Using Zoom for Lectures

- **Sign in using:**
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- **Please mute both:**
  - your video cameras for the entire lecture
  - your audio/mics unless asking or answering a question
- **Asking/answering a question, option 1:**
  - click on Participants
  - use the hand icon to raise your hand
  - I will call on you and ask you to unmute yourself
- **Asking/answering a question, option 2:**
  - click on Chat
  - type your question, and I will answer it

Today: Outline

- **Probabilistic Generative Models**
- **Linear Discriminant Analysis**

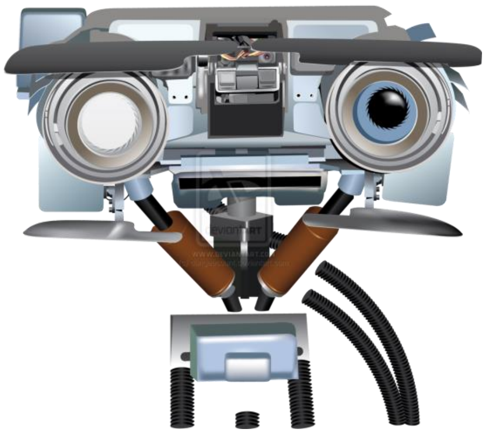
- **Reminders:** PS4 self score, due Apr 3

  Class Challenge will be posted Apr 3

  (3-week challenge)

  Midterm Exam, Apr 15 during class time

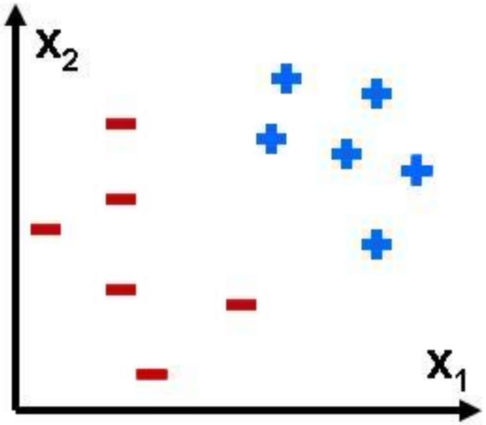
  (covering material up to and including Apr 3)



Probabilistic Generative Models

CS 542 Machine Learning

Probabilistic Classification



$$D = \left(x^{(i)}, y^{(i)}\right) : \text{data}$$
$$x \in \mathbb{R}^p$$
$$y \in \{k\}, k = 1, \dots, K$$

- Can model output value directly, but having a probability is often more useful
- Bayes classifier: minimizes the probability of misclassification

$$y = \underset{k}{\operatorname{argmax}}\, p(Y = k | X = x)$$

- Want to model conditional distribution, $\mathrm{p}(\mathrm{Y} = \mathrm{y}|X = x)$, then assign label based on it

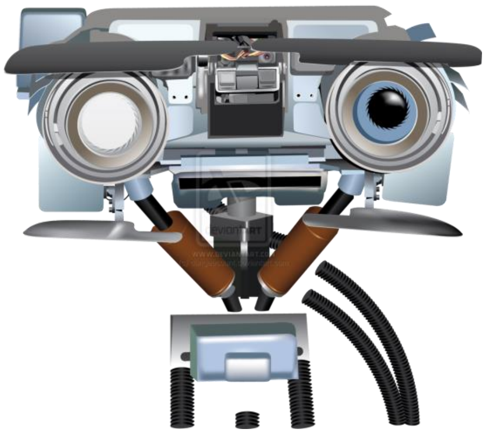
Two approaches to classification

- **Discriminative**: represent $\mathrm{p}(\mathrm{Y}|X)$ as function of parameters θ, then learn θ from training data

- **Generative**: use Bayes Rule

$$P\ (Y = k \mid X = x) = \frac{P(X = x \mid Y = k)P(Y = k)}{P(X = x)}$$

then learn parameters of class-conditional density $\mathrm{p}(\mathrm{X}|\mathrm{Y})$ and class prior $\mathrm{p}(\mathrm{Y})$ --- ignore $p(X)$



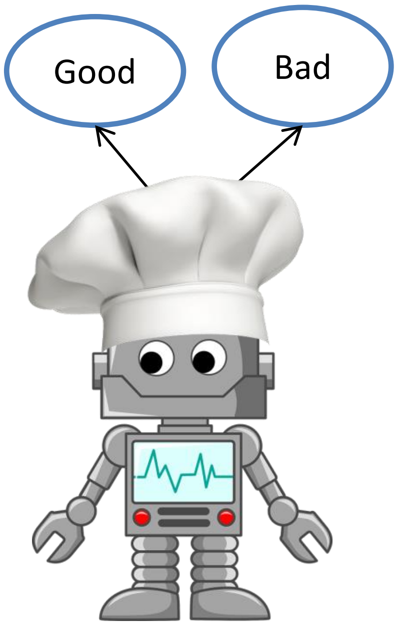
Generative *vs.* Discriminative

Intuition

Cookie Robots

- Suppose you own a cookie factory
- Want to detect bad cookies and discard them

Cookie Robots



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

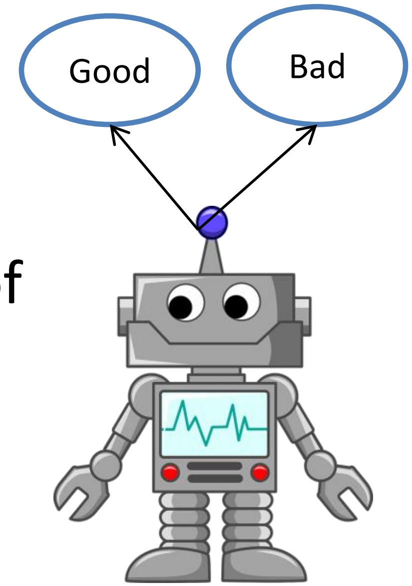
"The Chef"

– Can make good and bad cookies
– Compares new cookie to those
– Decides if it is good or bad

$$P(Y|X)$$

"The Critic"

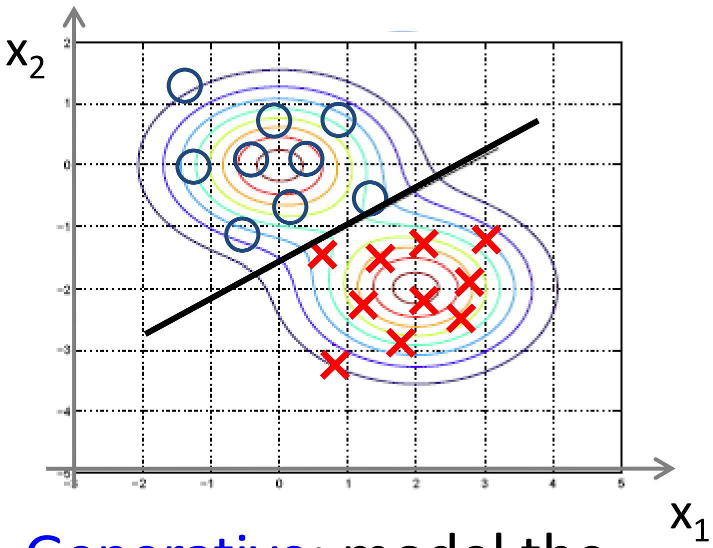
– Cannot make cookies
– Has seen lots of good and bad cookies
– Decides if it is good or bad



$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

Generative vs Discriminative

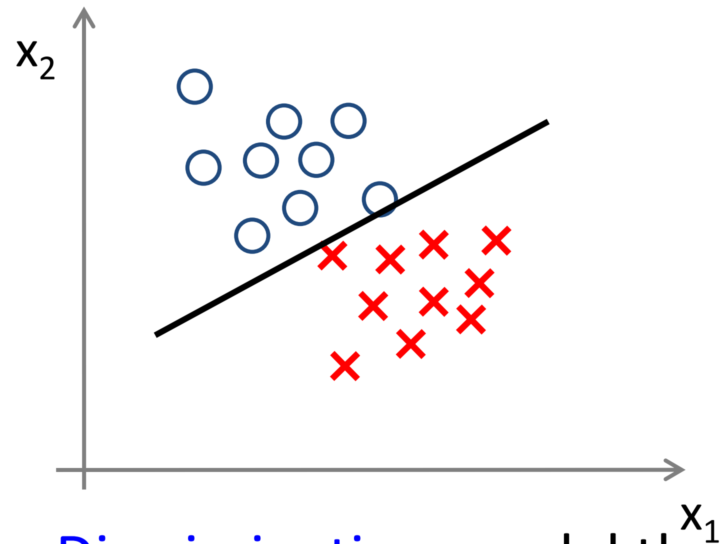
$P(X|Y), P(Y)$



- Generative: model the class-conditional distribution of features, e.g. LDA, Naïve Bayes

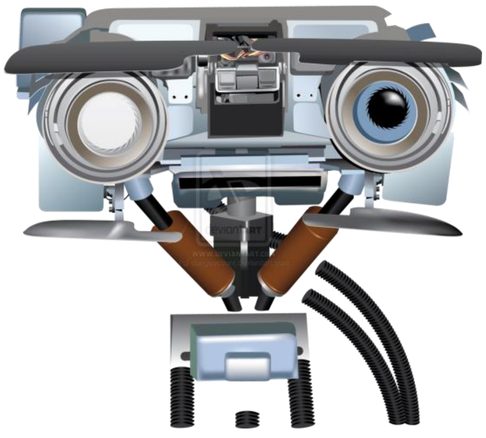
Can sample from distribution

$P(Y|X)$



- Discriminative: model the decision boundary directly, e.g. Logistic Regression, SVM

Cannot sample from distribution



Linear Discriminant Analysis Derivation

Slide credits: Sergio Bacallado

Bayes Classifier

Find an estimate $P(Y \mid X)$. Then, given an input x_0, we predict the output as in a Bayes classifier:

$$y_0 = argmax_y \, P(Y = y_0 \mid X = x_0).$$

Generative Classifier

Instead of estimating $P(Y \mid X)$, we will estimate:

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1. $P(X \mid Y)$: Given the category, what is the distribution of the inputs.

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Then, we use *Bayes rule* to obtain the estimate:

$$P(Y = k \mid X = x) = \frac{P(X = x \mid Y = k) P(Y = k)}{P(X = x)}$$

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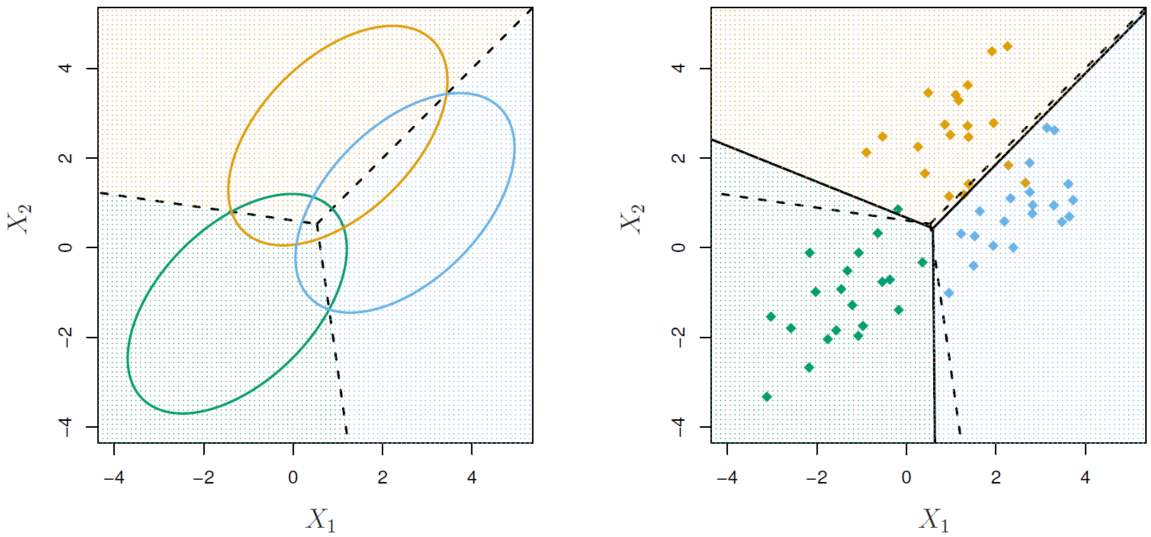
$$P(Y = k \mid X = x) = \frac{P(X = x \mid Y = k)P(Y = k)}{\sum_j P(X = x \mid Y = j)P(Y = j)}$$

Linear Discriminant Analysis (LDA)

Instead of estimating $P\,(Y \mid X)$, we will estimate:

1. We model $P(X = x|Y = k) = f_k(x)$ as a *Multivariate Normal Distribution*:



2. $P(Y = k) = \pi_k$ is estimated by the fraction of training samples of class k.

LDA prior and class-conditional density

Suppose that:

LDA prior and class-conditional density

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LDA prior and class-conditional density

Suppose that:

- We know $P(Y = k) = \pi_k$ exactly.
- $P(X = x|Y = k)$ is Mutivariate Normal with density:

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T\mathbf{\Sigma}^{-1}(x-\mu_k)}$$

LDA prior and class-conditional density

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Suppose that:

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μ_k : Mean of the inputs for category k.

$\boldsymbol{\Sigma}$: Covariance matrix (common to all categories).

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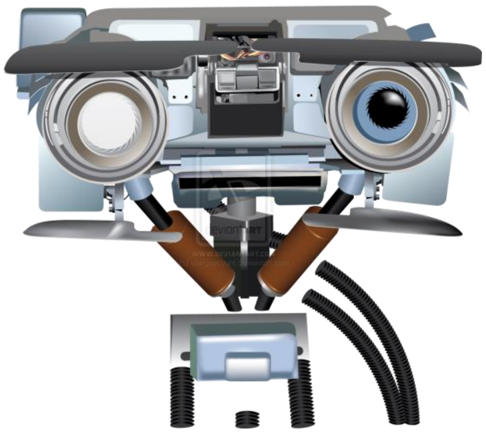
Then, what is the Bayes classifier?



LDA Solution

Slide credits: Sergio Bacallado

LDA has linear decision boundaries

By Bayes rule, the probability of category k, given the input x is:

$$P(Y = k \mid X = x) = \frac{f_k(x)\pi_k}{P(X = x)}$$

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$$P(Y = k \mid X = x) = C \times f_k(x)\pi_k$$

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Now, expanding $f_k(x)$:

$$P(Y = k \mid X = x) = \frac{C\pi_k}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

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Now, let us absorb everything that does not depend on k into a constant C':

$$P(Y=k \mid X=x) = C'\pi_k e^{-\frac{1}{2}(x-\mu_k)^T\mathbf{\Sigma}^{-1}(x-\mu_k)}$$

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and take the logarithm of both sides:

$$\log P(Y = k \mid X = x) = \log C' + \log \pi_k - \frac{1}{2}(x - \mu_k)^T \mathbf{\Sigma}^{-1}(x - \mu_k).$$

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So we want to find the maximum of this over k.

LDA has linear decision boundaries

Goal, maximize the following over k:

$$\log \pi_k - \frac{1}{2}(x - \mu_k)^T \mathbf{\Sigma}^{-1}(x - \mu_k).$$

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$$= C'' + \log \pi_k - \frac{1}{2}\mu_k^T \boldsymbol{\Sigma}^{-1} \mu_k + x^T \boldsymbol{\Sigma}^{-1} \mu_k$$

We define the objective:

$$\delta_k(x) = \log \pi_k - \frac{1}{2}\mu_k^T \boldsymbol{\Sigma}^{-1} \mu_k + x^T \boldsymbol{\Sigma}^{-1} \mu_k$$

At an input x, we predict the output with the highest $\delta_k(x)$.

LDA has linear decision boundaries

What is the decision boundary? It is the set of points in which 2 classes do just as well:

$$\delta_k(x) = \delta_l(x)$$

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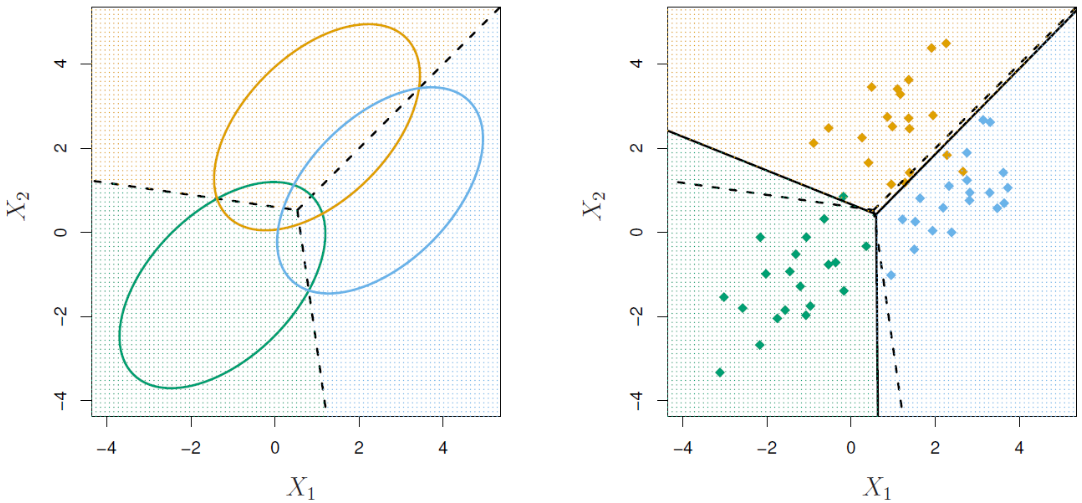
This is a linear equation in x.



Estimating π_k

$$\pi_k = \frac{\#\{i \; ; y_i = k\}}{n}$$

In English, the fraction of training samples of class k.

Estimating the parameters of $f_k(x)$

Estimate the center of each class μ_k:

$$\mu_k = \frac{1}{\#\{i; y_i = k\}} \sum_{i; y_i = k} x_i$$

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Estimate the common covariance matrix $\mathbf{\Sigma}$:

- One dimension ($p = 1$):

$$\sigma^2 = \frac{1}{n - K} \sum_{k=1}^{K} \sum_{i;\, y_i = k} (x_i - \mu_k)^2$$

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- Many dimensions ($p > 1$): Compute the vectors of deviations $(x_1 - \mu_{y_1}), (x_2 - \mu_{y_2}), \ldots, (x_n - \mu_{y_n})$ and use an estimate of its covariance matrix, $\mathbf{\Sigma}$.

LDA prediction

For an input x, predict the class with the largest:

$$\delta_k(x) = \log \pi_k - \frac{1}{2}\mu_k^T \boldsymbol{\Sigma}^{-1}\mu_k + x^T \boldsymbol{\Sigma}^{-1}\mu_k$$

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The decision boundaries are defined by:

$$\log \pi_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}^{-1}\mu_k + x^T \mathbf{\Sigma}^{-1}\mu_k = \log \pi_l - \frac{1}{2}\mu_l^T \mathbf{\Sigma}^{-1}\mu_l + x^T \mathbf{\Sigma}^{-1}\mu_l$$

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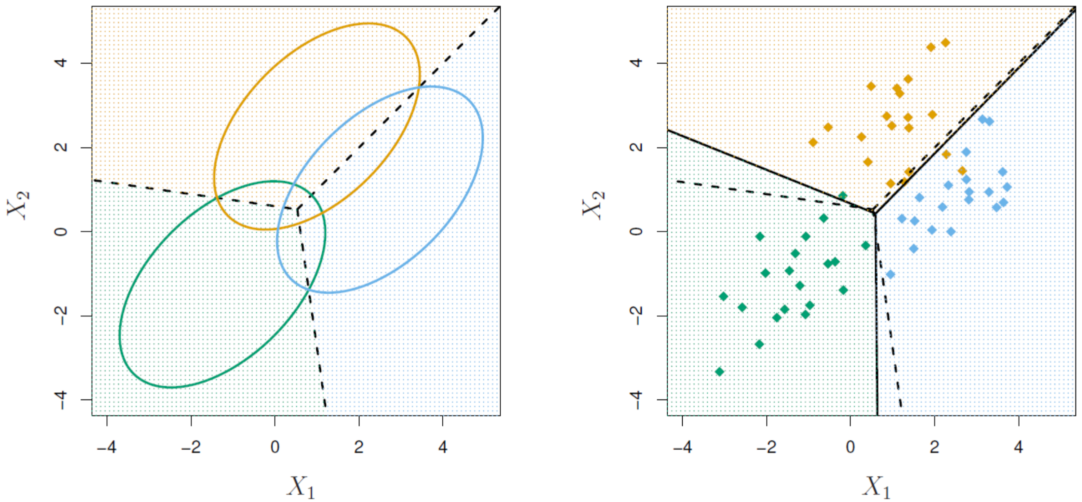
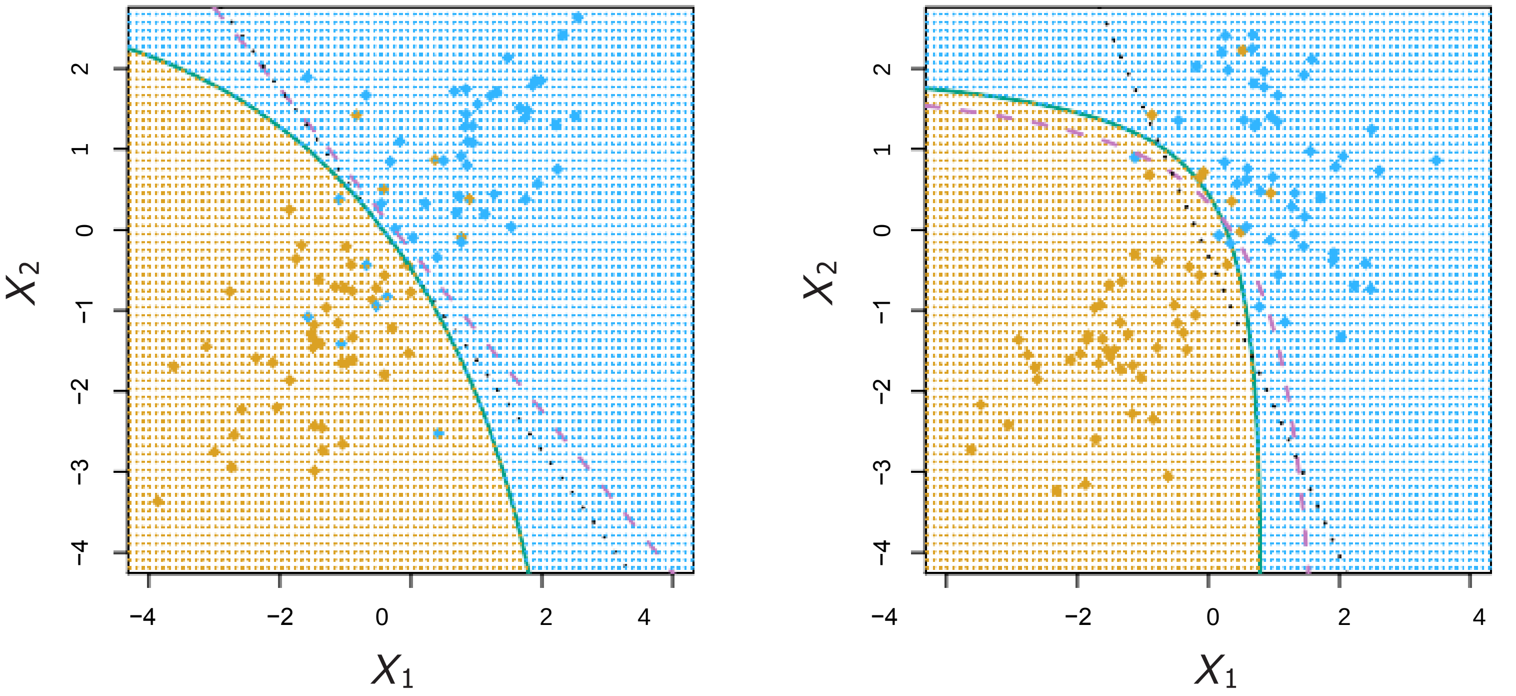
Solid lines in:



Quadratic discriminant analysis (QDA)

The assumption that the inputs of every class have the same covariance **Σ** can be quite restrictive:



Quadratic discriminant analysis (QDA)

In **quadratic discriminant analysis** we estimate a mean μ_k and a covariance matrix $\mathbf{\Sigma}_k$ for each class separately.

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Given an input, it is easy to derive an objective function:

$$\delta_k(x) = \log \pi_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}_k^{-1}\mu_k + x^T \mathbf{\Sigma}_k^{-1}\mu_k - \frac{1}{2}x^T \mathbf{\Sigma}_k^{-1}x - \frac{1}{2}\log|\mathbf{\Sigma}_k|$$

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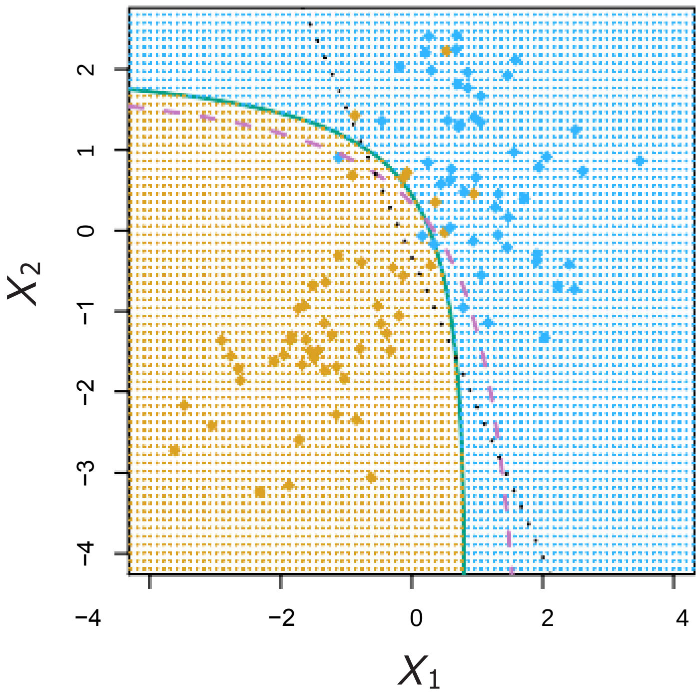
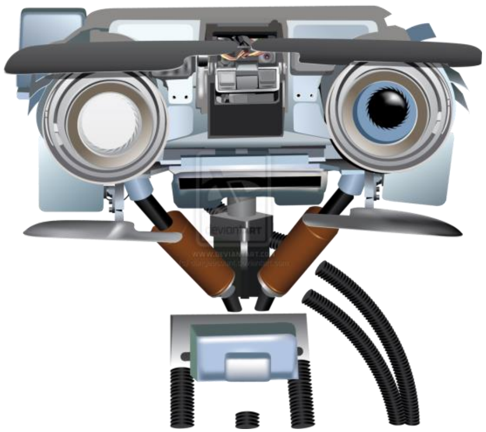
This objective is now quadratic in x and so are the decision boundaries.

Quadratic discriminant analysis (QDA)

- Bayes boundary (– – –)
- LDA (· · · · · · ·)
- QDA (——).





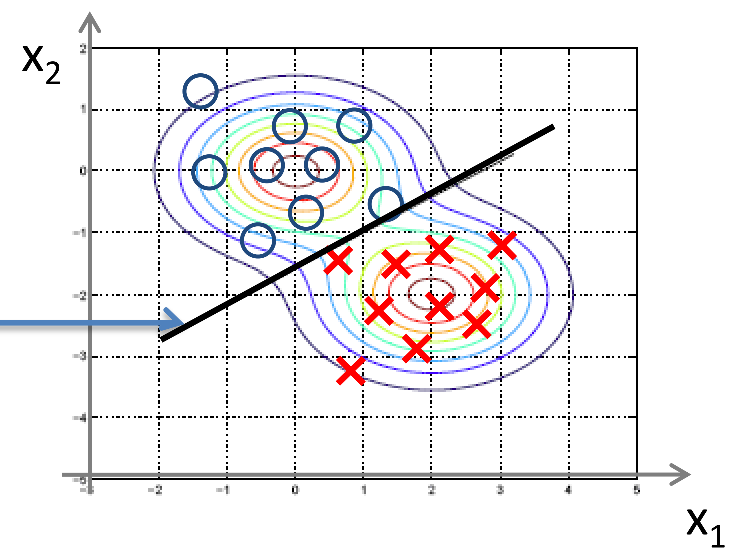
Linear Discriminant Analysis

More intuition

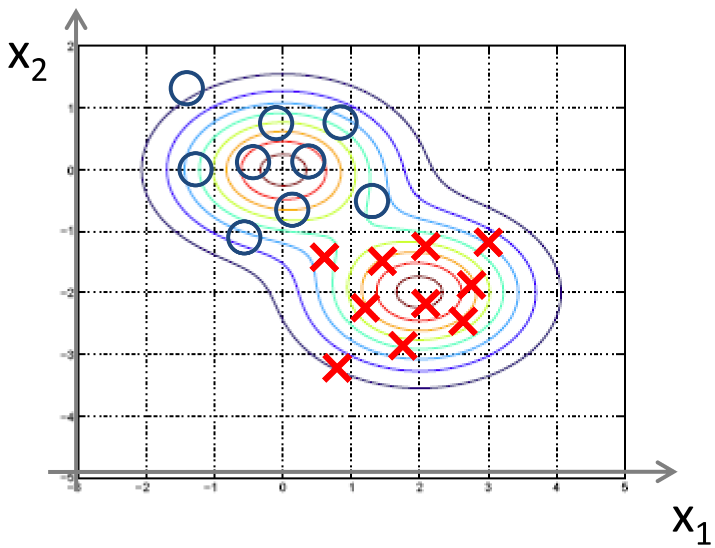
Illustration of Decision Boundary

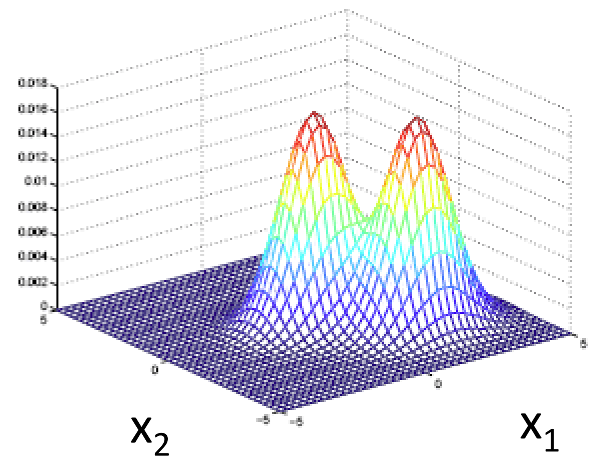
$$\underbrace{\log\frac{\pi_k}{\pi_l}}_{\text{class prior log-ratio}} - \underbrace{\frac{1}{2}(\mu_k+\mu_l)^T\Sigma^{-1}(\mu_k-\mu_l)}_{\text{constant}} + \underbrace{x^T}_{\text{input}}\underbrace{\Sigma^{-1}}_{\text{covariance}}\underbrace{(\mu_k-\mu_l)}_{\text{diff. in class means}} = 0$$

Can re-write as $\theta_0 + x^T\theta = 0$



Effect of Covariance Matrix





- covariance matrix determines the shape of the Gaussian density, so
- in LDA, the Gaussian densities for different classes have the same shape, but are shifted versions of each other (different mean vectors).

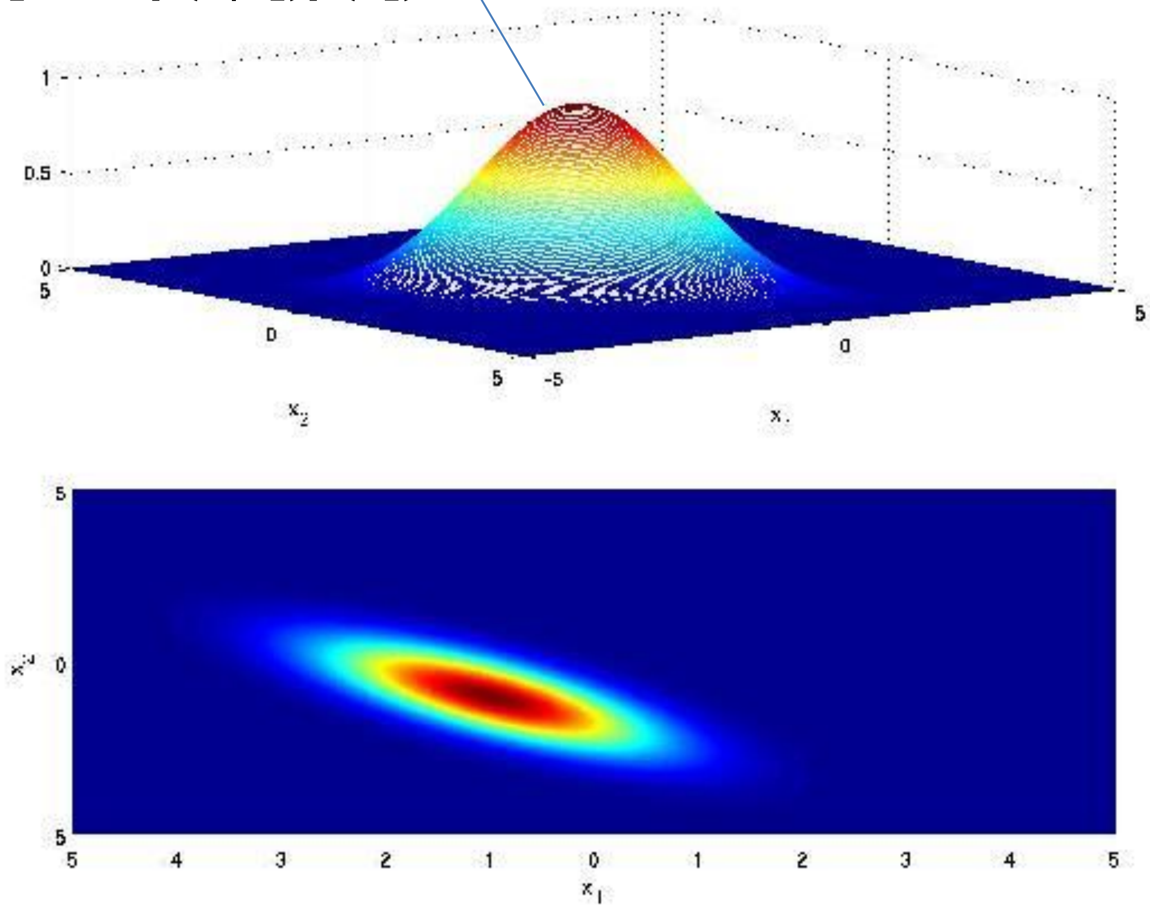
Effect of Class Prior

- What effect does the prior p(class), or π_k, have?
- Lets look at an example for 2 classes…

$$\boxed{\log \frac{\pi_k}{\pi_l}} - \boxed{\frac{1}{2}(\mu_k + \mu_l)^T \Sigma^{-1} (\mu_k - \mu_l)} + \boxed{x^T}\boxed{\Sigma^{-1}}\boxed{(\mu_k - \mu_l)} = 0$$

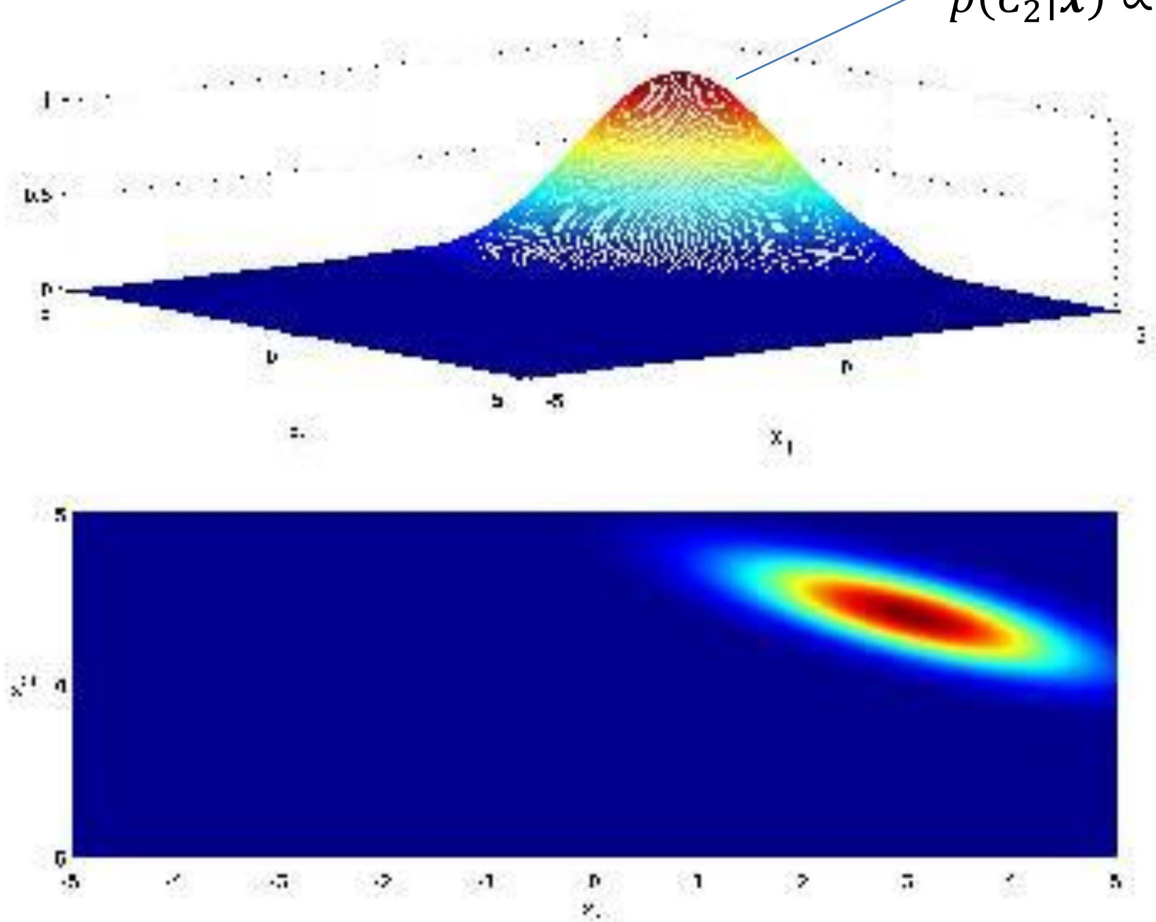
class prior
log-ratio

$p(C_1|\boldsymbol{x}) \propto p(\boldsymbol{x}|C_1)p(C_1)$



Model class-conditional probability of a 2D feature vector for class 1 as a multivariate Gaussian density.

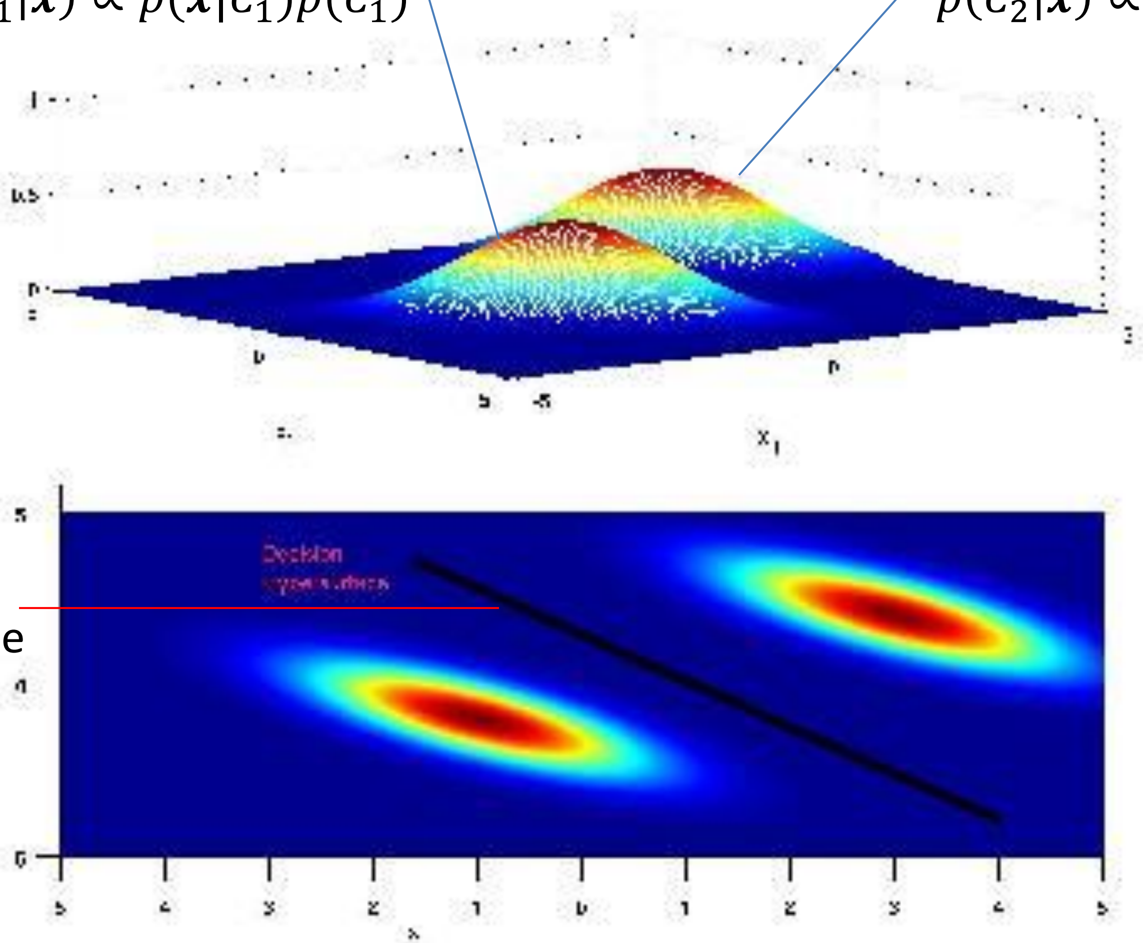
$p(C_2|\boldsymbol{x}) \propto p(\boldsymbol{x}|C_2)p(C_2)$



Now consider class 2 with a similar Gaussian conditional density, which has the same covariance but a different mean

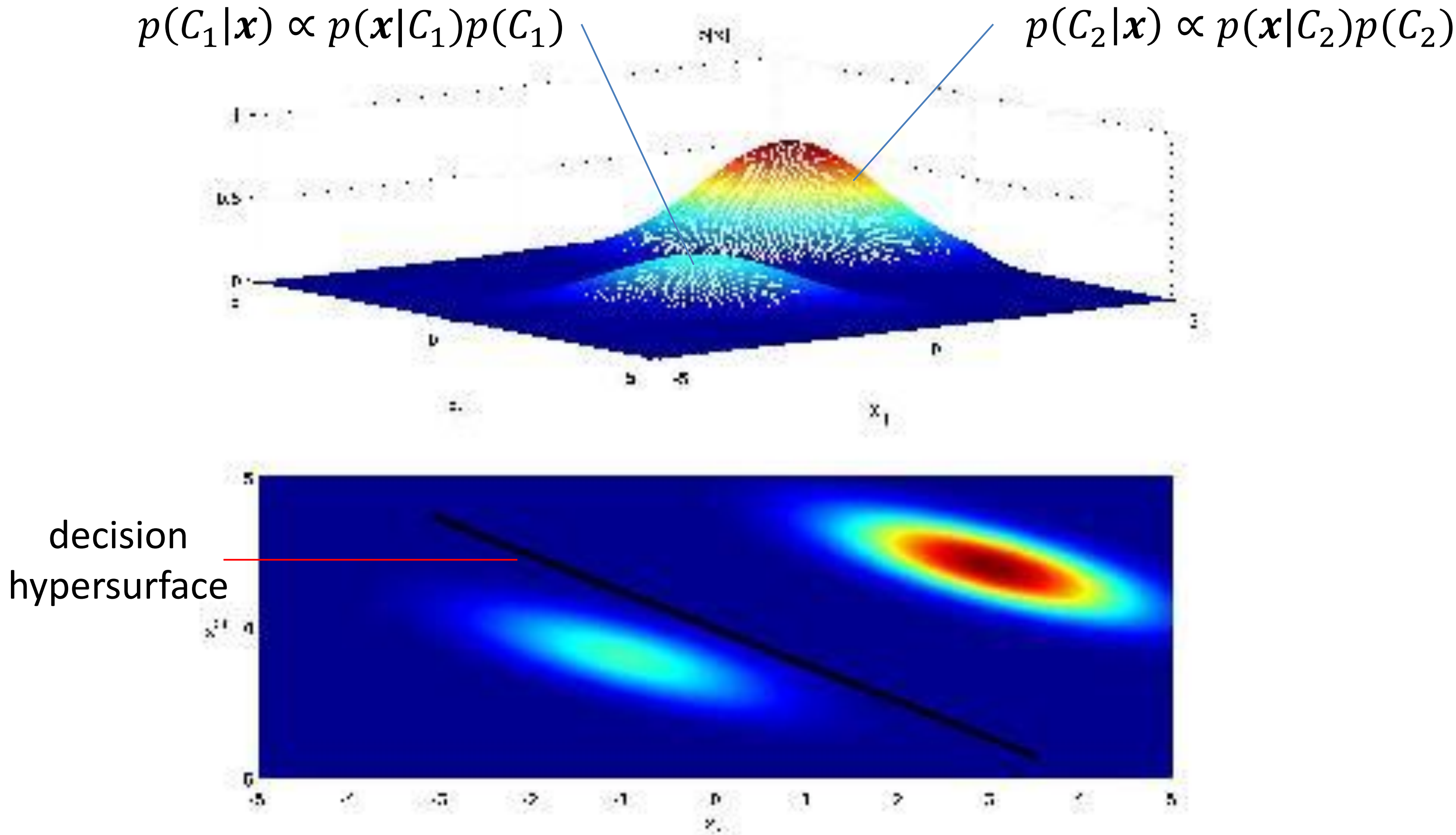
$p(C_1|\boldsymbol{x}) \propto p(\boldsymbol{x}|C_1)p(C_1)$

$p(C_2|\boldsymbol{x}) \propto p(\boldsymbol{x}|C_2)p(C_2)$



decision hypersurface

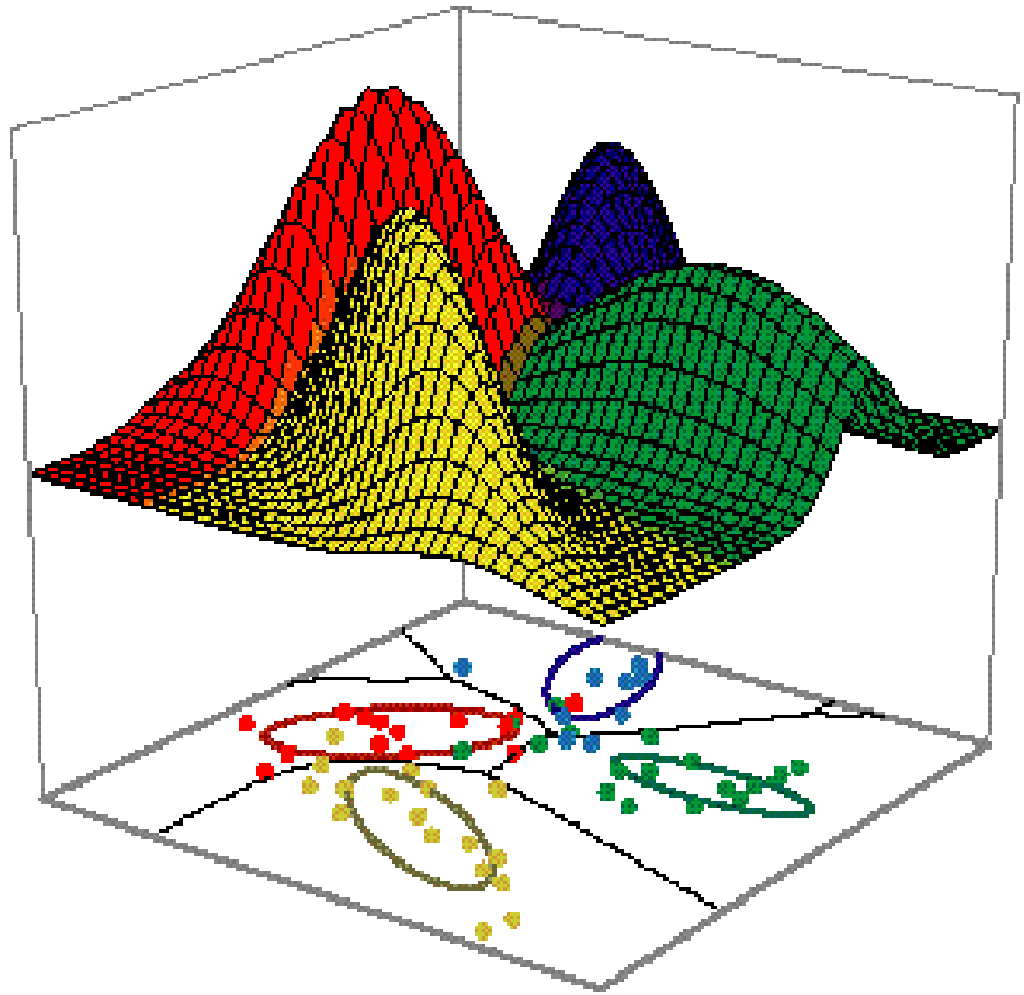
If the priors for each class are the same (i.e. 0.5), then the decision hypersurface cuts directly between the two means, with a direction parallel to the elliptical shape of the modes of the Gaussian densities shaped by their (identical) covariance matrices.



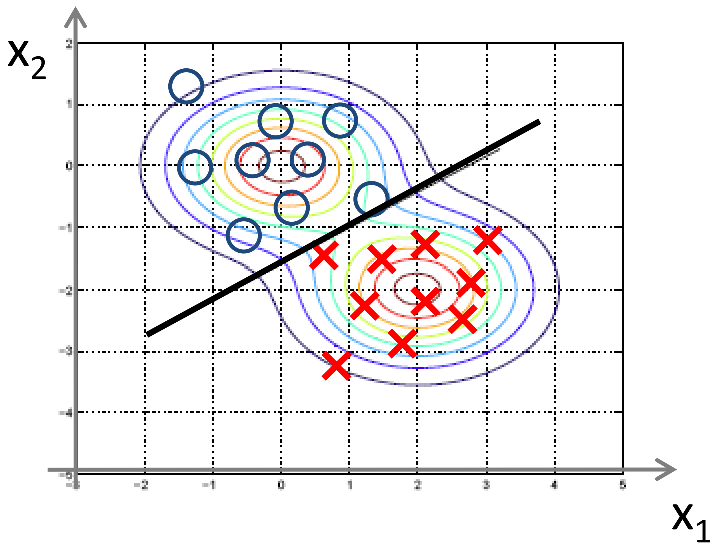
Now if the priors for each class are unequal, the decision hypersurface cuts between the two means with a direction as before, but now will be located further from the more likely class. This biases the predictor in favor of the more likely class.

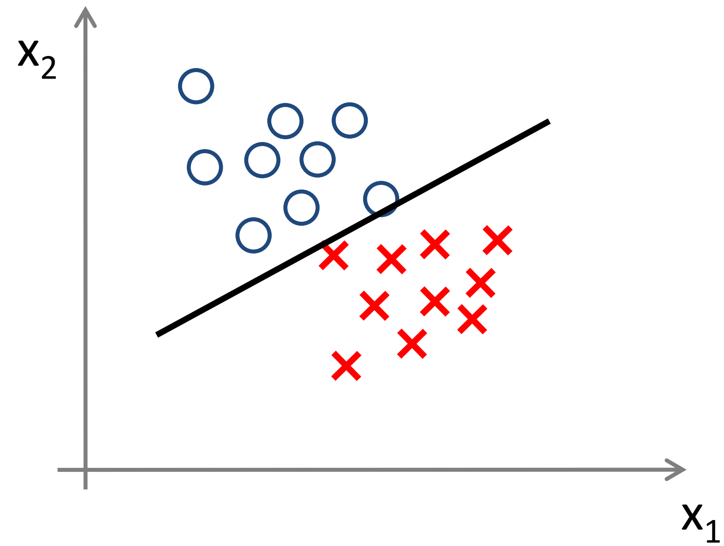
More than two classes, unequal covariances

- more general case of unequal covariances (here shown for four classes)
- QDA
- the decision hypersurface is no longer a hyperplane, i.e. it is nonlinear.



Generative vs Discriminative





- Generative: model the class-conditional distribution of features
- Can use it to generate new features

- Discriminative: model the decision boundary directly, e.g. Logistic Regression
- Cannot generate new features

Do they produce the same classifier?

- **Generative LDA approach**
  θ_j and θ_0 are functions of μ1,μ2, and Σ . In particular, θ_j and θ_0 are not completely independent.

- **Discriminative approach (logistic regression)**
  Directly estimates θ_j and θ_0, without assuming any constraints between them, by maximizing conditional likelihood p(y|x)

- The two methods will give **different** decision boundaries, even if both are linear.