

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)

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:

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

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

- Note that these probability sum to 1.

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

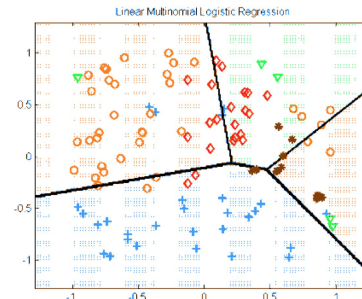
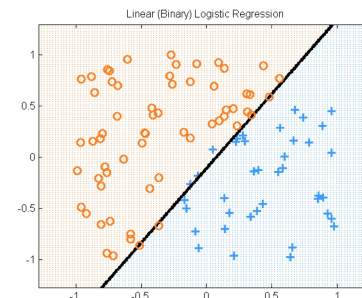
$$p(y = k \mid \mathbf{x}; \mathbf{w}) = \frac{\exp(\mathbf{w}_k^\top \phi(\mathbf{x}))}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^\top \phi(\mathbf{x}))}$$

$$p(y = K \mid \mathbf{x}; \mathbf{w}) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^\top \phi(\mathbf{x}))}$$

for $k = \{1, \dots, K-1\}$

equivalent to setting $\mathbf{w}_K = 0$

- Note that these probability sum to 1.



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

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

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

or

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

- Log-Likelihood

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

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

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

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 $p(\mathbf{x}, C_k)$

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*:

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

Gaussian Discriminant Analysis

Gaussian Discriminant Analysis

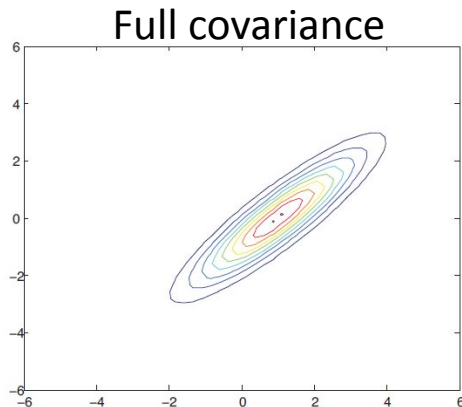
- Probability of class label
 - $p(C_k)$: Constant (e.g., Bernoulli)
- Conditional probability of data given a class
 - $p(\mathbf{x} \mid C_k)$: Gaussian distribution

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

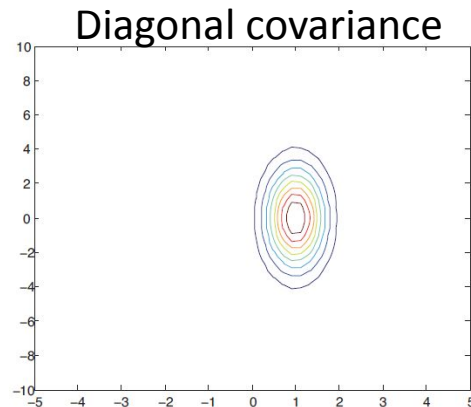
- Classification: use Bayes rule (previous slide)

Examples of Gaussian Distributions

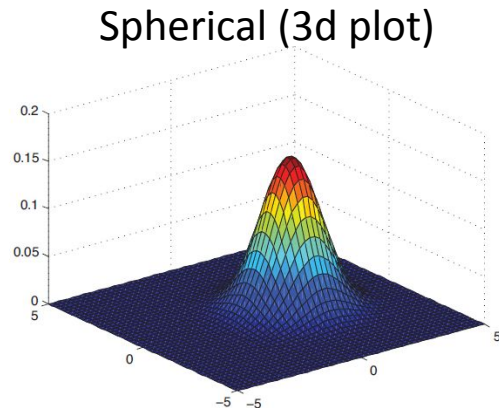
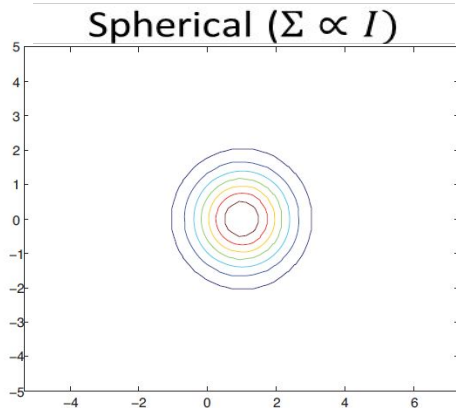
- Probability density $p(x)$ for 2 dimensional case



(a)

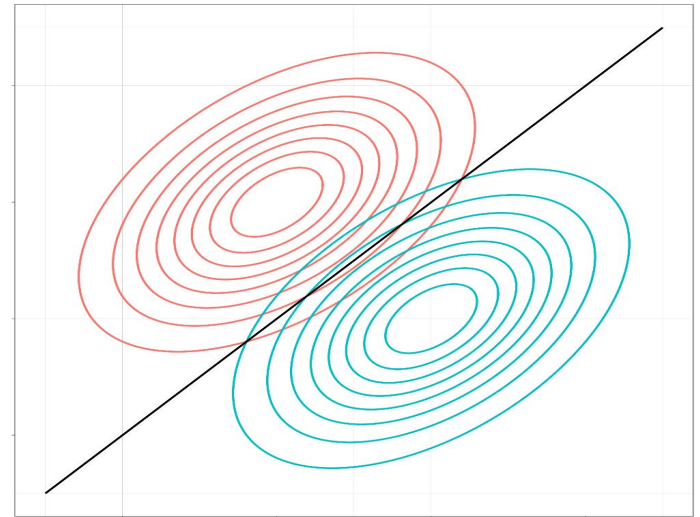
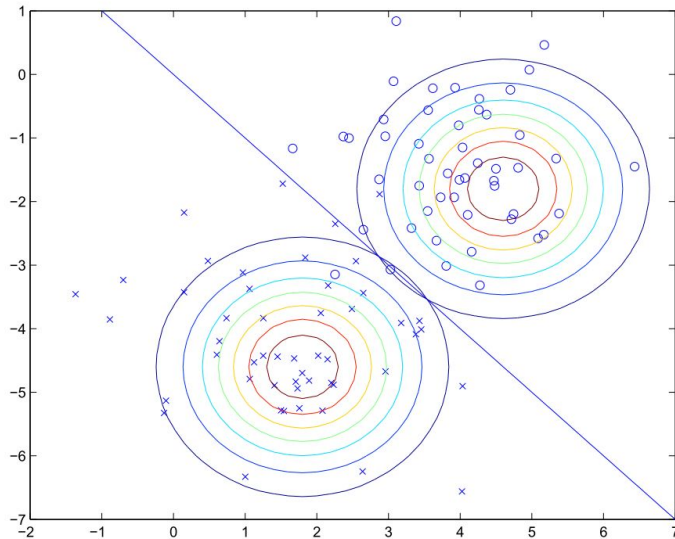


(b)



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!



Prediction: Class-Conditional Densities

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

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

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

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

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

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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$$\log \frac{P(C_1 | \mathbf{x})}{P(C_2 | \mathbf{x})} = \log \frac{P(C_1 | \mathbf{x})}{1 - P(C_1 | \mathbf{x})} \quad \text{“Log-odds”}$$

Derivation

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

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

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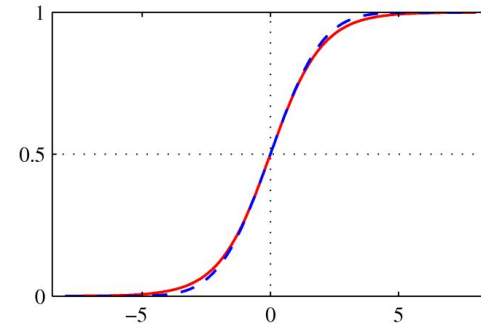
$$\begin{aligned} P(x, C_2) &= P(x | C_2) P(C_2) \\ &= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_2)^\top \Sigma^{-1} (x - \mu_2) \right\} P(C_2) \end{aligned}$$

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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):

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

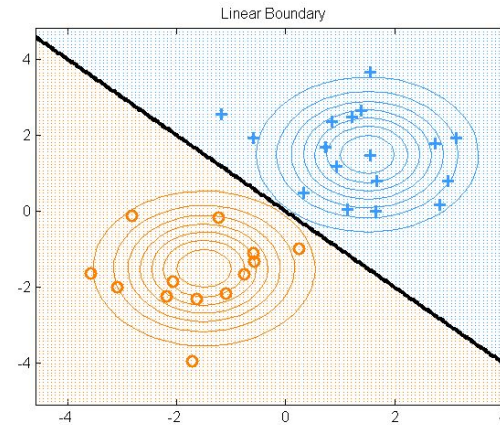
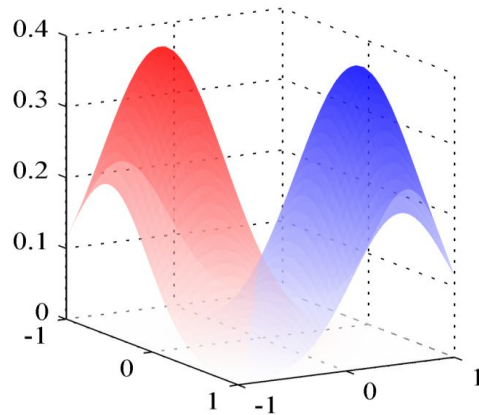
$$\text{where } w_0 = -\frac{1}{2}\mu_1^{\top} \boldsymbol{\Sigma}^{-1} \mu_1 + \frac{1}{2}\mu_2^{\top} \boldsymbol{\Sigma}^{-1} \mu_2 + \log \frac{p(C_1)}{p(C_2)}$$

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

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

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.



Likelihood function of generative models

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

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

Compact notation:
This is called joint likelihood.

Decomposition
of the joint
probability



$$= \prod_{i=1}^N P(\mathbf{x}^{(i)}|y^{(i)}, \mathbf{w})P(y^{(i)}|\mathbf{w})$$

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”)

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

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

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

Learning via maximum likelihood

- Maximum likelihood estimation (HW2):

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

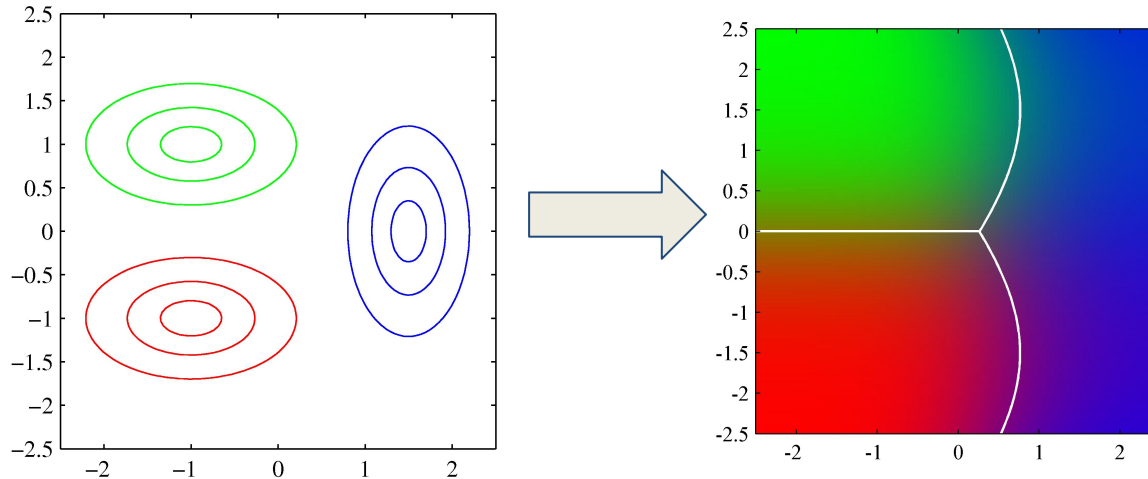
$$\mu_0 = \frac{\sum_{i=1}^N \mathbb{I}\{y^{(i)} = 0\} \mathbf{x}^{(i)}}{\sum_{i=1}^N \mathbb{I}\{y^{(i)} = 0\}}$$

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

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

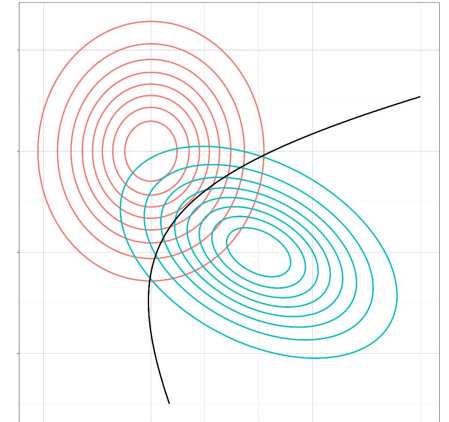
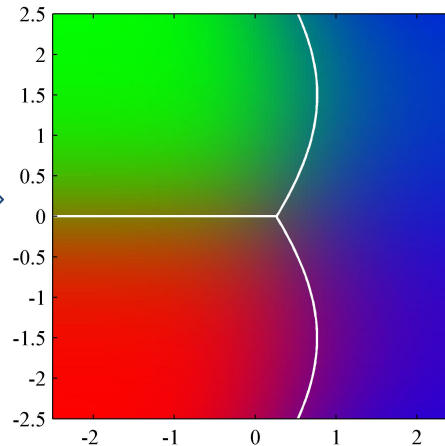
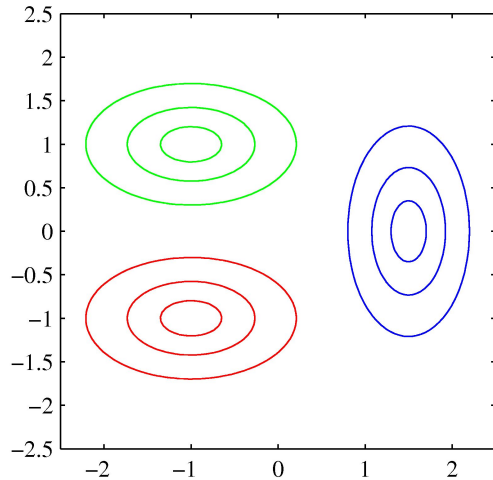
Different Covariance

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



Different Covariance

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



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.

Naive Bayes Classifier

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

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

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

Naive Bayes classifier

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

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

Naive Bayes classifier


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

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

Naive Bayes classifier

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

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

Naive Bayes assumption 

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!!

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)

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

(via **anonymous** google form: <https://forms.gle/fpYmiBtG9Me5qbP37>)



Change Log of lecture slides:

<https://docs.google.com/document/d/e/2PACX-1vSSIHJklypK7rKFSR1-5GYXyBCEW8UPtpSfCR9AR6M1I7K9ZQEmxfFwaWaW7kLDxusthsF8WlCyZJ-/pub>