Introduction to Machine Learning

Bayesian Classification

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Outline

Learning Probabilistic Classifiers

Training data, $D = [\langle \mathbf{x_i}, y_i \rangle]_{i=1}^{N}$

1. {circular,large,light,smooth,thick}, malignant
2. {circular,large,light,irregular,thick}, malignant
3. {oval,large,dark,smooth,thin}, benign
4. {oval,large,light,irregular,thick}, malignant
5. {circular,small,light,smooth,thick}, benign

- **Testing**: Predict y^* for $\mathbf{x}^*$
- Option 1: Functional Approximation

$$y^* = f(\mathbf{x}^*)$$

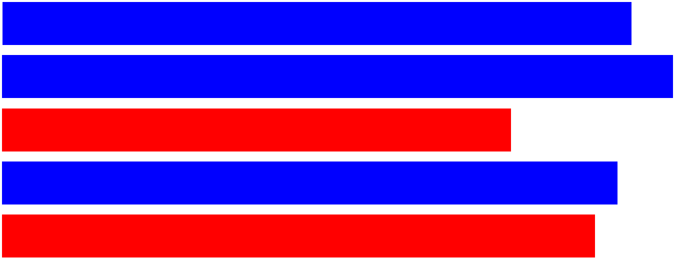
- Option 2: Probabilistic Classifier

$$P(Y = benign | \mathbf{X} = \mathbf{x}^*), P(Y = malignant | \mathbf{X} = \mathbf{x}^*)$$

Applying Bayes Rule

Training data, $D = [\langle \mathbf{x_i}, y_i \rangle]_{i=1}^{D}$

1.
2.
3.
4.
5.



- $\mathbf{x}^* =$ `circular,small, light,irregular,thin`
- What is $P(Y = benign|\mathbf{x}^*)$?
- What is $P(Y = malignant|\mathbf{x}^*)$?

Output Label – A Discrete Random Variable

- Y takes two values
- What is $p(Y)$?
  - $\sim Ber(\theta)$
  - How do you estimate θ?
  - Treat the labels in training data as binary samples
  - Posterior for θ

$$p(\theta) = \frac{\alpha_0 + N_1}{\alpha_0 + \beta_0 + N}$$

  - *Class 1 - Malignant; Class 2 - Benign*
  - Can we just use $p(y|\theta)$ for predicting future labels?
    - Just a prior for Y

Computing Posterior for Y

- What is probability of $\mathbf{x}^*$ to be malignant
  - $P(\mathbf{X} = \mathbf{x}^* | Y = \mathit{malignant})$?

Computing Posterior for Y

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  - $P(\mathbf{X} = \mathbf{x}^* | Y = \textit{malignant})$?
  - $P(Y = \textit{malignant})$?

Computing Posterior for Y

- What is probability of $\mathbf{x}^*$ to be malignant
  - $P(\mathbf{X} = \mathbf{x}^* | Y = malignant)$?
  - $P(Y = malignant)$?
  - $P(Y = malignant | \mathbf{X} = \mathbf{x}^*)$?

Computing Posterior for Y

- What is probability of $\mathbf{x}^*$ to be malignant
  - $P(\mathbf{X} = \mathbf{x}^* | Y = malignant)$?
  - $P(Y = malignant)$?
  - $P(Y = malignant | \mathbf{X} = \mathbf{x}^*)$?
  - $P(Y = malignant | \mathbf{X} = \mathbf{x}^*) = \frac{P(\mathbf{X}=\mathbf{x}^* | Y=malignant)P(Y=malignant)}{P(\mathbf{X}=\mathbf{x}^* | Y=malignant)P(Y=malignant)+P(\mathbf{X}=\mathbf{x}^* | Y=benign)P(Y=benign)}$

What is $P(\mathbf{X} = \mathbf{x}^* | Y = \mathit{malignant})$?

- Class conditional probability of random variable $\mathbf{X}$
- **Step 1**: Assume a probability distribution for $\mathbf{X}$ ($p(\mathbf{X})$)
- **Step 2**: Learn parameters from training data

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- But $\mathbf{X}$ is multivariate discrete random variable!
- How many parameters are needed?

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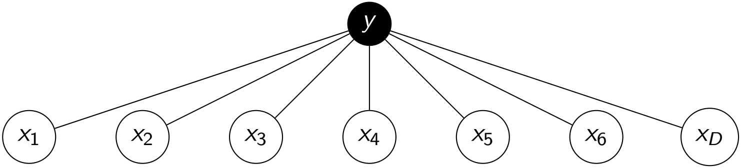
- $2(2^D - 1)$
- How much training data is needed?

Naive Bayes Assumption

- **All features are independent**
- Each variable can be assumed to be a Bernoulli random variable

$$P(\mathbf{X} = \mathbf{x}^* | Y = malignant) = \prod_{j=1}^{D} p(x_j^* | Y = malignant)$$

$$P(\mathbf{X} = \mathbf{x}^* | Y = benign) = \prod_{j=1}^{D} p(x_j^* | Y = benign)$$



- Only need $2D$ parameters

Example - Only binary features

- **Training a Naive Bayes Classifier**
- Find parameters that maximize likelihood of training data
  - What is a training example?
    - $\cancel{\mathbf{x}_i?}$
    - $\langle \mathbf{x_i}, y_i \rangle$
  - What are the parameters?
    - θ for Y (*class prior*)
    - $\boldsymbol{\theta}_{benign}$ and $\boldsymbol{\theta}_{malignant}$ (or $\boldsymbol{\theta}_1$ and $\boldsymbol{\theta}_2$)
  - Joint probability distribution of (X, Y)

$$\begin{aligned} p(\mathbf{x}_i, y_i) &= p(y_i|\theta)p(\mathbf{x}_i|y_i) \\ &= p(y_i|\theta)\prod_j p(x_{ij}|\theta_{jy_i}) \end{aligned}$$

Likelihood?

- Likelihood for D

$$l(D|\boldsymbol{\Theta}) = \prod_i \left(p(y_i|\theta) \prod_j p(x_{ij}|\theta_{jy_i}) \right)$$

- Log-likelihood for D

$$\begin{aligned} ll(D|\boldsymbol{\Theta}) &= N_1 \log\theta + N_2 \log(1-\theta) \\ &+ N_{1j} \log\theta_{1j} + (N_1 - N_{1j}) \log(1-\theta_{1j}) \\ &+ N_{2j} \log\theta_{2j} + (N_2 - N_{2j}) \log(1-\theta_{2j}) \end{aligned}$$

- N_1 - # malignant training examples, $N_2 = \#$ benign training examples
- N_{1j} - # malignant training examples with $x_j = 1$, $N_{2j} = \#$ benign training examples with $x_j = 2$

MLE?

- Maximize with respect to θ, assuming Y to be *Bernoulli*

$$\hat{\theta} = \frac{N_c}{N}$$

- Assuming each feature is binary $(x_j | (y = c) \sim \textit{Bernoulli}(\theta_{cj}),$ $c = \{1, 2\})$

$$\hat{\theta}_{cj} = \frac{N_{cj}}{N_c}$$

Algorithm 1 Naive Bayes Training for Binary Features

$N_c = 0,\ N_{cj} = 0, \forall j$
for $i = 1 : N$ **do**
    $c \leftarrow y_i$
    $N_c \leftarrow N_c + 1$
    for $j = 1 : D$ **do**
        if $x_{ij} = 1$ **then**
            $N_{cj} \leftarrow N_{cj} + 1$
        end if
    end for
end for
$\hat{\theta}_c = \frac{N_c}{N},\ \hat{\theta}_{cj} = \frac{N_{cj}}{N_c}$
return b

Adding Prior

- Add prior to θ and each θ_{cj}.
  - Beta prior for θ ($\sim Beta(a_0, b_0)$)
  - Beta prior for θ_{cj} ($\sim Beta(a, b)$)

Posterior Estimates

$$p(\theta|D) = Beta(N_1 + a_0, N - N_1 + b_0)$$

$$p(\theta_{cj}|D) = Beta(N_{cj} + a, N_c - N_{cj} + b)$$

Using Naive Bayes Model for Prediction

$$p(y = c|\mathbf{x}^*, D) \propto p(y = c|D) \prod_j p(x_j^*|y = c, D)$$

- MLE approach, MAP approach?
- Bayesian approach:

$$\begin{aligned} p(y = 1|\mathbf{x}, D) \quad \propto \quad & \left[\int Ber(y = 1|\theta)p(\theta|D)d\theta\right] \\ & \prod_j \left[\int Ber(x_j|\theta_{cj})p(\theta_{cj}|D)d\theta_{cj}\right] \end{aligned}$$

$$\bar{\theta} = \frac{N_1 + a_0}{N + a_0 + b_0}$$

$$\bar{\theta}_{cj} = \frac{N_{cj} + a}{N_c + a + b}$$

Example

#	Shape	Size	Color	Type
1	cir	large	light	malignant
2	cir	large	light	benign
3	cir	large	light	malignant
4	ovl	large	light	benign
5	ovl	large	dark	malignant
6	ovl	small	dark	benign
7	ovl	small	dark	malignant
8	ovl	small	light	benign
9	cir	small	dark	benign
10	cir	large	dark	malignant

- Test example: $\mathbf{x}^* = \{cir, small, light\}$

What if Attributes are Continuous?

- Naive Bayes is still applicable!
- Each variable is a univariate Gaussian (normal) distribution

$$
\begin{aligned}
p(y|\mathbf{x}) &\propto p(y)\prod_j p(x_j|y) = p(y)\prod_j \frac{1}{\sqrt{2\pi\sigma_j^2}} e^{-\frac{(x_j-\mu_j)^2}{2\sigma_j^2}} \\
&= p(y)\frac{1}{(2\pi)^{D/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{(\mathbf{x}-\boldsymbol{\mu})^\top \Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})}{2}}
\end{aligned}
$$

- Where $\mathbf{\Sigma}$ is a diagonal matrix with $\sigma_1^2, \sigma_1^2, \ldots, \sigma_D^2$ as the diagonal entries
- $\boldsymbol{\mu}$ is a vector of means
- Treating $\mathbf{x}$ as a multivariate Gaussian with zero covariance

What if Σ is not diagonal?

- Gaussian Discriminant Analysis
  - Class conditional density

$$p(\mathbf{x}|y=1) = \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$$

$$p(\mathbf{x}|y=2) = \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$$

  - Posterior density for y

$$p(y=1|\mathbf{x}) = \frac{p(y=1)\mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)}{p(y=1)\mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + p(y=2)\mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)}$$

Quadratic and Linear Discriminant Analysis

- Using non-diagonal covariance matrices for each class - **Quadratic Discriminant Analysis (QDA)**
  - Quadratic decision boundary
- If $\mathbf{\Sigma}_1 = \mathbf{\Sigma}_2 = \mathbf{\Sigma}$
- **Linear Discriminant Analysis (LDA)**
  - Parameter *sharing* or *tying*
  - Results in linear surface
  - No quadratic term

Alternative Interpretation of LDA

- Equivalent to computing the **Mahalanobis distance** of $\mathbf{x}$ to the two means.
- **Euclidean distance** is a special case of Mahalanobis distance when Σ is an identity matrix.

How to Train

MLE Training

- Estimate Bernoulli parameters for Y using MLE
- For each class, estimate MLE parameters for the multivariate normal distribution, i.e., $\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1$ and $\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2$
- For LDA, compute the MLE for $\boldsymbol{\Sigma}$ using all training data (ignoring the class label)

References

Murphy Book Chapters 9.1 - 9.3