=1}^{N} \log p(\vec{x}^{(i)}, y^{(i)} \mid A,B,C)$$

$$= \sum_{i=1}^{N} \Big[\underbrace{\log p(y_1^{(i)} \mid C)}_{\text{initial}} + \underbrace{\Big(\sum_{t=2}^{T} \log p(y_t^{(i)} \mid y_{t-1}^{(i)}, B)\Big)}_{\text{transition}} + \underbrace{\Big(\sum_{t=1}^{T} \log p(x_t^{(i)} \mid y_t^{(i)}, A)\Big)}_{\text{emission}} \Big]$$

MLE:

$$\hat{A}, \hat{B}, \hat{C} = \operatorname*{argmax}_{A,B,C} \ell(A,B,C)$$

$$\Rightarrow \hat{C} = \operatorname*{argmax}_{C} \sum_{i=1}^{N} \log p(y_1^{(i)} \mid C)$$

$$\hat{B} = \operatorname*{argmax}_{B} \sum_{i=1}^{N} \sum_{t=2}^{T} \log p(y_t^{(i)} \mid y_{t-1}^{(i)}, B)$$

$$\hat{A} = \operatorname*{argmax}_{A} \sum_{i=1}^{N} \sum_{t=1}^{T} \log p(x_t^{(i)} \mid y_t^{(i)}, A)$$

Can solve in closed form, which yields...

$$\hat{C}_k = \frac{\#(y_1^{(i)} = k)}{N} \quad \forall i,k$$

$$\hat{B}_{jk} = \frac{\#(y_t^{(i)} = k \text{ and } y_{t-1}^{(i)} = j)}{\#(y_{t-1}^{(i)} = j)} \quad \forall i, t>1, j, k$$

$$\hat{A}_{jk} = \frac{\#(x_t^{(i)} = k \text{ and } y_t^{(i)} = j)}{\#(y_t^{(i)} = j)} \quad \forall i,t,j,k$$

Hidden Markov Model

HMM Parameters:

Emission matrix, $\mathbf{A}$, where $P(X_t = k | Y_t = j) = A_{j,k}, \forall t, k$

Transition matrix, $\mathbf{B}$, where $P(Y_t = k | Y_{t-1} = j) = B_{j,k}, \forall t, k$

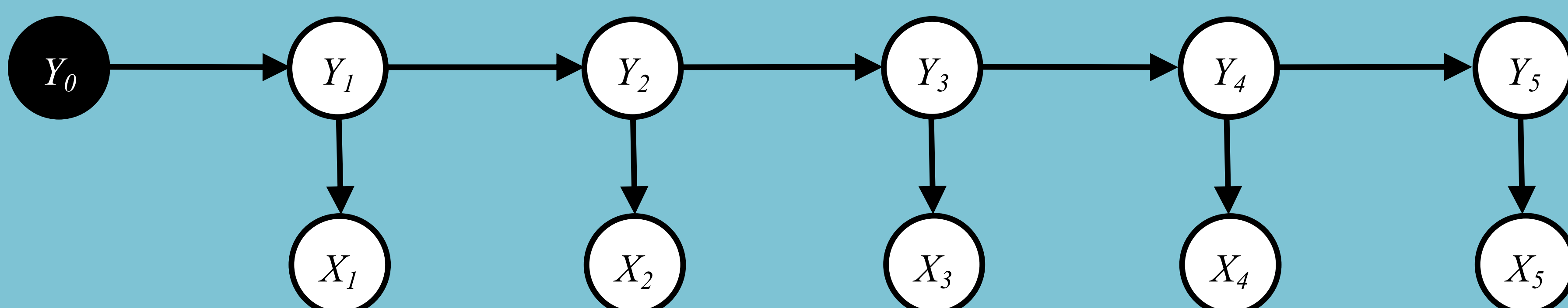
Assumption: $y_0 =$ START

Generative Story:

$$Y_t \sim \text{Multinomial}(\mathbf{B}_{Y_{t-1}}) \ \forall t$$

$$X_t \sim \text{Multinomial}(\mathbf{A}_{Y_t}) \ \forall t$$

For notational convenience, we fold the *initial probabilities* **C** into the *transition matrix* **B** by our assumption.



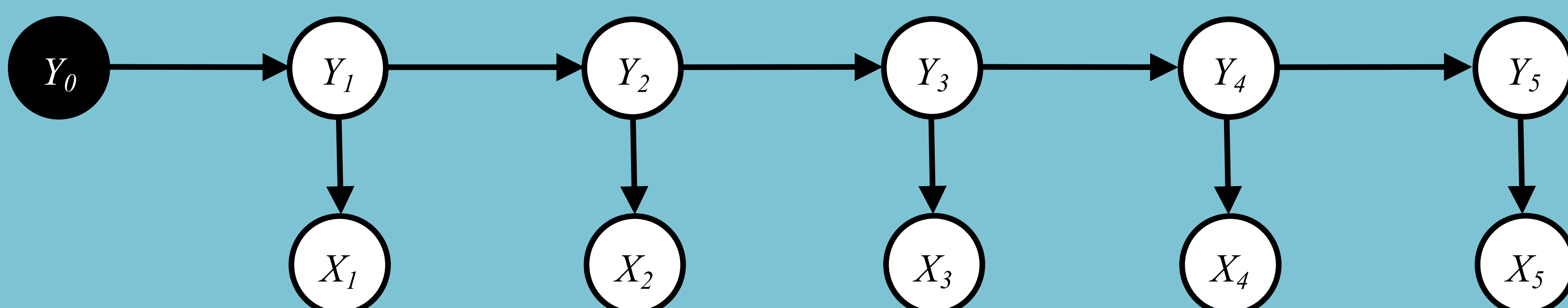
Hidden Markov Model

Joint Distribution:

$$y_0 = \text{START}$$

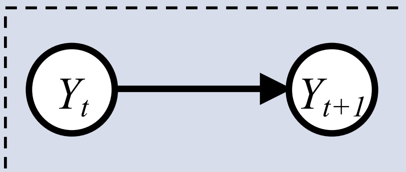
$$p(\mathbf{x}, \mathbf{y} | y_0) = \prod_{t=1}^{T} p(x_t | y_t) p(y_t | y_{t-1})$$

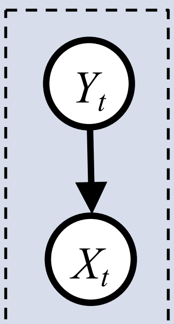
$$= \prod_{t=1}^{T} A_{y_t, x_t} B_{y_{t-1}, y_t}$$



Supervised Learning for HMMs

Learning an HMM decomposes into solving two (independent) Mixture Models





$$\mathcal{D} = \{(\vec{x}^{(i)}, \vec{y}^{(i)})\}_{i=1}^{N}$$

Likelihood:

$$\ell(A,B) = \sum_{i=1}^{N} \log p(\vec{x}^{(i)}, \vec{y}^{(i)})$$

$$= \sum_{i=1}^{N} \left[\sum_{t=1}^{T} \log p(y_t^{(i)} \mid y_{t-1}^{(i)}, B) + \log p(x_t^{(i)} \mid y_t^{(i)}, A) \right]$$

MLE:

$$\hat{A}, \hat{B} = \operatorname{argmax} \ell(A,B)$$

$$\hat{A} = \operatorname{argmax} \sum_{i=1}^{N} \left[\sum_{t=1}^{T} \log p(x_t^{(i)} \mid y_t^{(i)}, A) \right]$$

$$\hat{B} = \operatorname{argmax} \sum_{i=1}^{N} \left[\sum_{t=1}^{T} \log p(y_t^{(i)} \mid y_{t-1}^{(i)}, B) \right]$$

↑ can solve in closed form to get...

$$\hat{B}_{jk} = \frac{\#(y_t^{(i)} = k \text{ and } y_{t-1}^{(i)} = j)}{\#(y_{t-1}^{(i)} = j)}$$

$$\hat{A}_{jk} = \frac{\#(x_t^{(i)} = k \text{ and } y_t^{(i)} = j)}{\#(y_t^{(i)} = j)}$$

Unsupervised Learning for HMMs

- Unlike **discriminative** models p(y|x), **generative** models p(x,y) can maximize the likelihood of the data D = $\{x^{(1)}, x^{(2)}, \ldots, x^{(N)}\}$ where we don't observe any y's.
- This **unsupervised learning** setting can be achieved by finding parameters that maximize the **marginal likelihood**
- We optimize using the **Expectation-Maximization** algorithm

Since we don't observe y, we define the marginal probability:

$$p_{\theta}(\mathbf{x}) = \sum_{\mathbf{y} \in \mathcal{Y}} p_{\theta}(\mathbf{x}, \mathbf{y}) \quad (1)$$

The log-likelihood of the data is thus:

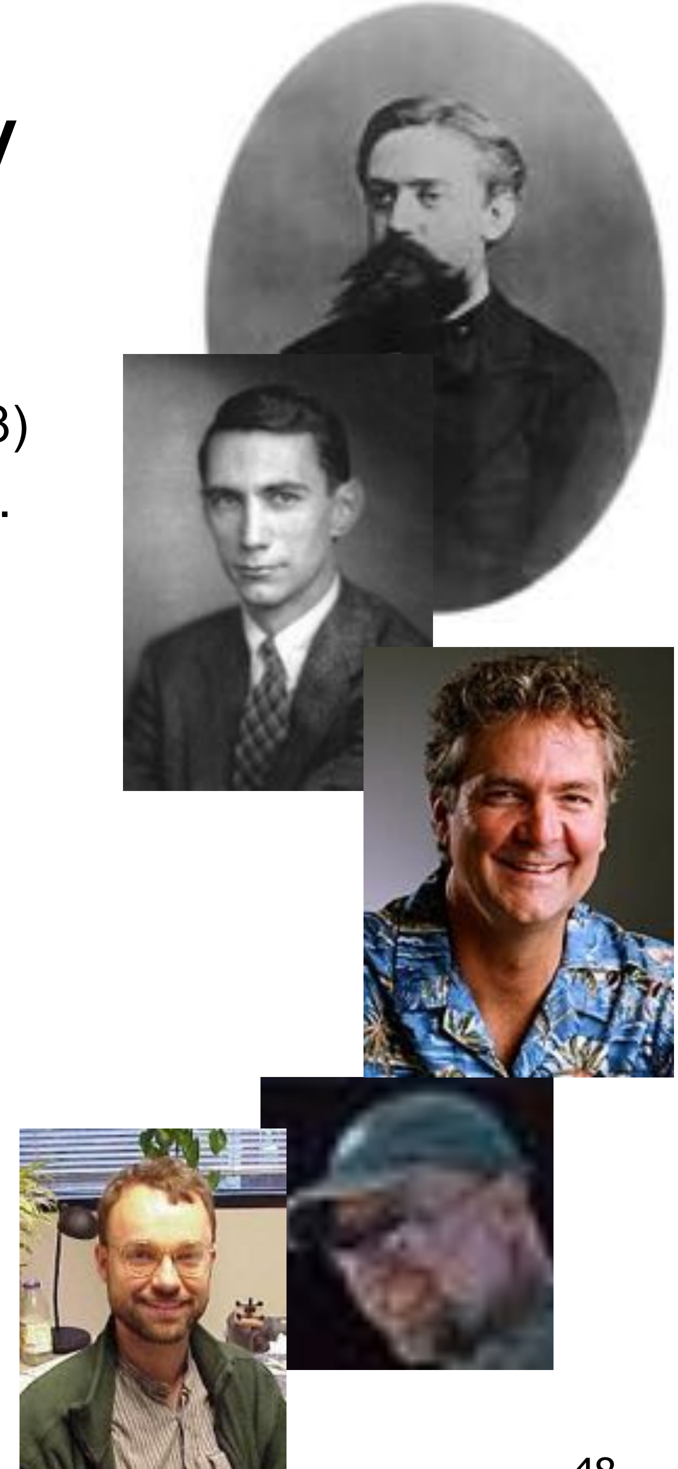
$$\ell(\theta) = \log \prod_{i=1}^{N} p_{\theta}(\mathbf{x}^{(i)})$$

$$= \sum_{i=1}^{N} \log \sum_{\mathbf{y} \in \mathcal{Y}} p_{\theta}(\mathbf{x}^{(i)}, \mathbf{y}) \quad (3)$$

Beyond the scope of today's lecture!

HMMs: History

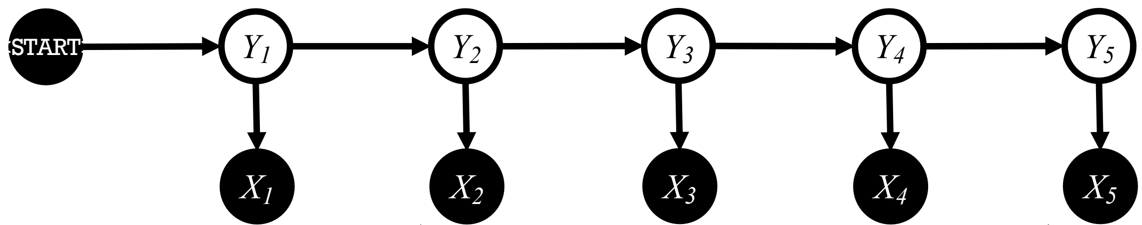
- Markov chains: Andrey Markov (1906)
  - Random walks and Brownian motion
- Used in Shannon's work on information theory (1948)
- Baum-Welsh learning algorithm: late 60's, early 70's.
  - Used mainly for speech in 60s-70s.
- Late 80's and 90's: David Haussler (major player in learning theory in 80's) began to use HMMs for modeling biological sequences
- Mid-late 1990's: Dayne Freitag/Andrew McCallum
  - Freitag thesis with Tom Mitchell on IE from Web using logic programs, grammar induction, etc.
  - McCallum: multinomial Naïve Bayes for text
  - With McCallum, IE using HMMs on CORA
- …



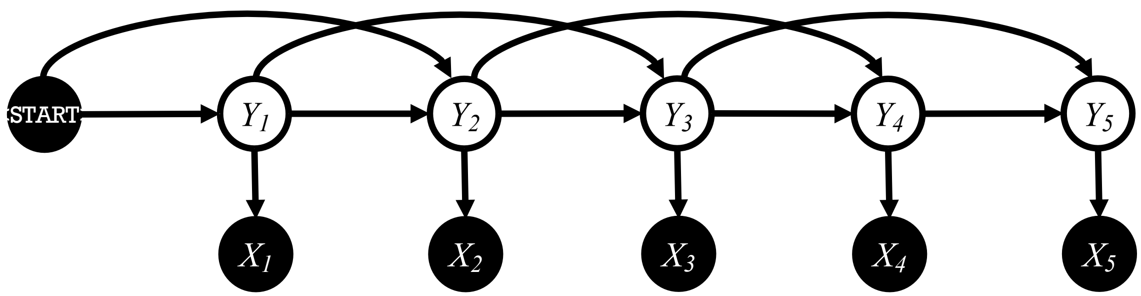
Slide from William Cohen

Higher-order HMMs

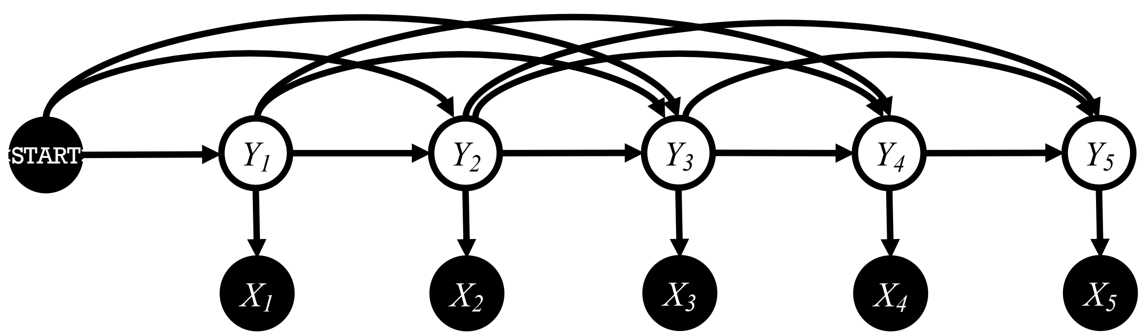
- 1st-order HMM (i.e. bigram HMM)



- 2nd-order HMM (i.e. trigram HMM)

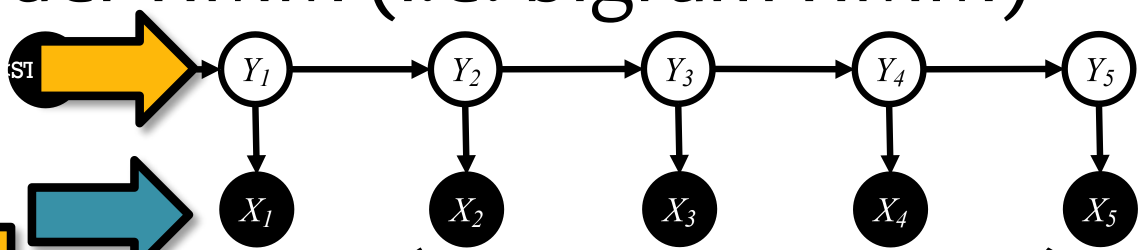


- 3rd-order HMM

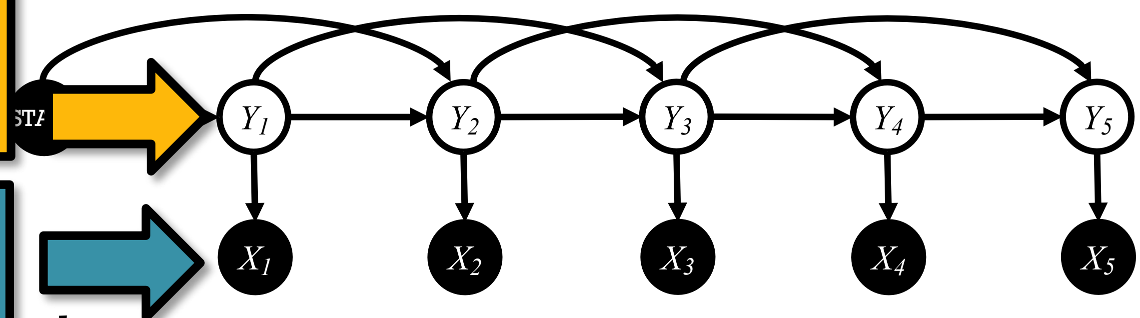


Higher-order HMMs

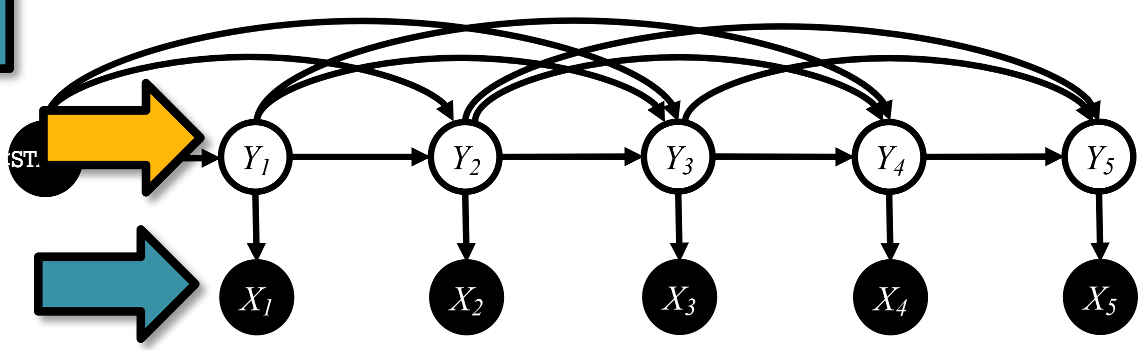
- 1^{st}-order HMM (i.e. bigram HMM)



- rder HMM (i.e. trigram HMM)



- rder HMM



Hidden States, **y**

Observa -tions, **x**