# Linear Classification Models

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# 2D Gaussians

A $p$-**dimensional Gaussian function** has the form:

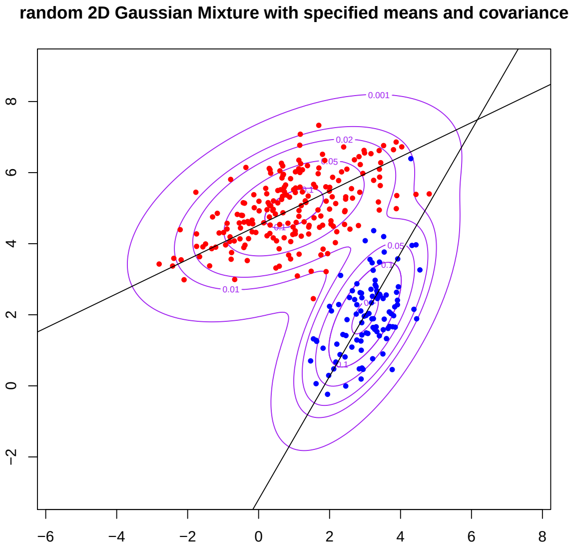
$$g(\mathbf{x}, \boldsymbol{\mu}, \Sigma) \quad = \quad \frac{1}{(2\,\pi)^{p/2}} \, \frac{1}{\sqrt{\det\, \Sigma}} \, \exp\left( -\tfrac{1}{2} \; (\mathbf{x} - \boldsymbol{\mu})' \; \Sigma^{-1} \; (\mathbf{x} - \boldsymbol{\mu}) \right).$$

where $\mathbf{x}$ be a $p$-dimensional value, $\mu$ is a $p$-dimensional vector of means, and $\Sigma$ is a positive definite $p \times p$ covariance matrix.
(We require $\Sigma$ to be positive definite so the determinant is positive.)

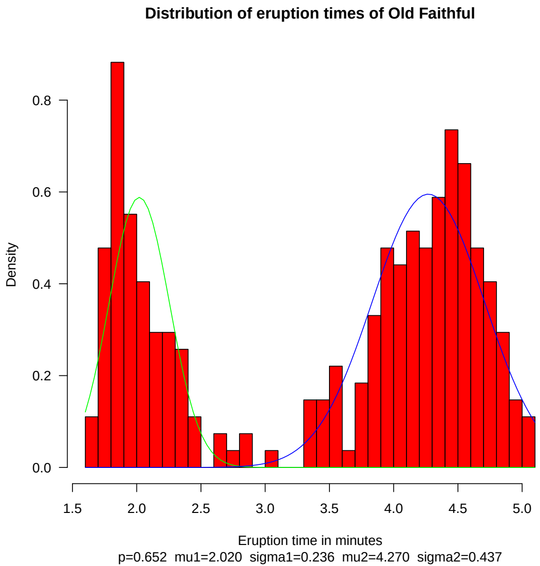
Equivalently, if $W = \Sigma^{-1}$:

$$g(\mathbf{x}, \boldsymbol{\mu}, W^{-1}) \quad = \quad \frac{1}{(2\,\pi)^{p/2}} \, \sqrt{\det\; W} \, \exp\left( -\tfrac{1}{2} \; (\mathbf{x} - \boldsymbol{\mu})' \; W \; (\mathbf{x} - \boldsymbol{\mu}) \right).$$

# Multiple Gaussians



# Old Faithful



# Mixture Models

To the distribution of geyser eruption times we can fit a *mixture model*

$$\text{Prob}[\,\text{eruption time} = x \mid \boldsymbol{\theta}\,] \;=\; (1-p)\, g(x, \mu_1, \sigma_1) \;+\; p\, g(x, \mu_2, \sigma_2).$$

This is a simple mixture of two gaussians, and so has five parameters: $p$, $\mu_1$, $\sigma_1$, $\mu_2$, $\sigma_2$.

If we can formalize the objective function, we can use an optimization method to find the optimal parameter vector

$$\boldsymbol{\theta} \;=\; (p,\, \mu_1,\, \sigma_1,\, \mu_2,\, \sigma_2)$$

A commonly-used objective function: **maximum likelihood**.

# Maximum Likelihood Estimation of Parameters

If the set of eruption times is $D = \{\ t_i \ \mid\ i = 1, \ldots, n\ \}$, then

$$\text{Likelihood}[\,\boldsymbol{\theta} \mid D\,] \;=\; \text{Prob}[\,D \mid \boldsymbol{\theta}\,] \;=\; \prod_{i=1}^{n} \text{Prob}[\,\text{eruption time} = t_i \ \mid\ \boldsymbol{\theta}\,]$$

and thus

$$\log\,\text{Likelihood}[\,\boldsymbol{\theta} \mid D\,] \;=\; \sum_{i=1}^{n} \log\left(\ (1-p)\ g(t_i, \mu_1, \sigma_1) \;+\; p\ g(t_i, \mu_2, \sigma_2)\ \right).$$

We give this objective function to an optimizer.

# Classification Models

A **classification** of a feature vector $\mathbf{x}$ is a value $y$ in a set $C$ of **classes**.

Given a training set of feature vectors $\mathbf{x}$ and classes $y$,
the **classification problem** is to find a function $f$ such that $y = f(\mathbf{x})$.

Given a $n \times p$ matrix/dataset $X$ ($n$ observations of $p$-feature vectors), and a $n \times 1$ vector $\mathbf{y}$ of classifications, find a **classification model** $y = f(\mathbf{x})$ that minimizes the **loss function**

$$L(\mathbf{y}, f(X)) \quad = \quad \|\mathbf{y} - f(X)\|.$$

This restates the classification problem as an optimization problem.

# Linear Discriminants

Using least squares we solve $X\boldsymbol{\beta} = \mathbf{y}$ for a $p \times 1$ vector of coefficients $\boldsymbol{\beta}$.

The classifier function can then be

$$y \quad = \quad f(\mathbf{x}) \quad = \quad \sigma(\langle\, \mathbf{x},\, \boldsymbol{\beta}\,\rangle)$$

where $\sigma$ is a function that 'rounds' or 'truncates' to an integer class value.

If a constant intercept $c$ is desired so $\boldsymbol{\beta} = (\mathbf{w}\ \ c)$, then

$$\langle\, (\mathbf{x}\ 1),\, (\mathbf{w}\ \ c)\,\rangle \quad = \quad \langle\, \mathbf{w},\, \mathbf{x}\,\rangle \ + \ c$$

— and the classifier is defined by the **hyperplane** $\langle\, \mathbf{w},\, \mathbf{x}\,\rangle \ = \ c$.

In the two-class case, for example, we could use:

$$\sigma(t) \quad = \quad \mathrm{sgn}(t) \quad = \quad \begin{cases} +1 & t > 0 \\ -1 & t < 0. \end{cases}$$

Input feature vectors $\mathbf{x}$ are given the classification $\sigma(\ \langle\, \mathbf{w},\, \mathbf{x}\,\rangle\ +\ c\ )$.

# Least Squares Linear Discriminants

We can find the coefficients **w** and $c$ via Least Squares as follows:

```
A = cbind( X, 1 )
#  add a column of '1' values for an intercept coefficient

wc = solve(t(A) %*% A) %*% t(A) %*% y
#  alternatively:   wc = lsfit(X, y)$coefficients
#  alternatively:   wc = lm(y ~ X)$coefficients

w = wc[1:2]
c = wc[3]
classifier = function(x, w, c) { 2 * ((x %*% w + c) > 0) - 1 }
                             # i.e., ((x %*% w + c) > 0) ? +1 : -1
                             #        where +1 = red and -1 = blue,
## classifier = function(x, w, c) { sign(x %*% w + c) }

# plot the discriminant
curve( -(w[1] * x + c)/w[2], col="green", add=TRUE )
```

# LDA (Linear Discriminant Analysis)

Assume our $k$ classes have a common covariance matrix $\Sigma$:

$$g_k(\mathbf{x}) \;=\; 1/(2\pi)^{p/2} \sqrt{\det(\Sigma^{-1})} \; \exp(\, -\tfrac{1}{2} \; (\mathbf{x} - \boldsymbol{\mu}_k)' \, \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) \; )$$

Given an input $\mathbf{x}$, we can estimate

$$\text{Prob}[\;\text{class} = k \mid \mathbf{x}\;] \;=\; \frac{g_k(\mathbf{x}) \; p_k}{\sum_\ell g_\ell(\mathbf{x}) \; p_\ell}$$

where $p_\ell$ is the (prior) probability of $\mathbf{x}$ belonging to class $i$. Then:

$$\begin{aligned}
\log \frac{\text{Prob}[\;\text{class} = k \mid \mathbf{x}\;]}{\text{Prob}[\;\text{class} = \ell \mid \mathbf{x}\;]} \;&=\; \log \frac{g_k(\mathbf{x})\, p_k}{g_\ell(\mathbf{x})\, p_\ell} \\
&=\; \log \frac{p_k}{p_\ell} - \tfrac{1}{2} \; ({\boldsymbol{\mu}_k}' \, \Sigma^{-1} \boldsymbol{\mu}_k \; + \; {\boldsymbol{\mu}_\ell}' \, \Sigma^{-1} \boldsymbol{\mu}_\ell) + (\boldsymbol{\mu}_k - \boldsymbol{\mu}_\ell)' \; \Sigma^{-1} \, \mathbf{x} \\
&=\; \langle \, \mathbf{w}, \, \mathbf{x} \, \rangle + c \qquad\qquad \text{where } \mathbf{w}' \;=\; (\boldsymbol{\mu}_k - \boldsymbol{\mu}_\ell)' \; \Sigma^{-1}
\end{aligned}$$

— a linear function of $\mathbf{x}$!

# LDA (Linear Discriminant Analysis)

We can equivalently define the discriminant function

$$d_k(\mathbf{x}) \;=\; \left(\log\; p_k \;-\; \tfrac{1}{2}\; \boldsymbol{\mu}_k{}'\; \Sigma^{-1}\; \boldsymbol{\mu}_k\right) \;+\; \boldsymbol{\mu}_k{}'\; \Sigma^{-1}\,\mathbf{x} \;=\; \langle\, \mathbf{w}_k,\, \mathbf{x}\,\rangle \;+\; c_k$$

so that: $\quad d_k(\mathbf{x}) > d_\ell(\mathbf{x}) \;\;\Leftrightarrow\;\; \mathrm{Prob}[\,\mathrm{class} = k \,|\, \mathbf{x}\,] \;>\; \mathrm{Prob}[\,\mathrm{class} = \ell \,|\, \mathbf{x}\,].$

Thus we can define a classifier function

$$f(\mathbf{x}) \;=\; \mathrm{argmax}_k\; d_k(\mathbf{x}).$$

For a training set $X$, if we are not given values for $p_k$, $\boldsymbol{\mu}_k$, or $\Sigma$:

- estimate $p_k$ as the proportion of training examples in class $k$
- estimate $\boldsymbol{\mu}_k$ as the average of the $\mathbf{x}$ examples in class $k$
- estimate $\Sigma$ to be the covariance matrix of the training set $X$.

# QDA (Quadratic Discriminant Analysis)

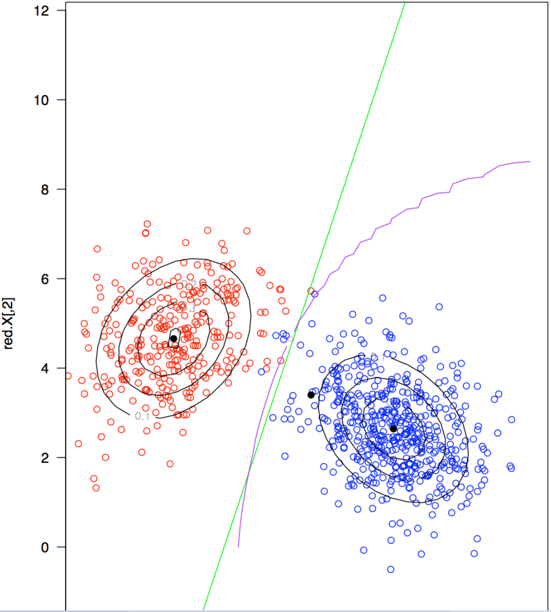
QDA generalizes on LDA by permitting discriminant functions of the form

$$d_k \;=\; \log\; p_k - \tfrac{1}{2}\,\log\;\det(\Sigma_k) - \tfrac{1}{2}\,\boldsymbol{\mu}_k{}'\,\Sigma_k^{-1}\boldsymbol{\mu}_k + (\mathbf{x}-\boldsymbol{\mu}_k)'\,\Sigma_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k)$$

where each class $k$ has its own covariance matrix $\Sigma_k$.

This is a quadratic function of $\mathbf{x}$.

# QDA



# Logistic Regression

Suppose there are two classes: $y = 0$ and $y = 1$.
We are given $\mathbf{x}$ and seek to find the best value of $y$.

Instead of using a normal regression model like

$$y = \langle \mathbf{w}, \mathbf{x} \rangle + c$$

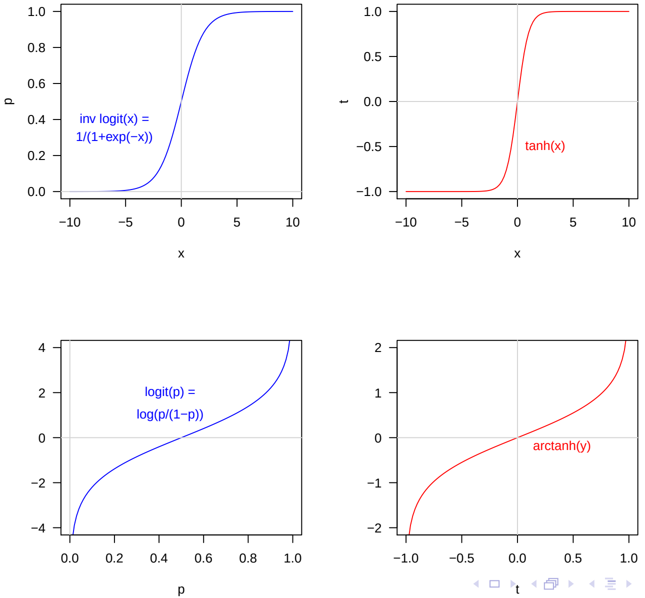
since $y$ is discrete we want to use a model like

$$y = \sigma( \langle \mathbf{w}, \mathbf{x} \rangle + c )$$

where $\sigma$ is a sigmoid function.

In **logistic regression**, $\sigma$ is the inverse logistic function ($\text{logit}^{-1}$).

# Sigmoid Functions



# Sigmoid Functions

We say $\sigma(x)$ is a **sigmoid** function if it resembles the sign function $sgn(x)$. Important examples:

$$\sigma(x) \;=\; \text{logit}^{-1}(c\,x) \;=\; \frac{1}{1+e^{-c\,x}}$$

$$\sigma(x) \;=\; \tanh(c\,x) \;=\; \frac{1-e^{-2\,c\,x}}{1+e^{-2\,c\,x}}$$

Here $c$ is a constant near 1 that can be used to 'tighten' the sigmoid.

These are both differentiable approximations of the sign function.

The logit function has an interesting property: it is the **log odds** function

$$\text{logit}(p) \;=\; \log\,\frac{p}{1-p}.$$

# Logistic Regression

Again, the target variable $y$ is a variable with discrete values 0 and 1.

Since $\text{Prob}[\,\text{class} = 1 \,|\, \mathbf{x}\,] \;=\; 1 - \text{Prob}[\,\text{class} = 0 \,|\, \mathbf{x}\,]$, we can compute

$$\log \; \frac{\text{Prob}[\;\text{class} = 1 \;|\; \mathbf{x}\;]}{1 \;-\; \text{Prob}[\;\text{class} = 1 \;|\; \mathbf{x}\;]}$$

and choose class 1 if it is positive, otherwise choose class 0.

In other words, using the logit function

$$\sigma^{-1}(p) \;=\; \text{logit}(p) \;=\; \log \; \frac{p}{1-p}$$

we want to pick class

$$\text{round}(\text{logit}(\;\text{Prob}[\;\text{class} = 1 \;|\; \mathbf{x}\;]\;)) \;\approx\; \sigma^{-1}(\;\text{Prob}[\;\text{class} = 1 \;|\; \mathbf{x}\;]\;).$$

# Logistic Regression

In general, if there are $K > 2$ classes, we consider all $K$ models of the form

$$\log \frac{\text{Prob}[\text{ class} = k \mid \mathbf{x} \text{ ]}}{1 \ - \ \text{Prob}[\text{ class} = k \mid \mathbf{x} \text{ ]}} \ = \ \langle \mathbf{w}_k, \mathbf{x} \rangle \ + \ c_k$$

with $\ell \neq k$ and $\sigma$ is the logistic function.

An equivalent formulation of these models is:

$$\text{Prob}[\text{ class} = k \mid \mathbf{x} \text{ ]} \ = \ \sigma(\ \langle \mathbf{w}_k, \mathbf{x} \rangle \ + \ c_k \ ).$$

# Logistic Regression