

# EECS 545: Machine Learning

## Lecture 5. Classification 2

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## Outline

- Probabilistic Discriminative models
  - Objective: maximize **conditional likelihood** over training data
 
$$\prod_i P(y^{(i)} | \mathbf{x}^{(i)}, \mathbf{w})$$
    - Logistic Regression (covered in previous lecture)
    - Softmax Regression: Multiclass extension of logistic regression
- Probabilistic Generative models
  - Objective: maximize **joint likelihood** over training data
 
$$\prod_i P(\mathbf{x}^{(i)}, y^{(i)} | \mathbf{w})$$
    - Gaussian Discriminant Analysis
    - Naive Bayes (part 1)

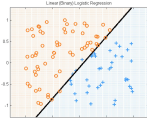
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## Softmax regression for multiclass classification

- For multiclass case, we can use softmax regression.
  - Softmax regression can be viewed as a generalization of logistic regression
- Recall that, logistic regression (binary classification) models class conditional probability as:

$$p(y = 1 | \mathbf{x}; \mathbf{w}) = \frac{\exp(\mathbf{w}^\top \phi(\mathbf{x}))}{1 + \exp(\mathbf{w}^\top \phi(\mathbf{x}))}$$

$$p(y = 0 | \mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(\mathbf{w}^\top \phi(\mathbf{x}))}$$

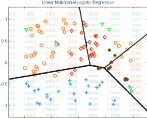


- Note that these probability sum to 1.

- For multiclass classification (with  $K$  classes), we use the following model

$$p(y = k | \mathbf{x}; \mathbf{w}) = \frac{\exp(\mathbf{w}_k^\top \phi(\mathbf{x}))}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^\top \phi(\mathbf{x}))} \quad \text{for } k = \{1, \dots, K-1\}$$

$$p(y = K | \mathbf{x}; \mathbf{w}) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^\top \phi(\mathbf{x}))} \quad \text{equivalent to setting } \mathbf{w}_K = 0$$



- Note that these probability sum to 1.

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## Softmax regression: Log-likelihood (objective function) and learning

- Defining  $\mathbf{w}_K = 0$ , we can write as:

$$p(y = k | \mathbf{x}; \mathbf{w}) = \frac{\exp(\mathbf{w}_k^\top \phi(\mathbf{x}))}{\sum_{j=1}^K \exp(\mathbf{w}_j^\top \phi(\mathbf{x}))}$$

or

$$p(y | \mathbf{x}; \mathbf{w}) = \prod_{k=1}^K \left[ \frac{\exp(\mathbf{w}_k^\top \phi(\mathbf{x}))}{\sum_{j=1}^K \exp(\mathbf{w}_j^\top \phi(\mathbf{x}))} \right]^{\mathbb{I}(y=k)}$$

- Log-Likelihood

$$\log p(D | \mathbf{w}) = \sum_i \log p(y^{(i)} | \mathbf{x}^{(i)}, \mathbf{w})$$

$$= \sum_i \log \prod_{k=1}^K \left[ \frac{\exp(\mathbf{w}_k^\top \phi(\mathbf{x}^{(i)}))}{\sum_{j=1}^K \exp(\mathbf{w}_j^\top \phi(\mathbf{x}^{(i)}))} \right]^{\mathbb{I}(y^{(i)}=k)}$$

- We can learn  $\mathbf{w}$  by gradient ascent for maximizing the log-likelihood or iterative Newton's method (IRLS).

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## Probabilistic Generative Models

## Learning the Classifier

- For classification, we want to compute  $p(C_k | \mathbf{x})$ 
  - (a) **Discriminative** models: Directly model  $p(C_k | \mathbf{x})$  and learn parameters from the training set.
    - Logistic regression
    - Softmax regression
  - (b) **Generative** models: Learn joint densities  $p(\mathbf{x}, C_k)$  by learning  $p(\mathbf{x} | C_k)$  and  $p(C_k)$ , and then use Bayes rule for predicting the class  $C_k$  given  $\mathbf{x}$ :
    - Gaussian Discriminant Analysis
    - Naive Bayes

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## Probabilistic Generative Models

- Bayes' theorem reduces the classification problem  $p(C_k | \mathbf{x})$  to estimating the distribution of the data:
 
$$p(C_k | \mathbf{x}) = \frac{p(\mathbf{x} | C_k) p(C_k)}{p(\mathbf{x})} = \frac{p(\mathbf{x} | C_k) p(C_k)}{\sum_{k'} p(\mathbf{x} | C_{k'}) p(C_{k'})}$$
- Density estimation can be decomposed into learning distributions from training data.
  - $p(C_k)$
  - $p(\mathbf{x} | C_k)$
- Maximum likelihood estimation for  $p(\mathbf{x}, C_k)$

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## Probabilistic Generative Models

- For two classes, Bayes' theorem says:

$$p(C_1 | \mathbf{x}) = \frac{p(\mathbf{x} | C_1) p(C_1)}{p(\mathbf{x} | C_1) p(C_1) + p(\mathbf{x} | C_2) p(C_2)}$$

- Use **log odds** (i.e., logit "score"):

$$a = \log \frac{p(C_1 | \mathbf{x})}{p(C_2 | \mathbf{x})} = \log \frac{p(\mathbf{x} | C_1) p(C_1)}{p(\mathbf{x} | C_2) p(C_2)}$$

- Then we can define the posterior via the **sigmoid**:

$$p(C_1 | \mathbf{x}) = \frac{1}{1 + \exp(-a)} = \sigma(a)$$

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# Gaussian Discriminant Analysis

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## Gaussian Discriminant Analysis

- Probability of class label
  - $p(C_k)$ : Constant (e.g., Bernoulli)
- Conditional probability of data given a class
  - $p(\mathbf{x} | C_k)$ : Gaussian distribution

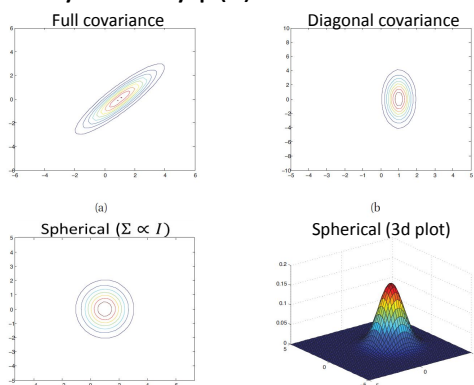
$$p(\mathbf{x} | C_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu_k)^\top \Sigma^{-1} (\mathbf{x} - \mu_k) \right\}$$

- Classification: use Bayes rule (previous slide)

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## Examples of Gaussian Distributions

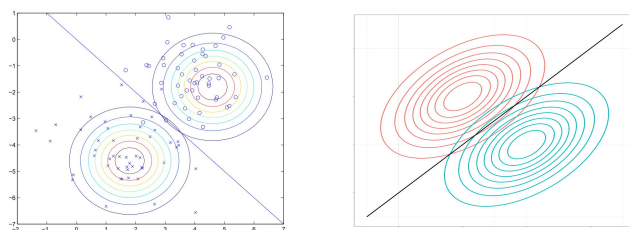
- Probability density  $p(\mathbf{x})$  for 2 dimensional case



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## Gaussian Discriminant Analysis

- Basic GDA assumes the same covariance for all classes
  - The figure below shows class-specific density and decision boundary. Note the linear decision boundary for any types of covariance matrices!



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## Prediction: Class-Conditional Densities

- Suppose we model  $p(\mathbf{x} | C_k)$  as Gaussians with the same covariance matrix.

$$p(\mathbf{x} | C_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu_k)^\top \Sigma^{-1} (\mathbf{x} - \mu_k) \right\}$$

- This gives us  $p(C_1 | \mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x} + w_0)$

– where  $\mathbf{w} = \Sigma^{-1}(\mu_1 - \mu_2)$

$$\text{and } w_0 = -\frac{1}{2} \mu_1^\top \Sigma^{-1} \mu_1 + \frac{1}{2} \mu_2^\top \Sigma^{-1} \mu_2 + \log \frac{p(C_1)}{p(C_2)}$$

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## Derivation

$$\begin{aligned} P(x, C_1) &= P(x | C_1) P(C_1) \\ &= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_1)^\top \Sigma^{-1} (x - \mu_1) \right\} P(C_1) \\ P(x, C_2) &= P(x | C_2) P(C_2) \\ &= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_2)^\top \Sigma^{-1} (x - \mu_2) \right\} P(C_2) \end{aligned}$$

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## Derivation

$$\begin{aligned} P(x, C_1) &= P(x | C_1) P(C_1) \\ &= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_1)^\top \Sigma^{-1} (x - \mu_1) \right\} P(C_1) \\ P(x, C_2) &= P(x | C_2) P(C_2) \\ &= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_2)^\top \Sigma^{-1} (x - \mu_2) \right\} P(C_2) \\ \log \frac{P(C_1 | \mathbf{x})}{P(C_2 | \mathbf{x})} &= \log \frac{P(C_1 | \mathbf{x})}{1 - P(C_1 | \mathbf{x})} \quad \text{"Log-odds"} \end{aligned}$$

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## Derivation

$$\begin{aligned} P(x, C_1) &= P(x | C_1) P(C_1) \\ &= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_1)^\top \Sigma^{-1} (x - \mu_1) \right\} P(C_1) \\ P(x, C_2) &= P(x | C_2) P(C_2) \\ &= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_2)^\top \Sigma^{-1} (x - \mu_2) \right\} P(C_2) \\ \log \frac{P(C_1 | \mathbf{x})}{P(C_2 | \mathbf{x})} &= \log \frac{P(C_1 | \mathbf{x})}{1 - P(C_1 | \mathbf{x})} \quad \text{"Log-odds"} \\ &= \log \frac{\exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu_1)^\top \Sigma^{-1} (\mathbf{x} - \mu_1) \right\}}{\exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu_2)^\top \Sigma^{-1} (\mathbf{x} - \mu_2) \right\}} + \log \frac{P(C_1)}{P(C_2)} \end{aligned}$$

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## Derivation

$$\begin{aligned}
 P(x, C_1) &= P(x | C_1) P(C_1) \\
 &= \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_1)^\top \Sigma^{-1} (x - \mu_1) \right\} P(C_1) \\
 P(x, C_2) &= P(x | C_2) P(C_2) \\
 &= \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_2)^\top \Sigma^{-1} (x - \mu_2) \right\} P(C_2) \\
 \log \frac{P(C_1 | \mathbf{x})}{P(C_2 | \mathbf{x})} &= \log \frac{P(C_1 | \mathbf{x})}{1 - P(C_1 | \mathbf{x})} \quad \text{"Log-odds"} \\
 &= \log \frac{\exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu_1)^\top \Sigma^{-1} (\mathbf{x} - \mu_1) \right\}}{\exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu_2)^\top \Sigma^{-1} (\mathbf{x} - \mu_2) \right\}} + \log \frac{P(C_1)}{P(C_2)} \\
 &= \left\{ -\frac{1}{2} (\mathbf{x} - \mu_1)^\top \Sigma^{-1} (\mathbf{x} - \mu_1) \right\} - \left\{ -\frac{1}{2} (\mathbf{x} - \mu_2)^\top \Sigma^{-1} (\mathbf{x} - \mu_2) \right\} + \log \frac{P(C_1)}{P(C_2)}
 \end{aligned}$$

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## Derivation

$$\begin{aligned}
 P(x, C_1) &= P(x | C_1) P(C_1) \\
 &= \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_1)^\top \Sigma^{-1} (x - \mu_1) \right\} P(C_1) \\
 P(x, C_2) &= P(x | C_2) P(C_2) \\
 &= \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_2)^\top \Sigma^{-1} (x - \mu_2) \right\} P(C_2) \\
 \log \frac{P(C_1 | \mathbf{x})}{P(C_2 | \mathbf{x})} &= \log \frac{P(C_1 | \mathbf{x})}{1 - P(C_1 | \mathbf{x})} \quad \text{"Log-odds"} \\
 &= \log \frac{\exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu_1)^\top \Sigma^{-1} (\mathbf{x} - \mu_1) \right\}}{\exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu_2)^\top \Sigma^{-1} (\mathbf{x} - \mu_2) \right\}} + \log \frac{P(C_1)}{P(C_2)} \\
 &= \left\{ -\frac{1}{2} (\mathbf{x} - \mu_1)^\top \Sigma^{-1} (\mathbf{x} - \mu_1) \right\} - \left\{ -\frac{1}{2} (\mathbf{x} - \mu_2)^\top \Sigma^{-1} (\mathbf{x} - \mu_2) \right\} + \log \frac{P(C_1)}{P(C_2)} \\
 &= (\mu_1 - \mu_2)^\top \Sigma^{-1} \mathbf{x} - \frac{1}{2} \mu_1^\top \Sigma^{-1} \mu_1 + \frac{1}{2} \mu_2^\top \Sigma^{-1} \mu_2 + \log \frac{P(C_1)}{P(C_2)}
 \end{aligned}$$

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## Derivation

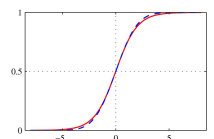
$$\begin{aligned}
 P(x, C_1) &= P(x | C_1) P(C_1) \\
 &= \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_1)^\top \Sigma^{-1} (x - \mu_1) \right\} P(C_1) \\
 P(x, C_2) &= P(x | C_2) P(C_2) \\
 &= \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_2)^\top \Sigma^{-1} (x - \mu_2) \right\} P(C_2) \\
 \log \frac{P(C_1 | \mathbf{x})}{P(C_2 | \mathbf{x})} &= \log \frac{P(C_1 | \mathbf{x})}{1 - P(C_1 | \mathbf{x})} \quad \text{"Log-odds"} \\
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 &= \left\{ -\frac{1}{2} (\mathbf{x} - \mu_1)^\top \Sigma^{-1} (\mathbf{x} - \mu_1) \right\} - \left\{ -\frac{1}{2} (\mathbf{x} - \mu_2)^\top \Sigma^{-1} (\mathbf{x} - \mu_2) \right\} + \log \frac{P(C_1)}{P(C_2)} \\
 &= (\mu_1 - \mu_2)^\top \Sigma^{-1} \mathbf{x} - \frac{1}{2} \mu_1^\top \Sigma^{-1} \mu_1 + \frac{1}{2} \mu_2^\top \Sigma^{-1} \mu_2 + \log \frac{P(C_1)}{P(C_2)} \\
 &= (\Sigma^{-1} (\mu_1 - \mu_2))^\top \mathbf{x} + w_0 \quad \text{where } w_0 = -\frac{1}{2} \mu_1^\top \Sigma^{-1} \mu_1 + \frac{1}{2} \mu_2^\top \Sigma^{-1} \mu_2 + \log \frac{P(C_1)}{P(C_2)}
 \end{aligned}$$

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## Prediction: Class-Conditional Densities for shared covariances

- $p(C_k | \mathbf{x})$  is a sigmoid function:

$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$



- with log-odds (*logit* function):

$$a = \log \left( \frac{\sigma}{1 - \sigma} \right) = (\Sigma^{-1} (\mu_1 - \mu_2))^\top \mathbf{x} + w_0$$

$$\text{where } w_0 = -\frac{1}{2} \mu_1^\top \Sigma^{-1} \mu_1 + \frac{1}{2} \mu_2^\top \Sigma^{-1} \mu_2 + \log \frac{P(C_1)}{P(C_2)}$$

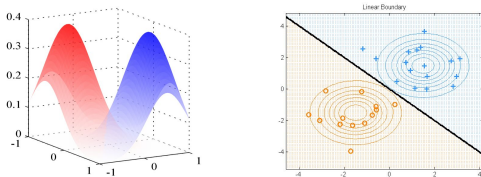
- Generalizes to *normalized exponential*, or *softmax*:

$$p_i = \frac{\exp(q_i)}{\sum_j \exp(q_j)}$$

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## Prediction: Linear Decision Boundaries

- At decision boundary, we have  $p(C_1 | \mathbf{x}) = p(C_2 | \mathbf{x})$
- With the same covariance matrices, the boundary  $p(C_1 | \mathbf{x}) = p(C_2 | \mathbf{x})$  is linear.
  - Different class  $p(C_1), p(C_2)$  just shift it around.



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## Likelihood function of generative models

- The likelihood of Data  $\{(\mathbf{x}^{(n)}, y^{(n)})\}$

$$\begin{aligned}
 P(D | \mathbf{w}) &= \prod_{i=1}^N P(\mathbf{x}^{(i)}, y^{(i)} | \mathbf{w}) \longrightarrow P(\mathbf{X}, \mathbf{y} | \mathbf{w}) \\
 &= \prod_{i=1}^N P(\mathbf{x}^{(i)} | y^{(i)}, \mathbf{w}) P(y^{(i)} | \mathbf{w})
 \end{aligned}$$

Decomposition of the joint probability

Compact notation: This is called joint likelihood.

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## Learning parameters via maximum likelihood

- Given training data  $\{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(N)}, y^{(N)})\}$  and a generative model ("shared covariance")

$$p(y) = \phi^y (1 - \phi)^{1-y}$$

$$p(\mathbf{x} | y = 0) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left( -\frac{1}{2} (\mathbf{x} - \mu_0)^\top \Sigma^{-1} (\mathbf{x} - \mu_0) \right)$$

$$p(\mathbf{x} | y = 1) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left( -\frac{1}{2} (\mathbf{x} - \mu_1)^\top \Sigma^{-1} (\mathbf{x} - \mu_1) \right)$$

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## Learning via maximum likelihood

- Maximum likelihood estimation (HW2):

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

$$\mu_0 = \frac{\sum_{i=1}^N \mathbb{I}\{y^{(i)} = 0\} \mathbf{x}^{(i)}}{\sum_{i=1}^N \mathbb{I}\{y^{(i)} = 0\}}$$

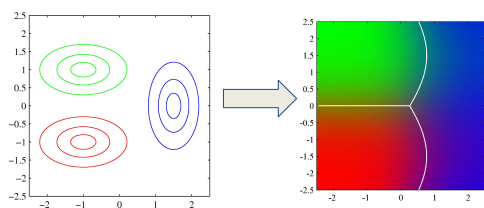
$$\mu_1 = \frac{\sum_{i=1}^N \mathbb{I}\{y^{(i)} = 1\} \mathbf{x}^{(i)}}{\sum_{i=1}^N \mathbb{I}\{y^{(i)} = 1\}}$$

$$\Sigma = \frac{1}{N} \sum_{i=1}^N (\mathbf{x}^{(i)} - \mu_{y^{(i)}})(\mathbf{x}^{(i)} - \mu_{y^{(i)}})^\top$$

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## Different Covariance

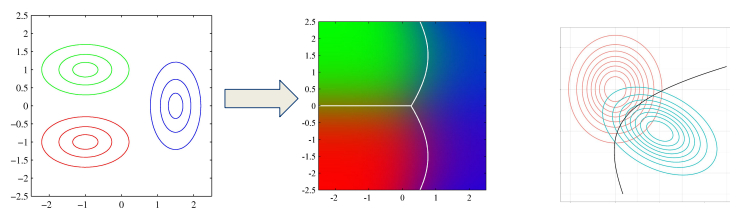
- Decision boundaries between some classes can be quadratic when they have **different** covariances.



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## Different Covariance

- Decision boundaries between some classes can be quadratic when they have **different** covariances.



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## Comparison between GDA and Logistic regression (or softmax regression)

- Logistic regression:
  - For an  $M$ -dimensional feature space, this model has  $M$  parameters to fit.
- Gaussian Discriminative Analysis
  - $2M$  parameters for the means of  $p(\mathbf{x} | C_1)$  and  $p(\mathbf{x} | C_2)$
  - $M(M+1)/2$  parameters for the shared covariance matrix
- Logistic regression has less parameters and is more flexible about data distribution.
- GDA has a stronger modeling assumption, and works well when the distribution follows the assumption.

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## Naive Bayes Classifier

(Brief Intro: to be continued in the next lecture)

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## Naive Bayes classifier

- Probability of class label:
  - $p(C_k)$ : Constant (e.g., Bernoulli)
- Conditional probability of data given the class
  - Naive Bayes assumption:  $p(\mathbf{x} | C_k)$  is factorized (Each coordinate of  $\mathbf{x}$  is conditionally independent of other coordinates given the class label)

$$P(x_1, \dots, x_M | C_k) = P(x_1 | C_k) \cdots P(x_M | C_k) = \prod_{j=1}^M P(x_j | C_k)$$

- Classification: use Bayes rule

$$(\text{binary}) \quad P(C_1 | \mathbf{x}) = \frac{P(C_1, \mathbf{x})}{P(\mathbf{x})} = \frac{P(C_1, \mathbf{x})}{P(C_1, \mathbf{x}) + P(C_2, \mathbf{x})}$$

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## Naive Bayes classifier

- When classifying, we can simply find the class  $C_k$  that maximizes  $P(C_k | \mathbf{x})$  using the Bayes rule:

$$\arg \max_k P(C_k | \mathbf{x}) = \arg \max_k P(C_k, \mathbf{x})$$

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## Naive Bayes classifier

- When classifying, we can simply find the class  $C_k$  that maximizes  $P(C_k | \mathbf{x})$  using the Bayes rule:

$$\begin{aligned} \arg \max_k P(C_k | \mathbf{x}) &= \arg \max_k P(C_k, \mathbf{x}) \\ &= \arg \max_k P(C_k) P(\mathbf{x} | C_k) \end{aligned}$$

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## Naive Bayes classifier

- When classifying, we can simply find the class  $C_k$  that maximizes  $P(C_k | \mathbf{x})$  using the Bayes rule:

$$\begin{aligned} \arg \max_k P(C_k | \mathbf{x}) &= \arg \max_k P(C_k, \mathbf{x}) \\ &= \arg \max_k P(C_k) P(\mathbf{x} | C_k) \\ \text{Naive Bayes assumption} &\rightarrow \\ &= \arg \max_k P(C_k) \prod_{j=1}^M P(x_j | C_k) \end{aligned}$$

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## Example: Naive Bayes for real-valued inputs

- Probability of class label:
  - $p(C_k)$ : Constant (e.g., Bernoulli)
- Conditional probability of data given the class
  - Naive Bayes assumption:  $P(\mathbf{x}|C_k)$  is factorized (e.g., 1D Gaussian)

$$\begin{aligned} P(x_1, \dots, x_M | C_k) &= P(x_1 | C_k) \cdots P(x_M | C_k) \\ &= \prod_{j=1}^M P(x_j | C_k) \\ &= \prod_{j=1}^M \frac{1}{\sqrt{2\pi\sigma_j^2}} \exp\left(-\frac{(x_j - \mu_j)^2}{2\sigma_j^2}\right) \end{aligned}$$

– Note: this is equivalent to GDA with diagonal covariance!!

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## Comparison: Discriminative vs. Generative

- The *generative* approach is typically model-based, and it can generate synthetic data from  $p(\mathbf{x} | C_k)$ .
  - By comparing the synthetic data and real data, we get a sense of how good the generative model is.
- The *discriminative* approach will typically have fewer parameters to estimate and have less assumptions about data distribution.
  - Linear (e.g. logistic regression) v/s quadratic (e.g., Gaussian discriminant analysis) in the dimension of the input.
  - Less generative assumptions about the data (however, constructing the features may require domain knowledge)

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### Any feedback (about lecture, slide, homework, project, etc.)?

(via anonymous google form: <https://forms.gle/fpYmi8tG9Me5qbP37>)



Change Log of lecture slides:

<https://docs.google.com/document/d/e/2PACX-1vSSIHjklvpk7rkFSR1-5GYXyBCEW8UPtpSfCR9AR6M17K9ZOEmxifwaWaW7kLDxusthsF8WICyZJ-/pub>

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