COMPSCI 589
Lecture 3: Naive Bayes, LDA, and Logistic Regression

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Created with support from National Science Foundation Award# IIS-1350522.

Outline

The Classification Task

Definition: The Classification Task

Given a feature vector $\mathbf{x} \in \mathbb{R}^D$ that describes an object that belongs to one of C classes from the set $\mathcal{Y}$, predict which class the object belongs to.

The Classifier Learning Problem

Definition: Classifier Learning

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : N\}$ where $\mathbf{x}_i \in \mathbb{R}^D$ is a feature vector and $y_i \in \mathcal{Y}$ is a class label, learn a function $f : \mathbb{R}^D \to \mathcal{Y}$ that accurately predicts the class label y for any feature vector $\mathbf{x}$.

Classification Error and Accuracy

Definition: Classification Error Rate

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : N\}$ and a function $f : \mathbb{R}^D \to \mathcal{Y}$, the classification error rate of f on $\mathcal{D}$ is:

$$Err(f, \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}(y_i \neq f(\mathbf{x}_i))$$

Definition: Classification Accuracy Rate

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : N\}$ and a function $f : \mathbb{R}^D \to \mathcal{Y}$, the classification accuracy rate of f on $\mathcal{D}$ is:

$$Acc(f, \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}(y_i = f(\mathbf{x}_i))$$

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Probabilistic Classification

- Suppose we know that the true probability of seeing a data case that belongs to class c is $P(Y = c) = \pi_c$ and the true probability density of seeing a data vector $\mathbf{x} \in \mathbb{R}^D$ that belongs to class c is $p(\mathbf{X} = \mathbf{x}|Y = c) = \phi_c(\mathbf{x})$.

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- We can use this information to compute the probability that the class of any observation $\mathbf{x}$ is c. How?
- Bayes Rule: $P(Y = c|\mathbf{X} = \mathbf{x}) = \dfrac{\phi_c(\mathbf{x})\pi_c}{\sum_{c' \in \mathcal{Y}} \phi_{c'}(\mathbf{x})\pi_{c'}}$

The Bayes Optimal Classifier

- The Bayes Optimal Classifier uses the classification function:

$$f_B(\mathbf{x}) = \arg\max_{c \in \mathcal{Y}} P(Y = c | \mathbf{X} = \mathbf{x})$$
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- The Bayes optimal classifier achieves the minimal possible expected error rate among all possible classifiers:

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- This is a nice result, but is it useful in practice?

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- The general form for the classification function is:

$$f_{NB}(\mathbf{x}) = \arg\max_{c \in \mathcal{Y}} \pi_c \prod_{d=1}^{D} \phi_{cd}(x_d)$$

Class Conditional Distributions

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- For general categorical values x_d, $p(X_d = x_d|Y = c)$ is a categorical distribution $\phi_{cd}(x_d) = \prod_{v \in \mathcal{X}_d} \theta_{vdc}^{[x_d = v]}$

Learning for Naive Bayes

- The class probabilities π_c and the parameters of the marginal class conditional distributions $\phi_{cd}(x_d)$ are learned by maximum likelihood on a sample of training data $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : n\}$.

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- Normal: $\mu_{dc} = \frac{\sum_{i=1}^{n} [y_i = c] x_{di}}{\sum_{i=1}^{n} [y_i = c]} \qquad \sigma^2_{dc} = \frac{\sum_{i=1}^{n} [y_i = c] (x_{di} - \mu_{dc})^2}{\sum_{i=1}^{n} [y_i = c]}$

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- Bernoulli: $\theta_{dc} = \frac{\sum_{i=1}^{n} [y_i=c] x_{di}}{\sum_{i=1}^{n} [y_i=c]}$ Categorical: $\theta_{vdc} = \frac{\sum_{i=1}^{n} [y_i=c][x_{di}=v]}{\sum_{i=1}^{n} [y_i=c]}$

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$$
\begin{aligned}
f_{NB}(\mathbf{x}) &= \arg\max_{c \in \mathcal{Y}} \pi_c \prod_{d=1}^{D} \phi_{cd}(x_d) \\
&= \arg\max_{c \in \mathcal{Y}} \log(\pi_c) + \sum_{d=1}^{D} \log(\phi_{cd}(x_d)) \\
&= \arg\max_{c \in \mathcal{Y}} \log(\pi_c) + \sum_{d=1}^{D} \left(-\frac{1}{2} \log(2\pi\sigma_{dc}^2) - \frac{1}{2\sigma_{dc}^2}(x_d - \mu_{dc})^2 \right)
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$$- \log(\pi_1) - \sum_{d=1}^{D} \left(-\frac{1}{2}\log(2\pi\sigma_{d1}^2) - \frac{1}{2\sigma_{d1}^2}(x_d - \mu_{d1})^2 \right) = 0$$

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- It's easy to see that the decision boundary is a quadratic function of $\mathbf{x}$ with the form: $\sum_{d=1}^{D} \left(a_d x_d^2 + b_d x_d \right) + c = 0$.

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- In the multi-class case, the decision boundary is piece-wise quadratic.

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- Data: Some care is needed in the estimation of parameters in the discrete case when data is scarce.

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- Instead of a product of independent Normals like in Naive Bayes, LDA assumes the class-conditional densities are multivariate normal with a common covariance matrix:

$$\phi_c(\mathbf{x}) = \mathcal{N}(\mathbf{x}; \mu_c, \Sigma) = \frac{1}{|2\pi\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu_c)^T\Sigma^{-1}(\mathbf{x}-\mu_c)\right)$$

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- The classification function is $f_{LDA}(\mathbf{x}) = \arg\max_{c\in\mathcal{Y}} \phi_c(\mathbf{x})\pi_c$

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- Class Means: $\mu_c = \frac{\sum_{i=1}^{n}[y_i=c]\mathbf{x}_i}{\sum_{i=1}^{n}[y_i=c]}$
- Shared Covariance: $\Sigma = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - \mu_{y_i})(\mathbf{x}_i - \mu_{y_i})^T$

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- We can cancel a large number of terms because of the common covariance matrix and obtain the following result:

$$\log(\pi_0) - \log(\pi_1) - 0.5\mu_0^T\Sigma^{-1}\mu_0 + 0.5\mu_1^T\Sigma^{-1}\mu_1 + (\mu_0-\mu_1)^T\Sigma^{-1}\mathbf{x} = 0$$

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- This shows that the decision boundary is actually linear in $\mathbf{x}$.

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- Data: LDA will generally need more data than NB since it needs to estimate the $O(D^2)$ parameters in the pooled covariance matrix Σ.

Outline

Generative vs Discriminative Classifiers

- The Bayes Optimal Classifier, Naive Bayes and LDA are said to be *generative* classifiers because they explicitly model the joint distribution $P(\mathbf{X}, Y)$ of the data vectors $\mathbf{x}$ and the labels y.

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- No, to build a probabilistic classifier, all we really need to model is $P(Y|\mathbf{X})$.
- Classifiers based on directly estimating $P(Y|\mathbf{X})$ are called *descriminative* classifiers because they ignore the distribution of $\mathbf{x}$ and focus only on the class labels y.

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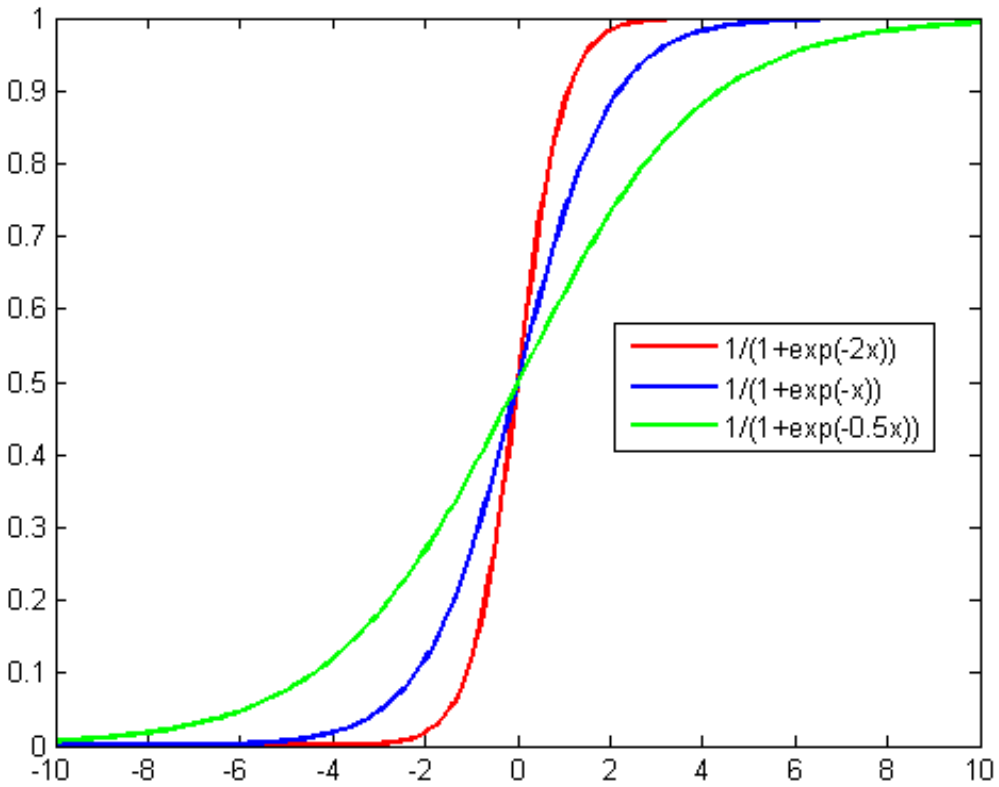
$$P(Y = 1|\mathbf{X}) = \frac{1}{1 + \exp(-(\mathbf{w}^T\mathbf{x} + b))}$$

- The classification function is: $f_{LR}(\mathbf{x}) = \arg\max_{c \in \mathcal{Y}} P(Y = c|\mathbf{x})$

Logistic Function



Multiclass Logistic Regression

- Logistic regression can also be extended to the multiclass case:

$$P(Y = c|\mathbf{x}) = \frac{\exp(\mathbf{w}_c^T \mathbf{x} + b_c)}{\sum_{c' \in \mathcal{Y}} \exp(-(\mathbf{w}_{c'}^T \mathbf{x} + b_{c'}))}$$

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- The classification function is still:

$$f_{LR}(\mathbf{x}) = \arg\max_{c \in \mathcal{Y}} P(Y = c|\mathbf{x})$$

Learning Logistic Regression

- The logistic regression model parameters $\theta = \{(\mathbf{w}_c, b_c), c \in \mathcal{Y}\}$ are selected to optimize the conditional log likelihood of the labels given a data set $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : n\}$:

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$$\theta_* = \arg\max_{\theta} \mathcal{L}(\theta|\mathcal{D}) = \arg\max_{\theta} \sum_{i=1}^{n} \log P(Y = y_i|\mathbf{X} = \mathbf{x}_i)$$

Learning Logistic Regression

- The logistic regression model parameters $\theta = \{(\mathbf{w}_c, b_c), c \in \mathcal{Y}\}$ are selected to optimize the conditional log likelihood of the labels given a data set $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : n\}$:

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- However, the function $\mathcal{L}(\theta|\mathcal{D})$ can not be maximized analytically. Learning the model parameters requires numerical optimization methods.

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- Interpretability: The "importance" of different feature variables x_d can be understood in terms of their weights w_{dc}.
- Accuracy: Tends to be better in high dimensions with limited data compared to LDA. Much worse than KNN in low dimensions with lots of data and non-linear decision boundaries.