Naïve Bayes

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Goals for the lecture

• understand the concepts
  • generative/discriminative models
  • examples of the two approaches
  • MLE (Maximum Likelihood Estimation)
• Naïve Bayes
  • Naïve Bayes assumption
  • model 1: Bernoulli Naïve Bayes
  • model 2: Multinomial Naïve Bayes
  • model 3: Gaussian Naïve Bayes
  • model 4: Multiclass Naïve Bayes
problem setting

- set of possible instances: $X$
- 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 $f$
  \[
  (x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}) \ldots (x^{(m)}, y^{(m)})
  \]

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 \( \theta \) such that \( h_\theta \in H \) best approximate the target

- different from nonparametric approaches like decision trees and nearest neighbor
- advantages: various hypothesis class; easier 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
  \[ h(x, y) = p(x, y) \]

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

- example: roll a weighted die
  - weights for each side ($\theta$) define how the data are generated
  - use MLE on the training data to learn $\theta$
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 vs. MAP

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

$$\theta^{MLE} = \arg\max_{\theta} \prod_{i=1}^N p(x^{(i)} | \theta)$$

Maximum Likelihood Estimate (MLE)
Background: MLE

Example: MLE of Exponential Distribution

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

Example: MLE of Exponential Distribution

- First write down log-likelihood of sample.

\[
\ell(\lambda) = \sum_{i=1}^{N} \log f(x^{(i)})
\]

\[
= \sum_{i=1}^{N} \log(\lambda \exp(-\lambda x^{(i)}))
\]

\[
= \sum_{i=1}^{N} \log(\lambda) + -\lambda x^{(i)}
\]

\[
= N \log(\lambda) - \lambda \sum_{i=1}^{N} x^{(i)}
\]
Background: MLE

Example: MLE of Exponential Distribution

- Compute first derivative, set to zero, solve for $\lambda$.

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

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

\[
\Rightarrow \lambda^{\text{MLE}} = \frac{N}{\sum_{i=1}^{N} x^{(i)}} \tag{3}
\]
MLE vs. MAP

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

$$\theta_{\text{MLE}} = \arg\max_{\theta} \prod_{i=1}^{N} p(x^{(i)} | \theta)$$

Maximum Likelihood Estimate (MLE)

$$\theta_{\text{MAP}} = \arg\max_{\theta} \prod_{i=1}^{N} p(x^{(i)} | \theta)p(\theta)$$

Maximum a posteriori (MAP) estimate

Prior
Spam News

The Economist

La paralización
Spain may be heading for its third election in a year

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

Sep 9th 2016 | MADRID | Europe

The Onion

ELECTION 2016

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 the belt carried him deeply beneath the factory floor, where Kaine found...
Model 0: Not-so-naïve Model?

Generative Story:
1. Flip a weighted coin ($Y$)
2. If heads, roll the **red** 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?

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

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

This model is computationally naïve!
Model 0: Not-so-naïve Model?

Flip weighted coin

If HEADS, roll red die

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

If TAILS, roll blue die

<table>
<thead>
<tr>
<th>y</th>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(x_3)</th>
<th>\ldots</th>
<th>(x_K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
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</tbody>
</table>
Naïve Bayes Assumption

Conditional independence of features:

\[
P(X_1, \ldots, X_K, Y) = P(X_1, \ldots, X_K | Y) P(Y) = \left( \prod_{k=1}^{K} P(X_k | Y) \right) P(Y)
\]
Assuming conditional independence, the conditional probabilities encode the **same information** as the joint table.

They are very convenient for estimating

\[ P( X_1, \ldots, X_n | Y) = P( X_1 | Y) \ast \ldots \ast P( X_n | Y) \]

They are almost as good for computing

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

\[
\forall x, y : P(Y = y | X_1, \ldots, X_n = x) = \frac{P(X_1, \ldots, X_n = x | Y)P(Y = y)}{P(X_1, \ldots, X_n = x)}
\]
Generic Naïve Bayes Model

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

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

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

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

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

**Classification:** Find the class that maximizes the posterior

\[
\hat{y} = \arg\max_y p(y|x)
\]
Generic Naïve Bayes Model

Classification:

\[
\hat{y} = \arg \max_y p(y|x) \quad \text{(posterior)}
\]

\[
= \arg \max_y \frac{p(x|y)p(y)}{p(x)} \quad \text{(by Bayes’ rule)}
\]

\[
= \arg \max_y p(x|y)p(y)
\]
Model 1: Bernoulli Naïve Bayes

**Support:** Binary vectors of length $K$

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

**Generative Story:**

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

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

**Model:**

$$p_{\phi,\theta}(x, y) = p_{\phi,\theta}(x_1, \ldots, x_K, y)$$

$$= p_{\phi}(y) \prod_{k=1}^{K} p_{\theta_k}(x_k|y)$$

$$= (\phi)^y (1 - \phi)^{(1-y)} \prod_{k=1}^{K} (\theta_{k,y})^{x_k} (1 - \theta_{k,y})^{(1-x_k)}$$
Model 1: Bernoulli Naïve Bayes

If HEADS, flip each red coin

If TAILS, flip each blue coin

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).
Model 1: Bernoulli Naïve Bayes

**Support:** Binary vectors of length $K$

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

**Generative Story:**

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

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

**Model:**

$$p_{\phi, \theta}(x, y) = (\phi)^y(1 - \phi)^{1-y} \prod_{k=1}^{K} \theta_k^{x_k}$$

**Classification:** Find the class that maximizes the posterior

$$\hat{y} = \arg\max_y p(y|x)$$
Generic Naïve Bayes Model

Classification:

\[ \hat{y} = \arg\max_y p(y|x) \quad \text{(posterior)} \]

\[ = \arg\max_y \frac{p(x|y)p(y)}{p(x)} \quad \text{(by Bayes’ rule)} \]

\[ = \arg\max_y p(x|y)p(y) \]
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.

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

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

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

$\forall k \in \{1, \ldots, K\}$
Model 2: Multinomial Naïve Bayes

Support:

Integer vector (word IDs)

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

Generative Story:

for \( i \in \{1, \ldots, N\} \):

\[ y^{(i)} \sim \text{Bernoulli}(\phi) \]

for \( j \in \{1, \ldots, M_i\} \):

\[ x_j^{(i)} \sim \text{Multinomial}(\theta_{y^{(i)}}, 1) \]

Model:

\[
p_{\phi, \theta}(\mathbf{x}, y) = p_{\phi}(y) \prod_{k=1}^{K} p_{\theta_k}(x_k | y) \]

\[ = (\phi)^y (1 - \phi)^{(1-y)} \prod_{j=1}^{M_i} \theta_{y, x_j} \]
Model 3: Gaussian Naïve Bayes

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

Model: Product of prior and the event model

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

Gaussian Naïve 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.

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

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

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