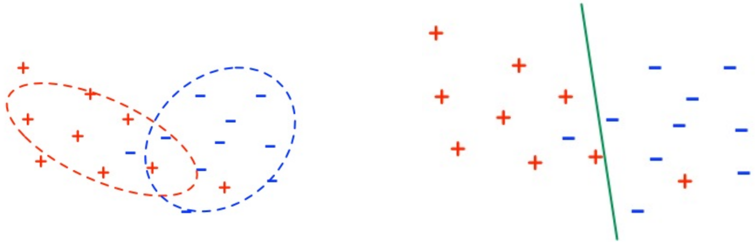
Classification with generative models II

DSE 210

Classification with parametrized models

Classifiers with a fixed number of parameters can represent a limited set of functions. Learning a model is about picking a good approximation.

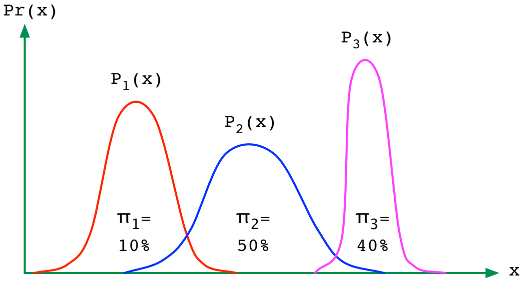
Typically the x's are points in p-dimensional Euclidean space, $\mathbb{R}^p$.



Two ways to classify:

- **Generative**: model the individual classes.
- **Discriminative**: model the decision boundary between the classes.

The Bayes-optimal prediction



Labels $\mathcal{Y} = \{1, 2, \ldots, k\}$, density $\Pr(x) = \pi_1 P_1(x) + \cdots + \pi_k P_k(x)$.

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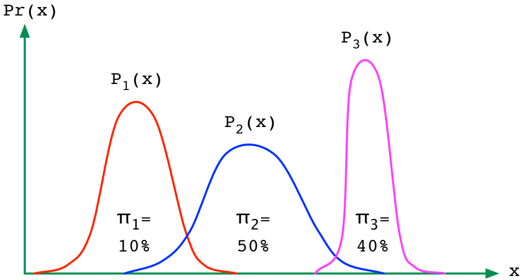

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For any $x \in \mathcal{X}$ and any label j,

$$\Pr(y = j | x) = \frac{\Pr(y = j)\Pr(x | y = j)}{\Pr(x)} = \frac{\pi_j P_j(x)}{\sum_{i=1}^{k} \pi_i P_i(x)}$$

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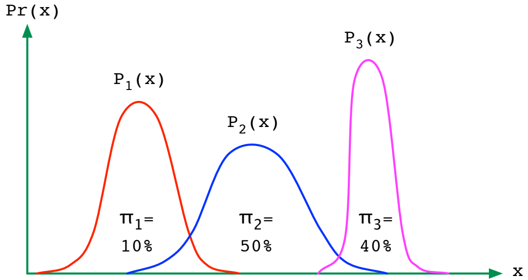

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Bayes-optimal prediction: $h^*(x) = \arg\max_j \pi_j P_j(x)$.

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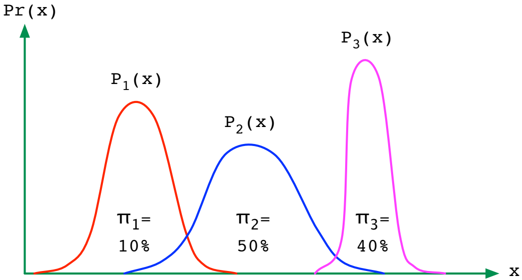

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Estimating the π_j is easy. Estimating the P_j is hard.

Estimating class-conditional distributions

Estimating an arbitrary distribution in $\mathbb{R}^p$:

- Can be done, e.g. with kernel density estimation.
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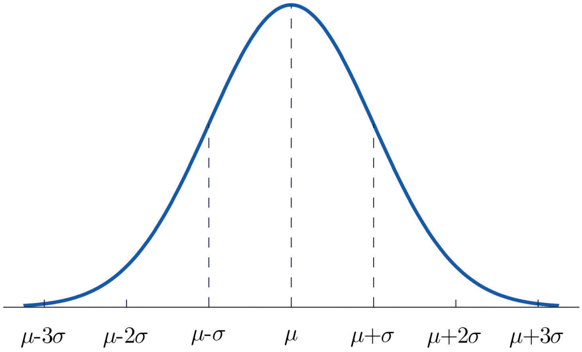
Instead: approximate each P_j with a simple, parametric distribution.

Some options:

- Product distributions.
  Assume coordinates are independent: naive Bayes.
- Multivariate Gaussians.
  Linear and quadratic discriminant analysis.
- More general graphical models.

The univariate Gaussian



The Gaussian $N(\mu, \sigma^2)$ has mean μ, variance σ^2, and density function

$$p(x) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right).$$

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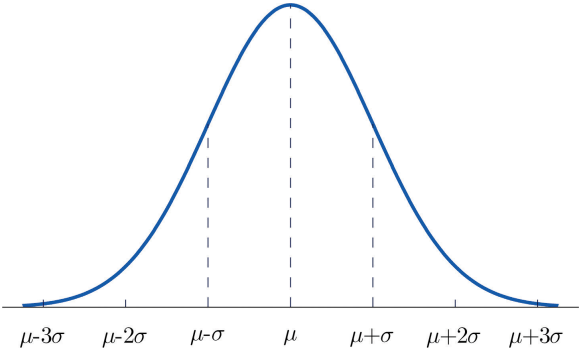

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But what if we have **two** variables?

Bivariate distributions

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Example: For a large collection of people, measure the two variables

$$H = \text{height}$$
$$W = \text{weight}$$

Independence would mean

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which would also imply $\mathbb{E}(HW) = \mathbb{E}(H)\mathbb{E}(W)$.

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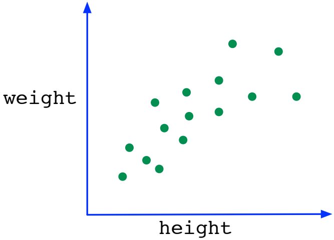
Is this an accurate approximation?
No: we'd expect height and weight to be **positively correlated**.

Types of correlation



H, W positively correlated.
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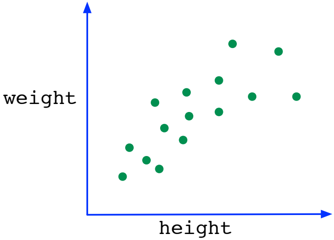

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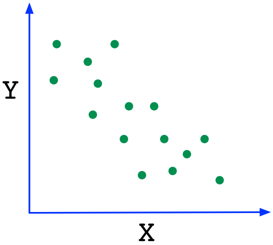
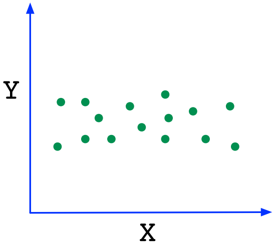
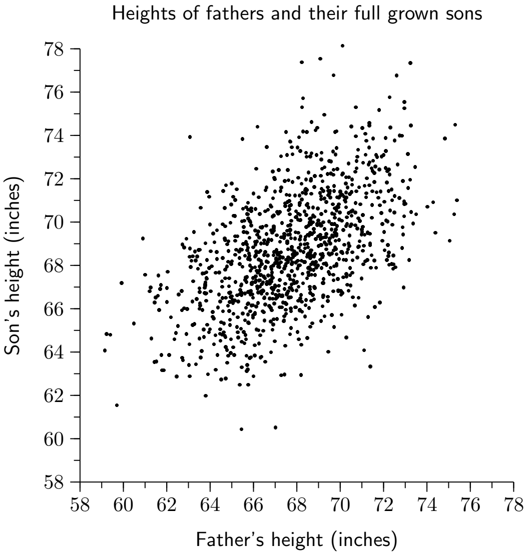


X, Y negatively correlated



X, Y uncorrelated

Pearson (1903): fathers and sons



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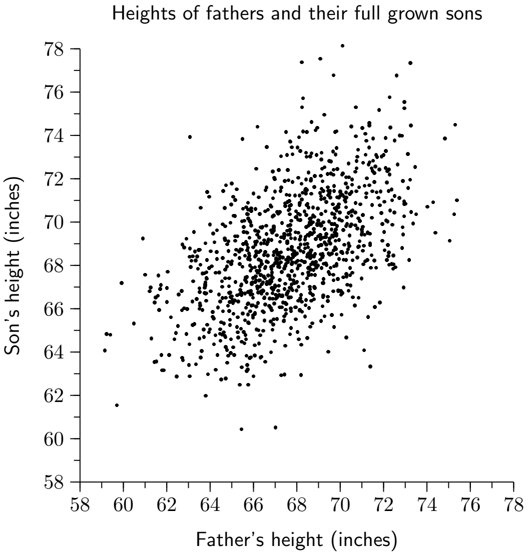
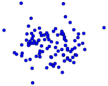


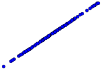
How to quantify the degree of correlation?

Correlation pictures

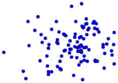
$r = 0$



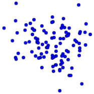
$r = 1$



$r = 0.25$



$r = -0.25$



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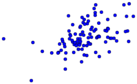
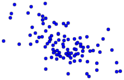
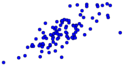


$r = -0.5$



$r = 0.75$



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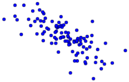

Covariance and correlation

Suppose X has mean μ_X and Y has mean μ_Y.

- Covariance

$$\mathrm{cov}(X, Y) = \mathbb{E}[(X - \mu_X)(Y - \mu_Y)] = \mathbb{E}[XY] - \mu_X \mu_Y$$

  Maximized when $X = Y$, in which case it is $\mathrm{var}(X)$.
  In general, it is at most $\mathrm{std}(X)\mathrm{std}(Y)$.

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- Correlation

  $$\text{corr}(X, Y) = \frac{\text{cov}(X, Y)}{\text{std}(X)\text{std}(Y)}$$

  This is always in the range $[-1, 1]$.

Covariance and correlation: example 1

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x	y	$\Pr(x, y)$
-1	-1	$1/3$
-1	1	$1/6$
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$$\begin{aligned} \mu_X &= \\ \mu_Y &= \\ \text{var}(X) &= \\ \text{var}(Y) &= \\ \text{cov}(X, Y) &= \\ \text{corr}(X, Y) &= \end{aligned}$$

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$$\begin{aligned} \mu_X &= 0 \\ \mu_Y &= -1/3 \\ \mathrm{var}(X) &= 1 \\ \mathrm{var}(Y) &= 8/9 \\ \mathrm{cov}(X, Y) &= 0 \\ \mathrm{corr}(X, Y) &= 0 \end{aligned}$$

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In this case, X, Y are independent. Independent variables always have zero covariance and correlation.

Covariance and correlation: example 2

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-1	-10	$1/6$
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$$\mu_X =$$

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$$\begin{aligned}
\mu_X &= 0 \\
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In this case, X and Y are negatively correlated.

The bivariate (2-d) Gaussian

A distribution over $(x, y) \in \mathbb{R}^2$, parametrized by:

- **Mean** $(\mu_x, \mu_y) \in \mathbb{R}^2$
- **Covariance matrix**

$$\Sigma = \begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{bmatrix}$$

where $\Sigma_{xx} = \text{var}(X),\ \Sigma_{yy} = \text{var}(Y),\ \Sigma_{xy} = \Sigma_{yx} = \text{cov}(X, Y)$

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Density $\quad p(x, y) = \dfrac{1}{2\pi|\Sigma|^{1/2}} \exp\left(-\dfrac{1}{2}\begin{bmatrix} x - \mu_x \\ y - \mu_y \end{bmatrix}^T \Sigma^{-1} \begin{bmatrix} x - \mu_x \\ y - \mu_y \end{bmatrix}\right)$

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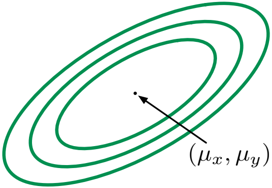
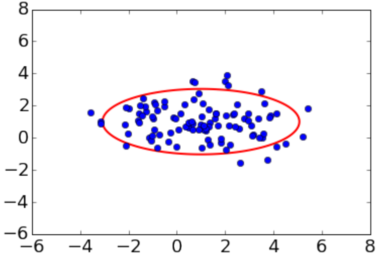
The density is highest at the mean, and falls off in ellipsoidal contours.

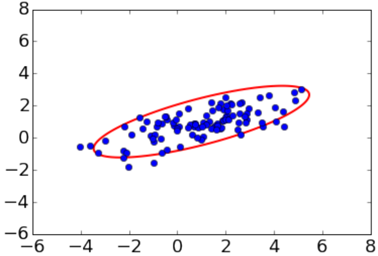


Bivariate Gaussian: examples

In either case, the mean is $(1, 1)$.

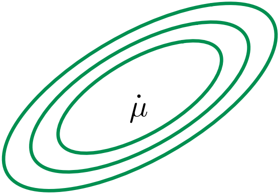


$$\Sigma = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\Sigma = \begin{bmatrix} 4 & 1.5 \\ 1.5 & 1 \end{bmatrix}$$

The multivariate Gaussian



$N(\mu, \Sigma)$: Gaussian in $\mathbb{R}^p$

- mean: $\mu \in \mathbb{R}^p$
- covariance: $p \times p$ matrix Σ

Density $\quad p(x) = \dfrac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\dfrac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$

Let $X = (X_1, X_2, \ldots, X_p)$ be a random draw from $N(\mu, \Sigma)$.

- μ is the vector of coordinate-wise means:

$$\mu_1 = \mathbb{E}X_1,\ \mu_2 = \mathbb{E}X_2, \ldots,\ \mu_p = \mathbb{E}X_p.$$

- Σ is a matrix containing all pairwise covariances:

$$\begin{aligned} \Sigma_{ij} = \Sigma_{ji} &= \text{cov}(X_i, X_j) \quad \text{if } i \neq j \\ \Sigma_{ii} &= \text{var}(X_i) \end{aligned}$$

- In matrix/vector form: $\mu = \mathbb{E}X$ and $\Sigma = \mathbb{E}(X-\mu)(X-\mu)^T$.

Special case: spherical Gaussian

The X_i are independent and all have the same variance σ^2. Thus

$$\Sigma = \sigma^2 I_p = \mathrm{diag}(\sigma^2, \sigma^2, \ldots, \sigma^2)$$

(off-diagonal elements zero, diagonal elements σ^2).

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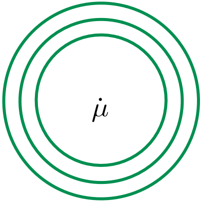
Density at a point depends only on its distance from μ:



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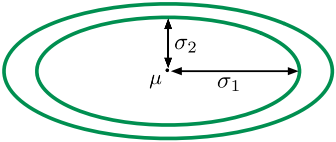
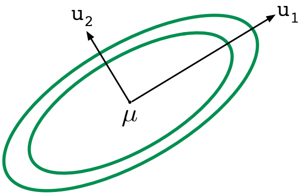
Contours of equal density are axis-aligned ellipsoids centered at μ:



The general Gaussian $N(\mu, \Sigma)$ in $\mathbb{R}^p$



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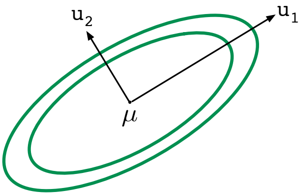

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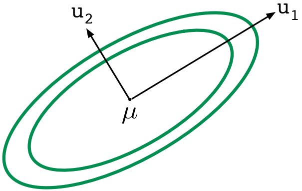

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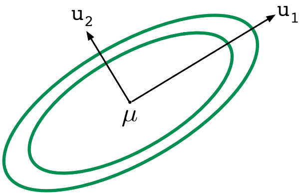

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If we write $S = \Sigma^{-1}$ then S is a $p \times p$ matrix and

$$(x-\mu)^T\Sigma^{-1}(x-\mu) \;=\; \sum_{i,j} S_{ij}(x_i-\mu_i)(x_j-\mu_j),$$

a **quadratic function** of x.

Binary classification with Gaussian generative model

Estimate class probabilities π_1, π_2 and fit a Gaussian to each class:

$$P_1 = N(\mu_1, \Sigma_1), \quad P_2 = N(\mu_2, \Sigma_2)$$

E.g. If data points $x^{(1)}, \ldots, x^{(m)} \in \mathbb{R}^p$ are class 1:

$$\mu_1 \; = \; \frac{1}{m}\left(x^{(1)} + \cdots + x^{(m)}\right) \quad \text{and} \quad \Sigma_1 \; = \; \frac{1}{m}\sum_{i=1}^{m}(x^{(i)} - \mu_1)(x^{(i)} - \mu_1)^T$$

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$\Sigma_1 = \Sigma_2$: **linear** decision boundary. Otherwise, **quadratic** boundary.

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When $\Sigma_1 = \Sigma_2 = \Sigma$: choose class 1 iff

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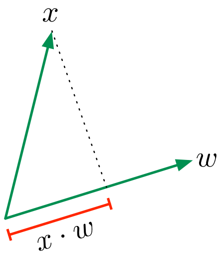
Geometrically: Suppose w is a unit vector (that is, $\|w\| = 1$). Then $x \cdot w$ is the projection of vector x onto direction w.



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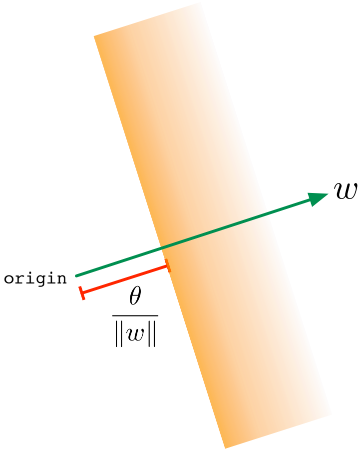
Let w be any vector in $\mathbb{R}^p$. What is meant by decision rule $w \cdot x \geq \theta$?



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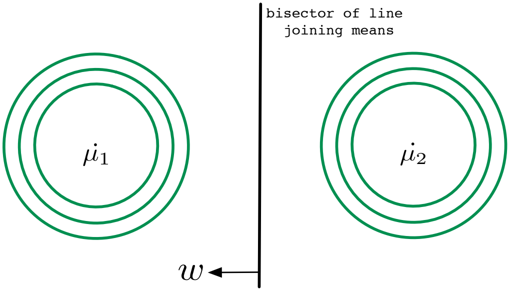
Example 1: Spherical Gaussians with $\Sigma = I_p$ and $\pi_1 = \pi_2$.



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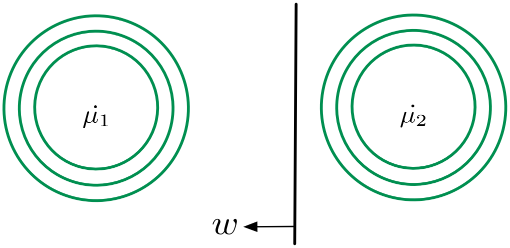

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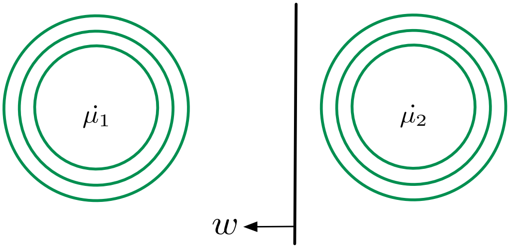
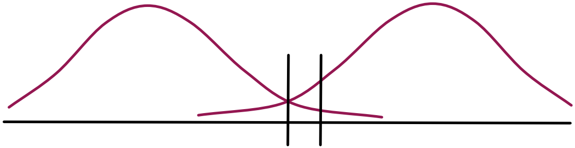


One-d projection onto w:



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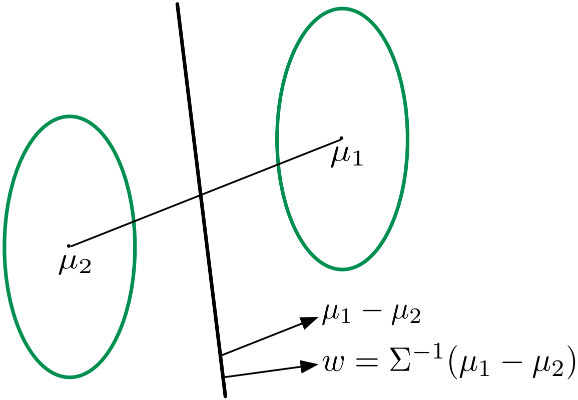

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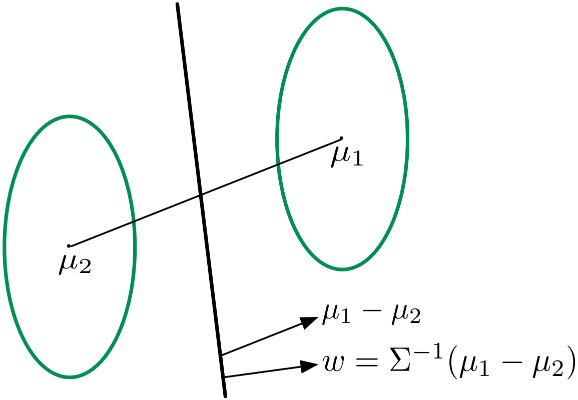

Rule: $w \cdot x \geq \theta$

- w, θ dictated by probability model, assuming it is a perfect fit
- Common practice: choose w as above, but fit θ to minimize training/validation error

Different covariances: $\Sigma_1 \neq \Sigma_2$

Quadratic boundary: choose class 1 iff $x^T M x + 2w^T x \geq \theta$, where:

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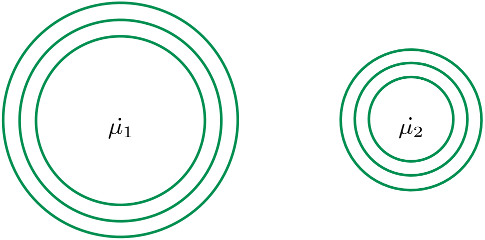

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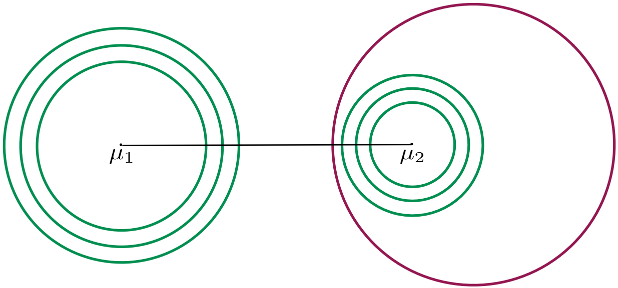

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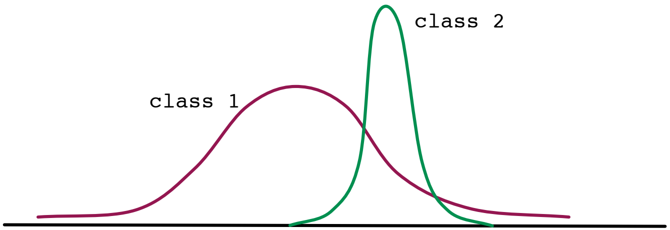

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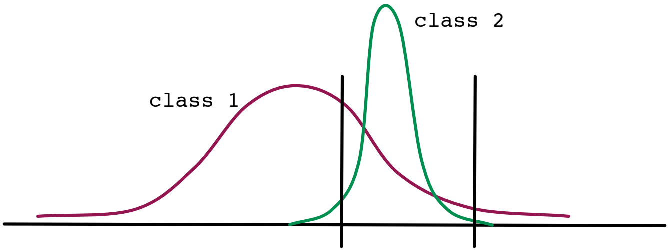

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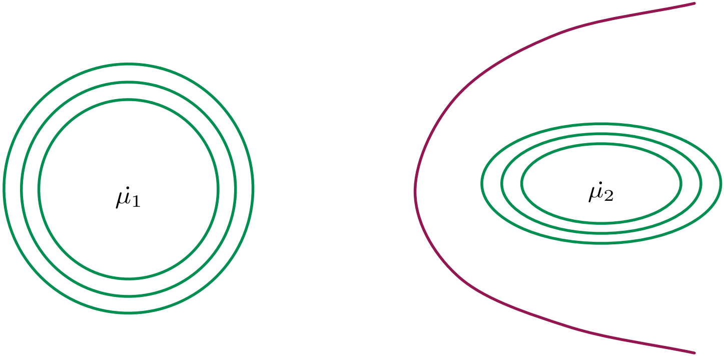

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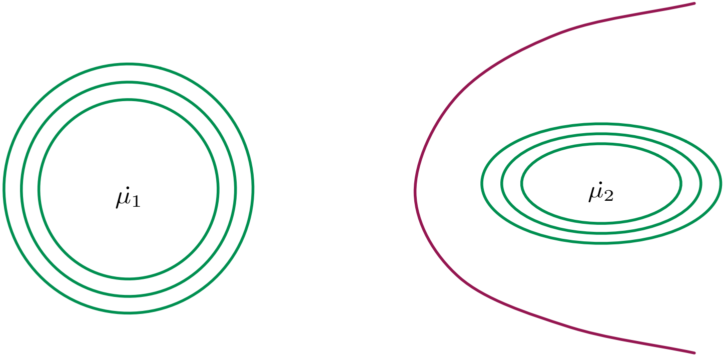

Many other possibilities!

Multiclass discriminant analysis

k classes: weights π_j, class-conditional distributions $P_j = N(\mu_j, \Sigma_j)$.

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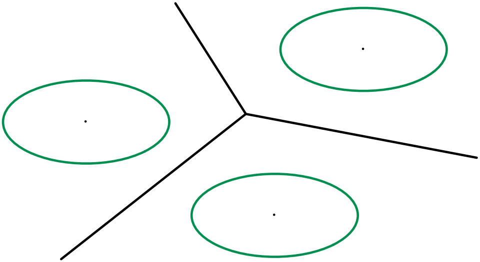
If $\Sigma_1 = \cdots = \Sigma_k$, the boundaries are **linear**.



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Data from three wineries from the same region of Italy

- 13 attributes: hue, color intensity, flavanoids, ash content, ...
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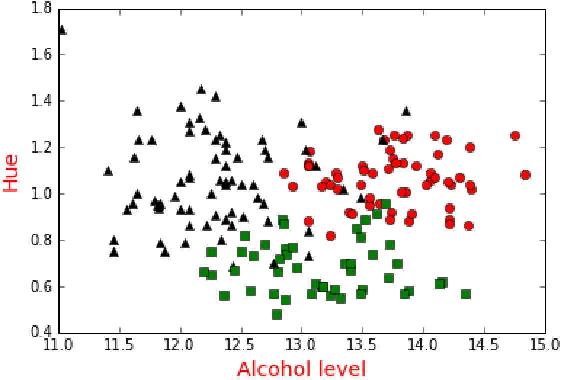

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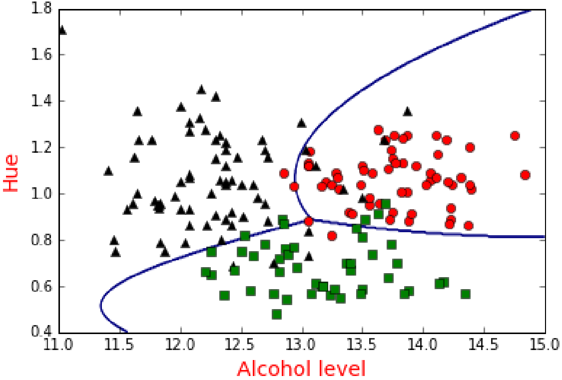

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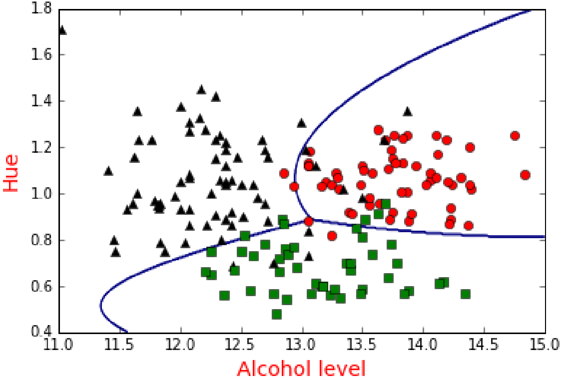

Test error using multiclass discriminant analysis: 1/60

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How to choose c? With a **validation set**.

- Divide original training set into a training set and a validation set.
- Fit parameters π_j, μ_j, Σ_j to training set
- Choose the constant c that yields lowest error rate on validation set

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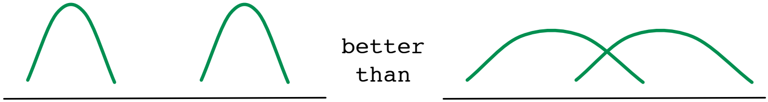

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Solution: $w \propto \Sigma^{-1}(\mu_1 - \mu_2)$. Look familiar?