

Classification with Generative Models

DSE 220

Previous Class..

- Introduction
 - Myself
 - TAs
 - Course
 - Machine Learning
 - ***Hands-On: Intro to scikit-learn***
- Nonparametric Methods
 - Decision Trees
 - ***Hands-On***
 - ***Self – practice***
 - kNN
 - ***Hands-On***
 - ***Self – practice***

Today

- Parametric Methods
 - Generative Models
 - Naive Bayes
 - Binary Features, Multinomial Features
 - ***Hands-On***
 - ***Self – practice***
 - Gaussian Generative Model
 - Fisher Linear Discriminant Analysis
 - ***Hands-On***
 - ***Self – practice***

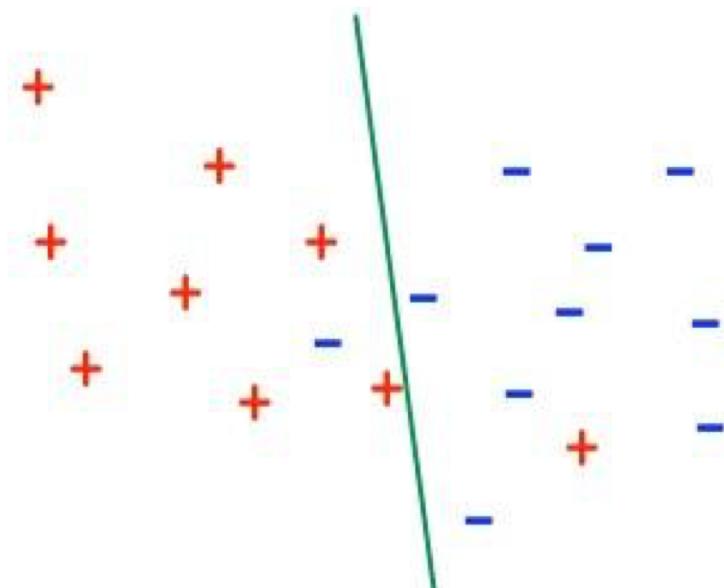
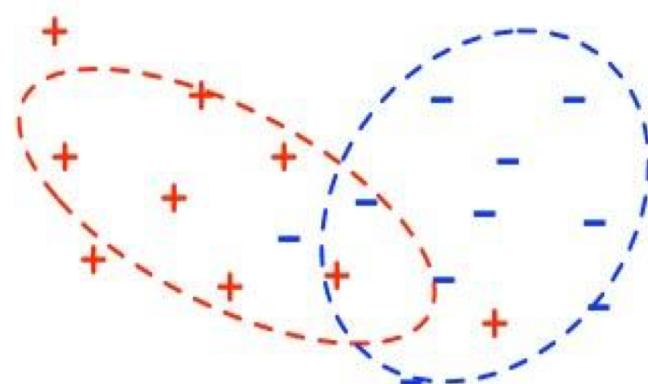
Today

- Regression Analysis
 - *Hands-On*
 - *Self – practice*
- Evaluation Metrics
 - Accuracy, Recall, Precision, Sensitivity, Specificity,...
 - ROC Curves
 - *Hands-On*
 - *Self – practice*

Classification with parametrized models

Classifiers with a fixed no. 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.

Quick review of conditional probability

Formula for conditional probability for any events A, B ,

$$\Pr(A|B) = \frac{\Pr(A \cap B)}{\Pr(B)}$$

Applied twice, this yields Bayes' rule:

$$\Pr(H|E) = \frac{\Pr(E|H)}{\Pr(E)} \Pr(H)$$

Example: Toss ten coins. What is the probability that the first is heads, given that nine of them are heads?

H = first coin is heads

E = nine of the ten coins are heads

$$\Pr(H|E) = \frac{\Pr(E|H)}{\Pr(E)} \cdot \Pr(H) = \frac{\binom{9}{8} \frac{1}{2^9}}{\binom{10}{9} \frac{1}{2^{10}}} \cdot \frac{1}{2} = \frac{9}{10}$$

Why Bayes' Rule?

$$\Pr(H|E) = \frac{\Pr(E|H)}{\Pr(E)} \Pr(H)$$

- describes the probability of an event based on prior knowledge of conditions that might be related to the event

Quick Quiz

- Suppose a disease is related to age. Probability of a patient having liver disease is 0.1, and the probability of an incoming patient being alcoholic is 0.05. If the probability of being alcoholic given that the person has liver disease is 0.07, then what is the probability of an incoming patient having liver disease given that he is alcoholic?

Quick Quiz

- Suppose a disease is related to age. Probability of a patient having liver disease is 0.1, and the probability of an incoming patient being alcoholic is 0.05. If the probability of being alcoholic given that the person has liver disease is 0.07, then what is the probability of an incoming patient having liver disease given that he is alcoholic?

A = Patient has liver disease

B = Patient is an alcoholic

$$P(A) = 0.10, P(B) = 0.05, P(B|A) = 0.07$$

$$P(A|B) = (0.07 * 0.1)/0.05 = 0.14$$

Disjoint and Independent Events

Disjoint or Mutually Exclusive

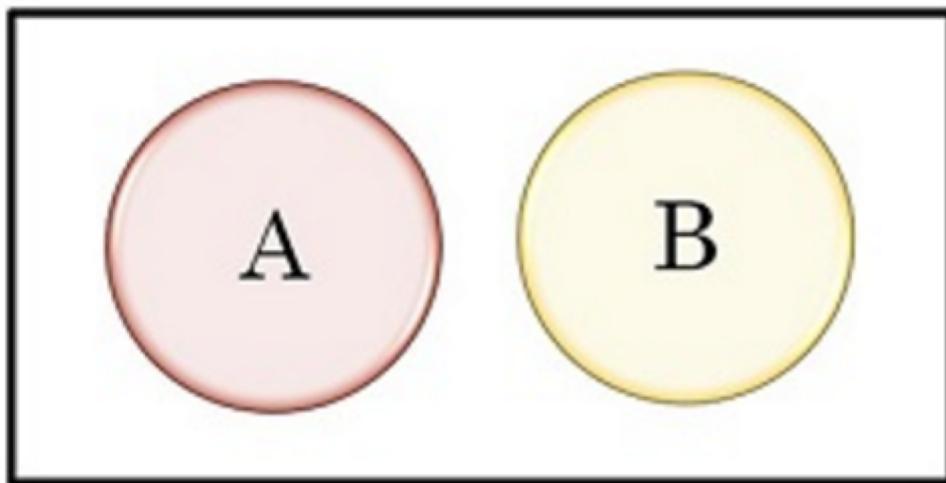
- Disjoint events cannot happen at the same time.
- e.g.: when tossing a coin, the result can either be heads or tails but cannot be both.

Independent

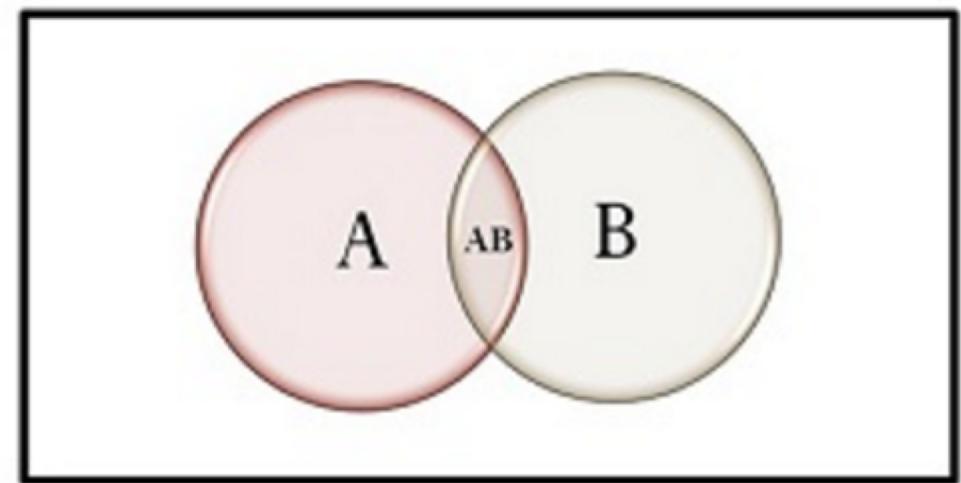
- Occurrence of one event does not influence the other(s).
- e.g.: when tossing two coins, the result of one flip does not affect the result of the other.

Disjoint and Independent Events

Disjoint Events



Independent Events



Summation rule

Suppose events A_1, \dots, A_k are disjoint events, one of which must occur. Then for any other event E ,

$$\begin{aligned}\Pr(E) &= \Pr(E \cap A_1) + \Pr(E \cap A_2) + \dots + \Pr(E \cap A_k) \\ &= \Pr(E|A_1)\Pr(A_1) + \Pr(E|A_2)\Pr(A_2) + \dots + \Pr(E|A_k)\Pr(A_k)\end{aligned}$$

Example: Sex bias in graduate admissions In 1969, there were 12673 applicants for graduate study at Berkeley. 44% of the male applicants were accepted, and 35% of the female applicants.

Over the sample space of applicants, define:

M = male

F = female

A = admitted

So: $\Pr(A|M) = 0.44$ and $\Pr(A|F) = 0.35$.

In every department, the accept rate for female applicants was at least as high as the accept rate for male applicants. How could this be?

Generative models

An unknown underlying distribution D over $X \times Y$.

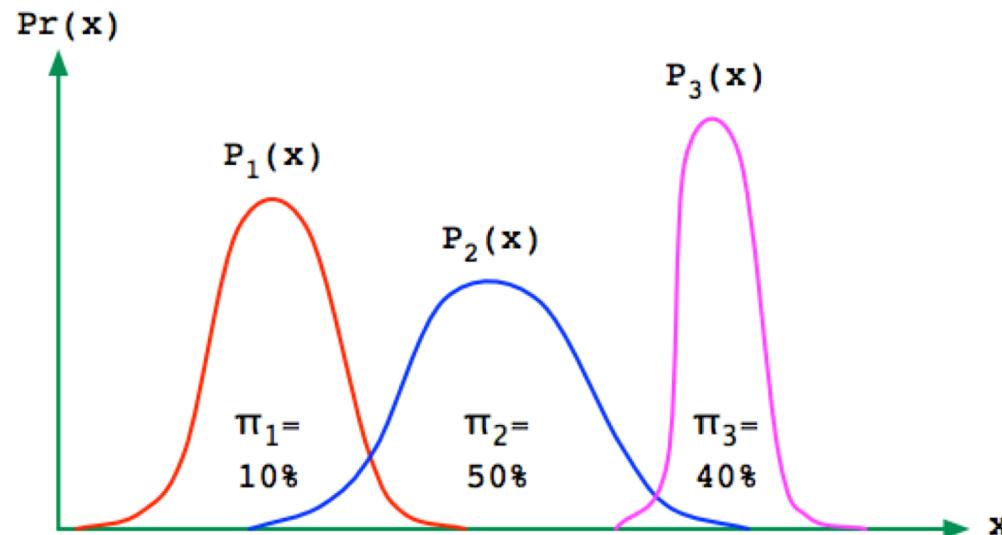
Generating a point (x, y) in two steps:

- ① When we were studying NN: first choose x , then choose y given x .
- ② Now: first choose y , then choose x given y .

Example:

$$X = \mathbb{R}$$

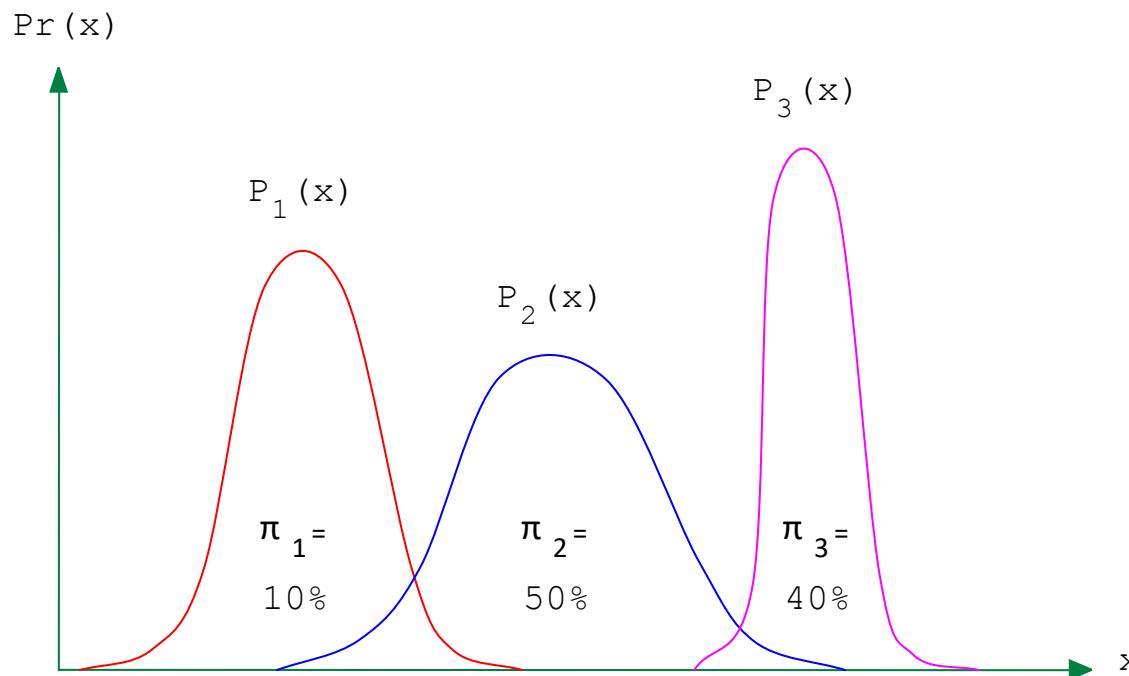
$$Y = \{1, 2, 3\}$$



The overall density is a mixture of the individual densities,

$$\Pr(x) = \pi_1 P_1(x) + \cdots + \pi_k P_k(x).$$

The Bayes-optimal prediction



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

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

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

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

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 hard.

Solution: 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.

Naive Bayes

- ① Probabilistic model (fits $P(\text{label} | \text{data})$)
- ② Makes a conditional independence assumption that features are independent given the label.

$$P(\text{feature}_i, \text{feature}_j | \text{label}) = P(\text{feature}_i | \text{label}) \cdot P(\text{feature}_j | \text{label})$$

$$\text{posterior} \quad \text{prior} \quad \text{likelihood}$$
$$p(\text{label} | \text{features}) = \frac{p(\text{label}) p(\text{features} | \text{label})}{p(\text{features})}$$

evidence

The diagram illustrates the components of the Naive Bayes posterior probability formula. The formula is $p(\text{label} | \text{features}) = \frac{p(\text{label}) p(\text{features} | \text{label})}{p(\text{features})}$. The word "posterior" is positioned above the equals sign and points to the result. The words "prior" and "likelihood" are positioned above the first term in the numerator and point to it. The word "evidence" is positioned below the denominator and points to it.

Naive Bayes

Due to the conditional independence assumption, we get

$$p(label|features) = \frac{p(label) \prod_i p(feature_i|label)}{p(features)}$$

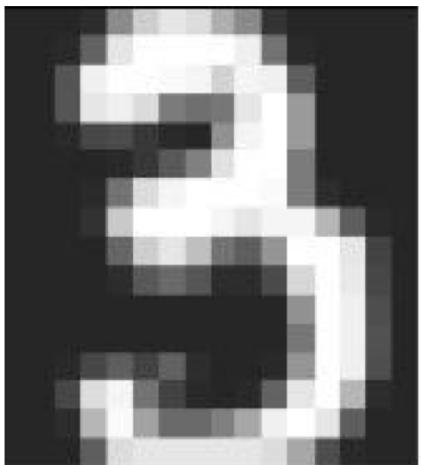
Denominator doesn't matter because we are interested in

$$p(label|features) \text{ vs. } p(\neg label|features)$$

both of which have same denominator

Naive Bayes

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



Binarized MNIST:

- $k = 10$ classes
- $X = \{0, 1\}^{784}$

Assume that **within each class**, the individual pixel values are independent.

$$P_j(x) = P_{j1}(x_1) \cdot P_{j2}(x_2) \cdots P_{j,784}(x_{784}).$$

Smoothed estimate of coin bias

Pick a class j and a pixel i . We need to estimate

$$p_{ji} = \Pr(x_i = 1 | y = j).$$

Out of a training set of size n ,

$$n_j = \# \text{ of instances of class } j$$

$$n_{ji} = \# \text{ of instances of class } j \text{ with } x_i = 1$$

Then the maximum-likelihood estimate of p_{ji} is

$$\hat{p}_{ji} = n_{ji} / n_j.$$

This causes problems if $n_{ji} = 0$. Instead, use “Laplace smoothing”:

$$\hat{p}_{ji} = \frac{n_{ji} + 1}{n_j + 2}.$$

Maximum Likelihood

Given observed values $X_1 = x_1, X_2 = x_2 \dots X_n = x_n$.

$\text{Likelihood}(\theta) = \text{probability of observing the given data as a function of } \theta$.

Maximum Likelihood estimate of $\theta = \text{value of } \theta \text{ that maximises } \text{Likelihood}(\theta)$.

Form of the classifier

Data space $X = \{0, 1\}^p$, label space $Y = \{1, \dots, k\}$. Estimate:

- $\{\pi_j : 1 \leq j \leq k\}$
- $\{p_{ji} : 1 \leq j \leq k, 1 \leq i \leq p\}$

Then classify point x as

$$\arg \max_j \pi_j \prod_{i=1}^p p_{ji}^{x_i} (1 - p_{ji})^{1-x_i}.$$

To avoid underflow: take the log:

$$\arg \max_j \log \pi_j + \underbrace{\sum_{i=1}^p (x_i \log p_{ji} + (1 - x_i) \log(1 - p_{ji}))}_{\text{of the form } w \cdot x + b}$$

A linear classifier!

$$w_i^{(j)} = \log(p_{ji}) - \log(1 - p_{ji}), b^{(j)} = \log(\pi_j) + \sum_i \log(1 - p_{ji})$$

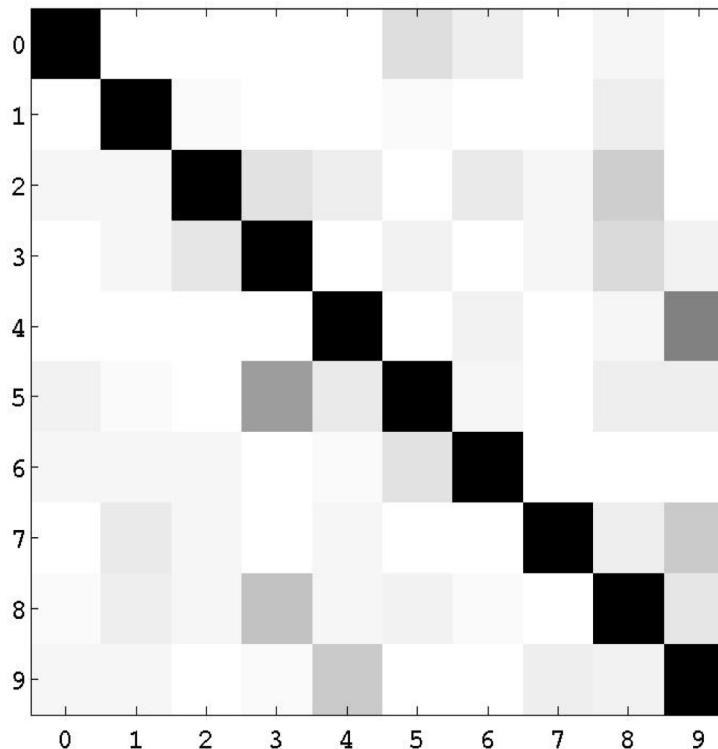
Example: MNIST

Result of training: mean vectors for each class.



Test error rate: 15.54%.

Visualization of the “confusion matrix” →



Other types of data

How would you handle data:

- Whose features take on more than two discrete values (such as ten possible colors)?
- Whose features are real-valued?
- Whose features are positive integers?
- Whose features are mixed: some real, some Boolean, etc?

How would you handle “missing data”: situations in which data points occasionally (or regularly) have missing entries?

- At train time: ???
- At test time: ???

Handling text data

Bag-of-words: vectorial representation of text documents.

It was the best of times, it was the worst of times, it was the age of wisdom, it was the age of foolishness, it was the epoch of belief, it was the epoch of incredulity, it was the season of Light, it was the season of Darkness, it was the spring of hope, it was the winter of despair, we had everything before us, we had nothing before us, we were all going direct to Heaven, we were all going direct the other way - in short, the period was so far like the present period, that some of its noisiest authorities insisted on its being received, for good or for evil, in the superlative degree of comparison only.



1	despair
2	evil
0	happiness
1	foolishness

- Fix $V = \text{some vocabulary}$.
- Treat each document as a vector of length $|V|$:

$$x = (x_1, x_2, \dots, x_{|V|}),$$

where $x_i = \# \text{ of times the } i\text{th word appears in the document.}$

A standard distribution over such document-vectors x : the **multinomial**.

Multinomial naive Bayes

Multinomial distribution over a vocabulary V :

$$p = (p_1, \dots, p_{|V|}), \text{ such that } p_i \geq 0 \text{ and } \sum_i p_i = 1$$

Document $x = (x_1, \dots, x_{|V|})$ has probability $\propto p_1^{x_1} p_2^{x_2} \cdots p_{|V|}^{x_{|V|}}$.

For naive Bayes: one multinomial distribution per class.

- Class probabilities π_1, \dots, π_k
- Multinomials $p^{(1)} = (p_{11}, \dots, p_{1|V|}), \dots, p^{(k)} = (p_{k1}, \dots, p_{k|V|})$

Classify document x as

$$\arg \max_j \pi_j \prod_{i=1}^{|V|} p_{ji}^{x_i}.$$

(As always, take log to avoid underflow: linear classifier.)

Bernoulli vs Multinomial

Naive Bayes using Bernoulli Distribution

$$\arg \max_j \pi_j \prod_{i=1}^p p_{ji}^{x_i} (1 - p_{ji})^{1-x_i}.$$

Naive Bayes using Multinomial Distribution

$$\arg \max_j \pi_j \prod_{i=1}^{|V|} p_{ji}^{x_i}.$$

Improving performance of multinomial naive Bayes

A variety of heuristics that are standard in text retrieval, such as:

① Compensating for burstiness.

Problem: Once a word has appeared in a document, it has a much higher chance of appearing again.

Solution: Instead of the number of occurrences f of a word, use $\log(1 + f)$.

② Downweighting common words.

Problem: Common words can have a unduly large influence classification

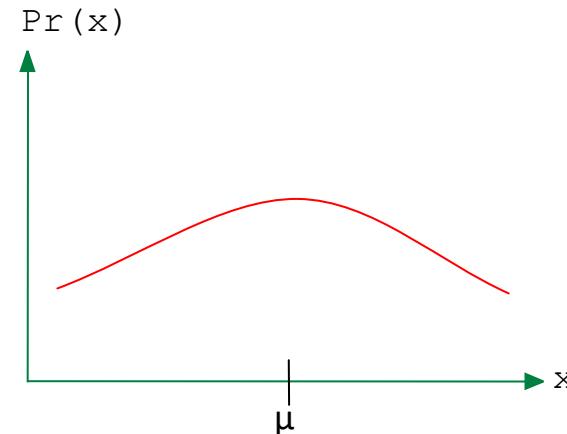
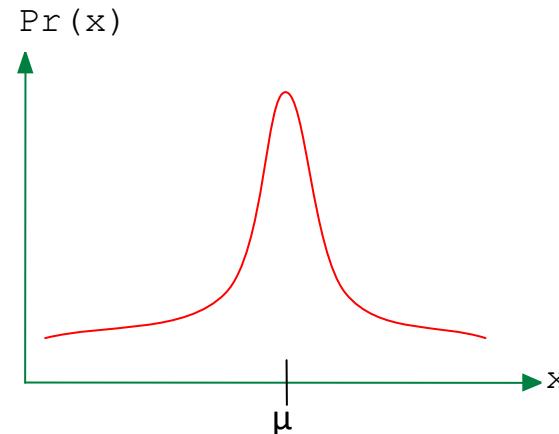
Solution: Weight each word w by **inverse document frequency**:

$$\log \frac{\# \text{ docs}}{\#(\text{docs containing } w)}$$

Variance

If you had to summarize the entire distribution of a r.v. X by a single number, you would use the mean (or median). Call it μ .

But these don't capture the *spread* of X :



What would be a good measure of spread? How about the average distance away from the mean: $E(|X - \mu|)$?

For convenience, take the square instead of the absolute value.

$$\text{Variance: } \text{var}(X) = E(X - \mu)^2 = E(X^2) - \mu^2,$$

where $\mu = E(X)$. The variance is always ≥ 0 .

Variance: example

Recall: $\text{var}(X) = \mathbf{E}(X - \mu)^2 = \mathbf{E}(X^2) - \mu^2$, where $\mu = \mathbf{E}(X)$.

Toss a coin of bias p . Let $X \in \{0, 1\}$ be the outcome.

$$\mathbf{E}(X) = p$$

$$\mathbf{E}(X^2) = p$$

$$\mathbf{E}(X - \mu)^2 = p^2 \cdot (1 - p) + (1 - p)^2 \cdot p = p(1 - p)$$

$$\mathbf{E}(X^2) - \mu^2 = p - p^2 = p(1 - p)$$

This variance is highest when $p = 1/2$ (fair coin).

The standard deviation of X is $\text{std}(X) = \sqrt{\text{var}(X)}$.

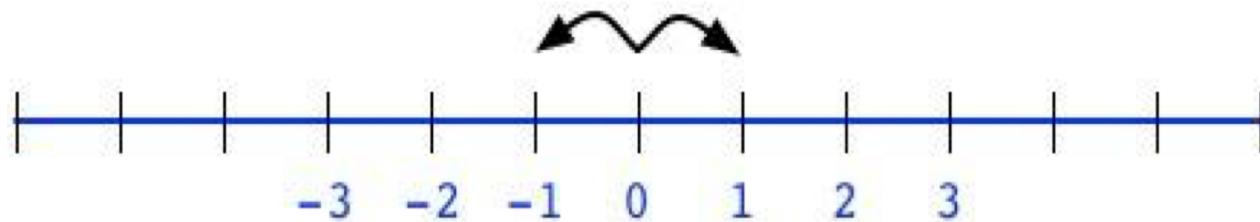
It is the average amount by which X differs from its mean.

It is the average amount by which X differs from its mean.

Variance of a sum

$\text{var}(X_1 + \dots + X_k) = \text{var}(X_1) + \dots + \text{var}(X_k)$ if the X_i are independent.

Symmetric random walk. A drunken man sets out from a bar. At each time step, he either moves one step to the right or one step to the left, with equal probabilities. Roughly where is he after n steps?



Let $X_i \in \{-1, 1\}$ be his i^{th} step. Then $E(X_i) = ?0$ and $\text{var}(X_i) = ?1$.

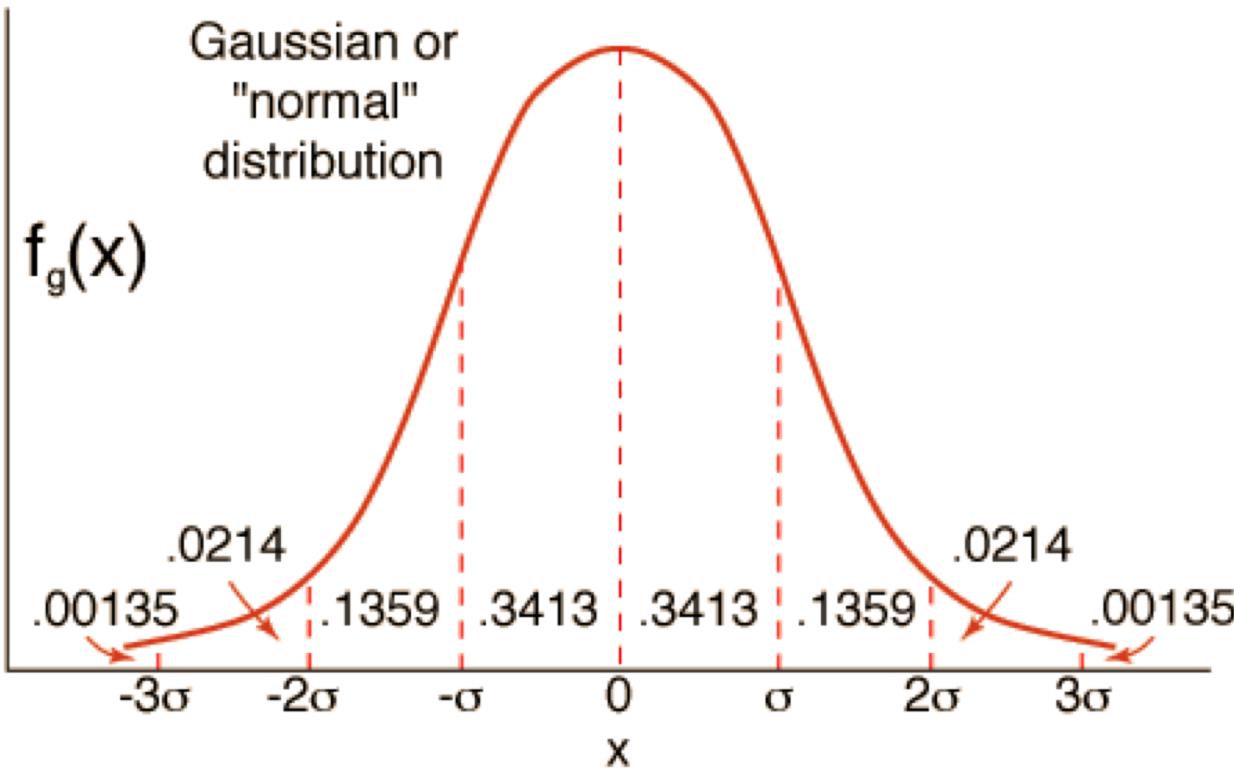
His position after n steps is $X = X_1 + \dots + X_n$.

$$E(X) = 0$$

$$\text{var}(X) = n$$

$$\text{stddev}(X) = \sqrt{n}$$

The univariate Gaussian



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

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

But what if we have two variables?

Bivariate distributions

Simplest option: treat each variable as independent.

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

H = height

W = weight

Independence would mean

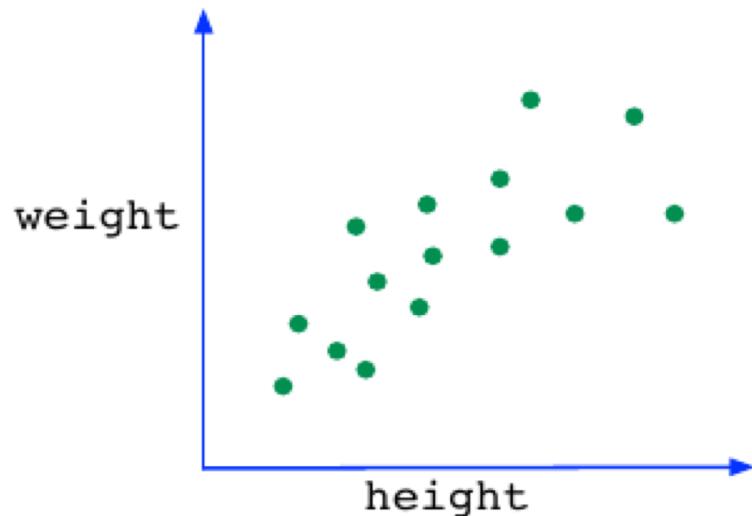
$$\Pr(H = h, W = w) = \Pr(H = h) \Pr(W = w),$$

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

Is this an accurate approximation?

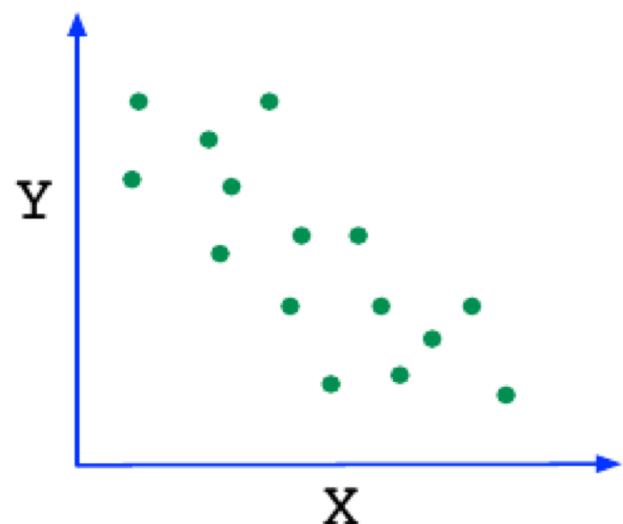
No: we'd expect height and weight to be **positively correlated**.

Types of correlation

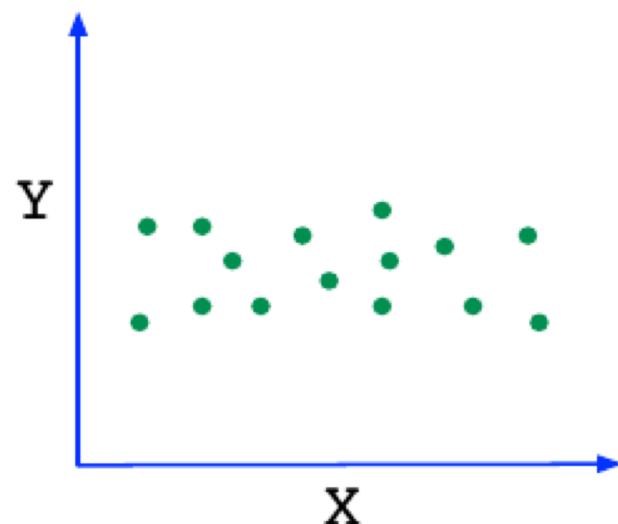


H, W positively correlated.
This also implies

$$\mathbb{E}(HW) > \mathbb{E}(H)\mathbb{E}(W).$$

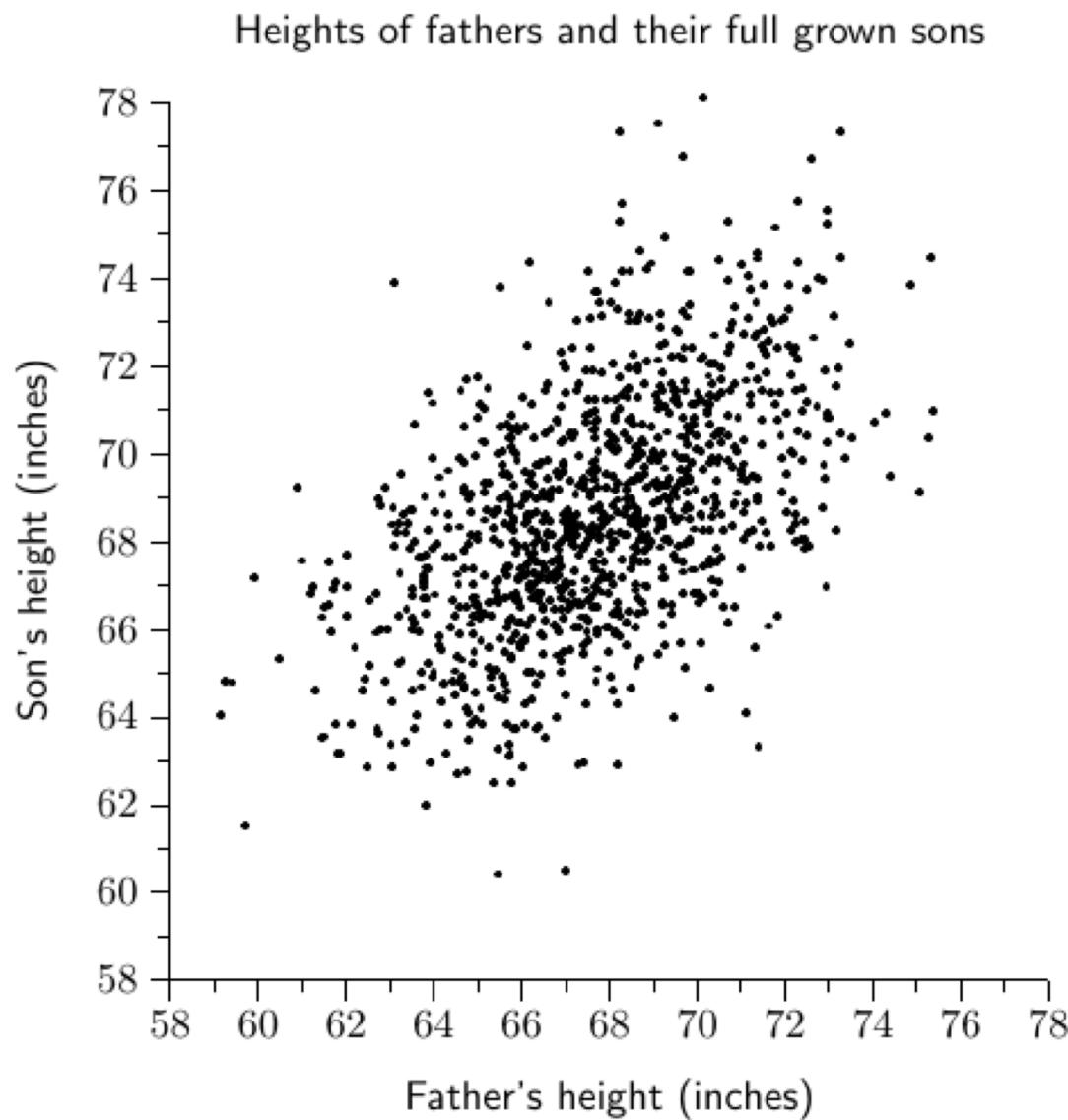


X, Y negatively correlated



X, Y uncorrelated

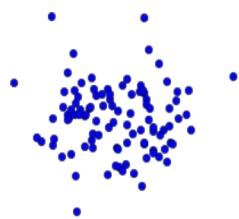
Pearson (1903): fathers and sons



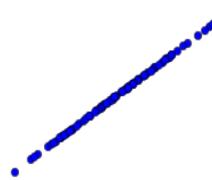
How to quantify the degree of correlation?

Correlation pictures

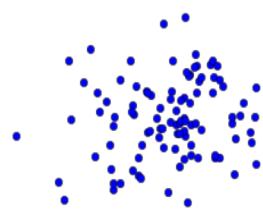
$r = 0$



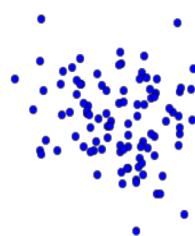
$r = 1$



$r = 0.25$



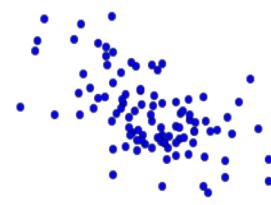
$r = -0.25$



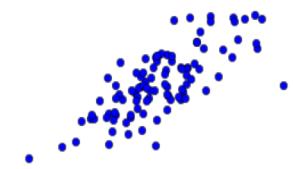
$r = 0.5$



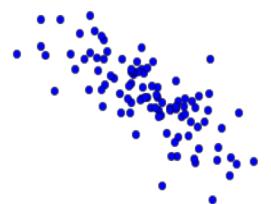
$r = -0.5$



$r = 0.75$



$r = -0.75$



Covariance and correlation

Suppose X has mean μ_x and Y has mean μ_Y

- Covariance

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

Maximized when $X = Y$, in which case it is $\text{var}(X)$.

In general, it is at most $\text{std}(X)\text{std}(Y)$.

- Correlation

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

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

Question

For variables X and Y, $\text{cov}(X, Y) = 0$.

Are X and Y independent?

Question

For variables X and Y, $\text{cov}(X,Y)=0$.

Are X and Y independent? No.

x	y	$P(x,y)$
-1	1	1/3
0	0	1/3
1	1	1/3

$$E[XY] = -1 \times 1/3 + 0 \times 1/3 + 1 \times 1/3 = 0$$

$$E[X] = 0$$

$$E[Y] = 2/3$$

$$\text{Cov}(X,Y) = E[XY] - E[X]E[Y] = 0$$

$$P(X=1, Y=1) = 1/3 \quad P(X=1) = 1/3, P(Y=1) = 2/3$$

$$P(X,Y) \neq P(X)P(Y)$$

Question

Random variables X and Y are uncorrelated.

Are X and Y independent?

Question

Random variables X and Y are uncorrelated.

Are X and Y independent? No.

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

Question

Random variables X and Y are independent.

Can X and Y be correlated?

Question

Random variables X and Y are independent.

Can X and Y be correlated? No.

$$P(X,Y) = P(X)P(Y)$$

$$E[XY] = E[X]E[Y]$$

$$\text{Cov}(X,Y) = E[XY] - E[X]E[Y] = 0$$

Covariance and correlation: example 1

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

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

x	y	$\Pr(x, y)$
-1	-1	1/3
-1	1	1/6
1	-1	1/3
1	1	1/6

$$\mu_X = 0$$

$$\mu_Y = -1/3$$

$$\text{var}(X) = 1$$

$$\text{var}(Y) = 8/9$$

$$\text{cov}(X, Y) = 0$$

$$\text{corr}(X, Y) = 0$$

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

Covariance and correlation: example 2

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

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

x	y	$\Pr(x, y)$	$\mu_X = 0$
-1	-10	1/6	$\mu_Y = 0$
-1	10	1/3	$\text{var}(X) = 1$
1	-10	1/3	$\text{var}(Y) = 100$
1	10	1/6	$\text{cov}(X, Y) = -10/3$
			$\text{corr}(X, Y) = -1/3$

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:

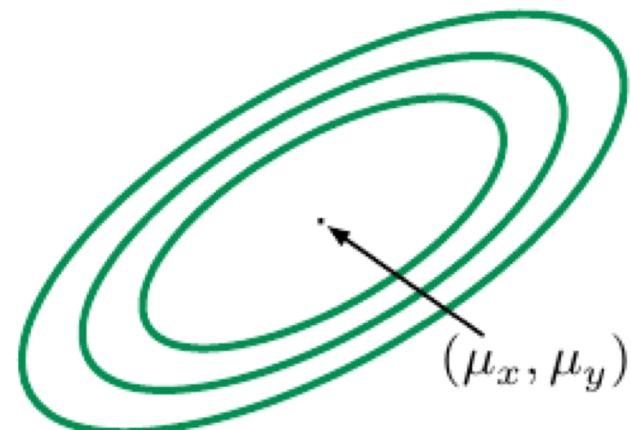
- **Mean** $(\mu_x, \mu_y) \in \mathbb{R}^2$
- **Covariance matrix**

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

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

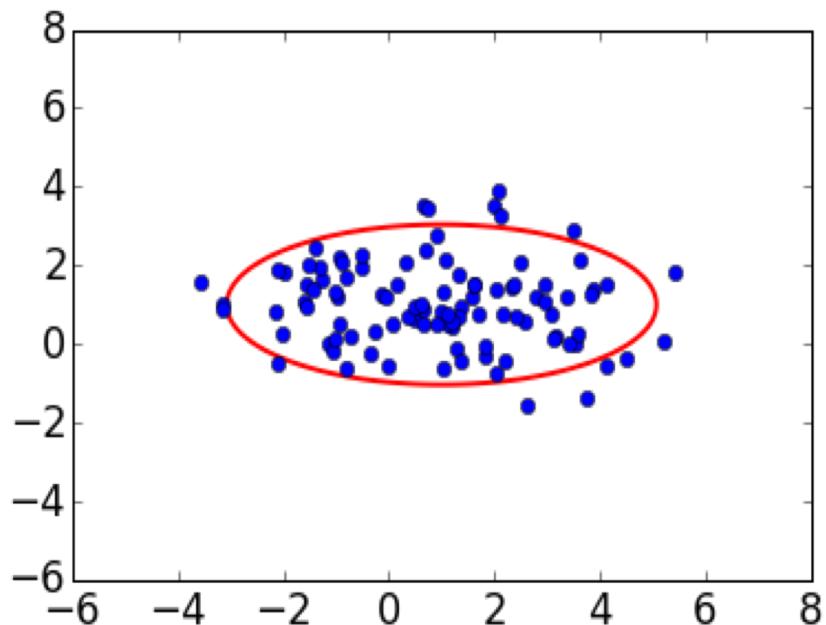
Density $p(x, y) = \frac{1}{2\pi|\Sigma|^{1/2}} \exp \left(-\frac{1}{2} \begin{bmatrix} x - \mu_x \\ y - \mu_y \end{bmatrix}^T \Sigma^{-1} \begin{bmatrix} x - \mu_x \\ y - \mu_y \end{bmatrix} \right)$

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

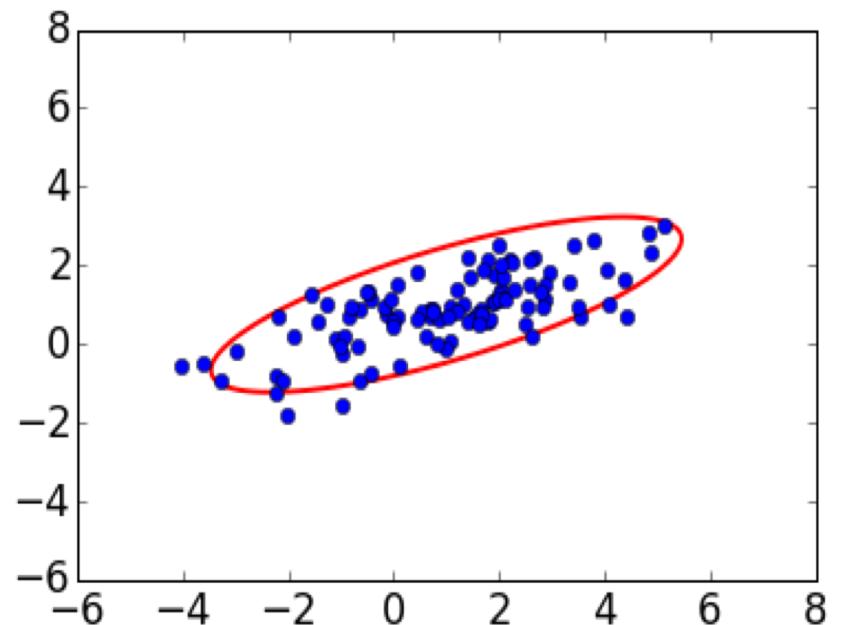


Bivariate Gaussian: examples

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

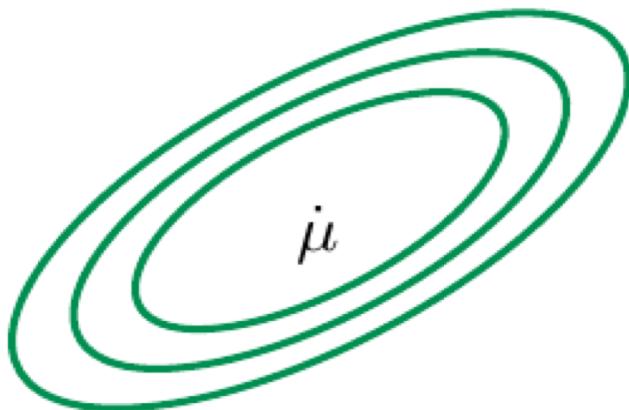


$$\Sigma = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$$



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

The multivariate Gaussian



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

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

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

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

- μ is the vector of coordinate-wise means:

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

- Σ is a matrix containing all pairwise covariances:

$$\Sigma_{ij} = \Sigma_{ji} = \text{cov}(X_i, X_j) \quad \text{if } i \neq j$$

$$\Sigma_{ii} = \text{var}(X_i)$$

- 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

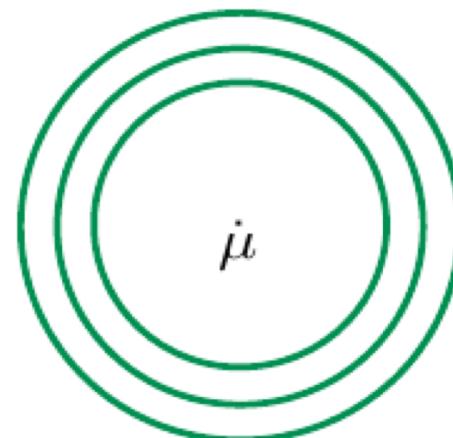
$$\Sigma = \sigma^2 I_p = \text{diag}(\sigma^2, \sigma^2, \dots, \sigma^2)$$

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

Each X_i is an independent univariate Gaussian $N(\mu_i, \sigma^2)$:

$$\Pr(x) = \prod_{i=1}^p \left(\frac{1}{\sigma \sqrt{2\pi}} e^{-(x_i - \mu_i)^2 / 2\sigma^2} \right) = \frac{1}{(2\pi)^{p/2} \sigma^p} \exp \left(-\frac{\|x - \mu\|^2}{2\sigma^2} \right)$$

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



Special case: diagonal Gaussian

The X_i are independent, with variances σ_i^2 . Thus

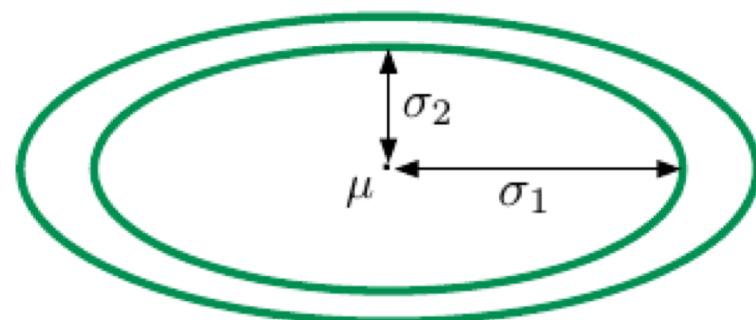
$$\Sigma = \text{diag}(\sigma_1^2, \dots, \sigma_p^2)$$

(all off-diagonal elements zero).

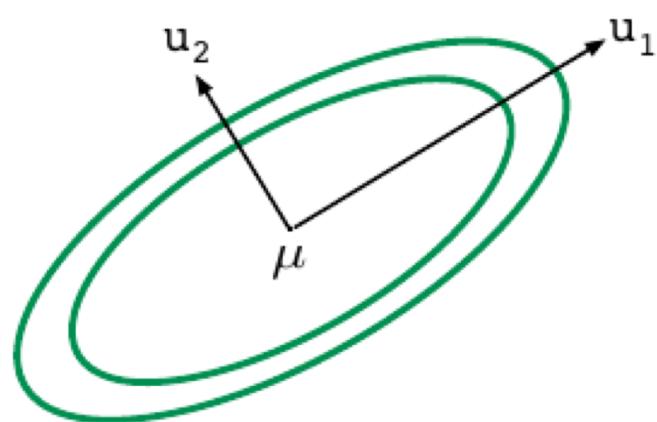
Each X_i is an independent univariate Gaussian $N(\mu_i, \sigma_i^2)$:

$$p(x) = \frac{1}{(2\pi)^{p/2}\sigma_1 \cdots \sigma_p} \exp\left(-\sum_{i=1}^p \frac{(x_i - \mu_i)^2}{2\sigma_i^2}\right)$$

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



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



Eigendecomposition of Σ yields:

- **Eigenvalues**
 $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p$
- Corresponding **eigenvectors**
 u_1, \dots, u_p

Recall density: $p(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp \left(-\frac{1}{2} \underbrace{(x - \mu)^T \Sigma^{-1} (x - \mu)}_{\text{What is this?}} \right)$

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:

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

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

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

Given a new point x , predict class 1 iff:

$$\pi_1 P_1(x) > \pi_2 P_2(x) \Leftrightarrow x^T M x + 2w^T x \geq \theta,$$

where:

$$M = \frac{1}{2} (\Sigma_2^{-1} - \Sigma_1^{-1})$$

$$w = \Sigma_1^{-1} \mu_1 - \Sigma_2^{-1} \mu_2$$

and θ is a constant depending on the various parameters.

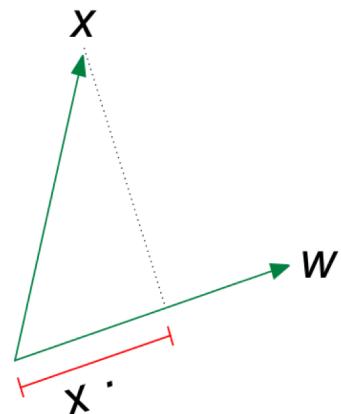
$\Sigma_1 = \Sigma_2$: linear decision boundary. Otherwise, quadratic boundary.

Linear decision boundary

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

$$x \cdot \underbrace{\Sigma^{-1}(\mu_1 - \mu_2)}_w \geq \theta.$$

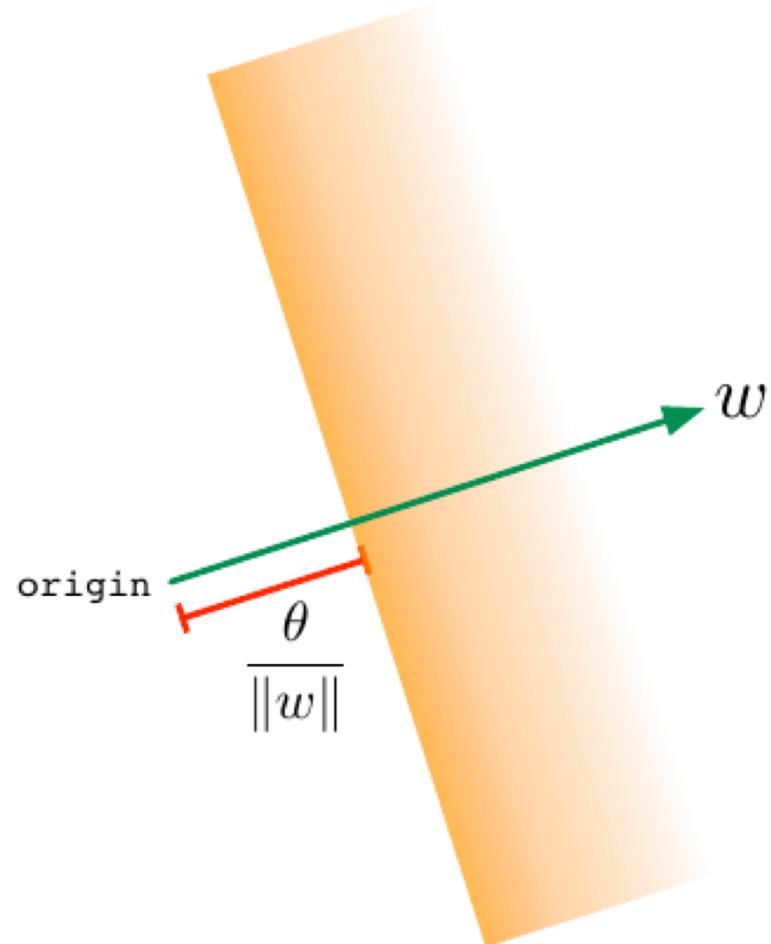
Geometric picture: Suppose w is a unit vector (that is, $\|w\| = 1$). Then $x \cdot w$ is the **projection** of vector x onto direction w .



And we can always make w a unit vector by dividing both sides of the inequality by $\|w\|$.

Linear decision boundary

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

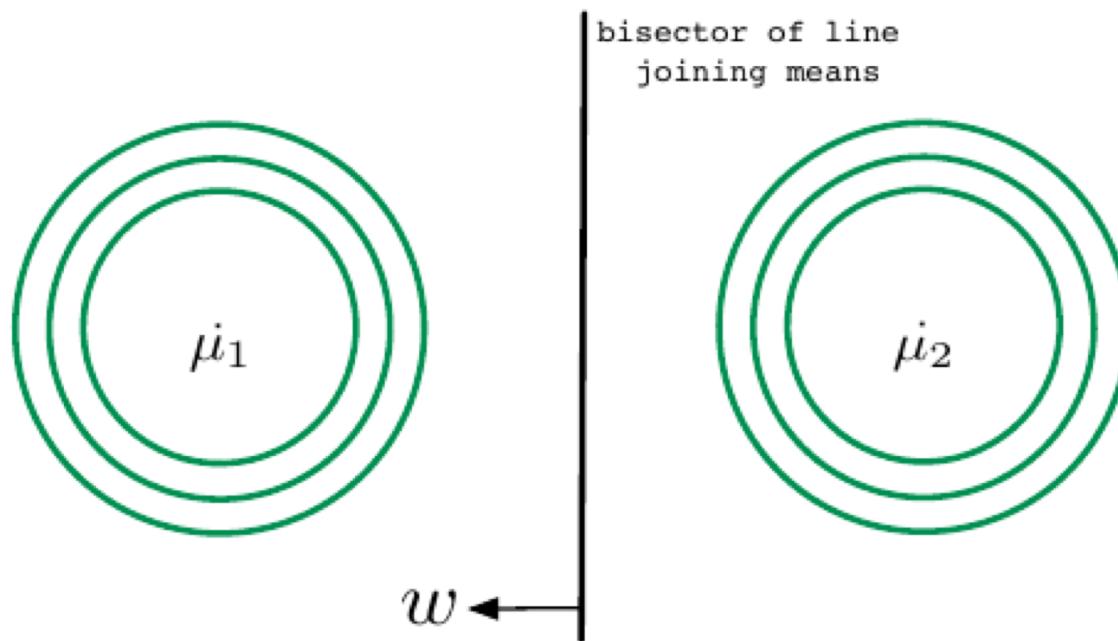


Common covariance: $\Sigma_1 = \Sigma_2 = \Sigma$

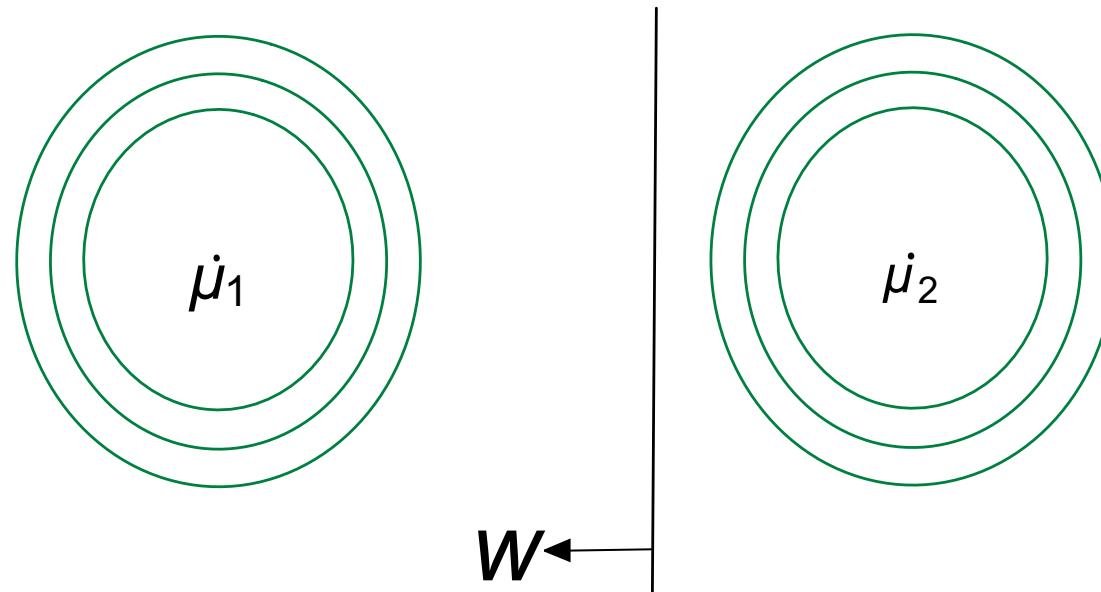
Linear decision boundary: choose class 1 iff

$$x \cdot \underbrace{\Sigma^{-1}(\mu_1 - \mu_2)}_w \geq \theta.$$

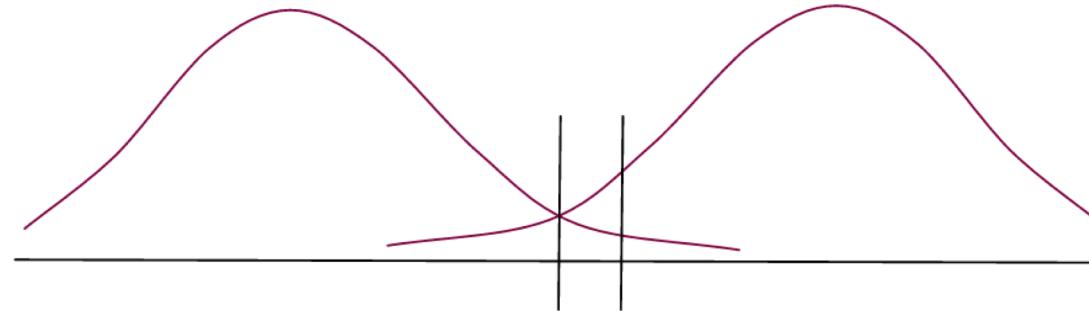
Example 1: Spherical Gaussians with $\Sigma = I_p$ and $\pi_1 = \pi_2$.



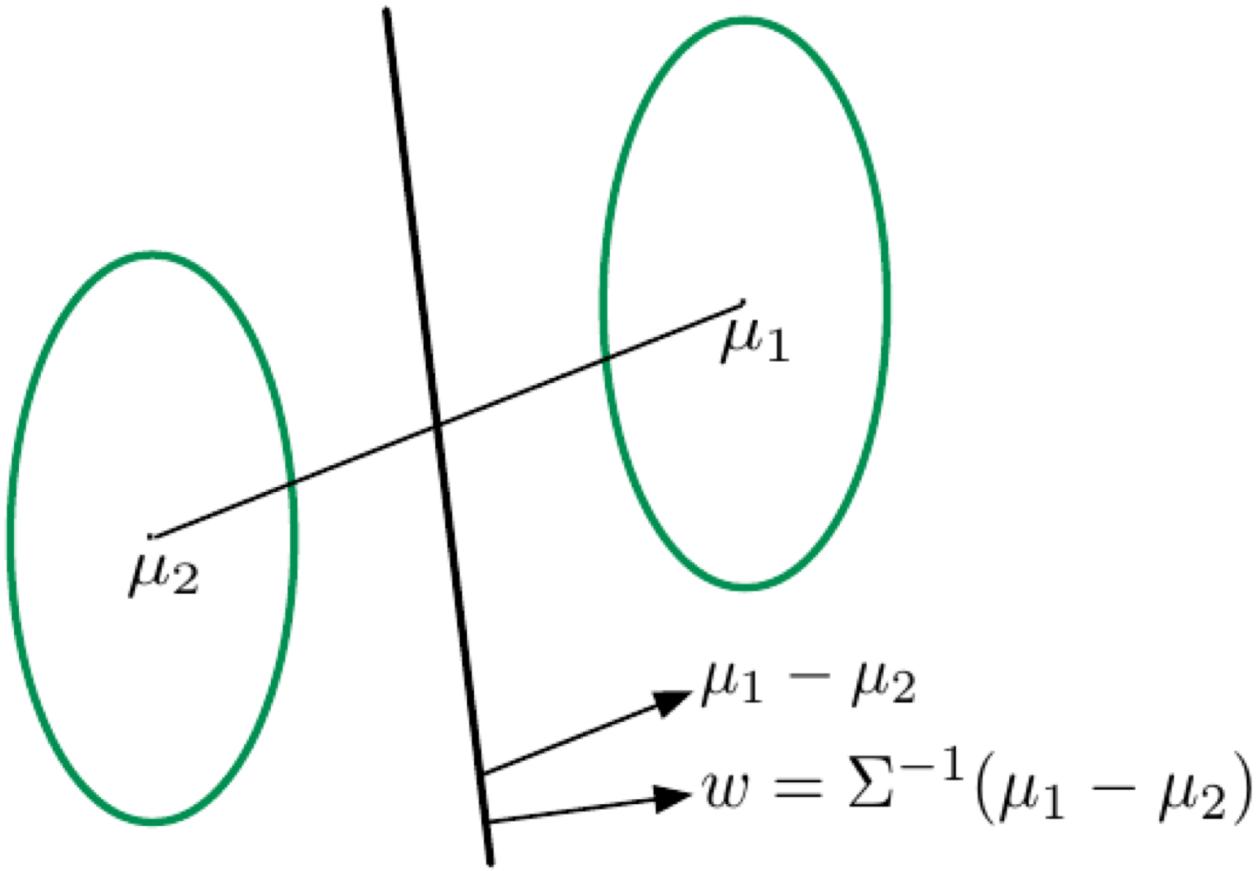
Example 2: Again spherical, but now $\pi_1 > \pi_2$.



One-d projection onto w :



Example 3: Non-spherical.



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

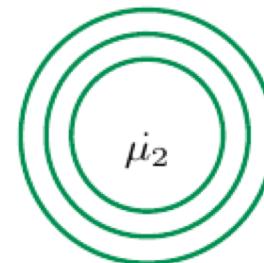
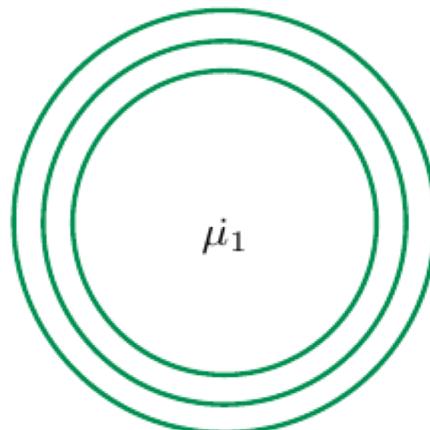
Different covariances: $\Sigma_1 \neq \Sigma_2$

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

$$M = \frac{1}{2}(\Sigma_2^{-1} - \Sigma_1^{-1})$$

$$w = \Sigma_1^{-1}\mu_1 - \Sigma_2^{-1}\mu_2$$

Example 1: $\Sigma_1 = \sigma_1^2 I_p$ and $\Sigma_2 = \sigma_2^2 I_p$ with $\sigma_1 > \sigma_2$



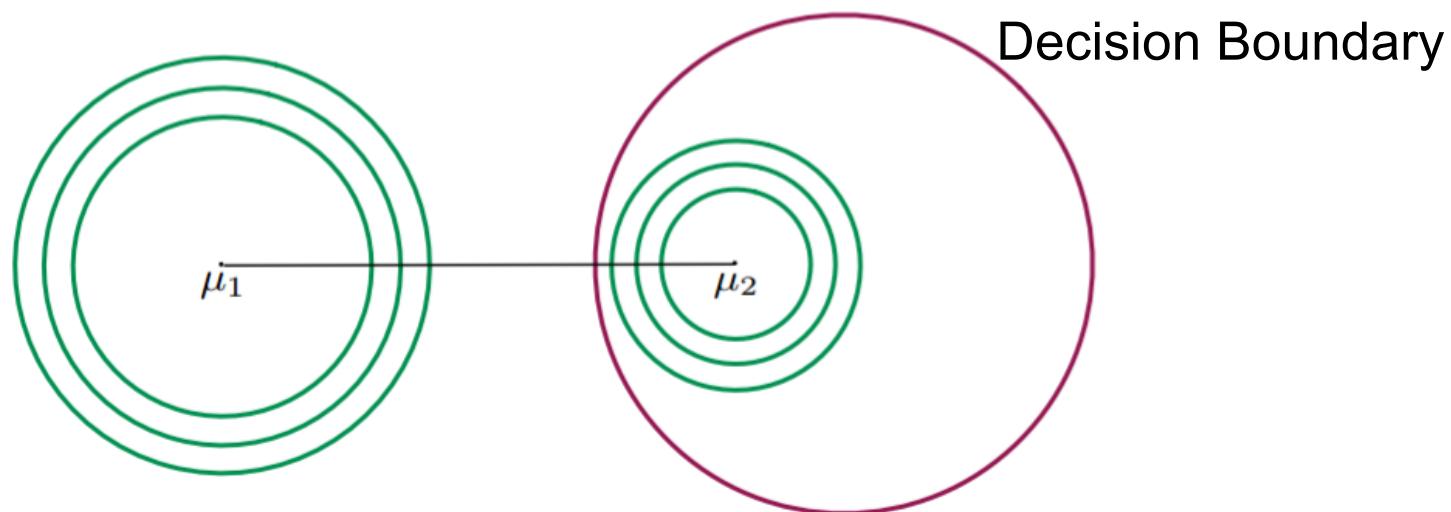
Different covariances: $\Sigma_1 \neq \Sigma_2$

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

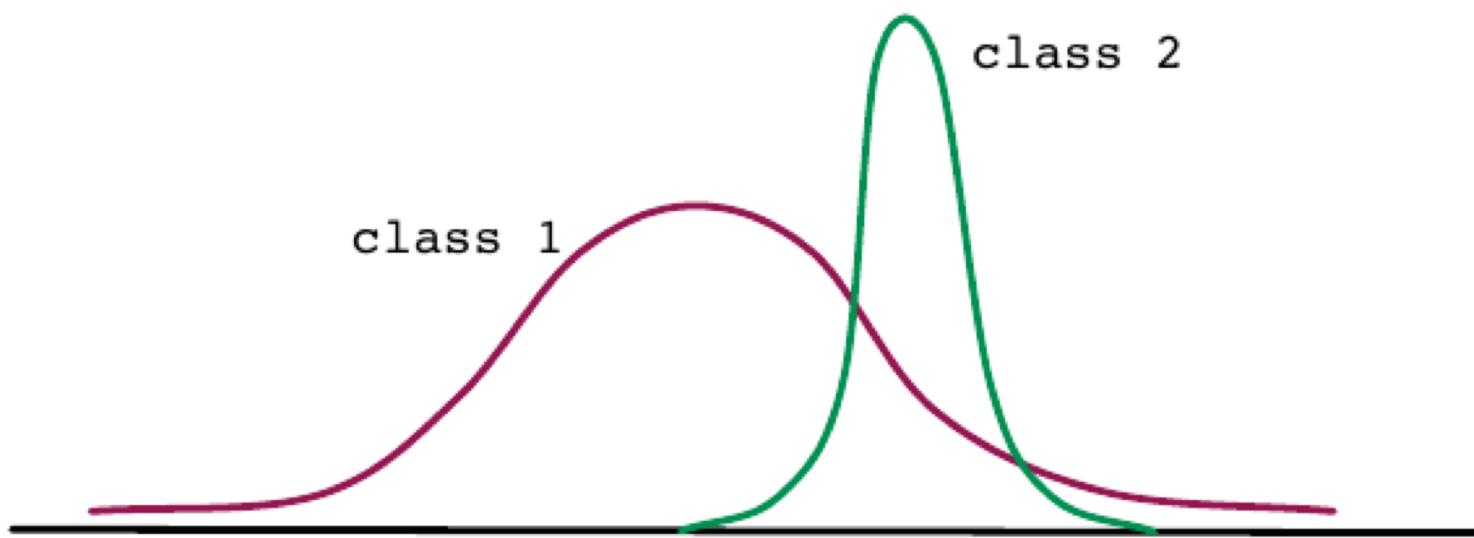
$$M = \frac{1}{2}(\Sigma_2^{-1} - \Sigma_1^{-1})$$

$$w = \Sigma_1^{-1}\mu_1 - \Sigma_2^{-1}\mu_2$$

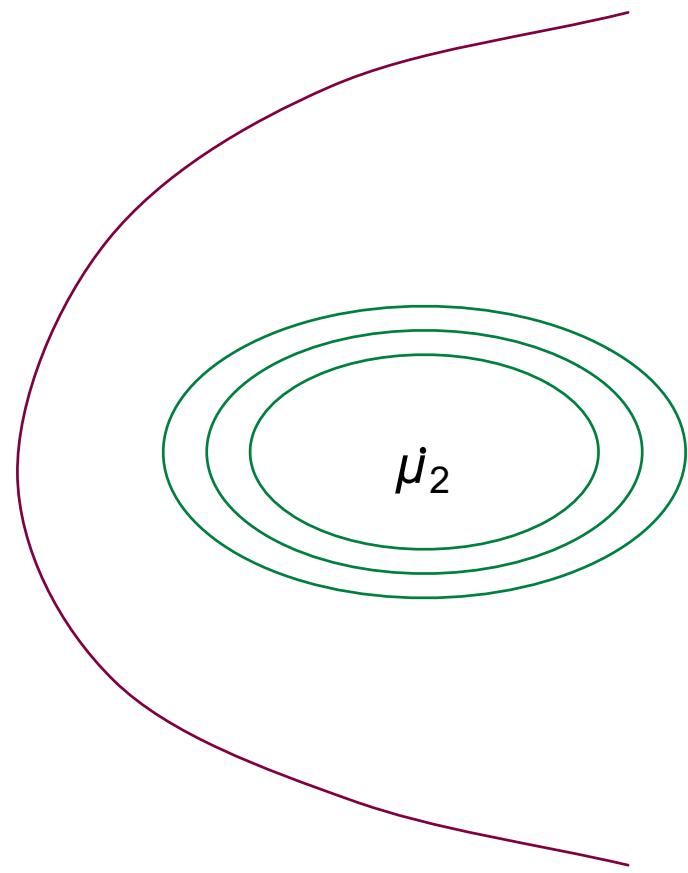
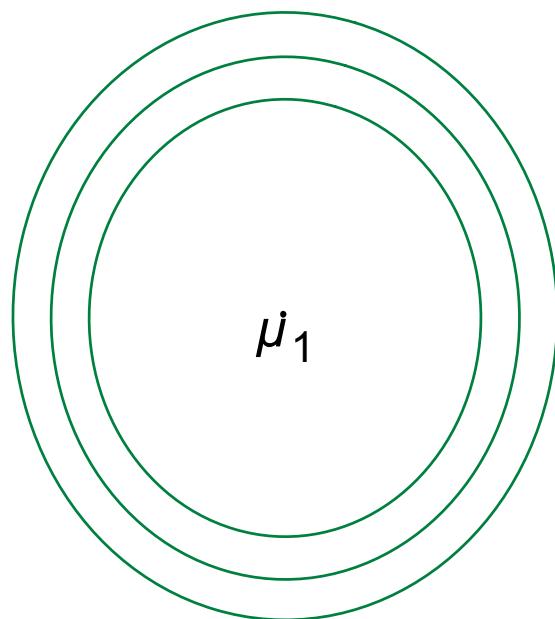
Example 1: $\Sigma_1 = \sigma_1^2 I_p$ and $\Sigma_2 = \sigma_2^2 I_p$ with $\sigma_1 > \sigma_2$



Example 2: Same thing in 1-d. $\mathcal{X} = \mathbb{R}$.



Example 3: A parabolic boundary.



Many other possibilities!

Multiclass discriminant analysis

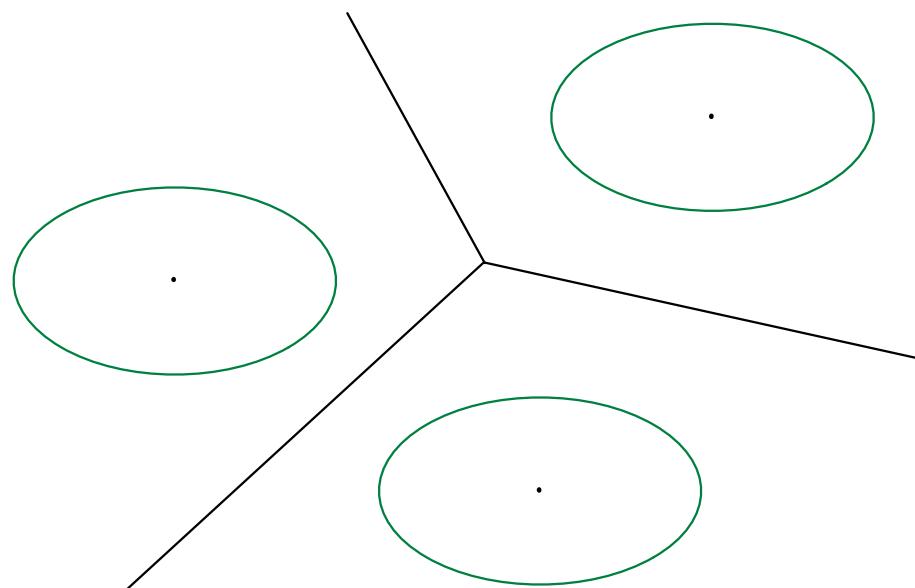
k classes: weights π_j , class-conditional distributions $P_j = N(\mu_j, \Sigma_j)$

Each class has an associated **quadratic** function

$$f_j(x) = \log (\pi_j P_j (x))$$

To class a point x , pick $\arg_j \max f_j(x)$.

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

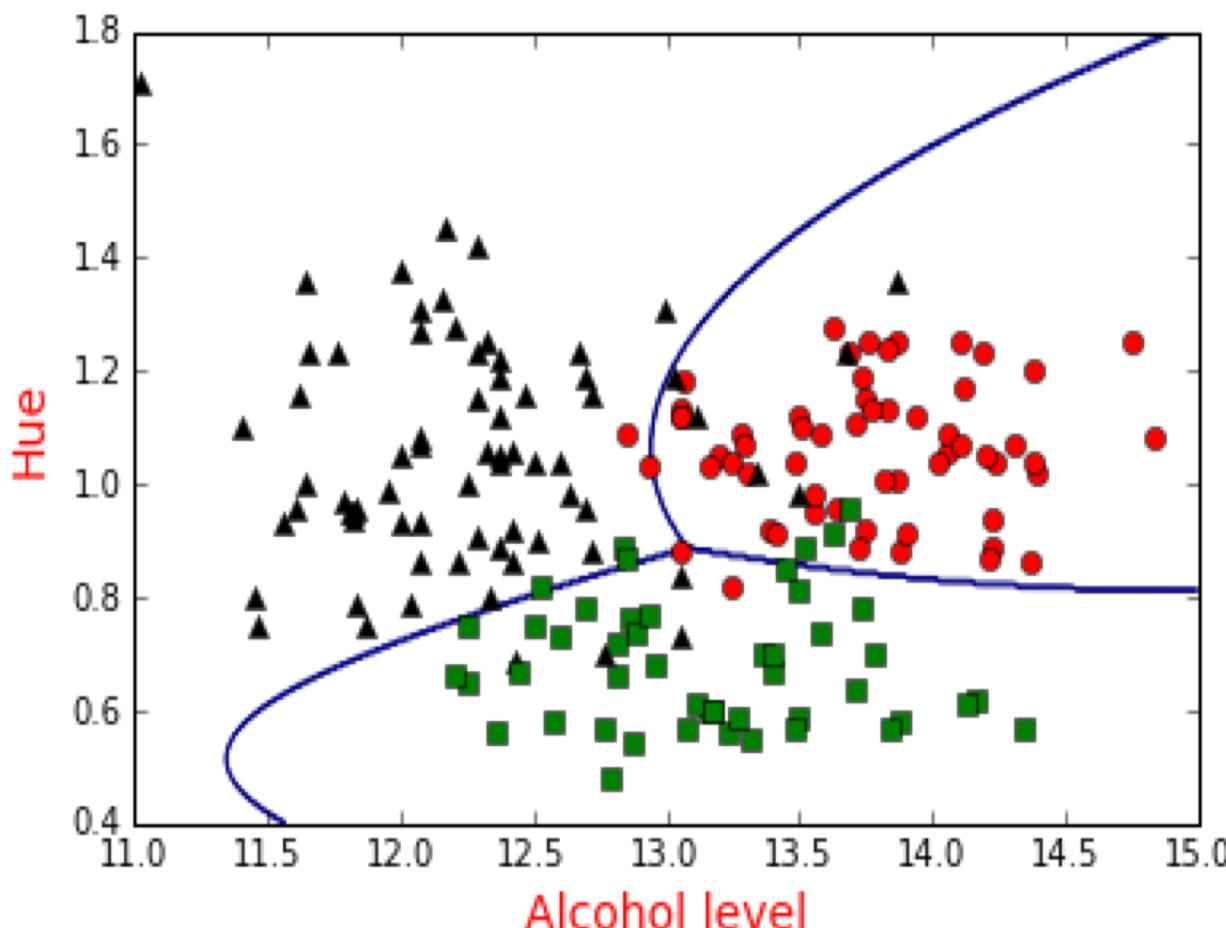


Example: “wine” data set

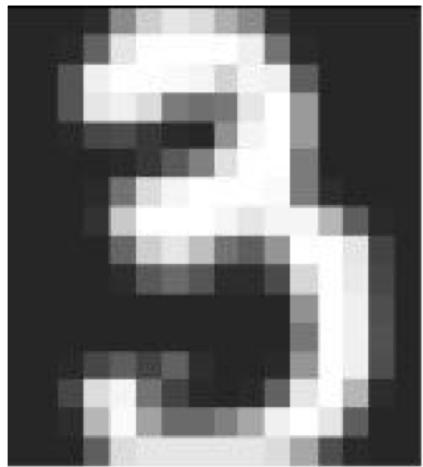
Data from three wineries from the same region of Italy

- 13 attributes: hue, color intensity, flavanoids, ash content, ...
- 178 instances in all: split into 118 train, 60 test

Test error using multiclass discriminant analysis: 1/60



Example: MNIST



To each digit, fit:

- class probability π_j
- mean $\mu_j \in \mathbb{R}^{784}$
- covariance matrix $\Sigma_j \in \mathbb{R}^{784 \times 784}$

Problem: formula for normal density uses Σ_j^{-1} , which is singular.

- Need to regularize: $\Sigma_j \rightarrow \Sigma_j + \sigma^2 I$
- This is a good idea even without the singularity issue

Fisher's linear discriminant

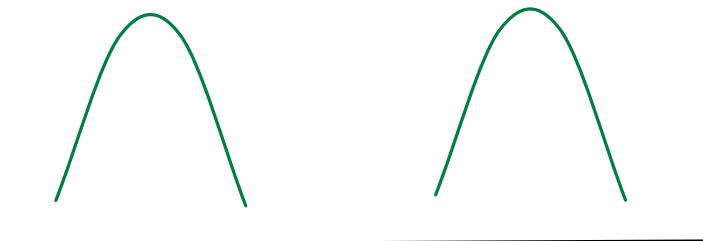
A framework for linear classification without Gaussian assumptions.

Use only first- and second-order statistics of the classes.

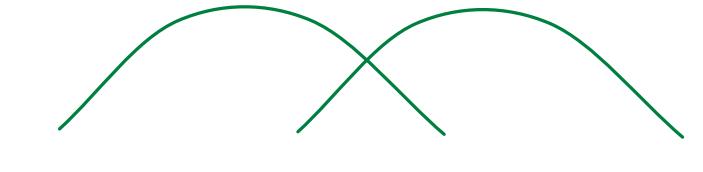
Class 1	Class 2
mean μ_1	mean μ_2
cov Σ_1	cov Σ_2
# pts n_1	# pts n_2

A linear classifier projects all data onto a direction w . Choose w so that:

- Projected means are well-separated, i.e. $(w \cdot \mu_1 - w \cdot \mu_2)^2$ is large.
- Projected within-class variance is small.



better
than



Fisher LDA (linear discriminant analysis)

Two classes: means μ_1, μ_2 ; covariances Σ_1, Σ_2 ; sample sizes n_1, n_2 .

Project data onto direction (unit vector) w .

- Projected means: $w \cdot \mu_1$ and $w \cdot \mu_2$
- Projected variances: $w^T \Sigma_1 w$ and $w^T \Sigma_2 w$
- Average projected variance:

$$\frac{n_1(w^T \Sigma_1 w) + n_2(w^T \Sigma_2 w)}{n_1 + n_2} = w^T \Sigma w,$$

where $\Sigma = (n_1 \Sigma_1 + n_2 \Sigma_2) / (n_1 + n_2)$.

Find w to maximize $J(w) = \frac{(w \cdot \mu_1 - w \cdot \mu_2)^2}{w^T \Sigma w}$

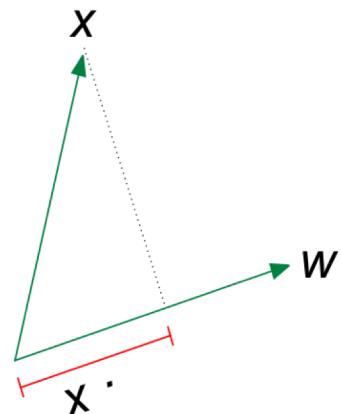
Solution: $w \propto \Sigma^{-1}(\mu_1 - \mu_2)$. Look familiar?

Recall: Linear decision boundary

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

$$x \cdot \underbrace{\Sigma^{-1}(\mu_1 - \mu_2)}_w \geq \theta.$$

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



And we can always make w a unit vector by dividing both sides of the inequality by $\|w\|$.

Fisher LDA: proof

Goal: find w to maximize $J(w) = \frac{(w \cdot \mu_1 - w \cdot \mu_2)^2}{w^T \Sigma w}$

- ① Assume Σ_1, Σ_2 are full rank; else project.
- ② Since Σ_1 and Σ_2 are p.d., so is their weighted average, Σ .
- ③ Write $u = \Sigma^{1/2}w$. Then

$$\begin{aligned}\max_w \frac{(w^T(\mu_1 - \mu_2))^2}{w^T \Sigma w} &= \max_u \frac{(u^T \Sigma^{-1/2}(\mu_1 - \mu_2))^2}{u^T u} \\ &= \max_{u: \|u\|=1} (u \cdot (\Sigma^{-1/2}(\mu_1 - \mu_2)))^2\end{aligned}$$

- ④ Solution: u is the unit vector in direction $\Sigma^{-1/2}(\mu_1 - \mu_2)$.
- ⑤ Therefore: $w = \Sigma^{-1/2} u \propto \Sigma^{-1}(\mu_1 - \mu_2)$.