Naïve Bayes

CS 760@UW-Madison

Goals for the lecture

- understand the concepts
  - generative/discriminative models
  - MLE (Maximum Likelihood Estimate) and MAP (Maximum A Posteriori)

  - Naïve Bayes
    - Naïve Bayes assumption
    - Generic Naïve Bayes
    - model 1: Bernoulli Naïve Bayes

  - Other Naïve Bayes
    - model 2: Multinomial Naïve Bayes
    - model 3: Gaussian Naïve Bayes
    - model 4: Multiclass Naïve Bayes

Review: supervised learning

problem setting

- set of possible instances (feature space): X
- unknown *target function* (concept): $f : X \rightarrow Y$
- set of *hypotheses* (hypothesis class): $H = \{ h \mid h : X \rightarrow Y \}$

given

- *training set* of instances of unknown target function f

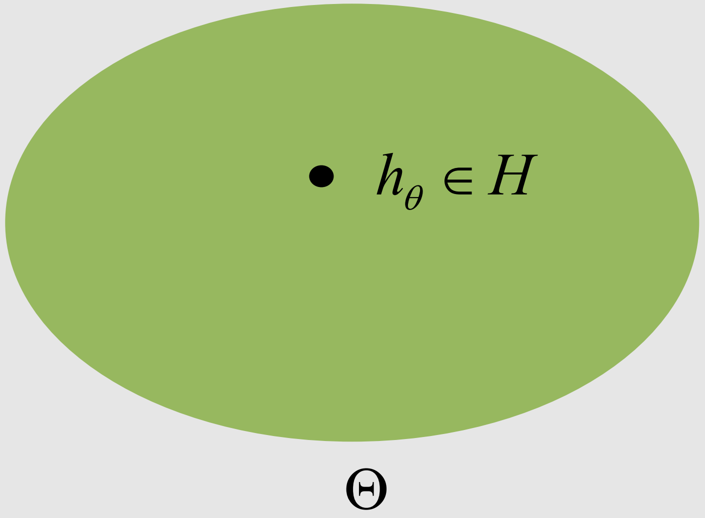
$$\left(\mathbf{x}^{(1)}, y^{(1)}\right), \left(\mathbf{x}^{(2)}, y^{(2)}\right) \ldots \left(\mathbf{x}^{(m)}, y^{(m)}\right)$$

output

- hypothesis $h \in H$ that best approximates target function

Parametric hypothesis class

- hypothesis $h \in H$ is indexed by parameter $\theta \in \Theta$
- learning: find the θ such that $h_\theta \in H$ best approximate the target



- different from "nonparametric" approaches like decision trees and nearest neighbor
- advantages: various hypothesis class encoding inductive bias/prior knowledge; easy to use math/optimization

Discriminative approaches

- hypothesis $h \in H$ directly predicts the label given the features

$$y = h(x) \text{ or more generally, } p(y \mid x) = h(x)$$

- then define a loss function $L(h)$ and find hypothesis with min. loss

- example: linear regression

$$h_\theta(x) = \langle x, \theta \rangle$$

$$L(h_\theta) = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Generative approaches

- hypothesis $h \in H$ specifies a **generative story** for how the data was created

$h(x, y) = p(x, y)$ or simply $h(x) = p(x)$

- then pick a hypothesis by maximum likelihood estimation (MLE) or Maximum A Posteriori (MAP)

- example: roll a weighted die
- weights for each side (θ) define how the data are generated
- use MLE on the training data to learn θ

Comments on discriminative/generative

- usually for supervised learning, parametric hypothesis class
- can also for unsupervised learning
  - k-means clustering (discriminative flavor) vs Mixture of Gaussians (generative)
- can also for nonparametric
  - nonparametric Bayesian: a large subfield of ML

- when discriminative/generative is likely to be better? Discussed in later lecture

- typical discriminative: linear regression, logistic regression, SVM, many neural networks (not all!), …
- typical generative: Naïve Bayes, Bayesian Networks, …

MLE and MAP

MLE vs. MAP

Suppose we have data $\mathcal{D} = \{x^{(i)}\}_{i=1}^{N}$

$$\boldsymbol{\theta}^{\text{MLE}} = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{N} p(\mathbf{x}^{(i)} | \boldsymbol{\theta})$$

Maximum Likelihood Estimate (MLE)

Background: MLE

Example: MLE of Exponential Distribution

- pdf of Exponential(λ): $f(x) = \lambda e^{-\lambda x}$
- Suppose $X_i \sim$ Exponential(λ) for $1 \leq i \leq N$.
- Find MLE for data $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$
- First write down log-likelihood of sample.
- Compute first derivative, set to zero, solve for λ.
- Compute second derivative and check that it is concave down at λ^{MLE}.

Background: MLE

Example: MLE of Exponential Distribution

- First write down log-likelihood of sample.

$$
\begin{aligned}
\ell(\lambda) &= \sum_{i=1}^{N} \log f(x^{(i)}) && (1)\\
&= \sum_{i=1}^{N} \log(\lambda \exp(-\lambda x^{(i)})) && (2)\\
&= \sum_{i=1}^{N} \log(\lambda) + -\lambda x^{(i)} && (3)\\
&= N \log(\lambda) - \lambda \sum_{i=1}^{N} x^{(i)} && (4)
\end{aligned}
$$

Background: MLE

Example: MLE of Exponential Distribution

- Compute first derivative, set to zero, solve for λ.

$$\frac{d\ell(\lambda)}{d\lambda} = \frac{d}{d\lambda} N \log(\lambda) - \lambda \sum_{i=1}^{N} x^{(i)} \tag{1}$$

$$= \frac{N}{\lambda} - \sum_{i=1}^{N} x^{(i)} = 0 \tag{2}$$

$$\boxed{\Rightarrow \lambda^{\text{MLE}} = \frac{N}{\sum_{i=1}^{N} x^{(i)}}} \tag{3}$$

MLE vs. MAP

Suppose we have data $\mathcal{D} = \{x^{(i)}\}_{i=1}^{N}$

$$\boldsymbol{\theta}^{\text{MLE}} = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{N} p(\mathbf{x}^{(i)} | \boldsymbol{\theta})$$

Maximum Likelihood Estimate (MLE)

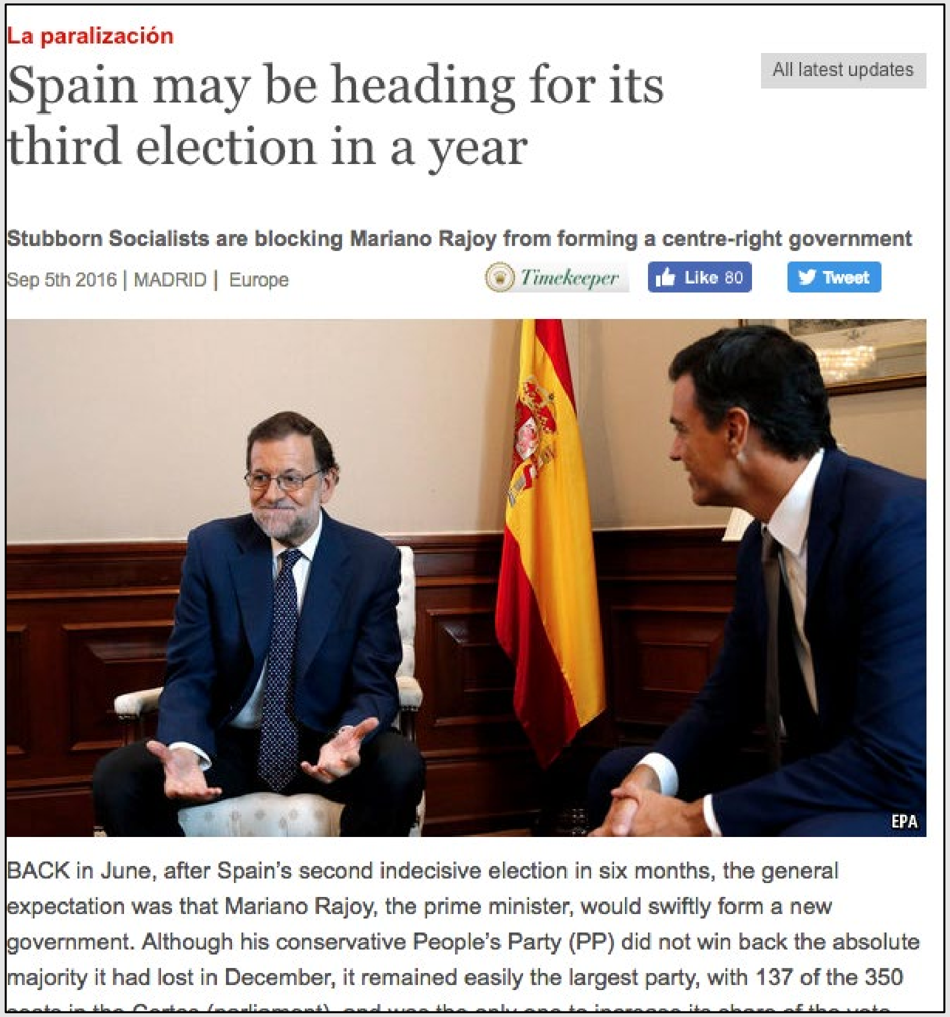
$$\boldsymbol{\theta}^{\text{MAP}} = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{N} p(\mathbf{x}^{(i)} | \boldsymbol{\theta}) \underbrace{p(\boldsymbol{\theta})}_{\text{Prior}}$$

Maximum *a posteriori* (MAP) estimate

Naïve Bayes

Spam News

The Economist



La paralización

All latest updates

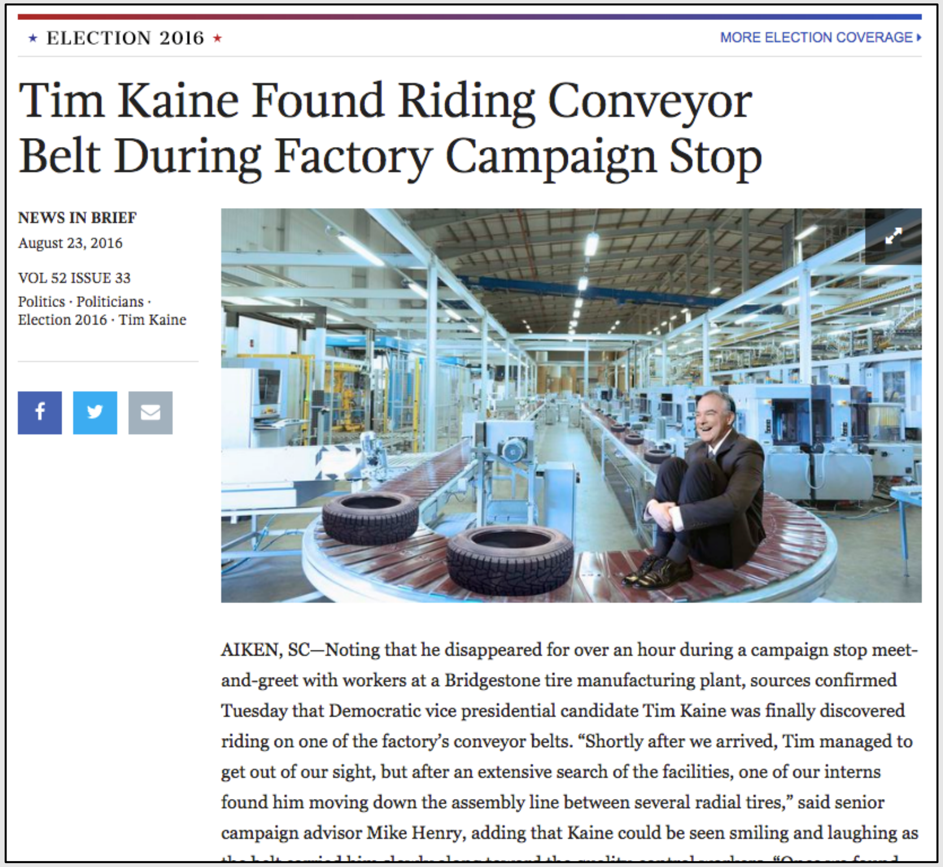
Spain may be heading for its third election in a year

Stubborn Socialists are blocking Mariano Rajoy from forming a centre-right government

Sep 5th 2016 | MADRID | Europe

BACK in June, after Spain's second indecisive election in six months, the general expectation was that Mariano Rajoy, the prime minister, would swiftly form a new government. Although his conservative People's Party (PP) did not win back the absolute majority it had lost in December, it remained easily the largest party, with 137 of the 350

The Onion



★ ELECTION 2016 ★

MORE ELECTION COVERAGE ▸

Tim Kaine Found Riding Conveyor Belt During Factory Campaign Stop

NEWS IN BRIEF

August 23, 2016

VOL 52 ISSUE 33

Politics · Politicians · Election 2016 · Tim Kaine

AIKEN, SC—Noting that he disappeared for over an hour during a campaign stop meet-and-greet with workers at a Bridgestone tire manufacturing plant, sources confirmed Tuesday that Democratic vice presidential candidate Tim Kaine was finally discovered riding on one of the factory's conveyor belts. "Shortly after we arrived, Tim managed to get out of our sight, but after an extensive search of the facilities, one of our interns found him moving down the assembly line between several radial tires," said senior campaign advisor Mike Henry, adding that Kaine could be seen smiling and laughing as

Model 0: Not-so-naïve Model?

Generative Story:

1. Flip a weighted coin (Y)
2. If heads, sample a document ID (X) from the Spam distribution
3. If tails, sample a document ID (X) from the Not-Spam distribution

$$P(X, Y) = P(X|Y)P(Y)$$

Model 0: Not-so-naïve Model?

Generative Story:

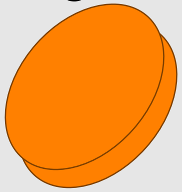
1. Flip a weighted coin (Y)
2. If heads, roll the **yellow** many sided die to sample a document vector (X) from the Spam distribution
3. If tails, roll the **blue** many sided die to sample a document vector (X) from the Not-Spam distribution

$$P(X_1, \ldots, X_K, Y) = P(X_1, \ldots, X_K | Y) P(Y)$$

This model is computationally naïve!

Model 0: Not-so-naïve Model?

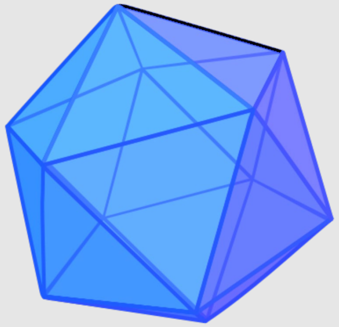
Flip weighted coin



If HEADS, roll yellow die

y	x_1	x_2	x_3	…	x_K
0	1	0	1	…	1
1	0	1	0	…	1
1	1	1	1	…	1
0	0	0	1	…	1
0	1	0	1	…	0
1	1	0	1	…	0

If TAILS, roll blue die



Each side of the die is labeled with a document vector (e.g. [1,0,1,…,1])

Naïve Bayes Assumption

Conditional independence of features:

$$
\begin{aligned}
P(X_1, \ldots, X_K, Y) &= P(X_1, \ldots, X_K | Y) P(Y) \\
&= \left(\prod_{k=1}^{K} P(X_k | Y) \right) P(Y)
\end{aligned}
$$

Estimating a joint from conditional probabilities

C	P(C)
0	0.33
1	0.67

$$P(A,B|C) = P(A|C) * P(B|C)$$

$$\forall a,bc : P(A=a \wedge B=b|C=c) = P(A=a|C=c) * P(B=b|C=c)$$

A	C	P(A|C)
0	0	0.2
0	1	0.5
1	0	0.8
1	1	0.5

B	C	P(B|C)
0	0	0.1
0	1	0.9
1	0	0.9
1	1	0.1

A	B	C	P(A,B,C)
0	0	0	…
0	0	1	…
0	1	0	…
0	1	1	
1	0	0	
1	0	1	
1	1	0	
1	1	1	

Estimating a joint from conditional probabilities

C	P(C)
0	0.33
1	0.67

A	C	P(A|C)
0	0	0.2
0	1	0.5
1	0	0.8
1	1	0.5

B	C	P(B|C)
0	0	0.1
0	1	0.9
1	0	0.9
1	1	0.1

D	C	P(D|C)
0	0	0.1
0	1	0.1
1	0	0.9
1	1	0.1

A	B	D	C	P(A,B,D,C)
0	0	0	0	…
0	0	1	0	…
0	1	0	0	…
0	1	1	0	
1	0	0	0	
1	0	1	0	
1	1	0	0	
1	1	1	0	
0	0	0	1	
0	0	1	0	
…	…	..	…	…

Estimating a joint from conditional probabilities

Assuming conditional independence, the conditional probabilities encode the **same information** as the joint table.

They are very convenient for estimating
$P(X_1,\ldots,X_n|Y)=P(X_1|Y)*\ldots*P(X_n|Y)$

They are almost as good for computing

$$P(Y|X_1,\ldots,X_n)=\frac{P(X_1,\ldots,X_n|Y)P(Y)}{P(X_1,\ldots,X_n)}$$

$$\forall \mathbf{x},y: P(Y=y|X_1,\ldots,X_n=\mathbf{x})=\frac{P(X_1,\ldots,X_n=\mathbf{x}|Y)P(Y=y)}{P(X_1,\ldots,X_n=\mathbf{x})}$$

Generic Naïve Bayes Model

Support: Depends on the choice of **event model,** $P(X_k|Y)$

Model: Product of **prior** and the event model

$$P(\mathbf{X}, Y) = P(Y) \prod_{k=1}^{K} P(X_k|Y)$$

Training: Find the **class-conditional** MLE parameters

For $P(Y)$, we find the MLE using the data. For each $P(X_k|Y)$ we condition on the data with the corresponding class.

Classification: Find the class that maximizes the posterior

$$\hat{y} = \underset{y}{\operatorname{argmax}}\, p(y|\mathbf{x})$$

Generic Naïve Bayes Model

Classification:

$$\hat{y} = \operatorname*{argmax}_y p(y|\mathbf{x}) \quad \text{(posterior)}$$

$$= \operatorname*{argmax}_y \frac{p(\mathbf{x}|y)p(y)}{p(x)} \quad \text{(by Bayes' rule)}$$

$$= \operatorname*{argmax}_y p(\mathbf{x}|y)p(y)$$

Various Naïve Bayes Models

Model 1: Bernoulli Naïve Bayes

Support: Binary vectors of length K

$$\mathbf{x} \in \{0,1\}^K$$

Generative Story:

$$Y \sim \text{Bernoulli}(\phi)$$

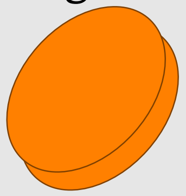
$$X_k \sim \text{Bernoulli}(\theta_{k,Y}) \ \forall k \in \{1, \ldots, K\}$$

Model:

$$\begin{aligned} p_{\phi,\boldsymbol{\theta}}(\boldsymbol{x}, y) &= p_{\phi,\boldsymbol{\theta}}(x_1, \ldots, x_K, y) \\ &= p_\phi(y) \prod_{k=1}^{K} p_{\boldsymbol{\theta}_k}(x_k|y) \\ &= (\phi)^y (1-\phi)^{(1-y)} \prod_{k=1}^{K} (\theta_{k,y})^{x_k} (1-\theta_{k,y})^{(1-x_k)} \end{aligned}$$

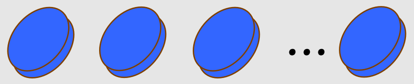
Model 1: Bernoulli Naïve Bayes

Flip weighted coin



If HEADS, flip each yellow coin

If TAILS, flip each blue coin



y	x_1	x_2	x_3	…	x_K
0	1	0	1	…	1
1	0	1	0	…	1
1	1	1	1	…	1
0	0	0	1	…	1
0	1	0	1	…	0
1	1	0	1	…	0

We can **generate** data in this fashion. Though in practice we never would since our data is **given.**

Instead, this provides an explanation of **how** the data was generated (albeit a terrible one).

Each red coin corresponds to an x_k

Model 1: Bernoulli Naïve Bayes

Support: Binary vectors of length K

$$\mathbf{x} \in \{0,1\}^K$$

Generative Story:

$$Y \sim \text{Bernoulli}(\phi)$$

$$X_k \sim \text{Bernoulli}(\theta_{k,Y}) \ \forall k \in \{1, \ldots, K\}$$

Model: $p_{\phi,\boldsymbol{\theta}}(\boldsymbol{x}, y) = (\phi)^y (1-\phi)^{(1-y)} \prod_{=1}$

Same as Generic Naïve Bayes

Classification: Find the class that maximizes the posterior

$$\hat{y} = \underset{y}{\operatorname{argmax}}\, p(y|\mathbf{x})$$

Generic Naïve Bayes Model

Recall...

Classification:

$$\hat{y} = \operatorname*{argmax}_y p(y|\mathbf{x}) \quad \text{(posterior)}$$

$$= \operatorname*{argmax}_y \frac{p(\mathbf{x}|y)p(y)}{p(x)} \quad \text{(by Bayes' rule)}$$

$$= \operatorname*{argmax}_y p(\mathbf{x}|y)p(y)$$

Model 1: Bernoulli Naïve Bayes

Training: Find the **class-conditional** MLE parameters

For *P(Y)*, we find the MLE using all the data. For each *P(X$_k$|Y)* we condition on the data with the corresponding class.

$$\phi = \frac{\sum_{i=1}^N \mathbb{I}(y^{(i)} = 1)}{N}$$

$$\theta_{k,0} = \frac{\sum_{i=1}^N \mathbb{I}(y^{(i)} = 0 \wedge x_k^{(i)} = 1)}{\sum_{i=1}^N \mathbb{I}(y^{(i)} = 0)}$$

$$\theta_{k,1} = \frac{\sum_{i=1}^N \mathbb{I}(y^{(i)} = 1 \wedge x_k^{(i)} = 1)}{\sum_{i=1}^N \mathbb{I}(y^{(i)} = 1)}$$

$$\forall k \in \{1, \ldots, K\}$$

Model 2: Multinomial Naïve Bayes

Support: Integer vector (word IDs)

$\mathbf{x} = [x_1, x_2, \ldots, x_M]$ where $x_m \in \{1, \ldots, K\}$ a word id.

Generative Story:

```
for $i \in \{1, \ldots, N\}$:
    $y^{(i)} \sim \text{Bernoulli}(\phi)$
    for $j \in \{1, \ldots, M_i\}$:        (Assume $M_i = M$ for all $i$)
        $x_j^{(i)} \sim \text{Multinomial}(\boldsymbol{\theta}_{y^{(i)}}, 1)$
```

Model:

$$p_{\phi,\boldsymbol{\theta}}(\boldsymbol{x}, y) = p_\phi(y) \prod_{k=1}^{K} p_{\boldsymbol{\theta}_k}(x_k|y)$$

$$= (\phi)^y (1-\phi)^{(1-y)} \prod_{j=1}^{M_i} \theta_{y,x_j}$$

Model 3: Gaussian Naïve Bayes

Support: $\mathbf{x} \in \mathbb{R}^K$

Model: Product of **prior** and the event model

$$p(\boldsymbol{x}, y) = p(x_1, \ldots, x_K, y)$$

$$= p(y) \prod_{k=1}^{K} p(x_k | y)$$

Gaussian Naive Bayes assumes that $p(x_k|y)$ is given by a Normal distribution.

Model 4: Multiclass Naïve Bayes

Model:

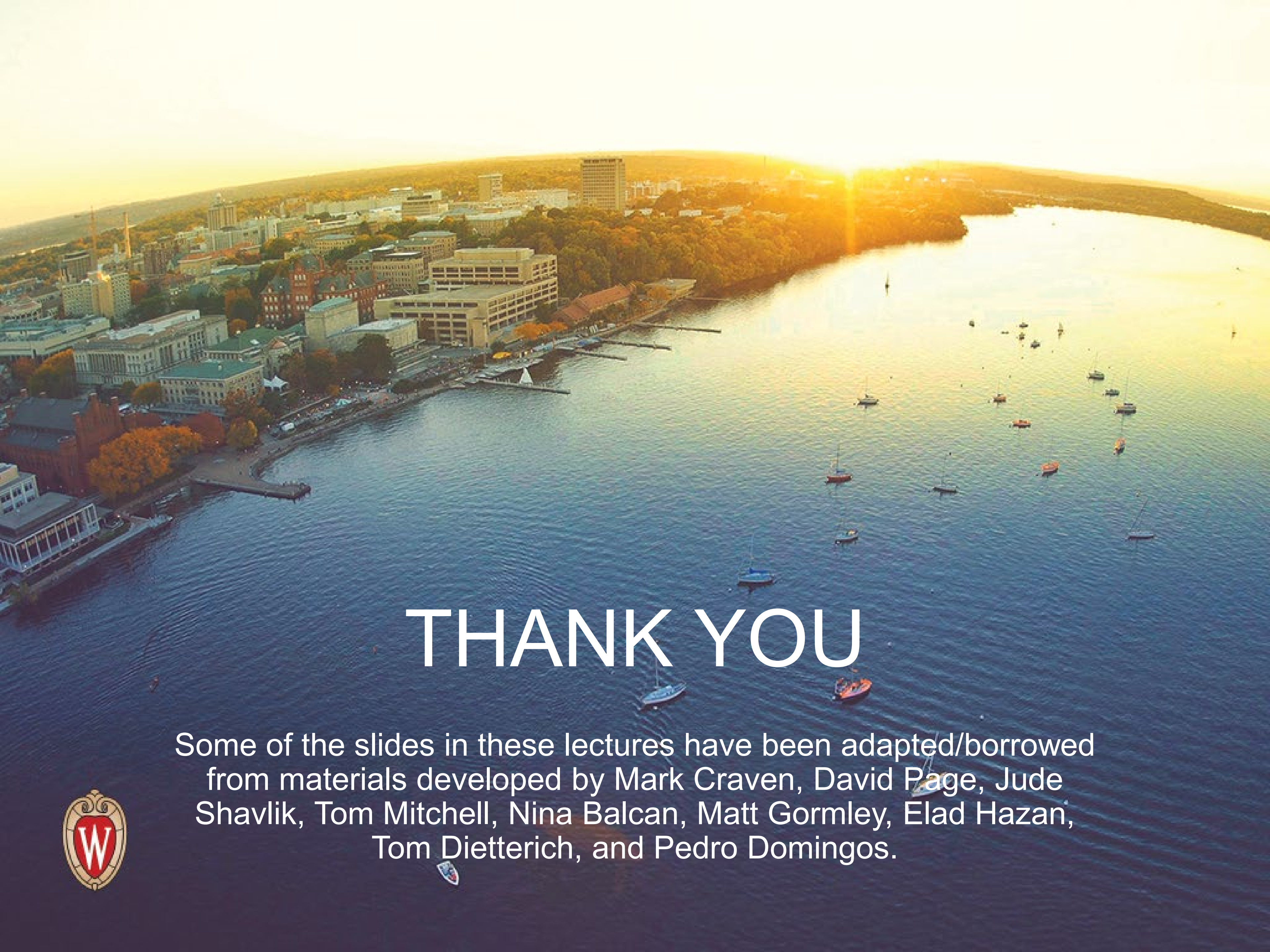
The only change is that we permit y to range over C classes.

$$p(\boldsymbol{x}, y) = p(x_1, \ldots, x_K, y)$$
$$= p(y) \prod_{k=1}^{K} p(x_k | y)$$

Now, $y \sim$ Multinomial$(\phi, 1)$ and we have a separate conditional distribution $p(x_k|y)$ for each of the C classes.

Summary: Generative Approach

- Step 1: specify the joint data distribution (generative story)
- Step 2: use MLE or MAP for training
- Step 3: use Bayes' rule for inference on test instances



THANK YOU

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