

# Machine learning notes

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## 1 Preliminary definitions

### 1.1 Trace of a matrix

The **trace** of a square matrix  $\mathbf{A}$ , denoted as  $\text{Tr}(\mathbf{A})$  is the sum of diagonal elements:

$$\text{Tr}(\mathbf{A}) = \sum_{d=1}^p A_{dd} \quad (1.1)$$

It follows that  $\text{Tr}(\mathbf{I}_d) = p$ . Also  $\text{Tr}(\mathbf{AB}) = \text{Tr}(\mathbf{BA})$  and  $\text{Tr}(\mathbf{x}^T \mathbf{x}) = \mathbf{x}^T \mathbf{x}$  the latter being a scalar.

### 1.2 Expectation

**Definition 1.1. Expectation** Let  $X$  be a random variable with a finite number of outcomes  $x_1, x_2, \dots, x_k$  occurring respectively with probabilities  $p_1, p_2, \dots, p_k$ . The expectation value is the summation of each outcome times its probability.

$$E[X] = \sum_k x_k \cdot p_k \quad (1.2)$$

In case of an infinite number of outcomes the summation is replaced with the integral:

$$E[X] = \int x \cdot p(x) dx \quad (1.3)$$

As explained here, when many random variables are involved, and there is no subscript in the  $E$  symbol, the expected value is taken with respect to their joint distribution:

$$E[h(X, Y)] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h(x, y) f_{XY}(x, y) dx dy$$

When a subscript is present, in some cases it tells us on which variable we should condition. So

$$E_X[h(X, Y)] = E[h(X, Y) | X] = \int_{-\infty}^{\infty} h(x, y) f_{h(X, Y)|X}(h(x, y) | x) dh$$

...But in other cases, it tells us which density to use for the "averaging"

$$E_X[h(X, Y)] = \int_{-\infty}^{\infty} h(x, y) f_X(x) dx$$

### 1.3 Variance

**Definition 1.2. Variance** The variance of a random variable X is the expected value of the squared deviation from the mean of X:

$$\text{Var}(X) = E[(X - \mu)^2] \quad (1.4)$$

Variance can be expressed in another way recalling  $\mu = E[X]$  and using the linearity property:

$$\begin{aligned} \text{Var}(X) &= E[(X - \mu)^2] = E[(X - E[X])^2] = \\ &= E[X^2 - 2 \cdot X \cdot E[X] + E[X]^2] \\ &= E[X^2] - 2 \cdot E[X \cdot \mu] + E[\mu^2] \\ &= E[X^2] - 2 \cdot \mu \cdot E[X] + \mu^2 \\ &= E[X^2] - \mu^2 = E[X^2] - E[X]^2 \end{aligned} \quad (1.5)$$

### 1.4 Median

**Definition 1.3. Median** For any probability distribution on the real line  $\mathbb{R}$  with cumulative distribution function F, regardless of whether it is any kind of continuous probability distribution, in particular an absolutely continuous distribution (which has a probability density function), or a discrete probability distribution, a median is by definition any real number m that satisfies

the inequalities:

$$P(x \leq m) \geq \frac{1}{2} \quad \text{and} \quad P(x \leq m) \geq \frac{1}{2} \quad (1.6)$$

(1.7)

or equivalently the inequalities

$$\int_{-\infty}^m F(x)dx \geq \frac{1}{2} \quad \text{and} \quad \int_m^\infty F(x)dx \geq \frac{1}{2} \quad (1.8)$$

## 1.5 Median as the minimizer of L<sub>1</sub> norm

Assume that S is a finite set, with say k elements. Line them up in order, as  $s_1 < s_2 < \dots < s_k$ .

If k is even there are (depending on the exact definition of median) many medians.  $|x - s_i|$  is the *distance* between x and  $s_i$ , so we are trying to minimize the sum of the distances. For example, we have k people who live at various points on the x-axis. We want to find the point(s) x such that the sum of the travel distances of the k people to x is a minimum.

Imagine that the  $s_i$  are points on the x-axis. For clarity, take k = 7. Start from well to the left of all the  $s_i$ , and take a tiny step, say of length  $\epsilon$ , to the right. Then you have gotten  $\epsilon$  closer to every one of the  $s_i$ , so the sum of the distances has decreased by  $7\epsilon$ .

Keep taking tiny steps to the right, each time getting a decrease of  $7\epsilon$ . This continues until you hit  $s_1$ . If you now take a tiny step to the right, then your distance from  $s_1$  increases by  $\epsilon$ , and your distance from each of the remaining  $s_i$  decreases by  $\epsilon$ . So there is a decrease of  $6\epsilon$ , and an increase of  $\epsilon$ , for a net decrease of  $5\epsilon$  in the sum.

This continues until you hit  $s_2$ . Now, when you take a tiny step to the right, your distance from each of  $s_1$  and  $s_2$  increases by  $\epsilon$ , and your distance from each of the five others decreases by  $\epsilon$ , for a net decrease of  $3\epsilon$ .

This continues until you hit  $s_3$ . The next tiny step gives an increase of  $3\epsilon$ , and a decrease of  $4\epsilon$ , for a net decrease of  $\epsilon$ .

This continues until you hit  $s_4$ . The next little step brings a total increase of  $4\epsilon$ , and a total decrease of  $3\epsilon$ , for an increase of  $\epsilon$ . Things get even worse when you travel further to the right. So the minimum sum of distances is reached at  $s_4$ , the median.

The situation is quite similar if k is even, say k = 6. As you travel to the right, there is a net decrease at every step, until you hit  $s_3$ . When you

are between  $s_3$  and  $s_4$ , a tiny step of  $\epsilon$  increases your distance from each of  $s_1$ ,  $s_2$ , and  $s_3$  by  $\epsilon$ . But it decreases your distance from each of the three others, for no net gain. Thus any  $x$  in the interval from  $s_3$  to  $s_4$ , including the endpoints, minimizes the sum of the distances.

In the even case, Some people prefer to say that any point between the two "middle" points is a median. So the conclusion is that the points that minimize the sum are the medians. Other people prefer to define the median in the even case to be the average of the two "middle" points. Then the median does minimize the sum of the distances, but some other points also do.

**In formulas** consider two  $x_i$ 's  $x_1$  and  $x_2$ , with  $x_2 > x_1$

•

$$\begin{aligned} x_1 \leq a \leq x_2 \\ \sum_{i=1}^2 |x_i - a| = |x_1 - a| + |x_2 - a| = a - x_1 + x_2 - a = x_2 - x_1 \end{aligned} \quad (1.9)$$

•

$$\begin{aligned} a < x_1 \\ \sum_{i=1}^2 |x_i - a| &= x_1 - a + x_2 - a = x_1 + x_2 - 2a \geq x_1 + x_2 - 2x_1 \\ &= x_2 - x_1 \end{aligned} \quad (1.10)$$

•

$$\begin{aligned} a \geq x_2 \\ \sum_{i=1}^2 |x_i - a| &= -x_1 + a - x_2 + a = -x_1 - x_2 + 2a \geq -x_1 - x_2 + 2x_2 \\ &= x_2 - x_1 \end{aligned} \quad (1.11)$$

$\implies$  for any two  $x_i$ 's the sum of the absolute values of the deviations is minimum when  $x_1 \leq a \leq x_2$  or  $a \in [x_1, x_2]$ .

When n is odd,

$$\begin{aligned} \sum_{i=1}^n |x_i - a| &= |x_1 - a| + |x_2 - a| + \cdots + \left| x_{\frac{n-1}{2}} - a \right| + \left| x_{\frac{n+1}{2}} - a \right| + \\ &\quad + \left| x_{\frac{n+3}{2}} - a \right| + \cdots + |x_{n-1} - a| + |x_n - a| \end{aligned} \quad (1.12)$$

consider the intervals  $[x_1, x_n], [x_2, x_{n-1}], [x_3, x_{n-2}], \dots, \left[ x_{\frac{n-1}{2}}, x_{\frac{n+3}{2}} \right]$ . If a is a member of all these intervals. i.e,  $\left[ x_{\frac{n-1}{2}}, x_{\frac{n+3}{2}} \right]$ ,

using the above theorem, we can say that all the terms in the sum except  $\left| x_{\frac{n+1}{2}} - a \right|$  are minimized. So

$$\begin{aligned} \sum_{i=1}^n |x_i - a| &= (x_n - x_1) + (x_{n-1} - x_2) + (x_{n-2} - x_3) + \cdots + \\ &\quad + \left( x_{\frac{n+3}{2}} - x_{\frac{n-1}{2}} \right) + \left| x_{\frac{n+1}{2}} - a \right| = \left| x_{\frac{n+1}{2}} - a \right| + \text{constant} \end{aligned} \quad (1.13)$$

To minimize also the term  $\left| x_{\frac{n+1}{2}} - a \right|$  it is clear we have to choose  $a = x_{\frac{n+1}{2}}$  to get 0 but this is the definition of the median.

$\implies$  When n is odd, the median minimizes the sum of absolute values of the deviations.

When n is even,

$$\begin{aligned} \sum_{i=1}^n |x_i - a| &= |x_1 - a| + |x_2 - a| + \cdots + \left| x_{\frac{n}{2}} - a \right| + \\ &\quad + \left| x_{\frac{n}{2}+1} - a \right| + \cdots + |x_{n-1} - a| + |x_n - a| \end{aligned} \quad (1.14)$$

If a is a member of all the intervals  $[x_1, x_n], [x_2, x_{n-1}], [x_3, x_{n-2}], \dots, \left[ x_{\frac{n}{2}}, x_{\frac{n}{2}+1} \right]$ , i.e,  $a \in \left[ x_{\frac{n}{2}}, x_{\frac{n}{2}+1} \right]$ ,

$$\begin{aligned} \sum_{i=1}^n |x_i - a| &= (x_n - x_1) + (x_{n-1} - x_2) + (x_{n-2} - x_3) + \cdots + \\ &\quad + \left( x_{\frac{n}{2}+1} - x_{\frac{n}{2}} \right) \end{aligned} \tag{1.15}$$

$\implies$  When  $n$  is even, any number in the interval  $[x_{\frac{n}{2}}, x_{\frac{n}{2}+1}]$ , i.e, including the median, minimizes the sum of absolute values of the deviations. For example consider the series: 2, 4, 5, 10, median,  $M = 4.5$ .

$$\sum_{i=1}^4 |x_i - M| = 2.5 + 0.5 + 0.5 + 5.5 = 9$$

If you take any other value in the interval  $[x_{\frac{n}{2}}, x_{\frac{n}{2}+1}] = [4, 5]$ , say 4.1

$$\sum_{i=1}^4 |x_i - 4.1| = 2.1 + 0.1 + 0.9 + 5.9 = 9$$

Taking for example 4 or 5 yields the same result:

$$\sum_{i=1}^4 |x_i - 4| = 2 + 0 + 1 + 6 = 9$$

$$\sum_{i=1}^4 |x_i - 5| = 3 + 1 + 0 + 5 = 9$$

This is because when summing the distance from  $a$  to the two middle points, you end up with the distance between them:  $a - x_{\frac{n}{2}} + (x_{\frac{n}{2}+1} - a) = x_{\frac{n}{2}+1} - x_{\frac{n}{2}}$

For any value outside the interval  $[x_{\frac{n}{2}}, x_{\frac{n}{2}+1}] = [4, 5]$ , say 5.2

$$\sum_{i=1}^4 |x_i - 5.2| = 3.2 + 1.2 + 0.2 + 4.8 = 9.4$$

## 1.6 Gaussian function and gaussian distribution

**Definition 1.4. Gaussian function** A Gaussian function is a mathematical function in the form:

$$f(x) = ae^{-\frac{(x-b)^2}{2c^2}} \quad (1.16)$$

The Gaussian function has three parameters  $a, b$  and  $c$ . The graph of a Gaussian function is the Bell curve. The parameter  $a$  is the height of the curve's peak,  $b$  is the position of the peak and  $c$  the *standard deviation* controls the width of the bell.

An important property of the Gaussian function is that the product of two Gaussian functions is still a Gaussian function:

$$\begin{aligned} f(x) \cdot g(x) &= ae^{-\frac{(x-b)^2}{2c^2}} a_1 e^{-\frac{(x-b_1)^2}{2c_1^2}} = (a \cdot a_1) e^{-\frac{x^2 - 2bx + b^2 + x^2 - 2b_1x + b_1^2}{2c^2 2c_1^2}} = \\ &= (a \cdot a_1) e^{-\frac{2x^2 - 2x(b+b_1) + b^2 + b_1^2}{2c^2 2c_1^2}} = (a \cdot a_1) e^{-\frac{x^2 - 2x \frac{b+b_1}{2} + \frac{b^2 + b_1^2}{2}}{2c^2 c_1^2}} = \\ &= (a \cdot a_1) e^{-\frac{x^2 - 2x \frac{b+b_1}{2} + \frac{b^2 + b_1^2}{2}}{2c^2 c_1^2}} e^{-\frac{\left(\frac{b+b_1}{2}\right)^2 - \left(\frac{b+b_1}{2}\right)^2}{2c^2 c_1^2}} = \\ &= (a \cdot a_1) e^{-\frac{x^2 - 2x \frac{b+b_1}{2} + \left(\frac{b+b_1}{2}\right)^2}{2c^2 c_1^2}} e^{-\frac{\left(\frac{b+b_1}{2}\right)^2 - \frac{b^2 + b_1^2}{2}}{2c^2 c_1^2}} = \quad (1.17) \\ &= (a \cdot a_1) e^{-\frac{\left(x - \frac{b+b_1}{2}\right)^2}{2c^2 c_1^2}} e^{-\frac{\left(\frac{b+b_1}{2}\right)^2 - \frac{b^2 + b_1^2}{2}}{2c^2 c_1^2}} = \\ &= a_2 e^{-\frac{\left(x - \frac{b+b_1}{2}\right)^2}{2c^2 c_1^2}} = a_2 e^{-\frac{(x-b_2)^2}{2c_2^2}} \end{aligned}$$

**Definition 1.5. Gaussian distribution** A normalized Guassian function or normal distribution is a Gaussian function with an area under the curve equal to 1. Hence it can be interpreted as a probability distribution.

To find the formula let us force the curve to have area 1:

$$\int_{-\infty}^{\infty} ae^{-\frac{(y-b)^2}{2c^2}} dy = a \int_{-\infty}^{\infty} e^{-\frac{(y-b)^2}{2c^2}} dy \quad (1.18)$$

and performing a change of integration variable:

$$\begin{aligned} \frac{y-b}{\sqrt{2c}} = x \Rightarrow dx = dy \frac{1}{\sqrt{2c}} dx \Rightarrow dy = \sqrt{2c} dx \\ a \int_{-\infty}^{\infty} e^{-\frac{(y-b)^2}{2c^2}} dy = \sqrt{2c} a \int_{-\infty}^{\infty} e^{-x^2} dx \end{aligned} \quad (1.19)$$

where  $\sqrt{2c}$  is a constant so that it can be moved out of the integral. From now on we will focus just on the integral.

Unfortunately the integral has not solutions with elementary functions (Liouville theorem, see Abstract Algebra). However the definite integral exists (demonstration is skipped) and it is:

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} \quad (1.20)$$

To have area equal to 1 we must have:

$$ac\sqrt{2\pi} = 1 \Rightarrow a = \frac{1}{\sqrt{2\pi}c} \quad (1.21)$$

So now the function is defined by just 2 parameters.

Normally  $b = \mu$  and is the mean of the function while  $c = \sigma$  is the standard deviation.

As opposed to the Gaussian function, multiplying two of these functions we do not get another gaussian distribution, but a scaled gaussian distribution. If the Gaussian functions have 0-mean and  $\sigma^2 = 1$  then the product is still Gaussian distribution with 0-mean and  $\sigma^2 = 1$ .

**Definition 1.6. Standard Normal Gaussian distribution** A Standard Normal Gaussian distribution is a Gaussian distribution with 0 mean and standard deviation 1.

## 2 Statistical Decision Theory

### 2.1 Expected prediction error

Let  $X \in \mathbb{R}^P$  denote a real valued random input vector, and  $Y \in \mathbb{R}^P$  a real valued random output variable, with joint distribution  $Pr(X, Y)$ . We seek

a function  $f(X)$  for predicting  $Y$  given values of the input  $X$ . This theory requires a loss function  $L(Y, f(X))$  for penalizing errors in prediction, and by far the most common and convenient is squared error loss:  $L(Y, f(X)) = (Y - f(X))^2$ .

The estimated prediction error is

$$\begin{aligned} \text{EPE}(f) &= \mathbf{E} \left[ (Y - f(X))^2 \right] = \int (y - f(x))^2 p(x, y) dx dy \\ &= \int_x \int_y (y - f(x))^2 p(x, y) dx dy \end{aligned} \quad (2.1)$$

Recalling  $p(x, y) = p(y|x)p(x)$ :

$$\begin{aligned} \text{EPE}(f) &= \int_x \int_y (y - f(x))^2 p(y|x)p(x) dx dy \\ &= \int_x \int_y ((y - f(x))^2 p(y|x) dy) p(x) dx \\ &= \int_x \mathbf{E}_{Y|X} [(y - f(X))^2 | X = x] p(x) dx \\ &= \mathbf{E}_X [\mathbf{E}_{Y|X} [(y - f(X))^2 | X = x]] \end{aligned} \quad (2.2)$$

So to minimize the prediction error:

$$f(x) = \arg \min_c \mathbf{E}_{Y|X} [(y - c(x))^2 | X = x] \Rightarrow f(x) = \mathbf{E}[Y|X = x] \quad (2.3)$$

The *Nearest Neighbour* algorithm, assigns labels to points by counting and averaging the labels of the points belonging to a given neighbourhood:

$$\hat{f}(x) = \text{Ave} (y_i | x_i \in N_k(x)) \quad (2.4)$$

where  $N_k(x)$  contains the  $k$  points closest to  $x$ . This presents **two approximations**

- expectation is approximated by averaging
- conditioning at a point is relaxed to conditioning on some region centred at the target point.

With  $k$  sufficiently large, the average gets more stable and with large  $N$  the points will be more likely close to  $x$ . If  $k, N \rightarrow \infty$  with  $k/N \rightarrow 0$  the average becomes the expectation and we have the best possible estimator.

Unfortunately often we do not have so much data and some other times we might want exploit the supposed structure of data (linear, polynomial etc.).

However there is even a bigger problem when there are too many dimensions (i.e.,  $p$  is large). Consider a uniformly distributed input in a  $p$  dimensional unit hypercube. Consider a hypercube neighbourhood around the target point capturing a fraction  $r$  of the total observations distributed among the unit hypercube. The edge of the neighbour hypercube will be  $e_p(r) = r^{1/p}$ . In 10 dimensions, using a neighborhood capturing 1% of the data we have  $r(0.01) = 0.63$  so we must use 63% of the total data for one target.

On the contrary the linear regression is a **model-based approach**, i.e., one assumes that the function  $f(x)$  is approximately linear:

$$f(x) \approx x^T \beta \quad (2.5)$$

Putting this in the EPE equation:

$$\begin{aligned} f(x) &= \arg \min_c E_{Y|X} \left[ (y - c(x))^2 | X = x \right] \\ &= \arg \min_{\beta} E_{Y|X} \left[ (y - x^T \beta)^2 | X = x \right] \\ \Rightarrow \beta &= \left[ E[X \cdot X^T] \right]^{-1} \cdot E[X \cdot Y] \end{aligned} \quad (2.6)$$

The minimum of a quadratic function is given by deriving and setting its derivative to 0.

If instead of a  $L_2$  loss function we use  $L_1$

$$\begin{aligned} EPE(f) &= E[|Y - f(X)|] = \int |y - f(x)| p(x, y) dx dy \\ &= \int_x \int_y |y - f(x)| p(x, y) dx dy \end{aligned} \quad (2.7)$$

Recalling  $p(x, y) = p(y|x)p(x)$ :

$$\begin{aligned}
EPE(f) &= \int_x \int_y |y - f(x)| p(y|x)p(x) dx dy \\
&= \int_x \int_y |(y - f(x))| p(y|x) dy p(x) dx \\
&= \int_x E_{Y|X} [|y - f(X)| |X = x] p(x) dx \\
&= E_X [E_{Y|X} [|y - f(X)| |X = x]]
\end{aligned} \tag{2.8}$$

$$f(x) = \arg \min_c E_{Y|X} [|y - c(x)| |X = x] \tag{2.9}$$

and as already seen in 1.5, the minimizer for the sum of distances is the median.

### 2.1.1 Loss function for categorical variables

For categorical output variables  $\mathbb{G}_k$  we have:

$$EPE = E \left[ L \left( G, \hat{G}(X) \right) \right] = E_x \sum_{k=1}^K L \left[ \mathbb{G}_k, \hat{G}(X) \right] \Pr(\mathbb{G}_k | X) \tag{2.10}$$

where the expectation is again taken with respect to the joint distribution  $\Pr(G, X)$ . Conditioning again we can write:

$$EPE = E_x \sum_{k=1}^K L \left[ \mathbb{G}_k, \hat{G}(X) \right] \Pr(\mathbb{G}_k | X) \tag{2.11}$$

where the integral over  $y$  has been substituted with the summation due to the categorical nature of the variable.

The minimizer is given by:

$$\hat{G}(x) = \arg \min_{g \in \mathbb{G}} \sum_{k=1}^K L(\mathbb{G}_k, g) \Pr(\mathbb{G}_k | X = x) \tag{2.12}$$

Often the *zero-one loss function* is used for categorical variables and the above simplifies to:

$$\hat{G}(x) = \arg \min_{g \in \mathbb{G}} [1 - \Pr(g|X=x)] = \arg \max_{g \in \mathbb{G}} [\Pr(g|X=x)] \quad (2.13)$$

This is known as *Bayes classifier* because **it classifies to the most probable class, using conditional discrete probability distribution.**

**Note:** When models or loss functions use additional parameters that penalize complexity (Lasso, Ridge and others) we cannot use the training data to determine these parameters, since we would pick those that gave interpolating fits with zero residuals but it will be unlikely to predict future data.

## 2.2 Bias-Variance trade-off

$$\begin{aligned} EPE(f) &= \mathbf{E} [(Y - f(X))^2] = \\ &= \mathbf{E} [Y^2] - 2\mathbf{E}[Y]\mathbf{E}[f(X)] + \mathbf{E}[f(X)^2] \\ &= Y^2 - 2Y\mathbf{E}[f(X)] + \mathbf{E}[f(X)^2] \end{aligned} \quad (2.14)$$

Recalling

$$\begin{aligned} \text{BIAS}(Y, \mathbf{E}[f(X)]) &= |Y - \mathbf{E}[f(X)]| \\ \Rightarrow \text{BIAS}(Y, f(X))^2 &= (Y - \mathbf{E}[f(X)])^2 \\ &= Y^2 - 2Y\mathbf{E}[f(X)] + \mathbf{E}[f(X)]^2 \end{aligned} \quad (2.15)$$

EPE can be expressed using also the Variance definition in 1.3

$$\begin{aligned} EPE(f) &= Y^2 - 2Y\mathbf{E}[f(X)] + \mathbf{E}[f(X)]^2 - \mathbf{E}[f(X)]^2 \\ &= \text{BIAS}(Y, f(X))^2 + \text{Var}(Y, f(x)) \end{aligned} \quad (2.16)$$

The bias is given by the distance of our predictions from real points. Complex models have more degrees of freedom and are able to fit closer real points hence they tend to have low bias. However, they present higher variance. On the contrary simple models (i.e., linear) have lower variance but higher bias.

The error due to variance is the amount by which the prediction, over one training set, differs from the expected predicted value, over all the training sets. As with bias, you can repeat the entire model building process multiple times. To paraphrase Manning et al (2008), variance measures how inconsistent are the predictions from one another, over different training sets, not whether they are accurate or not. A learning algorithm with low bias must be "flexible" so that it can fit the data well. But if the learning algorithm is too flexible, it will fit each training data set differently, and hence have high variance.

For linear models fit by ordinary least squares, the estimation bias is zero. For restricted fits, such as ridge regression, it is positive, and we trade it off with the benefits of a reduced variance.

## 3 Linear Regression Models

We start from the *univariate linear regression*, i.e., each output consists of a single value while the input is a vector of values.

### 3.1 Univariate linear regression

Univariate means single output, i.e,  $y$  is a number. The basic form is

$$f(X) = \beta_0 + \sum_{j=1}^p X_j \beta_j \quad (3.1)$$

The most popular estimation method for a linear model is the least square:

$$RSS(\beta) = \sum_{i=1}^p (y_i - f(x_i))^2 = (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \quad (3.2)$$

where  $\mathbf{X}$  is a  $N \times (p + 1)$  matrix with each row being an input vector,  $\mathbf{y}$  a  $N$  vector (we must have  $N$  input-output pairs, in this case the output is considered mono-dimensional).

By minimizing we get:

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \quad (3.3)$$

Geometrically we are projecting  $\mathbf{y}$  onto the hyperplane spanned by  $\mathbf{X}$  and the projections is referred to as  $\hat{\mathbf{y}}$ :

$$\hat{\mathbf{y}} = \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} = \mathbf{H} \mathbf{Y} \quad (3.4)$$

where  $\mathbf{H}$  is called the *hat* matrix.

### 3.2 Equivalence of Ordinary least squares and maximum likelihood

We are using an additive model, assuming a Gaussian white noise:

$$\mathbf{y} = \beta^T \mathbf{x} + \epsilon \quad (3.5)$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2) \quad (3.6)$$

Adding a constant to a Gaussian random variable is equivalent to another Gaussian random variable with the mean shifted:

$$\Pr(\mathbf{y}) \sim \mathcal{N}(\beta^T \mathbf{x}, \sigma^2) \quad (3.7)$$

Considering the matrix  $\mathbf{X}$  and the output vector  $\mathbf{y}$  representing the training set, used to estimate the coefficients, we have:

$$\Pr(\mathbf{y} | \mathbf{X}, \beta, \sigma^2) = \prod_{i=1}^N \Pr(y_i | \mathbf{x}_i, \beta, \sigma^2) = \prod_{i=1}^N \mathcal{N}(\beta^T \mathbf{x}_i, \sigma^2) \quad (3.8)$$

where we have assumed each observation is independent. A product of univariate Gaussian can be rewritten as a multivariate Gaussian:

$$\begin{aligned} \Pr(\mathbf{y} | \mathbf{X}, \beta, \sigma^2) &= \prod_{i=1}^N \mathcal{N}(\beta^T \mathbf{x}_i, \sigma^2) = \prod_{i=1}^N \frac{1}{(2\pi)^{\frac{1}{2}} \sigma} e^{-\frac{(y_i - \beta^T \mathbf{x}_i)^2}{2\sigma^2}} = \\ &= \frac{1}{(2\pi)^{\frac{p}{2}} \sigma} \prod_{i=1}^N e^{-\sum_{i=1}^N \frac{(y_i - \beta^T \mathbf{x}_i)^2}{2\sigma^2}} = \\ &= \frac{1}{(2\pi)^{\frac{p}{2}} \sigma^{|I|}} e^{-\frac{1}{2} (\mathbf{y} - \beta^T \mathbf{X})^T (\sigma^2 \mathbf{I})^{-1} (\mathbf{y} - \beta^T \mathbf{X})} = \mathcal{N}(\beta^T \mathbf{X}, \sigma^2 \mathbf{I}) \end{aligned} \quad (3.9)$$

If the variables are not independent the more general form is:

$$\mathcal{N}(\beta^T \mathbf{X}, \Sigma) = \frac{1}{(2\pi)^{\frac{p}{2}} |\Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2} (\mathbf{y} - \beta^T \mathbf{X})^T \Sigma^{-1} (\mathbf{y} - \beta^T \mathbf{X})} \quad (3.10)$$

**Definition of likelihood** The quantity  $\Pr(\mathbf{y}|\mathbf{x}, \beta, \sigma^2)$  is called **likelihood** and tell us how much it is likely the outcome  $y_i$  in the dataset given the input  $\mathbf{x}$  and the parameters.

A different approach to find a model that fits the data is to maximize the *likelihood* of the whole dataset:

$$L = \Pr(\mathbf{y}|\mathbf{X}, \beta, \sigma^2) = \frac{1}{(2\pi)^{\frac{p}{2}} |\Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(\mathbf{y} - \beta^T \mathbf{X})^T \Sigma^{-1} (\mathbf{y} - \beta^T \mathbf{X})} \quad (3.11)$$

Actually maximizing the likelihood is equivalent to maximizing its logarithmic, the *log-likelihood*:

$$\begin{aligned} \log L &= \sum_{i=1}^N \log \left[ \frac{1}{(2\pi)^{\frac{1}{2}} \sigma} e^{-\frac{(y_i - \beta^T x_i)^2}{2\sigma^2}} \right] \\ &= \sum_{i=1}^N -\frac{1}{2} \log 2\pi - \log \sigma - \frac{(y_i - \beta^T x_i)^2}{2\sigma^2} = \\ &= -\frac{1}{2} \log 2\pi - \log \sigma - \frac{1}{2\sigma^2} \sum_{i=1}^N (y_i - \beta^T x_i)^2 \end{aligned} \quad (3.12)$$

As already done for OLS, taking the derivative w.r.t.  $\beta$  and setting it to 0:

$$\begin{aligned} \frac{\partial \log L}{\partial \beta} &= -\frac{1}{2\sigma^2} (-2) (y_i - \beta^T x_i) = 0 \\ \Rightarrow (y - \beta^T \mathbf{X}) &= 0 \Rightarrow \beta = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \end{aligned} \quad (3.13)$$

This is the same solution of the OLS: the two models are equivalent.

**The two models are equivalent assuming a normal distribution.**

### 3.3 Expectation of the parameter estimation: unbiased estimator

Computing the expectation of  $\hat{\beta}$ :

$$\begin{aligned}
E_{Pr(y|X,\beta,\sigma^2)}[\hat{\beta}] &= \sum \hat{\beta} Pr(y|X, \beta, \sigma^2) = \\
&= (X^T X)^{-1} X^T \sum y Pr(y|X, \beta, \sigma^2) = \\
&= (X^T X)^{-1} X^T E_{Pr(y|X,\beta,\sigma^2)}[y] = \\
&= (X^T X)^{-1} X^T X \beta = \beta
\end{aligned} \tag{3.14}$$

This is an **unbiased estimator**.

Now let us calculate the covariance matrix:

$$\begin{aligned}
\text{Cov}[\hat{\beta}] &= \\
&= E_{Pr(y|X,\beta,\sigma^2)} \left[ (\hat{\beta} - E_{Pr(y|X,\beta,\sigma^2)}[\beta]) (\hat{\beta} - E_{Pr(y|X,\beta,\sigma^2)}[\beta])^T \right] = \\
&= E_{Pr(y|X,\beta,\sigma^2)} \left[ (\hat{\beta} - \beta) (\hat{\beta} - \beta)^T \right] = \\
&= E_{Pr(y|X,\beta,\sigma^2)} [\hat{\beta} \hat{\beta}^T] - \beta \beta^T
\end{aligned} \tag{3.15}$$

and

$$\begin{aligned}
E_{Pr(y|X,\beta,\sigma^2)}[\hat{\beta} \hat{\beta}^T] &= \\
&= E_{Pr(y|X,\beta,\sigma^2)} \left[ \left( (X^T X)^{-1} X^T y \right) \left( (X^T X)^{-1} X^T y \right)^T \right] = \\
&= (X^T X)^{-1} X^T E_{Pr(y|X,\beta,\sigma^2)}[y y^T] X (X^T X)^{-1}
\end{aligned} \tag{3.16}$$

and recalling from 3.9  $Pr(y) \sim \mathcal{N}(\beta^T X, \sigma^2 I)$

$$\begin{aligned}
\text{Cov}[y] &= \sigma^2 I = \\
&= E_{Pr(y|X,\beta,\sigma^2)}[y y^T] - E_{Pr(y|X,\beta,\sigma^2)}[y] E_{Pr(y|X,\beta,\sigma^2)}[y^T]
\end{aligned} \tag{3.17}$$

Rearranging

$$\begin{aligned}
& \Rightarrow E_{Pr(y|\mathbf{X}, \beta, \sigma^2)} [yy^T] = \sigma^2 \mathbf{I} + E_{Pr(y|\mathbf{X}, \beta, \sigma^2)} [y] E_{Pr(y|\mathbf{X}, \beta, \sigma^2)} [y^T] = \\
& = \sigma^2 \mathbf{I} + E_{Pr(y|\mathbf{X}, \beta, \sigma^2)} [\mathbf{X}\beta] E_{Pr(y|\mathbf{X}, \beta, \sigma^2)} [\beta^T \mathbf{X}^T] = \\
& = \sigma^2 \mathbf{I} + \mathbf{X}\beta\beta^T\mathbf{X}^T
\end{aligned} \tag{3.18}$$

Substituting:

$$\begin{aligned}
E_{Pr(y|\mathbf{X}, \beta, \sigma^2)} [\hat{\beta}\hat{\beta}^T] &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T (\sigma^2 \mathbf{I} + \mathbf{X}\beta\beta^T\mathbf{X}^T) \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} = \\
&= \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1}
\end{aligned} \tag{3.19}$$

and finally variance-covariance matrix of the least square parameters is

$$Cov [\hat{\beta}] = (\mathbf{X}^T \mathbf{X})^{-1} \sigma^2 \tag{3.20}$$

$$\text{Var}(\hat{\beta}) = (\mathbf{X}^T \mathbf{X})^{-1} \sigma^2 \tag{3.21}$$

### 3.4 Noise variance estimation

We can find an estimation of the noise variance from the maximum likelihood model using the same procedure used to find the parameters, i.e., taking the derivative and equating it to 0:

$$\begin{aligned}
\frac{\partial \log L}{\partial \sigma} &= \sum_{i=1}^N -\frac{1}{\sigma} + \frac{1}{\sigma^3} (y_i - \mathbf{x}_i^T \beta)^2 = 0 \Rightarrow \frac{N}{\sigma} + \frac{1}{\sigma^3} \sum_{i=1}^N (y_i - \mathbf{x}_i^T \beta)^2 = 0 \\
\Rightarrow \hat{\sigma}^2 &= \frac{1}{N} \sum_{i=1}^N (y_i - \mathbf{x}_i^T \beta)^2
\end{aligned} \tag{3.22}$$

This can be re-expressed as

$$\begin{aligned}
\Rightarrow \hat{\sigma}^2 &= \frac{1}{N} \sum_{i=1}^N \left( y_i - \mathbf{x}_i^T \hat{\beta} \right)^2 = \frac{1}{N} \sum_{i=1}^N \left( y_i - \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \right)^2 = \\
&= \frac{1}{N} \left( \mathbf{y} - \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \right)^T \left( \mathbf{y} - \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \right) = \\
&= \mathbf{y}^T \mathbf{y} - 2 \mathbf{y}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} + \mathbf{y}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \cancel{\mathbf{X}^T} \cancel{\mathbf{X}} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \\
&= \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \left( \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} \hat{\beta} \right)
\end{aligned} \tag{3.23}$$

Taking the expectation w.r.t.  $\Pr(\mathbf{y}|\mathbf{X}, \beta, \sigma^2)$ :

$$\begin{aligned}
\mathbf{E}_{\Pr(\mathbf{y}|\mathbf{X}, \beta, \sigma^2)} [\hat{\sigma}^2] &= \frac{1}{N} \mathbf{E}_{\Pr(\mathbf{y}|\mathbf{X}, \beta, \sigma^2)} [\mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} \hat{\beta}] = \\
&= \frac{1}{N} \mathbf{E}_{\Pr(\mathbf{y}|\mathbf{X}, \beta, \sigma^2)} [\mathbf{y}^T \mathbf{y}] - \frac{1}{N} \mathbf{E}_{\Pr(\mathbf{y}|\mathbf{X}, \beta, \sigma^2)} [\mathbf{y}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}]
\end{aligned} \tag{3.24}$$

Suppose  $\mathbf{t} \sim \mathcal{N}(\mu, \Sigma)$ , then  $\mathbf{E}_{p(\mathbf{t})} (\mathbf{t}^T \mathbf{A} \mathbf{t}) = \text{Tr}(\mathbf{A} \Sigma) + \mu^T \mathbf{A} \mu$  with  $\mu = \mathbf{X} \beta$

$$\begin{aligned}
E_{Pr(y|X,\beta,\sigma^2)} [\hat{\sigma}^2] &= \frac{1}{N} E_{Pr(y|X,\beta,\sigma^2)} [y^T y] + \\
&- \frac{1}{N} E_{Pr(y|X,\beta,\sigma^2)} [y^T X (X^T X)^{-1} X^T y] = \\
&= \frac{1}{N} E_{Pr(y|X,\beta,\sigma^2)} [y^T I_N y] + \\
&- \frac{1}{N} E_{Pr(y|X,\beta,\sigma^2)} [y^T X (X^T X)^{-1} X^T y] = \\
&= \frac{1}{N} (\text{Tr} (\sigma^2 I_N) + \beta^T X^T X \beta) + \\
&- \frac{1}{N} (\text{Tr} [\sigma^2 X (X^T X)^{-1} X^T] + \beta^T X^T X (X^T X)^{-1} X^T \beta) = \\
&= \frac{1}{N} (N \sigma^2 + \beta^T X^T X \beta) - \frac{1}{N} (\sigma^2 \text{Tr} [X (X^T X)^{-1} X^T] + \beta^T X^T X \beta) = \\
&= \sigma^2 + \frac{1}{N} \cancel{\beta^T X^T X \beta} - \frac{\sigma^2}{N} \text{Tr} [X (X^T X)^{-1} X^T] \cancel{- \frac{1}{N} \beta^T X^T X \beta} = \\
&= \sigma^2 - \frac{\sigma^2}{N} \text{Tr} [(X^T X)^{-1} X^T X] = \sigma^2 - \frac{\sigma^2}{N} \text{Tr} [I_p] \\
&\Rightarrow E_{Pr(y|X,\beta,\sigma^2)} [\hat{\sigma}^2] = \sigma^2 \left(1 - \frac{p}{N}\right)
\end{aligned} \tag{3.25}$$

where lastly we have used the product property of the trace (see 1.1).

Normally  $p < N$  hence the estimate of the variance is smaller than the true variance, so this estimator is **biased**. The estimate gets closer to the real value when  $p/N$  is small, i.e., assuming  $p$  is fixed, increasing the samples used.

This result might be strange. First of all notice from 3.22 that the closer the model gets to the data, the smaller  $\hat{\sigma}^2$ . By definition the parameter estimates are the ones that minimise the noise and hence  $\hat{\sigma}^2$ . As a consequence, when using the true parameters we would get equal or higher variance.

To estimate the true variance we can use the following formula:

$$\hat{\sigma}^2 = \frac{1}{N-p-1} \sum_{i=1}^N (y_i - \hat{y}_i)^2 \tag{3.26}$$

$N-p-1$  makes this estimation unbiased i.e.,  $\frac{1}{N-p-1} E[\hat{\sigma}^2] = \sigma^2$ .

### 3.5 Interpretation of covariance

Consider a covariance matrix of size  $2 \times 2$  for a two parameter model (i.e., a line on the plane) and suppose the first diagonal element, corresponding to the variable  $\hat{\beta}_0$  is much bigger than the second one corresponding to  $\hat{\beta}_1$ . This means that we can change  $\hat{\beta}_0$  a little without affecting too much the model. On the contrary if the variance is small, small changes will affect significantly the model. Sometimes this happens when one variable has a much higher absolute value.

If the values on the off-diagonals are negative, then when increasing one coefficient i.e.,  $\hat{\beta}_0$ , the other must be decreased to have the line to pass as close as possible to all points. For example in 2D, increasing  $\hat{\beta}_0$  reduces the coefficient value: if it is positive, the line will be "more horizontal", if negative it becomes steeper, "more vertical".

### 3.6 Z-score

Let us assume data were really generated by a linear model but were corrupted by Gaussian noise with 0 mean and variance  $\sigma^2$ :

$$Y = \beta_0 + \sum_i^p \beta_i X_i + \epsilon \quad (3.27)$$

where  $\epsilon \sim \mathcal{N}(0, \sigma^2)$ . The estimated parameters will still be a normal distribution:

$$\hat{\beta} \sim \mathcal{N}(\beta, (\mathbf{X}^T \mathbf{X})^{-1} \sigma^2) \quad (3.28)$$

**Definition 3.1. Z-score** A Z-score is a numerical measurement used in statistics of a value's relationship to the mean (average) of a group of values, measured in terms of standard deviations from the mean. If a Z-score is 0, it indicates that the data point's score is identical to the mean score. A Z-score of 1.0 would indicate a value that is one standard deviation from the mean. Z-scores may be positive or negative, with a positive value indicating the score is above the mean and a negative score indicating it is below the mean. Z-scores are measures of an observation's variability

$$z_j = \frac{x - \mu}{\sigma} \quad (3.29)$$

In machine learning the z-value is the regression coefficient divided by its standard error. It is also sometimes called the z-statistic. If the z-value is too big in magnitude (i.e., either too positive or too negative), it indicates that the corresponding true regression coefficient is not 0 and the corresponding X-variable matters. A good rule of thumb is to use a cut-off value of 2 which approximately corresponds to a two-sided hypothesis test with a significance level of  $\alpha = 0.05$ .

Z-values are computed as the test statistic for the hypothesis test that the true corresponding regression coefficient  $\beta$  is 0. In hypothesis testing, we assume the null hypothesis is true, and then see if the data provide evidence against it. So in this case, we assume  $\beta$  is 0. That is, we assume the expectation of the fitted regression coefficient  $\hat{\beta}$  is 0:

$$z_j = \frac{\hat{\beta}_j}{\hat{\sigma}_{\sqrt{v_j}}} \quad (3.30)$$

where the denominator is the variance of the parameter (from 3.28) with  $v_j$  being the diagonal element of  $(X^T X)^{-1}$ .

**Theorem 1 (The Gauss-Markov theorem).** Among all linear unbiased estimators, the least square estimates of the parameters are the ones having smallest variance and consequently from 2.16 is the one with the smallest mean squared error (the bias-squared term for unbiased estimator is by definition 0).

*Proof.* Let  $\hat{\beta} = Cy$  be another linear estimator of  $\beta$  with  $C = (X^T X)^{-1} X^T + D$

$$\mathbf{E} [\hat{\beta}] = \mathbf{E} [Cy] = \mathbf{E} \left[ \left( (X^T X)^{-1} X^T + D \right) (X\beta + \epsilon) \right] = \quad (3.31)$$

$$= \left( (X^T X)^{-1} X^T X \beta + D X \beta \right) + \underbrace{\left( (X^T X)^{-1} X^T + D \right)}_{\mathbf{E}[\epsilon]} = \quad (3.32)$$

$$= (\beta + D X \beta) = (I + D X) \beta \quad (3.33)$$

$$(3.34)$$

where  $\mathbf{E}[\epsilon] = 0$ .

To be an unbiased estimator  $\mathbf{D}\mathbf{X} = 0$ , then

$$\begin{aligned}
\text{Var}(\hat{\beta}) &= \text{Var}(\mathbf{C}\mathbf{y}) = \mathbf{C}\text{Var}(\mathbf{y})\mathbf{C}^T = \sigma^2 \mathbf{C}\mathbf{C}^T = \\
&= \sigma^2 \left( (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T + \mathbf{D} \right) \left( (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T + \mathbf{D} \right)^T = \\
&= \sigma^2 \left( (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T + \mathbf{D} \right) \left( \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} + \mathbf{D}^T \right) = \\
&= \sigma^2 \left( \cancel{(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T} \cancel{\mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1}} + (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{D}^T + \right. \\
&\quad \left. + \mathbf{D}\mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} + \mathbf{D}\mathbf{D}^T \right) = \\
&= \sigma^2 \left( \cancel{(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T} \cancel{\mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1}} + (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{D}\mathbf{X})^T + \right. \\
&\quad \left. + \mathbf{D}\mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} + \mathbf{D}\mathbf{D}^T \right) \\
&\mathbf{D}\mathbf{X} = 0 \\
\Rightarrow \text{Var}(\tilde{\beta}) &= \sigma^2 \left( (\mathbf{X}^T \mathbf{X})^{-1} + \cancel{(\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{D}\mathbf{X})^T} + \cancel{\mathbf{D}\mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1}} + \mathbf{D}\mathbf{D}^T \right) \\
\text{Var}(\tilde{\beta}) &= \text{Var}(\hat{\beta}) + \sigma^2 \mathbf{D}\mathbf{D}^T
\end{aligned} \tag{3.35}$$

□

### 3.7 Orthogonalization

Normally inputs are not perpendicular but can be orthogonalized. The goal is to define a new orthogonal basis for the data. The procedure, named **Grand-Schmidt procedure** is the following:

When inputs are correlated, the residual will be close to zero generating instabilities in the coefficients  $\hat{\beta}_j$  and the z-score will be small.

The algorithm in matrix form is

$$\mathbf{X} = \mathbf{Z}\Gamma$$

where  $\mathbf{z}_j$  are the column vectors of  $\mathbf{Z}$  and  $\Gamma$  is upper triangular. Introducing the diagonal matrix  $\mathbf{D}$  with  $j$ -th diagonal element  $D_{jj} = \|\mathbf{z}_j\|$  we get:

---



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initialize  $z_0 = x_0 = \mathbf{1}$  where  $\mathbf{1}$  is a vector of all ones;  
 For  $j = 1, \dots, p$  regress  $x_j$  on  $z_0, \dots, z_{p-1}$  to produce the coefficients  
 $\hat{\gamma}_{lj} = \frac{\langle z_l, x_j \rangle}{\langle z_l, z_l \rangle}$  for  $l = 0, \dots, j-1$ ;  
 Calculate the residual vectors as  $z_j = x_j - \sum_{k=0}^{j-1} \hat{\gamma}_{kj} z_k$ ;  
 Regress  $y$  on the residual  $z_p$  to get the estimate  $\hat{\beta}_p = \frac{\langle z_p, y \rangle}{\langle z_p, z_p \rangle}$

---

$$\mathbf{X} = \mathbf{ZD}^{-1}\mathbf{D}\boldsymbol{\Gamma} = \mathbf{QR} \quad (3.36)$$

where  $Q$  is an orthogonal,  $Q^T Q = I$ ,  $N \times (p+1)$  matrix and  $R$  is a  $(p+1)(p+1)$  upper triangular matrix.

The least square solution becomes

$$\hat{\boldsymbol{\beta}} = R^{-1} Q^T y \hat{y} = Q Q^T y \quad (3.37)$$

### 3.8 Multivariate output

We can rewrite the equation in matrix form:

$$Y = XB + E \quad (3.38)$$

where  $Y$  is a  $N \times K$  matrix,  $X$  is  $N \times (p+1)$ ,  $B$  is  $(p+1) \times K$ ,  $E$  has the same dimensions of  $Y$ . The root squared error is

$$\begin{aligned} \text{RSS}(B) &= \sum_{k=1}^K \sum_{i=1}^N (y_{ik} - f(x_i))^2 = \text{tr} \left[ (Y - XB)^T (Y - XB) \right] \\ &\Rightarrow B = (X^T X)^{-1} X^T Y \end{aligned} \quad (3.39)$$

Multiple outputs do not affect one another's least square estimates.

### 3.9 Subset selection

Least square estimates sometimes show low bias but high variance resulting in a non-satisfactory prediction accuracy. This can be improved by setting some coefficients to 0 to sacrifice a little of bias to reduce significantly the variance.

Other times it is useful to reduce the input dimensionality for easiness of interpretation or for computation purposes.

### 3.9.1 Best subset selection

This algorithm finds for each  $k \in 0, 1, 2, \dots, p$ , the subset of size  $k$  that gives the smallest residual sum of squares. Note that if a variable is in the best subset of size  $m$ , it might not be in the subsets of larger size (and of course neither in the smallest ones).

### 3.9.2 Forward stepwise selection

Searching for all the subsets is too computationally intensive (and infeasible for  $p > 40$ ). The *forward stepwise* algorithm starts with the intercept and then sequentially adds to the model the predictor that most improves the fit. QR decomposition can be exploited to choose the next candidate.

This algorithm is a greedy sub-optimal algorithm. Statistically it will have lower variance but higher bias.

### 3.9.3 Backward stepwise selection

*Backward stepwise* selection starts with the full model and sequentially removes the predictor having least impact on the model, i.e., having the smallest Z-score.

**Note:** this algorithm can only be applied when  $N > p$  while *forward stepwise* can always be used.

### 3.9.4 Implementations

[From ESLII pg. 60] Some software packages implement hybrid stepwise-selection strategies that consider both forward and backward moves at each step, and select the "best" of the two. For example in the R package the step function uses the AIC criterion for weighing the choices, which takes proper account of the number of parameters fit; at each step an add or drop will be performed that minimizes the AIC score.

Other more traditional packages base the selection on  $F$ -statistics, adding "significant" terms, and dropping "non-significant" terms. These are out of fashion.

### 3.9.5 Forward stagewise regression

As forward stepwise, it starts with the intercept. At each step the algorithm identifies the variable most correlated with the residual and computes the linear regression coefficient of the residual on this chosen variable and then adds it to the current coefficient for that variable. This is continued till none of the variables have correlation with the residual.

At each step only one coefficient is updated by a small step so that the number of steps is bigger than  $p$ . This slow-fitting pays in high dimensions.

**Note:** forward stagewise is very competitive in

## 3.10 Shrinkage methods

Subset selection methods either keep or remove a predictor. It has higher variance. Shrinkage or regularization methods are more continuous. They force the model to keep the weights as small as possible.

### 3.10.1 Ridge regression

Ridge regression shrinks the coefficients by imposing a penalty on their size. The ridge coefficients minimize a penalized residual sum of squared errors

$$\hat{\beta}^{\text{ridge}} = \arg \min_{\beta} \left\{ \sum_{i=1}^N \left( y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^p \beta_j^2 \right\} \quad (3.40)$$

where  $\lambda$  is a parameter controlling the amount of shrinkage: the bigger the value the greater the amount of shrinkage. This concept is also used in the Neural Networks. Another way to express 3.40 is the following:

$$\begin{aligned} \hat{\beta}^{\text{ridge}} &= \arg \min_{\beta} \left\{ \sum_{i=1}^N \left( y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 \right\} \\ &\text{subject to } \sum_{j=1}^p \beta_j^2 \leq t \end{aligned} \quad (3.41)$$

where there is a one-to-one correspondence between  $\lambda$  and  $t$ . Note that the penalization term does not consider  $\beta_0$  otherwise the procedure will depend on the chosen origin for  $Y$ .

This algorithm solves the problem of high variance in case of correlated inputs when big coefficients of correlated variables can be cancelled out. With a constraints on the coefficients this problem is alleviated.

The coefficients are not preserved when the input is scaled. Generally inputs are standardized before applying the algorithm.

$$\text{RSS}(\lambda, \beta) = (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) + \lambda\beta^T\beta \quad (3.42)$$

$$\hat{\beta}^{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1} \mathbf{X}^T\mathbf{y} \quad (3.43)$$

Now even if  $\mathbf{X}$  is not full rank, the problem is non singular (the inverse exists). In case of orthonormal inputs, the ridge coefficients are the same of least square but scaled:  $\hat{\beta}^{\text{ridge}} = \frac{\hat{\beta}}{1+\lambda}$ .

The parameter  $\lambda$  can also be derived assuming a prior distribution  $y_i \sim \mathcal{N}(\beta_0 + x_i^T\beta, \sigma^2)$  and the parameters  $\beta_j$  are distributed as  $\mathcal{N}(0, \tau^2)$ . Then from 3.40  $\lambda = \frac{\sigma^2}{\tau^2}$ .

Applying the SVD decomposition of the matrix  $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T$  where  $\mathbf{X}$  is  $N \times p$ ,  $\mathbf{U}$  is  $N \times p$  and  $\mathbf{V}$  is  $p \times p$ , the latter two both orthogonal with the columns of  $\mathbf{U}$  spanning the column space of  $\mathbf{X}$  and the columns of  $\mathbf{V}$  spanning the row space of  $\mathbf{X}$ .  $\mathbf{D}$  is a  $p \times p$  diagonal matrix with the elements  $d_1 \geq d_2 \geq \dots \geq d_p \geq 0$  called singular value decomposition of  $\mathbf{X}$ . If any  $d_j = 0$  then  $\mathbf{X}$  is singular.

The least squares equation can be rewritten as

$$\mathbf{X}\hat{\beta}^{\text{ls}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{U}\mathbf{U}^T\mathbf{y} \quad (3.44)$$

In case of the ridge regression, the coefficients are

$$\begin{aligned} \mathbf{X}\hat{\beta}^{\text{ridge}} &= \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{U}\mathbf{U}^T\mathbf{y} = \\ &= \sum_{j=1}^p \mathbf{u}_j \frac{d_j^2}{d_j^2 + \lambda} \mathbf{u}_j^T \mathbf{y} \end{aligned} \quad (3.45)$$

where  $\mathbf{u}_j$  are the column vectors. So ridge regression first computes the coordinates of  $\mathbf{y}$  with respect to the orthonormal basis  $\mathbf{U}$ , it then shrinks those coordinates since  $\lambda \geq 0$ . A greater amount of shrinkage is applied to the coordinates of basis vector with smaller  $d_j$ , corresponding to elements with small variance.

### 3.10.2 Lasso regression

The lasso regression is similar to ridge regression but it uses a  $L_1$  penalization instead of  $L_2$ .

$$\hat{\beta}^{\text{lasso}} = \arg \min_{\beta} \left\{ \sum_{i=1}^N \left( y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^p |\beta_j| \right\} \quad (3.46)$$

or equivalently

$$\begin{aligned} \hat{\beta}^{\text{lasso}} &= \arg \min_{\beta} \left\{ \sum_{i=1}^N \left( y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 \right\} \\ &\text{subject to } \sum_{j=1}^p |\beta_j| \leq t \end{aligned} \quad (3.47)$$

If  $t > t_0 = \sum_1^p |\beta_j|$  where  $\beta_j$  are the least square coefficients, then the lasso coefficients are the same of the least squares ones. If  $t = t_0/2$  then the least square coefficients are shrunk by 50% on average. Making  $t$  sufficiently big will cause some of the coefficients to be exactly 0.

In 3.1, the blue areas show the constraints for the estimates of ridge and lasso regressions, while the ellipses are contours of the residual sum of squares, centered at  $\beta^{\text{ls}}$ , in case of only two coefficients. For the lasso one of the coefficients is 0 when it hits one of the corner. In higher dimensions the figure becomes a rhomboid with many corners (and faces) so it becomes easy to hit a corner.

Also other penalization factors can be chosen, 3.2

### 3.10.3 Least angle regression

It is similar to forward stepwise. At first it identifies the variable most correlated with the response but instead of fitting it completely, it moves the variable toward its least squares value. As soon as another value gets correlated to the residual as the previous variable, the process is paused. The second variable joins the active set and their coefficients are moved together in a way that keeps their correlations tied and decreasing. The process is continued until all the variables are in the model. After  $\min(N - 1, p)$  steps

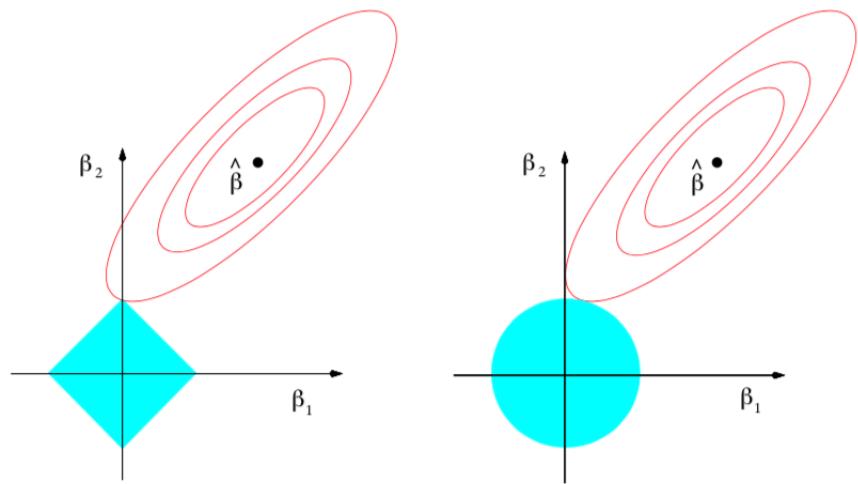
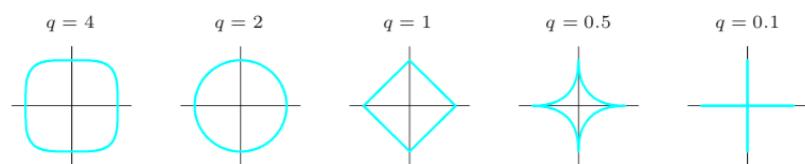


Figure 3.1: Constraints of ridge and lasso regression.



**FIGURE 3.12.** Contours of constant value of  $\sum_i |\beta_i|^q$  for given values of  $q$

Figure 3.2: Shapes of different penalization factors.

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standardize the predictors to have 0 mean and unit norm;  
 $\mathcal{A}_k \leftarrow \emptyset$ ;  
 $r \leftarrow y - \bar{y}$ ,  $\beta_i = 0$  for  $i \neq 0$ ;  
**while**  $|\mathcal{A}_k| < p$  **do**  
 | find the predictor most correlated to  $r$ ;  
 | insert the predictor in the active set  $\mathcal{A}_k$ ;  
 | move the coefficients of the predictors in the active set to the  
 | direction defined by their joint least squares coefficient of the  
 | current residual, i.e.,  

$$\delta_k = \left( X_{\mathcal{A}_k}^T X_{\mathcal{A}_k} \right)^{-1} X_{\mathcal{A}_k}^T r_k \quad (3.48)$$
  
 | (where  $\mathcal{A}_k$  is the current active set of variables) until some other  
 | competitor  $x_l$  has as much correlation with the current residual;  
 |  $r_k \leftarrow y - X_{\mathcal{A}_k} \beta_{\mathcal{A}_k}$

---

we arrive at the full least squares solution. The coefficient profile evolves as

$$\beta_{\mathcal{A}_k} = \beta_{\mathcal{A}_k} + \alpha \delta_k \quad (3.49)$$

If to the LAR algorithm we add the following rule i.e.,

*If a non-zero coefficient hits 0, drop its variable from the active set of variables and recompute the current joint least squares direction.*

we get the same coefficient path of the lasso and this is called LAR(lasso). So this become an efficient solution to compute the Lasso problem, especially with  $N \gg p$  since Lasso can take more than  $p$  steps while LAR require  $p$  steps and it is efficient since it requires the same complexity as that of a single least squares fit using the  $p$  predictors.

### 3.11 Derived input directions methods

When a large number of inputs is present, often there is a high correlation among them. In this case is convenient to regress on a new set inputs obtained form a linear combination of the original input.

### 3.11.1 Principal component analysis

First input must be standardized since this analysis depends on the scaling. The principal components are defined as

$$z_i = Xv_i \quad (3.50)$$

where  $v_i$  are the column vectors of  $V$  from the SVD decomposition of  $X = UDV^T$  (recall that  $z_m$  are orthogonal). The algorithm then regresses  $X$  on  $z_1, \dots, z_M$  for  $M \leq p$  and we have:

$$\hat{y}_{(M)}^{\text{PCR}} = \bar{y}\mathbf{1} + \sum_{m=1}^M \hat{\theta}_m z_m \quad (3.51)$$

where  $\hat{\theta}_m = \langle z_m, y \rangle / \langle z_m, z_m \rangle$ . Since  $z_m$  are linear combination of the original predictors  $x_j$ , we can express the solution as

$$\hat{\beta}^{\text{PCR}}(M) = \sum_{m=1}^M \hat{\theta}_m v_m \quad (3.52)$$

With  $M = p$  we get the usual least squares. Principal component analysis discards the  $p - M$  smallest eigenvalue components.

The value  $M$  is suggested by cross-validation.

### 3.11.2 Partial least squares

This technique uses a set of linear combinations of  $y$  in addition to  $X$  for the construction. It is not scale invariant so each  $x_j$  must be standardized.

Since PLS uses  $y$  to construct its directions, its solution path is not linear in  $y$ . It seeks direction with high variance and high correlation with the response while PCR only with high variance.

## 3.12 Multioutput shrinkage and selection

To apply selection and shrinkage methods in the multiple output case, one could apply a univariate technique individually to each outcome or simultaneously to all outcomes, i.e., different  $\lambda$  in Ridge or Lasso can be used for each output or the same value can be adopted.

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standardize  $x_j$  to 0 mean and 1 variance;

$$\hat{y}^{(0)} \leftarrow \bar{y}\mathbf{1};$$

$$x_j^{(0)} \leftarrow x_j;$$

**for**  $m = 1, \dots, p$  **do**

$z_m = \sum_{j=1}^p \hat{\phi}_{mj} x_j^{(m-1)}$ where $\hat{\phi}_{mj} = \langle x_j^{(m-1)}, y \rangle$ ; $\hat{\theta}_m = \frac{\langle z_m, y \rangle}{\langle z_m, z_m \rangle};$ $\hat{y}^m = \hat{y}^{(m-1)} + \hat{\theta}_m z_m;$ orthogonalize each $x_j^{m-1}$ w.r.t. $z_m : x_j^{(m)} = x_j^{(m-1)} - \frac{\langle z_m, x_j^{(m-1)} \rangle}{\langle z_m, z_m \rangle} z_m, j = 1, \dots, p;$
---

Output the sequence of fitted vectors  $\{\hat{y}^m\}_1^p$ . Since  $z_1^m$  are linear in  $x_j$ , so is  $\hat{y}^{(m)} = X\hat{\beta}^{pls}(m)$ . These coefficients can be recovered from the sequence of PLS transformations.

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### 3.13 Other derived algorithms

#### 3.13.1 Incremental forward stagewise

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$r \leftarrow y$  ;  
 $\beta_i = 0$  for  $i \neq 0$ ;  
 find the (standardized) predictor  $x_j$  most correlated with the residual ;  
 $\beta_j \leftarrow \beta_j + \delta_j$  where  $\delta_j = \epsilon \text{sign} [\langle x_j, r \rangle]$  and  $\epsilon > 0$  small;  
 $r \leftarrow r - \delta_j x_j$ ;  
 Repeat the steps many times until the residuals are uncorrelated with the predictors.

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#### 3.13.2 The Dantzig selector

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### 3.13.3 The Grouped Lasso

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## 4 Bayesian inference

### 4.1 Introduction to Bayes' theorem

Bayes' theorem is a formula that describes how to update the probabilities of hypotheses when given evidence. It follows simply from the axioms of conditional probability, but can be used to powerfully reason about a wide range of problems involving belief updates.

Given a hypothesis  $H$  and evidence  $E$ , Bayes' theorem states that the relationship between the probability of the hypothesis  $\Pr(H)$ , before getting the evidence, and the probability of the hypothesis after getting the evidence  $\Pr(H|E)$  is

$$\Pr(H|E) = \frac{\Pr(E|H)\Pr(H)}{\Pr(E)} \quad (4.1)$$

Often there are competing hypothesis and the task is to determine which is the most probable.

This formula relates the probability of the hypothesis before getting the evidence  $\Pr(H)$ , to the probability of the hypothesis after getting the evidence,  $\Pr(H|E)$ : this term is generally what we want to know. For this reason,  $\Pr(H)$  is called the **prior probability**, while  $\Pr(H|E)$  is called the **posterior probability**. The factor that relates the two,  $\frac{\Pr(E|H)}{\Pr(E)}$ , is called the **likelihood ratio** and  $\Pr(E|H)$  is called **likelihood** which indicates the compatibility of the evidence with the given hypothesis.  $\Pr(H|E)$  and  $\Pr(E|H)$  are called conditional probabilities. A conditional probability is an expression of how probable one event is given that some other event occurred (a fixed value) and Bayes' theorem centers on relating different conditional probabilities.

$\Pr(E)$  is sometimes called **marginal likelihood** or model evidence this factor is the same for all the hypotheses being considered.

## 4.2 Bayes inference

Bayesian inference is a method of statistical inference in which Bayes' theorem is used to update the probability for a hypothesis as more evidence or information becomes available. Bayesian inference assumes the data were generated by a model with unknown parameters. From this, it tries to come up with beliefs about the likely "true values" of the parameters of the model. The Bayesian approach differs from the standard ("frequentist") method for inference in its use of a prior distribution to express the uncertainty present before seeing the data, and to allow the uncertainty remaining after seeing the data to be expressed in the form of a posterior distribution.

For this reason when writing down the Bayes theorem in these cases, formally also the conditional on the choice of the model should be written down:

$$\Pr(\theta|\mathbf{X}, M) = \frac{\Pr(\mathbf{X}|\theta, M)\Pr(\theta|M)}{\Pr(\mathbf{X}|M)} \quad (4.2)$$

Here the hypothesis described in the previous paragraph is represented by a set of values for the parameters.

Once the model is stipulated,  $\Pr(\mathbf{X}|\theta)$  can be evaluated for any given set of parameters: in this sense the likelihood is fixed once the model is fixed.  $\Pr(\mathbf{X}|M)$  can be reexpressed as  $\Pr(\mathbf{X}|M) = \int \Pr(\mathbf{X}|\theta, M)\Pr(\theta|M)d\theta$ . In this way it can be re-thought as a normalization factor of the sets of parameters since it is a summation over the all parameter space. However note that it **does depend** on the choice of the model. It can be seen also as asking the question *how much is it probable to see the data we have seen given that the model M, without any claim about its parameters, generated those data?*

## 4.3 Types of estimation

It is the moment to clarify different types of estimation. We have already seen the Ordinary Least Square (OLS) estimation, and other types of estimation based on the definition of an error function.

We have also seen the **Maximum Likelihood Estimation (MLE)** approach, which maximizes the likelihood of the Bayes expression and how it is equivalent to OLS estimation in case of linear regression. (To be precise almost always the log-likelihood is maximized, first of all because of analytical convenience since many times we deal with exponentials coming from

Gaussian distribution. Secondly for numerical precision: we are dealing with probabilities, numbers between 0 and 1 and since the range is quite small, underflow might be a problem.) The logarithmic instead extends the range by mapping numbers close to 0 to  $\infty$ , resulting in a better precision.

The **Maximum A-Priori (MAP)** estimation maximizes the numerator of the Bayes expression, i.e., the likelihood times the prior, which means the likelihood is weighted by weights coming from the prior. When using a uniform distribution for the prior, MAP turns into MLE since we are assigning equal weights for each possible value. For example suppose we can assign six possible values to  $\beta$  and assume  $P(\beta_i) = 1/6$ :

$$\begin{aligned}\beta_{\text{MAP}} &= \arg \max_{\beta} \sum_i \Pr(x_i|\beta) + \log P(\beta) = \\ &= \arg \max_{\beta} \sum_i \Pr(x_i|\beta) + \text{const} = \arg \max_{\beta} \sum_i \Pr(x_i|\beta) = \beta_{\text{MLE}}\end{aligned}\tag{4.3}$$

When using a different prior, i.e., the simplification does not hold anymore.

## 4.4 Conjugate distributions

**Definition 4.1. Conjugate distributions** In Bayesian probability theory, if the posterior distribution  $\Pr(\theta|X, M)$  is in the same probability space as the prior probability distribution  $\Pr(\theta|M)$ , then the prior and posterior are called **conjugate distributions**, and the prior is called **conjugate prior for the likelihood function**.

As example consider the Gaussian distribution: **the Gaussian family is conjugate to itself (or self-conjugate) with respect to a Gaussian likelihood function.** If the likelihood is Gaussian, choosing Gaussian prior will ensure that also the posterior distribution is a Gaussian (see 1.6). This means that the Gaussian distribution is a conjugate prior for the likelihood that is also Gaussian.

Consider the general problem of inferring a (continuous) distribution for a parameter  $\theta$  given some datum or data  $x$ . From Bayes' theorem, the posterior distribution is equal to the product of the likelihood function  $p(x|\theta, M)$  and the prior  $p(\theta|M)$ . Let the likelihood function be considered fixed; the likelihood function is usually well-determined from a statement of the data-generating process. It is clear that different choices of the prior distribution

$p(\theta|M)$  may make the integral more or less difficult to calculate, and the product  $p(x|\theta, M) \times p(\theta|M)$  may take one algebraic form or another. For certain choices of the prior, the posterior has the same algebraic form as the prior (generally with different parameter values). Such a choice is a conjugate prior. A conjugate prior is an algebraic convenience, giving a closed-form expression for the posterior; otherwise numerical integration may be necessary. Further, conjugate priors may give intuition, by more transparently showing how a likelihood function updates a prior distribution. All members of the exponential family have conjugate priors.

In case of **classification** we are given a training set with input and output data. Once we have stipulated a model that could have generated output data, we want to find the best parameters of the model such that when those inputs are fed to the model we get those outputs. So the question becomes *what is the best set of parameters  $\theta$  for the model  $M$  that could have generated the output  $y$  when the model has been fed with input data  $\mathbf{X}$ ?*

In formula:

$$\Pr(\theta|y, \mathbf{X}, M) = \frac{\Pr(y|\theta, \mathbf{X}, M)\Pr(\theta|\mathbf{X}, M)}{\Pr(y|\mathbf{X}, M)} \quad (4.4)$$

#### 4.4.1 Dataset likelihood

4.4.1 To be precise the likelihood is the likelihood of an entire dataset, since we are interested in all  $y$  and not in a single value  $y$ .  $\Pr(y|\theta, \mathbf{X}, M)$  is then a joint density over all the responses in our dataset:  $\Pr(y_1, y_2, \dots, y_N|\theta, \mathbf{X}, M)$ . Evaluating this density at the observed points gives a single likelihood value for the whole dataset. Assuming that the noise at each data point is independent we can factorize as:

$$\Pr(y|\theta, \mathbf{X}, M) = \prod_{n=1}^N \Pr(y_n|x_n, \theta) \quad (4.5)$$

We have not say that  $y_n$ 's are completely independent as otherwise it would not be worth trying to model the data at all. Rather, they are **conditionally independent** given a value  $\theta$ , i.e., the deterministic model. Basically the model incorporates the dependency. Consider the following example, we have a set of data  $(y, \mathbf{X})$  from which we want to predict the output  $y_n$  given a new  $x_n$ . Recalling from conditional probability that  $P(A|B) = \frac{P(A \cap B)}{P(B)}$  we

have:

$$P(y_n|y, \mathbf{x}_n, \mathbf{X}) = \frac{Pr(y_n \cap y|\mathbf{x}_n, \mathbf{X})}{Pr(y|\mathbf{x}_n, \mathbf{X})} \quad (4.6)$$

Note that actually  $y$  does not depend on  $\mathbf{x}_n$ :  $Pr(y|\mathbf{x}_n, \mathbf{X}) = Pr(y|\mathbf{X})$ . Using independence:

$$P(y_n|y, \mathbf{x}_n, \mathbf{X}) = \frac{Pr(y_n \cap y|\mathbf{x}_n, \mathbf{X})}{Pr(y|\mathbf{X})} = \frac{Pr(y|\mathbf{X})Pr(y_n|\mathbf{x}_n, \mathbf{X})}{Pr(y|\mathbf{X})} = \quad (4.7)$$

[TO BE CONTINUED WAITING ON ANSWER ON CROSS-VALIDATED STACK EXCHANGE]

## 5 Linear Classification

For classification problem, in this section we assume the classification boundaries are linear, i.e., in the input hyperspace the points belonging to different classes can be separated by hyperplanes.

### 5.1 Linear regression of an Indicator matrix

Suppose we have  $K$  classes. For a single output we build a vector  $\mathbf{y} = (y_1, \dots, y_k)$  where  $y_k = 1$  if the class it belongs is the  $k$  class. As output we will have the matrix  $\mathbf{Y}$  of 0 and 1 with each row having a single 1. We fit a linear regression model to each of the columns of  $\mathbf{Y}$  simultaneously:

$$\hat{\mathbf{Y}} = \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$$

We get a coefficient vector for each response column  $y_k$ , and hence a  $(p+1) \times K$  matrix  $\hat{\mathbf{B}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$ , where  $\mathbf{X}$  will have  $p+1$  columns with a leading column of 1 for the intercept.

Suppose we are given a new input  $x$ . Then the classification problem becomes:

*compute the output  $\hat{f}(x)^T = (1, x^T) \hat{\mathbf{B}}$  which is a  $k$  vector identify the largest component  $\hat{G}(x) = \arg \max_{k \in \mathcal{G}} \hat{f}_k(x)$ .*

With this approach we are basically estimating a conditional expectation, i.e., given the inputs  $\mathbf{x}$  what is the probability the output is of class  $k$ ? Mathematically  $E(y_k|X=x) = Pr(G=k|X=x)$  since  $y_k=1$ .

Although the linear model guarantees  $\sum_{k \in \mathcal{G}} \hat{f}_k = 1$ , as long as there is an intercept in the model,  $\hat{f}_k(x)$  can be negative or bigger than one, especially when making predictions outside the hull of training data. Although this fact, this approach still works in many cases.

**An important limitation** is when  $K \geq 3$ . Even if the classes can still be separated by more than one linear boundaries, linear regression cannot find linear boundaries (because they are more than one?).

Quadratic regression might solve the problem, but a general rule is that if  $k \geq 3$  classes are lined up (their centroids are in the same line), a polynomial term with degree up to  $k - 1$  is needed to solve the problem, and since the direction is arbitrary, cross-products terms might be needed too.

## 5.2 Linear Discriminant analysis

For optimal classification we have to know the class posteriors  $\Pr(G|X)$ . Let  $\pi_k$  be the prior probability of class  $k$  with  $\sum_k^K \pi_k = 1$ . Suppose  $f_k(x)$  is the class conditional density. From the Bayes theorem (?) we get

$$\Pr(G = k|X = x) = \frac{\Pr(X = x|G = k)\Pr(G = k)}{\Pr(X = x)} \quad (5.1)$$

$\Pr(G = k)$  is the prior probability  $\pi_k$ ,  $\Pr(X = x|G = k)$  is the class conditional density while the denominator can be rewritten using the **Total Probability Theorem** as

$$\Pr(X = x) = \sum_{l=1}^K \Pr(X = x|G = l)\Pr(G = l) = \sum_{l=1}^K \Pr(X = x|G = l)\pi_l \quad (5.2)$$

$$\Rightarrow \Pr(G = k|X = x) = \frac{f_k(x)\pi_k}{\sum_{l=1}^K f_l(x)\pi_l} \quad (5.3)$$

The goodness of classification mostly rely on  $f_k(x)$  and many techniques use models for class densities:

- linear and quadratic discriminant analysis use Gaussian densities;
- mixtures of Gaussians allow for non-linear boundaries;
- Naive Bayes models assume that each class density is a product of marginal densities i.e., inputs are conditionally independent in each class.

Modelling each class density as a multivariate Gaussian we have

$$f_k(x) = \frac{1}{(2\pi)^{\frac{p}{2}} |\sum_k|^{\frac{1}{2}}} e^{-\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1} (x-\mu_k)} \quad (5.4)$$

**Linear Discriminant analysis assumes equal covariance matrices for all classes.** Taking as comparison between two classes the log-ratio, we have

$$\begin{aligned} \log \frac{\Pr(G=k|X=x)}{\Pr(G=l|X=x)} &= \log \frac{f_k(x)\pi_k}{f_l(x)\pi_l} = \log \frac{\pi_k}{\pi_l} + \log \frac{f_k(x)}{f_l(x)} = \\ &= \log \frac{\pi_k}{\pi_l} + \log \frac{e^{-\frac{1}{2}(x-\mu_k)^T \Sigma^{-1} (x-\mu_k)}}{e^{-\frac{1}{2}(x-\mu_l)^T \Sigma^{-1} (x-\mu_l)}} = \\ &= \log \frac{\pi_k}{\pi_l} - \frac{1}{2} (x - \mu_k)^T \Sigma^{-1} (x - \mu_k) - \left( -\frac{1}{2} \right) (x - \mu_l)^T \Sigma^{-1} (x - \mu_l) = \\ &= \log \frac{\pi_k}{\pi_l} - \frac{1}{2} \left[ (x - \mu_k)^T \Sigma^{-1} (x - \mu_k) + (x - \mu_l)^T \Sigma^{-1} (\mu_l - x) \right] = \\ &= \log \frac{\pi_k}{\pi_l} - \frac{1}{2} \left[ (2x - \mu_k - \mu_l)^T \Sigma^{-1} (\mu_l - \mu_k) \right] = \\ &= \log \frac{\pi_k}{\pi_l} + \frac{1}{2} x^T \Sigma^{-1} (\mu_k - \mu_l) - \frac{1}{2} (\mu_k + \mu_l)^T \Sigma^{-1} (\mu_k - \mu_l) = \end{aligned} \quad (5.5)$$

which is linear in  $x$ , so all decision boundaries are linear (i.e., they are hyperplanes in  $p$  dimensions). If the common covariance matrix is spherical, i.e.,  $\Sigma = \sigma^2 I$  and the class priors are equal, each boundary that separates two classes is the perpendicular bisector of the segment joining the centroids of the two classes.

The linear discriminant functions of each class are

$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T + \log \pi_k \quad (5.6)$$

We do not know the parameters of the Gaussian distribution and we must

estimate them from the training data:

$$\hat{\pi}_k = \frac{N_k}{N} \quad (5.7)$$

$$\hat{\mu}_k = \sum_{g_i=k} \frac{x_i}{N_k} \quad (5.8)$$

$$\hat{\Sigma} = \sum_{k=1}^K \frac{(x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T}{(N - K)} \quad (5.9)$$

**Note** that LDA does not use Gaussian assumption for the features.

### 5.2.1 Decision rule

Consider two classes 1 and 2. LDA classifies to class 1 if

$$x^T \hat{\Sigma}^{-1} \hat{\mu}_1 - \frac{1}{2} \hat{\mu}_1^T \hat{\Sigma}^{-1} \hat{\mu}_1 + \log \hat{\pi}_1 > x^T \hat{\Sigma}^{-1} \hat{\mu}_2 - \frac{1}{2} \hat{\mu}_2^T \hat{\Sigma}^{-1} \hat{\mu}_2 + \log \hat{\pi}_2 \quad (5.10)$$

to class 2 if  $<$  holds. In such case there is a correspondence between LDA and linear regression classification if the two classes are coded with +1 and -1. In this case the coefficient vector from least squares is proportional to the LDA direction. However unless  $N_1 = N_2$ , the intercepts are different and so are the decision rules.

With more than 2 classes, linear regression is not able to classify correctly while LDA does.

## 5.3 Quadratic Discriminant analysis

If we do not assume equal covariance, the squared term in  $x$  does not cancel out and we get quadratic discriminant functions:

$$\delta_k(x) = -\frac{1}{2} \log |\Sigma_k| - \frac{1}{2} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) + \log \pi_k \quad (5.11)$$

The decision boundaries between two classes are quadratic functions.

**Note:** QDA does not differ much from LDA applied the enlarged quadratic polynomial input space but generally QDA is preferred in this case.

The estimates are similar but the covariance matrix must be estimated for each class. When  $p$  is large, this means a dramatic increase in the number of parameters, considering we only need the differences  $\delta_k(x) - \delta_l(x)$ . LDA needs  $(K - 1) \times (p + 1)$  parameters, while QDA needs  $(K - 1) \times (p(p + 3)/2 + 1)$ .

## 5.4 Regularized discriminant analysis

This method shrinks the separate covariances of QDA towards a common covariance as in LDA. In a way it is similar to ridge regression. The regularized covariance matrices have the form:

$$\hat{\Sigma}_k(\alpha) = \alpha \hat{\Sigma}_k + (1 - \alpha) \hat{\Sigma} \quad (5.12)$$

with  $\alpha \in [0, 1]$ , the two extremes being LDA and QDA.  $\alpha$  can be chosen on the validation data or by cross-validation.

Similarly we can allow  $\hat{\Sigma}$  to be shrunk toward the scalar covariance:

$$\hat{\Sigma}(\gamma) = \gamma \hat{\Sigma} + (1 - \gamma) \hat{\sigma}^2 I \quad (5.13)$$

with  $\gamma \in [0, 1]$  so we get a more general family of covariances

$$\hat{\Sigma}_k(\alpha, \gamma) = \alpha \hat{\Sigma}_k + (1 - \alpha) \left( \gamma \hat{\Sigma} + (1 - \gamma) \hat{\sigma}^2 I \right) \quad (5.14)$$

## 5.5 Computation

Computation of LDA and QDA is simplified by diagonalizing the covariance matrices with the singular value decomposition  $\hat{\Sigma}_k = U_k D_k U_k^T$ . The terms in 5.11 become

$$\begin{aligned} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) &= (x - \mu_k)^T \left( U_k D_k U_k^T \right)^{-1} (x - \mu_k) = \\ &= (x - \mu_k)^T U_k D_k^{-1} U_k^T (x - \mu_k) = \left[ U_k^T (x - \mu_k) \right]^T D_k^{-1} \left[ U_k^T (x - \mu_k) \right] \end{aligned} \quad (5.15)$$

$$\log |\hat{\Sigma}_k| = \sum_l \log d_{kl} \quad (5.16)$$

Considering the above steps, LDA classifier can be seen as performing the following steps:

- sphere the data w.r.t. the common covariance estimate:  $X^* \leftarrow D^{-\frac{1}{2}} U^T X$ . The common covariance estimate for  $X^*$  will now be the identity.
- Classify to the closest centroid in the transformed space, modulo the effect of the class prior probability  $\pi_k(?)$

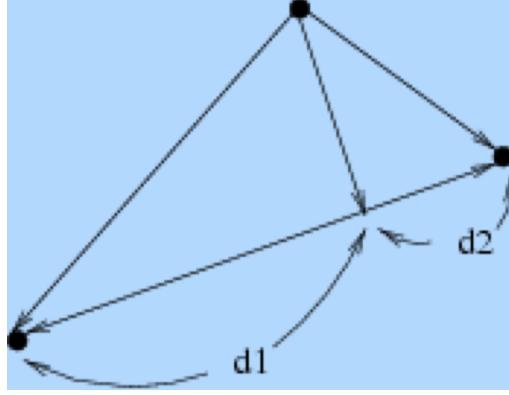


Figure 5.1: ...

## 5.6 Regularized-rank linear discriminant analysis

Consider  $K = 2$  with two centroids and the input is 2, i.e., input points are on a plane. Given an input point, for classification purposes what matters is not the distance in the  $p$  space of such point from the two centroids but rather the distance from the two centroids of the projection of this point on the line joining them (5.1). So basically instead of using the 2 dimensions, we are calculating the distance in one dimension, a line. If  $K = 3$  then the points are projected onto a plane (2d), of course in this case it is convenient if  $p > 2$ .

More generally the  $K$  centroids in  $p$ -dimensional input, lie in an affine subspace of dimensions  $\leq K - 1$  and if  $p >$  is much larger than  $K$  this will be a considerable drop in dimension.

If  $K > 3$  we can look for a  $L < K - 1$  dimensional subspace optimal for LDA. Fisher defined *optimal* such that the projected centroids were spread out as much as possible in terms of variance. This problem, finding the principal component subspaces of the centroids, involves the following steps:

- compute the  $k \times p$  matrix of class centroids  $M$  and the common covariance matrix  $W$  for within-class covariance;
- compute  $M^* = MW^{-\frac{1}{2}}$  using the eigen-value decomposition;
- compute  $B^*$ , the covariance matrix of  $M^*$  ( $B$  for between class covariance) and its eigenvalue decomposition  $B^* = V^* D_B V^{*T}$ . The columns  $v_1^*$  from the first to the last define the coordinates of optimal subspaces.

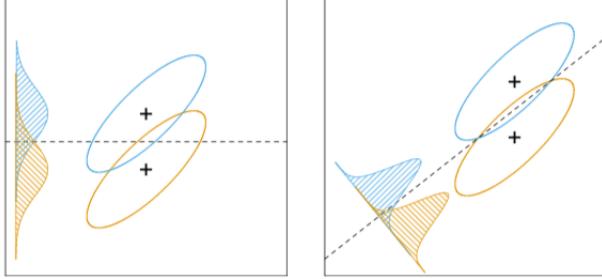


Figure 5.2: Covariance.

The  $l$ th discriminant variable is given by  $Z_l = v_l^T X$  with  $v_l = W^{-\frac{1}{2}}v_l^*$ . Although the direction joining the centroids separates the means as much as possible (maximizes the between class covariance), there is an overlap between the projected classes due to the nature of covariances. Taking the covariances into account reduce the overlap and that is what we are doing (5.2).

The between-class variance  $Z$  is  $a^T B a$  and the within class variance is  $a^T W a$ , with  $B + W = T$ , the total covariance matrix of  $X$ . Fisher's problem maximizes the *Rayleigh quotient*:

$$\max_a \frac{a^T B a}{a^T W a} \quad (5.17)$$

This is a generalized eigenvalue problem, with  $a$  given by the largest eigenvalue. Similarly one can find the next direction  $a_2$ , orthogonal in  $W$  to  $a_1$ , such that  $a_2^T B a_2 / a_2^T W a_2$  is maximized; the solution is  $a_2 = v_2$ , and so on.  $a_l$  are the *discriminant coordinates* or *canonical variates*, different from discriminant functions.

The reduced subspaces can be used both for visualization and classification by limiting the distance between centroids to the chosen subspace. However, when doing this, due to the Gaussian classification, a correction factor of  $\log \pi_k$  is needed. The misclassification is given by the overlapping area in 5.2 between the two densities. When both classes have the same priors  $\pi_k$  as in the figure, the optimal cut-point is the midway between projected means, if not the cut-point is moved towards the smaller class to have a better error rate.

For 2 classes one can derive the linear rule using LDA, and then choosing the cut-point to minimize misclassification error.

## 5.7 Logistic regression

The idea behind logistic regression is to still exploit a linear model  $x^T \beta$  but having its output representing a probability, i.e., constrained between 0 and 1. This part is performed using the sigmoid function

$$p = \sigma(q) = \frac{1}{1 + e^{-q}} \quad (5.18)$$

Inverting the terms we get

$$q = -\log \frac{1-p}{p} = \log \frac{p}{1-p} \quad (5.19)$$

5.19 is called **logit function**. As  $q$  increases to  $\infty$ , the output of the sigmoid gets closer to 1; instead when it diverges to  $-\infty$  we get 0. Suppose we have just 2 classes or equivalently a binary classifier that tells the probability of an event to happen:  $Y_n = 1$  when the event happens and  $Y_n = 0$  when it does not. We can express the probabilities output by our classifier when new input data  $x_{\text{new}}$  are observed as:

$$\begin{aligned} P(G = 1|x_n, \beta) &= \frac{1}{1 + e^{-\beta^T x_{\text{new}}}} \\ P(G = 0|x_n, \beta) &= 1 - \frac{1}{1 + e^{-\beta^T x_{\text{new}}}} = \frac{e^{-\beta^T x_{\text{new}}}}{1 + e^{-\beta^T x_{\text{new}}}} \end{aligned} \quad (5.20)$$

These equations can be combined in a single equation:

$$P(G = g|x_n, \beta) = P(G = 1|x_n, \beta)^g P(G = 0|x_n, \beta)^{g-1} \quad (5.21)$$

Taking the log-ratio between the two probabilities we have:

$$\log \frac{P(Y_n = 0|x_n, \beta)}{P(Y_n = 1|x_n, \beta)} = \log \frac{\frac{e^{-\beta^T x_{\text{new}}}}{1 + e^{-\beta^T x_{\text{new}}}}}{\frac{1}{1 + e^{-\beta^T x_{\text{new}}}}} = -\beta^T x_{\text{new}} \quad (5.22)$$

So we are using lines (or hyperplanes) to separate the two classes.

### 5.7.1 Multinomial logistic regression: more than 2 classes

Now suppose we have more than two classes and we still want to separate those classes with linear functions, which means we will have a hyperplane separating two classes. We have  $K$  possible outcomes. We can think to run  $K - 1$  independent binary logistic regressions with one class chosen as **pivot**, generally the one corresponding to class  $K$ , and with the other  $K - 1$  classes separately regressed against the pivot:

$$\begin{aligned} \log \frac{\Pr(G = 1|X = x)}{\Pr(G = K|X = x)} &= \beta_1^T x \\ \log \frac{\Pr(G = 2|X = x)}{\Pr(G = K|X = x)} &= \beta_2^T x \\ &\vdots \\ \log \frac{\Pr(G = K-1|X = x)}{\Pr(G = K|X = x)} &= \beta_{(K-1)}^T x \end{aligned} \tag{5.23}$$

The choice of the pivot class used as denominator is arbitrarily and the estimates are equivalent under different choices.

Summing the probability of each class we must get 1:

$$\begin{aligned} \sum_{l=1}^K \Pr(G = l|X = x) &= 1 \Rightarrow \Pr(G = K|X = x) + \sum_{l=1}^{K-1} \Pr(G = l|X = x) = 1 \\ \Rightarrow \Pr(G = K|X = x) &+ \sum_{l=1}^{K-1} \Pr(G = K|X = x) e^{\beta_l^T x} = 1 \\ \Rightarrow \Pr(G = K|X = x) &= \frac{1}{1 + \sum_{l=1}^{K-1} e^{\beta_l^T x}} \end{aligned} \tag{5.24}$$

So we can re-express the probabilities as:

$$\Pr(G = k|X = x) = \frac{e^{\beta_k^T x}}{1 + \sum_{l=1}^{K-1} e^{\beta_l^T x}} \tag{5.25}$$

**Softmax function** We do not have anymore the sigmoid function, instead we have used another function named **softmax** that as the sigmoid takes

any real value as input and outputs a value between 0 and 1. The difference mostly relies on the denominator used for normalization factor since the sigmoid is a 2D curve while the softmax can have higher dimensionality (for 2D it corresponds to the sigmoid).

### 5.7.2 Fitting logistic regression

From now on we will consider a logistic regression for just two classes.

As seen in 4.4, we want to find the best parameters for the chosen model according to some criteria. First let us apply the Bayes theorem:

$$\Pr(\beta|y, \mathbf{X}, M) = \frac{\Pr(y|\beta, \mathbf{X}, M) \Pr(\beta, M)}{\Pr(y|\mathbf{X}, M)} \quad (5.26)$$

**From now on we will not write the conditional on the model for seek of brevity but we know it exists.**

This formula tells we want to find the coefficients given some input and output data. Let us analyse each term:

- **Pr( $\beta$ ) (prior distribution):** this is the prior belief about the parameters without seeing the data. As prior, we will use a Gaussian distribution with 0 mean:  $\mathcal{N}(0, \sigma^2 \mathbf{I})$ . In this way the parameters will depend on  $\sigma^2$ : more formally we should write  $\Pr(\beta|\sigma)$  but we will skip. Although the choice of the Gaussian distribution with 0 mean is analytically convenient as seen in 4.4, we will not rely on conjugacy.
- **Pr( $y|\beta, \mathbf{X}$ ) (likelihood):** we will assume  $y$  are conditionally independent (4.4.1):

$$\Pr(y|\mathbf{X}, \beta) = \prod_{n=1}^N \Pr(y_n|x_n, \beta) \quad (5.27)$$

Since in this case we have a binary variable, instead of a Gaussian random variable, suitable for real values distribution, we will consider a binary random variable  $Y_n$  characterised by the probability of the second class:

$$\Pr(y|\mathbf{X}, \beta) = \prod_{n=1}^N \Pr(Y_n = y_n|x_n, \beta) \quad (5.28)$$

- $\Pr(\mathbf{y}|\mathbf{X})$  (**marginal likelihood**): It can be expressed as

$$\Pr(\mathbf{y}|\mathbf{X}) = \int \Pr(\mathbf{y}|\beta, \mathbf{X}) \Pr(\beta) d\beta \quad (5.29)$$

So the numerator can be calculated and results in a Gaussian function not in standard form (1.6). The denominator, or marginal likelihood, as we have seen can be expressed as  $\Pr(\mathbf{y}|\mathbf{X}) = \int \Pr(\mathbf{y}|\beta, \mathbf{X}) \Pr(\beta) d\beta$ . Mathematically this integral has no close solution since (again see 1.6) and the impossibility of the integral of  $e^{-x^2}$ , unless an ad-hoc prior distribution is chosen.

When we cannot directly compute the posterior density (due to the denominator), we have three options:

1. find the single value  $\beta$  that correspond to the highest value of the posterior. This is equivalent to find the value  $\beta$  that maximize the numerator since the denominator is not a function of  $\beta$  but a numerical value.
2. Approximate  $\Pr(\beta|\mathbf{X}, \mathbf{y})$  with some other density that we can compute analytically.
3. Sample directly from the posterior  $\Pr(\beta|\mathbf{X}, \mathbf{y})$  knowing only the numerator.

The first method is simple and hence popular but it is not very "Bayesian", since we will make predictions of new data based on a single value and not a distribution. The whole Bayesian theory is based on making an hypothesis and getting feedback from the data that can validate or not that hypothesis. Also when using a distribution we get also measures on how confident we are about the estimated model. For example when estimating a Gaussian distribution, we estimate the coefficients  $\mu$  and  $\sigma^2$ : the smaller the latter value the more confident we are about the model. When using a single value we loose this piece of information.

With the second method we get a density easy to work with but if the chosen density is very different from the posterior our model will not be very reliable.

The third method samples from the posterior and hence to get a good approximation but it can be difficult.

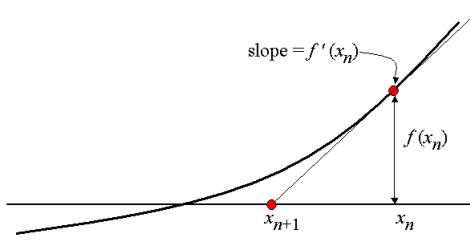


Figure 5.3: Newton-Raphson example.

### 5.7.3 First method: point estimation, the MAP solution

We have seen that in some cases we cannot compute the posterior but we can compute the numerator of the expression, i.e., the prior multiplied by the likelihood. The value that maximizes the posterior is also the value that maximizes the numerator. We have already seen a likelihood maximization procedure in ??; here we are maximizing the likelihood times the prior. This solution is the **maximum a posteriori (MAP)** estimate.

**The Newton-Raphson method** The Newton-Raphson method finds the points where  $f(x) = 0$ . Starting from an estimation  $x_n$  of such points, the estimation is updated by moving to the point where the tangent to the function at  $x_n$  passes through the x-axis. This point is computed by approximating the gradient as a change in  $f(x)$  divided by a change in  $x$ :

$$\begin{aligned} f'(x_n) &= -\frac{f(x_n) - 0}{x_n - x_{n+1}} \\ \Rightarrow x_{n+1} &= x_n - \frac{f(x_n)}{f'(x_n)} \end{aligned} \tag{5.30}$$

Instead of finding the point for which  $f(x) = 0$ , we want to find the point where its derivative is 0. Hence we substitute  $f(x)$  with  $f'(x)$  and  $f'(x)$  with  $f''(x)$ . In this way the method can be used to find points where the gradient passes through 0, i.e., minima, maxima and points of inflections:

$$\begin{aligned} f''(x_n) &= -\frac{f'(x_n) - 0}{x_n - x_{n+1}} \\ \Rightarrow x_{n+1} &= x_n - \frac{f'(x_n)}{f''(x_n)} \end{aligned} \tag{5.31}$$

When dealing with vectors,  $f'(x)$  is replaced by the vector of partial derivatives evaluated at  $x_n$  and  $\frac{1}{f''(x_n)}$  is replaced by the inverse of the Hessian matrix  $\frac{\partial^2 f(x)}{\partial x \partial x^T}$ .

**Derivation** As already done, instead of maximizing the function itself, we maximize its logarithmic. Apart from the mathematical convenience this is also the advantage of avoiding underflow: we are dealing with probabilities, number between 0 and 1 and these might be too small to have a sufficient numerical precision. The logarithmic, as the numbers go to 0, makes the number goes to infinity, guaranteeing a better numerical precision. Since we cannot compute the derivative and set it to 0, we use the Newton-Raphson procedure. Let us call the numerator  $g(\beta, \mathbf{X}, \mathbf{y}) = \Pr(\mathbf{y}|\beta, \mathbf{X})\Pr(\beta|\mathbf{X})$ :

$$\beta' = \beta - \left( \frac{\partial^2 \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta \partial \beta^T} \right)^{-1} \frac{\partial \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta} \quad (5.32)$$

The procedure is iterative and stops when the gradient is 0. To check the point we have converged to corresponds to a minimum we check the Hessian matrix is negative definite.

Before computing the derivatives we re-express  $g(\beta, \mathbf{X}, \mathbf{y})$ .

$$\begin{aligned} \log g(\beta, \mathbf{X}, \mathbf{y}) &= \sum_{n=1}^N \log \Pr(Y_n = y_n | \mathbf{x}_n, \beta) + \log \Pr(\beta | \sigma^2) = \\ &= \sum_{n=1}^N \log \left[ \left( \frac{1}{1 + e^{-\beta^T \mathbf{x}_n}} \right)^{y_n} \left( \frac{e^{-\beta^T \mathbf{x}_n}}{1 + e^{-\beta^T \mathbf{x}_n}} \right)^{1-y_n} \right] + \log \Pr(\beta | \sigma^2) = \end{aligned} \quad (5.33)$$

We denote  $P_n = P(Y_n = 1 | \beta, \mathbf{x}_n) = \frac{1}{1 + e^{-\beta^T \mathbf{x}_n}}$ :

$$\log g(\beta, \mathbf{X}, \mathbf{y}) = \sum_{n=1}^N \log P_n^{y_n} + \log(1 - P_n)^{1-y_n} + \log \Pr(\beta | \sigma^2) = \quad (5.34)$$

Racalling

$$\begin{aligned}
\Pr(\beta|\sigma^2) &= \frac{1}{\sqrt{(2\pi)^D |\Sigma|}} e^{-\frac{(\beta-\mu)^T(\beta-\mu)}{2\sigma^2}} \\
\Rightarrow \log g(\beta, \mathbf{X}, \mathbf{y}) &= \sum_{n=1}^N \log P_n^{y_n} + \log(1-P_n)^{1-y_n} - \frac{D}{2} \log(2\pi) - D \log \sigma + \\
&\quad - \frac{1}{2\sigma^2} \beta^T \beta
\end{aligned} \tag{5.35}$$

Now we can take the derivative:

$$\begin{aligned}
\frac{\partial \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta} &= -\frac{1}{\sigma^2} \beta + \sum_{n=1}^N \frac{y_n}{P_n} \frac{\partial P_n}{\partial \beta} + \frac{1-y_n}{1-P_n} \frac{\partial(1-P_n)}{\partial \beta} = \\
&= \frac{\partial \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta} = -\frac{1}{\sigma^2} \beta + \sum_{n=1}^N \frac{y_n}{P_n} \frac{\partial P_n}{\partial \beta} - \frac{1-y_n}{1-P_n} \frac{\partial P_n}{\partial \beta}
\end{aligned} \tag{5.36}$$

Now we must calculate  $\frac{\partial P_n}{\partial \beta}$ :

$$\begin{aligned}
\frac{\partial P_n}{\partial \beta} &= \frac{\partial}{\partial \beta} \frac{1}{1+e^{-\beta^T \mathbf{x}_n}} = \frac{\partial}{\partial \beta} \left(1+e^{-\beta^T \mathbf{x}_n}\right)^{-1} = \\
&= \frac{1}{\left(1+e^{-\beta^T \mathbf{x}_n}\right)^2} \frac{\partial}{\partial \beta} \left(1+e^{-\beta^T \mathbf{x}_n}\right) = \\
&= -\mathbf{x}_n \frac{e^{-\beta^T \mathbf{x}_n}}{\left(1+e^{-\beta^T \mathbf{x}_n}\right)^2} = -\mathbf{x}_n \frac{1}{\left(1+e^{-\beta^T \mathbf{x}_n}\right)} \frac{e^{-\beta^T \mathbf{x}_n}}{\left(1+e^{-\beta^T \mathbf{x}_n}\right)} = \\
&= -\mathbf{x}_n P_n (1-P_n)
\end{aligned} \tag{5.37}$$

Substituting in 5.36:

$$\begin{aligned}
\frac{\partial \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta} &= -\frac{1}{\sigma^2} \beta + \sum_{n=1}^N \frac{y_n}{P_n} \frac{\partial P_n}{\partial \beta} - \frac{1-y_n}{1-P_n} \frac{\partial P_n}{\partial \beta} = \\
&= -\frac{1}{\sigma^2} \beta + \sum_{n=1}^N \frac{y_n}{P_n} [-\mathbf{x}_n P_n (1-P_n)] + \\
&\quad - \frac{1-y_n}{1-P_n} [-\mathbf{x}_n P_n (1-P_n)] = \\
&= -\frac{1}{\sigma^2} \beta + \sum_{n=1}^N -y_n \mathbf{x}_n (1-P_n) - (1-y_n) (-\mathbf{x}_n P_n) = \\
&= -\frac{1}{\sigma^2} \beta + \sum_{n=1}^N \mathbf{x}_n (y_n - P_n)
\end{aligned} \tag{5.38}$$

Now we must compute the Hessian matrix:

$$\begin{aligned}
\frac{\partial^2 \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta \partial \beta^T} &= \frac{\partial}{\partial \beta^T} \left( -\frac{1}{\sigma^2} \beta + \sum_{n=1}^N \mathbf{x}_n (y_n - P_n) \right) = \\
&= -\frac{1}{\sigma^2} \mathbf{I} - \sum_{n=1}^N \mathbf{x}_n \frac{\partial P_n}{\partial \beta^T} = -\frac{1}{\sigma^2} \mathbf{I} - \sum_{n=1}^N \mathbf{x}_n \mathbf{x}_n^T P_n (1-P_n)
\end{aligned} \tag{5.39}$$

where we used the result from 5.37.

Note that the 2 terms are negative definite, hence the Hessian is always negative definite. Therefore there can only be one optimum and it must be the minimum.

The decision boundary is the one for which  $\Pr(Y_n = 1 | \mathbf{x}, \hat{\beta} = 0.5)$ .

The steps above can be done for any prior and likelihood combination. In some cases the posterior might have several maxima and or some minima and it become difficult to know if the maximum is a global optimum.

The *Elements of Statistical Learning* book instead of maximizing posterior (or equivalently the numerator), it maximizes the likelihood. Let us express  $\Pr(G = k | X = x) = p_k(x, \theta)$  with  $\theta = \{\beta_{10}, \beta_1^T, \dots, \beta_{(K-1)0}, \beta_{K-1}^T\}$

and let us define the log-likelihood

$$\ell(\theta) = \sum_{i=1}^N \log p_{g_i}(x_i, \theta) \quad (5.40)$$

Consider just two classes with responses 0, 1 and let  $p_1(x, \theta) = p(x, \theta)$  and  $p_2(x, \theta) = 1 - p(x, \theta)$ . Recall that having two classes  $\sum_{l=1}^{K-1} e^{\beta_{l0} + \beta_l^T x_i} = e^{\beta_{10} + \beta_1^T x_i}$ . The log-likelihood can be written as:

$$\begin{aligned} \ell(\beta) &= \sum_{i=1}^N \{y_i \log p(x_i, \beta) + (1 - y_i) \log (1 - p(x_i, \beta))\} = \\ &= \sum_{i=1}^N y_i \log \frac{e^{\beta_{10} + \beta_1^T x_i}}{1 + \sum_{l=1}^{K-1} e^{\beta_{l0} + \beta_l^T x_i}} + \\ &\quad + \sum_{i=1}^N (1 - y_i) \log \left( 1 - \frac{e^{\beta_{10} + \beta_1^T x_i}}{1 + \sum_{l=1}^{K-1} e^{\beta_{l0} + \beta_l^T x_i}} \right) = \\ &= \sum_{i=1}^N y_i \log \frac{e^{\beta_{10} + \beta_1^T x_i}}{1 + e^{\beta_{10} + \beta_1^T x_i}} + \\ &\quad + \sum_{i=1}^N (1 - y_i) \log \left( 1 - \frac{e^{\beta_{10} + \beta_1^T x_i}}{1 + e^{\beta_{10} + \beta_1^T x_i}} \right) = \\ &= \sum_{i=1}^N y_i \left( \log e^{\beta_{10} + \beta_1^T x_i} - \log \left( 1 + e^{\beta_{10} + \beta_1^T x_i} \right) \right) + \\ &\quad + \sum_{i=1}^N (1 - y_i) \log \frac{1}{1 + e^{\beta_{10} + \beta_1^T x_i}} = \\ &= \sum_{i=1}^N y_i \left( \log e^{\beta_{10} + \beta_1^T x_i} - \log \left( 1 + e^{\beta_{10} + \beta_1^T x_i} \right) \right) + \\ &\quad - \sum_{i=1}^N (1 - y_i) \log \left( 1 + e^{\beta_{10} + \beta_1^T x_i} \right) = \\ &= \sum_{i=1}^N \left\{ y_i \left( \beta_{10} + \beta_1^T x_i \right) - \log \left( 1 + e^{\beta_{10} + \beta_1^T x_i} \right) \right\} \end{aligned} \quad (5.41)$$

Here  $\beta = [\beta_{10}, \beta_1]$ . To maximize the log-likelihood we set the derivative to 0:

$$\frac{\partial \ell(\beta)}{\partial \beta} = \sum_{i=1}^N x_i(y_i - p(x_i, \beta)) = 0 \quad (5.42)$$

Using the *Newton-Raphson* algorithm that requires the second-derivative:

$$\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} = - \sum_{i=1}^N x_i x_i^T p(x_i, \beta)(1 - p(x_i, \beta)) \quad (5.43)$$

$$\Rightarrow \beta^{\text{new}} = \beta^{\text{old}} - \left( \frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} \right)^{-1} \frac{\partial \ell(\beta)}{\partial \beta} \quad (5.44)$$

Using the matrix notation,

$$\frac{\partial \ell(\beta)}{\partial \beta} = X^T(y - p) \quad (5.45)$$

$$\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} = -X^T W X \quad (5.46)$$

So the Newton step becomes

$$\begin{aligned} \beta^{\text{new}} &= \beta^{\text{old}} + (X^T W X)^{-1} X^T(y - p) = \\ &= (X^T W X)^{-1} X^T W \left( X \beta^{\text{old}} + W^{-1}(y - p) \right) = \\ &= (X^T W X)^{-1} X^T W z \end{aligned} \quad (5.47)$$

with

$$z = X \beta^{\text{old}} + W^{-1}(y - p) \quad (5.48)$$

sometimes known as the adjusted response. This algorithm is known as **iteratively reweighted least squares (IRLS)** since each iteration solves the weighted least square problem:

$$\beta^{\text{new}} \leftarrow \arg \min_{\beta} (z - X\beta)^T W (z - X\beta) \quad (5.49)$$

$\beta = 0$  seems a good starting value. Convergence is never guaranteed but typically the algorithm does converge, since the log-likelihood is concave but

overshooting can occur. In the rare cases that the log-likelihood decreases, step size halving will guarantee convergence.

For  $K > 2$  we still use the iteration procedure but we will have a  $K - 1$  vector response and a non-diagonal weight matrix per observation. In this case it is better to work with the vector  $\theta$  directly.

#### 5.7.4 Second method: Laplace approximation

There are many approximation methods but the most common is the Laplace approximation. The idea is to approximate the density of interest with a Gaussian.

Choosing a Gaussian means choosing a proper variance and mean value. The Laplace approximation method fixes one of the two parameters, i.e., the mean to the value maximizing the posterior,  $\beta$ . We approximate  $\log g(\beta, \mathbf{X}, \mathbf{y})$  with the Taylor expansion around  $\hat{\beta}$ :

$$\begin{aligned} \log g(\beta, \mathbf{X}, \mathbf{y}) &\approx \log g(\hat{\beta}, \mathbf{X}, \mathbf{y}) + \frac{\partial \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta} \Big|_{\hat{\beta}} (\beta - \hat{\beta}) + \\ &+ \frac{\partial^2 \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta^2} \Big|_{\hat{\beta}} (\beta - \hat{\beta})^2 = \\ &= \log g(\hat{\beta}, \mathbf{X}, \mathbf{y}) + \frac{\partial^2 \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta^2} \Big|_{\hat{\beta}} \frac{(\beta - \hat{\beta})^2}{2} \end{aligned} \quad (5.50)$$

where the second term is the gradient evaluated at the maximum point that therefore must be 0.

The Gaussian density and its log are the following:

$$\begin{aligned} &\frac{1}{2\pi} e^{-\frac{(\beta-\hat{\beta})^2}{2\sigma^2}} \\ &\Rightarrow \log \text{const} - \frac{1}{2\sigma^2} (\beta - \mu)^2 \end{aligned} \quad (5.51)$$

which is similar to 5.50. By analogy of the two equations:

$$\begin{aligned} \mu &= \hat{\beta} \\ -\frac{1}{\sigma^2} &= -\frac{\partial^2 \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta^2} \Big|_{\hat{\beta}} \end{aligned} \quad (5.52)$$

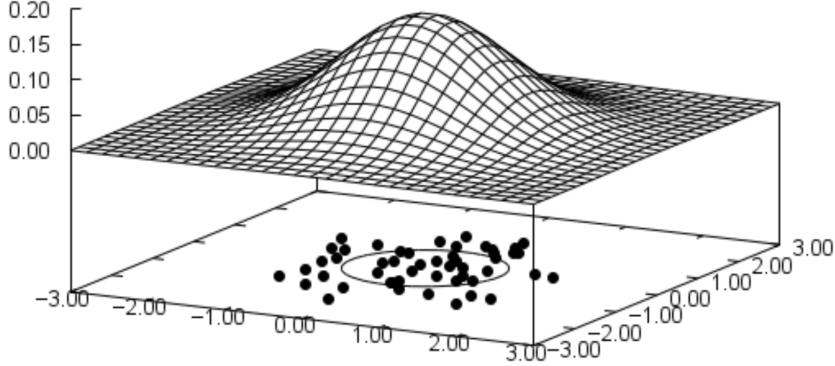


Figure 5.4: Example of multinomial Gaussian.

It can be applied also to multivariate densities  $\Pr(\beta, \mathbf{X}, \mathbf{y}) \approx \mathcal{N}(\mu, \Sigma)$ :

$$\begin{aligned}\mu &= \hat{\beta} \\ \Sigma^{-1} &= -\frac{\partial^2 \log g(\beta, \mathbf{X}, \mathbf{y})}{\partial \beta \partial \beta^T} \Big|_{\hat{\beta}}\end{aligned}\quad (5.53)$$

Consider a multinomial 2D Gaussian function (dimensionality of  $\beta$  is 2) as in 5.4 and suppose to project on the plane the points of the curve having the same value (the ellipses in the figure). The ellipses will be the combination of coefficients giving the same function value.

In figure 5.5 the Laplace approximation of the posterior (darker lines) is shown while the lighter lines are the true unnormalised posterior. The centre point corresponds to the maximum point  $\hat{\beta}$ . Note how the approximation is good around  $\hat{\beta}$  and it diverges going further from it.

We use the approximate posterior to compute predictions. But now we have a density and not a single value: the prediction is computed by averaging over this density: it is like averaging over all possible values of  $\beta$ . We should calculate the expected value  $\Pr(Y_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \beta)$  with respect to the approximate posterior denoted as  $\mathcal{N}(\mu, \Sigma)$ :

$$\Pr(Y_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \beta) = \mathbf{E}_{\mathcal{N}(\mu, \Sigma)} \{ \Pr(T_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \beta) \} \quad (5.54)$$

However, we cannot compute the integral (of the expectation), but we can

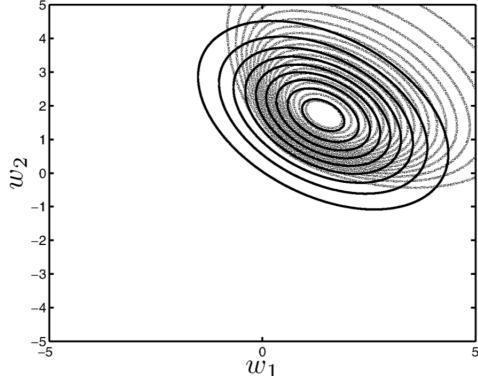


Figure 5.5: The axis are the parameters. The Laplace approximation of the posterior (darker lines) is shown while the lighter lines are the true un-normalised posterior. The centre point corresponds to the maximum point  $\hat{\beta}$ .

sample from  $\mathcal{N}(\mu, \Sigma)$  and approximate the expectation with a sum:

$$\Pr(Y_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \beta) = \frac{1}{N_s} \sum_{s=1}^{N_s} \frac{1}{1 + e^{-\beta_s^T \mathbf{x}_{\text{new}}}} \quad (5.55)$$

**Comparison between the decision boundaries of MAP and Laplace method.** In case of MAP estimation we get a single separating line as in 5.6a for the example of two classes. In case of Laplace approximation we don't have a single separating line but a density distribution. 5.6b shows 20 boundaries (i.e., set of coefficients) sampled randomly from the distribution. All or almost all separates the classes quite well but in the area from the graph further from the classes (or from the centroids or clusters) there is a lot of variability. This variability represents the uncertainty of the classifier in those area far from the classes, where no event (in the sense of data entry) was observed.

This is made clearer by looking at the decision boundaries in 5.6c and 5.6d. In case of MAP it is quite obvious: the probability increases or decreases just moving close to or far from to the boundary. In case of Laplace approximation the contours are no longer straight lines. The probability are now close to 0.5 in all the area except those closes to the two classes. It is like the classifier is unable to take a decision in those areas, that are the ones

where no event has been noted.

On the contrary the classifier resulting from MAP approximation is always sure about its work: it can only classify either with one or the other class except in on the points on the boundaries. This result from the fact that it is the result of a single point and not a distribution: i.e., the amount of confidence on the result is left out.

### 5.7.5 Third method: sampling technique

The reason of estimating the posterior density with Laplace approximation or any other method is to take into account uncertainties in  $\beta$  when making predictions. Using the Gaussian approximation we were able to sample as in equation 5.55 directly from data. When deciding we take the conditional probability by averaging all over the potential values  $\beta$  by taking the expectation:

$$\Pr(T_{\text{new}} = 1 | x_{\text{new}}, \mathbf{X}, \mathbf{y}, \sigma^2) = E_{\Pr(\beta | \mathbf{X}, \mathbf{y}, \sigma^2)}(\Pr(T_{\text{new}} = 1 | x_{\text{new}}, \beta)) \quad (5.56)$$

In these types of approximations we cut off the approximation step and sample directly from the posterior. A set of samples from the true posterior could be substituted directly into equation 5.55 to compute the desired predictive probability  $\Pr(y_i | x_i, \mathbf{X}, \beta)$ . A popular sampling technique is the **Metropolis-Hastings** algorithm.

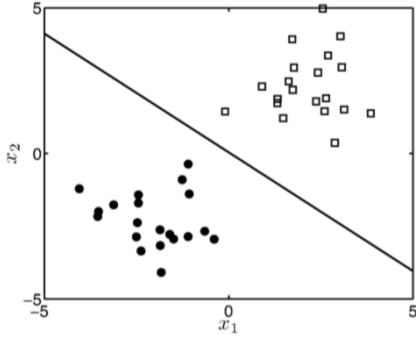
Drawing from the posterior does not mean we can write it down but that we sample directly the system (physical or whatever) generating the data.

**The metropolis-Hastings algorithms** The objective is to sample from  $\Pr(\beta | \mathbf{X}, \mathbf{y}, \sigma^2)$  to approximate the following expectation:

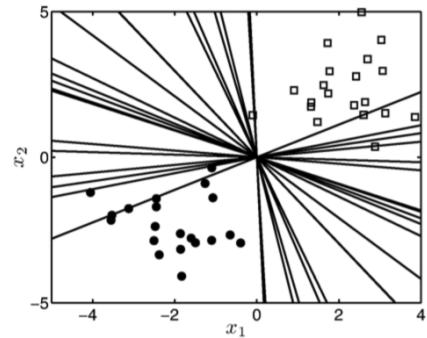
$$\begin{aligned} \Pr(Y_{\text{new}} = 1 | x_{\text{new}}, \mathbf{X}, \mathbf{y}, \sigma^2) &= E_{\Pr(\beta | \mathbf{X}, \mathbf{y}, \sigma^2)} [\Pr(T_{\text{new}} = 1 | x_{\text{new}}, \beta)] \\ &= \int \Pr(Y_{\text{new}} = 1 | x_{\text{new}}, \beta) \Pr(\beta | \mathbf{X}, \mathbf{y}, \sigma^2) d\beta \end{aligned} \quad (5.57)$$

with

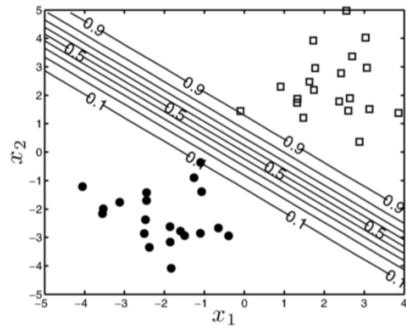
$$\Pr(Y_{\text{new}} = 1 | x_{\text{new}}, \mathbf{X}, \mathbf{y}, \sigma^2) \approx \frac{1}{N_s} \sum_{s=1}^{N_s} \Pr(Y_{\text{new}} = 1 | x_{\text{new}}, \beta_s) \quad (5.58)$$



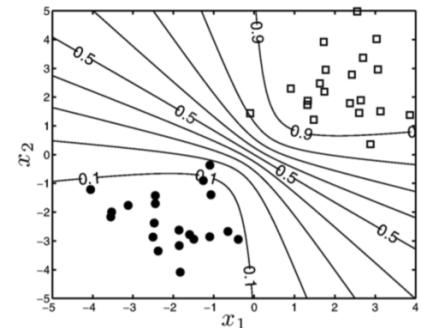
(a) Decision boundary for MAP estimation.



(b) Decision boundary for Laplace approximation estimation.



(c) Contours of probability of belonging to class 1 in case of MAP estimation.



(d) Contours of probability of belonging to class 1 in case of Laplace approximation estimation computed with a sample based approximation.

Figure 5.6: Comparison between MAP and Laplace approximation contours and probability densities.

The algorithm generates a sequence of samples  $\beta_1, \beta_2, \dots$ . First all the algorithm is independent from the starting point, as long as we sample long enough: it is guaranteed the sequence converges.

**The generation of new samples** happens in this way. Suppose we have the sample  $s - 1$ , we will propose a new sample  $\tilde{\beta}_s$  and define the density  $\Pr(\tilde{\beta}_s | \beta_{s-1})$ . This density is unrelated with the posterior  $\Pr(\beta | \mathbf{X}, \mathbf{y}, \sigma^2)$  and we can define it as we please but it will affect the convergence time. A common choice is to use a Gaussian centred on the current sample,  $\beta_{s-1}$ :

$$\Pr(\tilde{\beta}_s | \beta_{s-1}, \Sigma) = \mathcal{N}(\beta_{s-1}, \Sigma) \quad (5.59)$$

Generally  $\sigma$  is taken diagonal with same values. The smaller the elements on the diagonal, the smaller the distance at each step.

Such a sequence creates a **random walk**. The choice of the Gaussian is justified by the ease of sampling from the Gaussian and by its symmetry: moving from  $\tilde{\beta}_{s-1}$  to  $\tilde{\beta}_s$  is just as likely to move from  $\tilde{\beta}_s$  to  $\tilde{\beta}_{s-1}$ :

$$\Pr(\tilde{\beta}_s | \beta_{s-1}, \Sigma) = \Pr(\tilde{\beta}_{s-1} | \beta_s, \Sigma) \quad (5.60)$$

**Accepting or rejecting the candidate**  $\tilde{\beta}_s$  is performed by calculating the following quantity:

$$r = \frac{\Pr(\tilde{\beta}_s | \mathbf{X}, \mathbf{y}, \sigma^2)}{\Pr(\beta_{s-1} | \mathbf{X}, \mathbf{y}, \sigma^2)} \frac{\Pr(\beta_{s-1} | \tilde{\beta}_s, \Sigma)}{\Pr(\hat{\beta}_s | \beta_{s-1}, \Sigma)} \quad (5.61)$$

The expression is the product of the ratio of the posterior density at the proposed sample to that at the old sample times the ratio of the proposed densities. For the Gaussian symmetry discussed above, this term is 1 when using Gaussian densities. Note that we cannot compute exactly the densities, but being a ratio the normalisation constant (the denominator in Bayes expression) simplifies and only the likelihoods times the priors are left:

$$r = \frac{\Pr(\tilde{\beta}_s | \sigma^2)}{\Pr(\beta_{s-1} | \sigma^2)} \frac{\Pr(\mathbf{y} | \mathbf{X}, \tilde{\beta}_s, \sigma^2)}{\Pr(\mathbf{y} | \mathbf{X}, \beta_{s-1}, \sigma^2)} \quad (5.62)$$

If  $r > 1$ , i.e, we get a higher posterior density, we accept the candidate otherwise we accept the candidate with probability equal to  $r$ . The complete algorithm is depicted in 5.7 where a uniform distribution in  $[0, 1]$  is used as

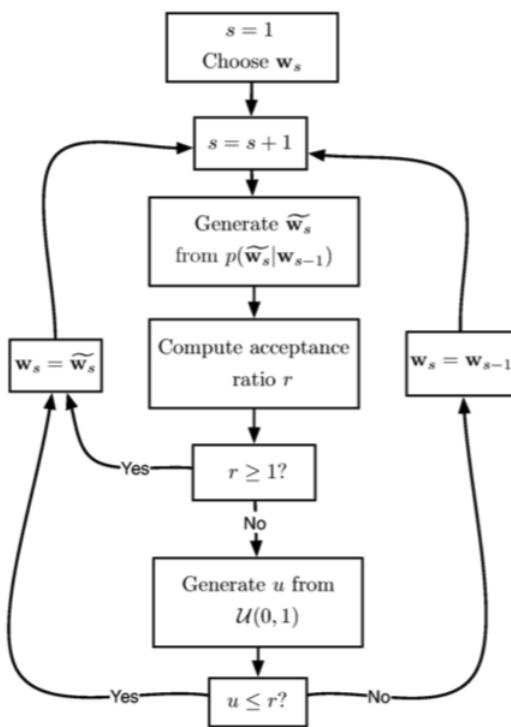
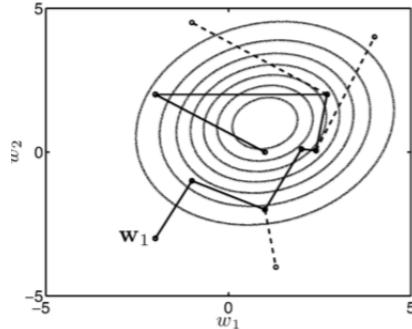


Figure 5.7: The steps of the Metropolis-Hastings algorithm.  $U$  is a uniform distribution in  $[0, 1]$



(e) After ten samples.

Figure 5.8: Example of Metropolis-Hastings iterations: solid lines are accepted coefficients, dashed lines are the rejected ones.

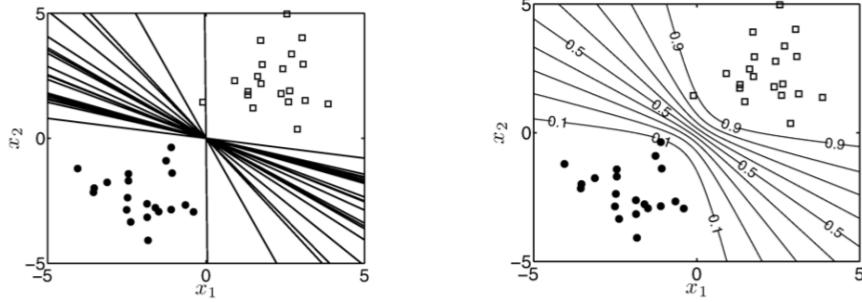
decision rule in case  $r < 1$ . Being a uniform distribution, the probability that  $u \leq r$  is  $r$ .

5.8 shows a 10-iteration process of the algorithms where solid lines are accepted coefficients, dashed lines are the rejected ones. Note that even the third sample causes a decrease in the posterior  $r < 1$ , nevertheless in this specific case the decision rule accepted it. On the contrary the 4-th sample causes a huge decrease hence it is very unlikely it is accepted and in fact it is not, so  $\beta_4 = \beta_3$ . After  $N$  samples we compute the sample based approximations to the mean and covariance

$$\begin{aligned}\mu' &= \frac{1}{N_s} \sum_{s=1}^{N_s} \beta_s \\ S' &= \frac{1}{N_s} \sum_{s=1}^{N_s} (\beta_s - \mu')(\beta_s - \mu')^T\end{aligned}\tag{5.63}$$

**Definition 5.1. Burn-in** It is the time interval between the starting of the algorithm and the convergence.

It cannot be determined: to overcome this problem, a method for determining convergence (to a distribution, not to a value) should be established. For example, in the algorithm above, we do not know if the starting point belongs to an area from which we are supposed to sample: it might be very



(a) Predictive probability contours of (b) Decision boundaries created from  
classifying objects as square. randomly selected MH samples.

Figure 5.9: Example of Metropolis-Hastings algorithm results.

far from the posterior. Including these samples in the approximation might result in a not good value. That is why the first samples (ranging from few samples to thousands) should be discarded.

A popular method is to start several samplers simultaneously from different starting points. When all the samplers are generating samples with similar mean and variance, it suggests they converged all to the same distributions.

**Definition 5.2. convergence** In this case we are talking about the convergence to a given distribution, not a single point. The convergence to a distribution is characterized to the convergence of its parameters: in case of the Gaussian the mean and variance.

We can even look at each coefficient independently:

$$\Pr(\beta_1 | \mathbf{X}, \mathbf{y}, \sigma^2) = \int \Pr(\beta_1, \beta_2 | \mathbf{X}, \mathbf{y}, \sigma^2) d\beta_2 \quad (5.64)$$

**To calculate the predictive probability** using the obtained set of samples, we can do what already done with the Laplace approximation:

$$\Pr(Y_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{y}, \sigma^2) = \frac{1}{N_s} \sum_{s=1}^{N_s} \frac{1}{1 + e^{-\beta_s^T \mathbf{x}_{\text{new}}}} \quad (5.65)$$

5.9a and 5.9b show an example of possible shapes of contours: it does not look too different from the Laplace ones. The only difference is that these

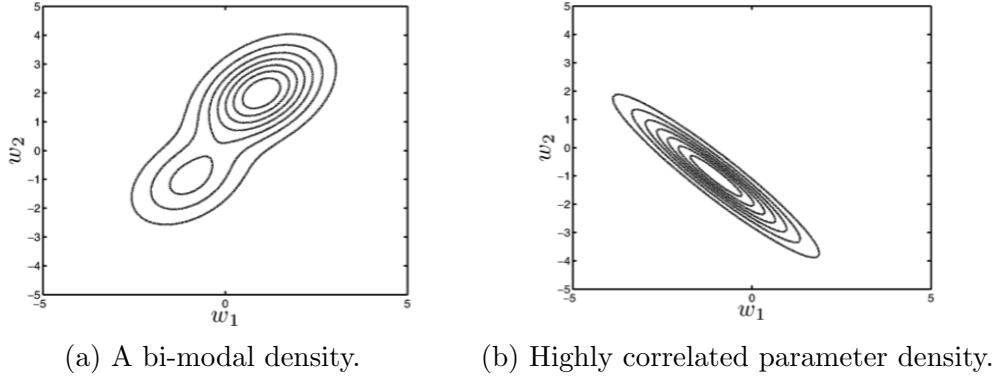


Figure 5.10: Example of Metropolis-Hastings algorithm results.

contours are not so tight as the Laplace's ones. This suggests the probability decreases more slowly.

**Limitations** The difficult mostly lies in the unknown shape of the density. When a density has two or more modes, MH moves towards the modes as these moves increase the posterior density and hence are always accepted. When close to a mode, many steps are required to move from one mode to another and this is very unlikely. We might end up exploring a mode without even knowing the other exists (see 5.10a). Another problem arises when the variables are strongly correlated (see 5.10b). Let us pick any position and propose a movement from a Gaussian with diagonal covariance (i.e., having circular contours). The shapes are very different and many samples will be rejected: the majority of moves that we sample from our proposal will involve moving steeply down the probability gradient. There are even other problems.

### 5.7.6 Usage

LR is used as data analysis tool where the goal is to understand the role of the input variables in explaining the outcome. Typically many models are fit in a search for a parsimonious model involving a subset of the variables, possibly with some interactions terms.

It is widely used in biostatistical applications where binary responses (two classes) occur quite frequently. For example, patients survive or die, have heart disease or not, or a condition is present or absent.

## 5.8 Regularized Logistic regression

We can use the  $L_1$  penalty for variable selection and shrinkage:

$$\arg \max_{\beta_0, \beta_1} \left\{ \sum_{i=1}^N y_i (\beta_0 + \beta^T x_i) - \log(1 + e^{\beta_0 + \beta^T x_i}) - \lambda \sum_{j=1}^p |\beta_j| \right\} \quad (5.66)$$

This function is concave and can be solved using a nonlinear programming method.

## 5.9 Logistic vs LDA

The difference between the models relies on how the linear coefficients are estimated. The logistic regression model is more general since it makes less assumptions.

LDA is not robust to outliers since observations far from the decision boundary are used to estimate the common covariance matrix, while they are scaled down in the Logistic regression.

## 5.10 Perceptron learning algorithm

It tries to find a separate hyperplane by minimizing the distance of misclassified points to the decision boundary. If a response  $y_i = 1$  is misclassified, then  $x_i^T \beta + \beta_0 < 0$ , and the opposite for a misclassified response with  $y_i = -1$ . The goal is to minimize

$$D(\beta, \beta_0) = - \sum_{i \in \mathcal{M}} y_i (x_i^T \beta + \beta_0) \quad (5.67)$$

where  $\mathcal{M}$  is the set of misclassified points. The gradient is

$$\frac{\partial D(\beta, \beta_0)}{\partial \beta} = - \sum_{i \in \mathcal{M}} y_i x_i \quad (5.68)$$

$$\frac{\partial D(\beta, \beta_0)}{\partial \beta_0} = - \sum_{i \in \mathcal{M}} y_i \quad (5.69)$$

where the algorithm uses the stochastic gradient descent where the coefficients are updated by the gradient value weighted by a step  $\rho$ . There are many problems though:

- when data are separable, there are many solutions which depend on the starting value;
- many steps might be required;
- when data are not separable, the algorithm will not converge;

## 5.11 Optimal separating hyperplanes

The optimal separating hyperplane separates the two classes and maximizes the distance to the closest point from either class (Vapnik, 1996). Not only does this provide a unique solution to the separating hyperplane problem, but by maximizing the margin between the two classes on the training data, this leads to better classification performance on test data.

Suppose  $M$  is the distance. Then

$$\begin{aligned} & \max_{\beta, \beta_0, \|\beta\|=1} M \\ & y_i(x_i^T \beta + \beta_0) \geq M \end{aligned} \quad (5.70)$$

We can move the constrain on the module  $\|\beta\| = 1$  to the condition  $\frac{1}{\|\beta\|} y_i(x_i^T \beta + \beta_0) \geq M$ , which redefines  $\beta_0$ .

For a pair of coefficients satisfying this inequalities, any positively scaled multiple satisfies them too, so we can set arbitrarily set  $\|\beta\| = \frac{1}{M}$ :

$$\begin{aligned} & \min_{\beta, \beta_0} \frac{1}{2} \|\beta\|^2 \\ & \text{subject to } y_i(x_i^T \beta + \beta_0) \geq 1 \end{aligned} \quad (5.71)$$

With this constraint, a margin around the decision boundary with thick  $\frac{1}{\|\beta\|}$  is present. We choose  $\beta$  to maximize the thickness of margin margin. This is a convex optimization problem. The Lagrange primal function to be minimized is:

$$L_p = \frac{1}{2} \|\beta\|^2 = \sum_{i=1}^N \alpha_i [y_i(x_i^T \beta + \beta_0)] \quad (5.72)$$

and setting the derivatives to 0:

$$\beta = \sum_{i=1}^N \alpha_i y_i x_i^0 = \sum_{i=1}^N \alpha_i y_i \quad (5.73)$$

and substituting in 5.72:

$$L_D = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{k=1}^N \alpha_i \alpha_k y_i y_k x_i^T x_k \quad (5.74)$$

*subject to  $\alpha_i \geq 0$  and  $\sum_{i=1}^N \alpha_i y_i = 0$*

The optimal hyperplane focuses more on points that counts, i.e., close to the border. For this reason it is more robust. LDA depends on all the data, even points faraway. If classes are really Gaussian LDA is optimal and separating hyperplane will pay a price for focusing on noisier data. For logistic regression, if a separate hyperplane exists, since the log-likelihood can be driven to 0.

When data are not separable there will be no feasible solution and an alternative formulation is needed.

## 6 Basis expansion and regularization

To extend the flexibility of linear model, a transformation of  $\mathbf{X}$  can be performed and then use a linear model to the derived input features. Denoting the transformation  $h_m(\mathbf{X}) : \mathcal{R}^p \rightarrow \mathcal{R}$  for a single input  $m$ , we have the model:

$$f(\mathbf{X}) = \sum_{m=1}^M \beta_m h_m(\mathbf{X}) \quad (6.1)$$

$h()$  are called **basis function** Any kind of transformation can be applied: square-roots, squared (on single inputs i.e,  $x_i^2$  or among different inputs  $x_i x_j$ ), logarithmic, power functions, trigonometric, etc.

Polynomials are more widely used but they have a limitation due to its global nature: when tweaking the parameters to achieve a desired behaviour in a specific region, problems might arise in another region.

A solution is to consider **piecewise-polynomials** and **splines**.

### 6.1 Piecewise Polynomials and splines

For the moment  $X$  is assumed one-dimensional. A piecewise polynomial function is obtained by dividing the domain of  $X$  into contiguous intervals

and use a different  $f$  in each interval.

Given a sequence  $a = t_0 < t_1 < \dots < t_{m+1} = b$ , the piecewise polynomials are delimited by an adjacent pair in the sequence. So we have the following sequence of intervals:

$$I_l = [t_{l-1}, t_l] \text{ for } 1 \leq l \leq m \text{ and } [t_m, t_{m+1}] \quad (6.2)$$

So the piecewise polynomials, having basis functions:  $h_0(X) = 1, h_1(X) = X, h_2(X) = X^2$  and so on, is:

$$f(x) = \begin{cases} g_0(x) = \beta_{0,0} + \beta_{0,1}X + \dots + \beta_{0,k-1}X^{k-1} & X \in I_1 \\ \vdots \\ g_{m-1}(x) = \beta_{m-1,0} + \beta_{m-1,1}X + \dots + \beta_{m-1,k-1}X^{k-1} & X \in I_{k+1} \end{cases} \quad (6.3)$$

In this way we get discontinuities at the boundaries. Note that discontinuity means we get completely different values for almost the same input. More often we would like to have continuity at the boundaries or knots:  $f(\xi^+) = f(\xi^-)$  which implies the condition:  $\beta_1 + \xi\beta_2 = \beta_3 + \xi_1\beta_4$  which removes one degree of freedom.

These constraints, one for each knot, can be embedded in additional basis functions of the type  $h(X) = (X - \xi)_+$  where  $(\cdot)_+ = \max(\cdot, 0)$  i.e., the basis function is 0 for  $X - \xi < \xi$ ,  $X - \xi$  otherwise

$$h(X) = (X - \xi)_+ = \max(X - \xi, 0) = \begin{cases} 0 & X - \xi < 0 \\ X - \xi & X - \xi \geq 0 \end{cases} \quad (6.4)$$

Using the previous and these basis functions we can reexpress the global function as:

$$\begin{aligned} f(x) = & \beta_{0,0} + \beta_{0,1}X + \dots + \beta_{0,k-1}X^{k-1} + \\ & + \beta_{1,0}(X - \xi_0)_+^0 + \beta_{1,1}(X - \xi_0)_+^1 + \dots + \beta_{1,k-1}(X - \xi_0)_+^{k-1} + \\ & + \dots \\ & + \beta_{m-1,0}(X - \xi_{m-1})_+^0 + \dots + \beta_{m-1,k-1}(X - \xi_{m-2})_+^{k-1} \end{aligned} \quad (6.5)$$

**To force continuity between two regions** we set the terms  $\beta_{1,0}(X - \xi_j)_+^0$  to 0:

For example forcing continuity at the first knot:

$$\begin{aligned}\beta_{1,0}(X - \xi_0)_+^0 &= \beta_{0,0} + \beta_{0,1}\xi_0 \\ \Rightarrow \beta_{1,0} &= \beta_{0,0} + \beta_{0,1}\xi_0\end{aligned}\tag{6.6}$$

In this way we don't have a jump at the boundaries:

$$\begin{aligned}f(x) = &\beta_{0,0} + \beta_{0,1}X + \cdots + \beta_{0,k-1}X^{k-1} + \\ &+ \beta_{1,1}(X - \xi_0)_+^1 + \cdots + \beta_{1,k-1}(X - \xi_0)_+^{k-1} + \\ &+ \vdots \\ &+ \beta_{m-1,1}(X - \xi_{m-1})_+^1 + \cdots + \beta_{m-1,k-1}(X - \xi_{m-1})_+^{k-1}\end{aligned}\tag{6.7}$$

In this way we have removed  $m - 1$  parameters.

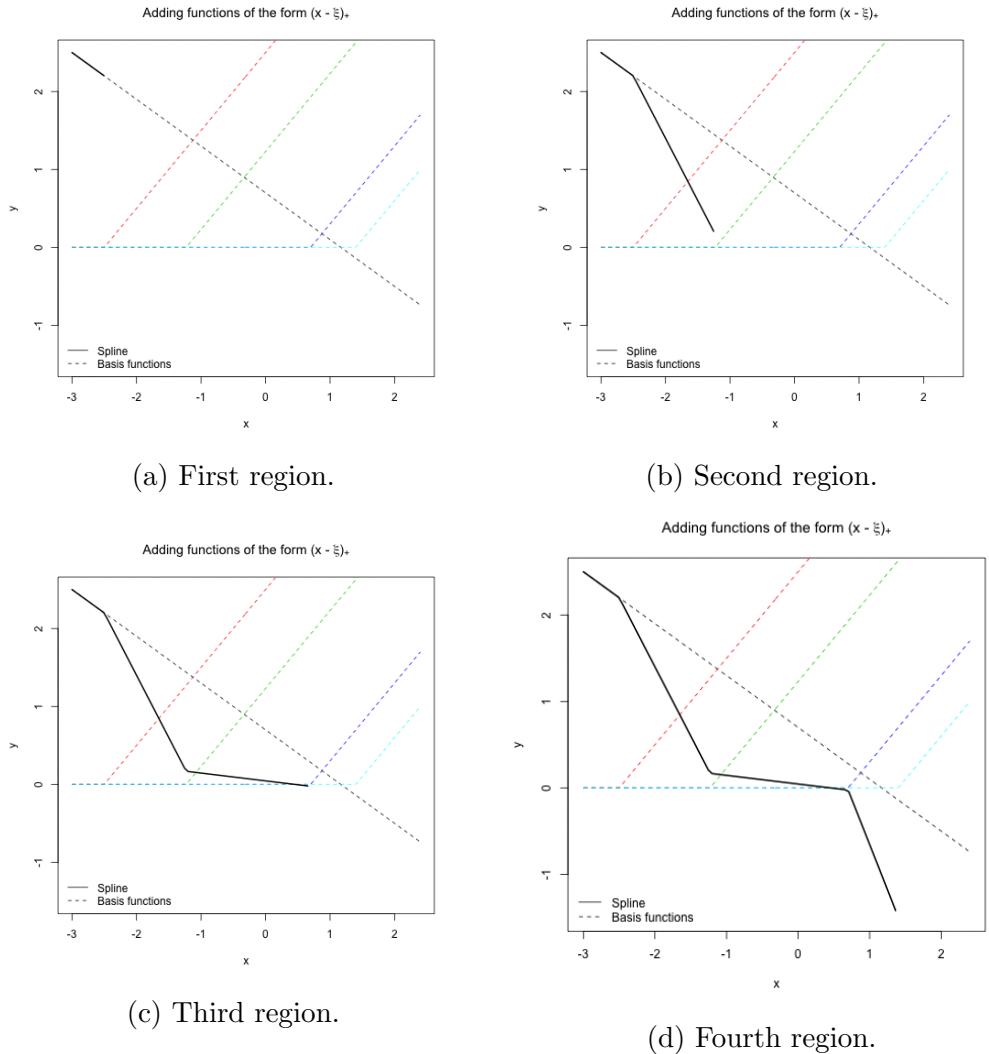
There is a difference in this representation: before we have to select a polynomial function for a specific region where the fit to the global function was given by the fit of the parameters specific to that region, now we have a global function that works a little differently. In the first region, the only non-null terms are  $\beta_{0,j}$  as before. When reaching the second region, the terms  $\beta_{1,j}$  becomes non-null. Now the coefficients of the polynomial are the sum of the coefficients of these two region: i.e., in the second region we have:

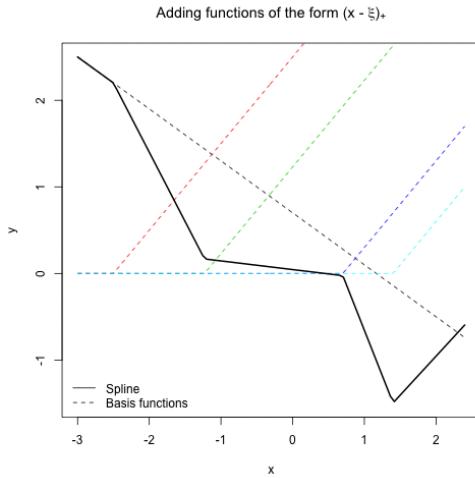
$$\begin{aligned}f(x) = &\beta_{0,0} - (\beta_{1,1} + \cdots + \beta_{1,k-1})\xi_0 + (\beta_{0,1} + \beta_{1,1})X + \\ &+ \cdots + (\beta_{0,k-1} + \beta_{1,k-1})X^{k-1}\end{aligned}\tag{6.8}$$

6.1 shows the global function, solid line, given by the sum of basis functions, dashed lines, when traversing the graph from left to right. At each knot, a new basis function is activated and summed to the global function.

The basis functions can be seen as a correction to the global polynomial for that specific region and the knots are those points where the correction starts. At the knot  $X = \xi_j$  so the correction starts very gently and the continuity is preserved.

Generally, smoother functions are preferred and these are achieved by increasing the order of the local polynomials and increasing the order of continuity (continuity first derivative, second derivative). It is claimed that cubic splines are the lowest-order spline for which the discontinuity is not visible to the human eye and seldom higher degrees are needed, unless smooth derivatives are required.





(e) Fifth region.

Figure 6.1: Linear splines. The solid line is the global function while the dashed lines are the basis functions.

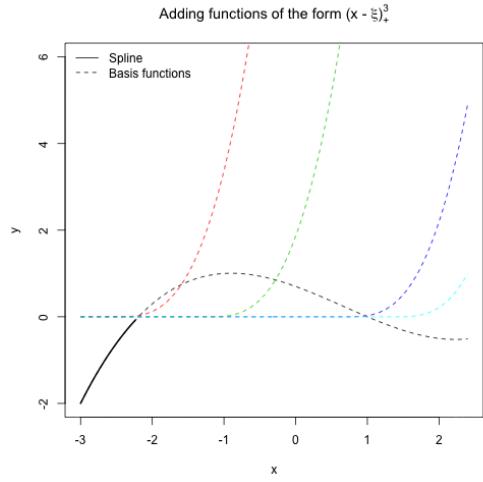
The spline order, number of knots and their positions must be selected. Generally the position of the knots is chosen according the observation, while the order is chosen a-priori.

## 6.2 Natural cubic splines

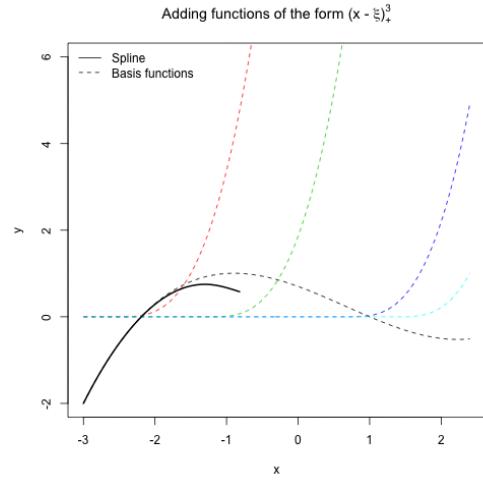
Polynomial fits to data tends to be erratic at the boundaries and additionally splines behave even more widely than the global polynomial beyond the boundaries. This is shown by the point-wise variance (the variance of the estimator at one point:  $\text{Var}[\hat{f}(x_0)]$ ) in 6.3. Note the variance explosion close to the boundaries, especially for cubic splines.

A **natural cubic spline** adds additional constraints by forcing linearity beyond the boundary knots. These frees up four degrees of freedom (2 in both boundary regions), that can be used more profitably by sprinkling more knots in the interior region. There will be a price to pay in terms of bias near the boundaries, but in these regions we have less information anyway so assuming the function is linear here is reasonable.

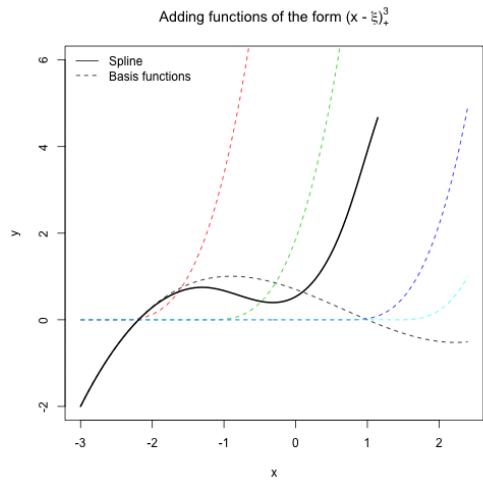
A natural cubic spline with  $K$  knots is represented by  $K$  basis functions. One can start from the basis of a cubic spline and then derive the reduce



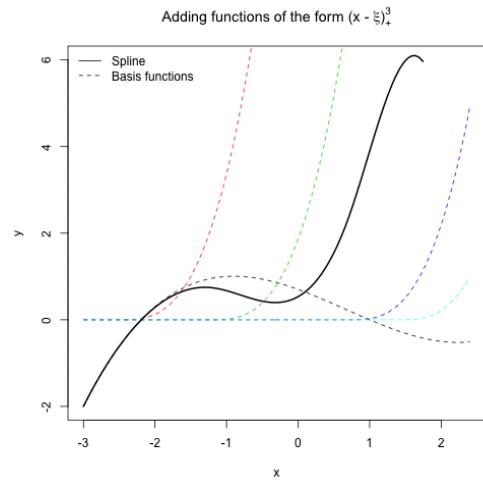
(a) First region.



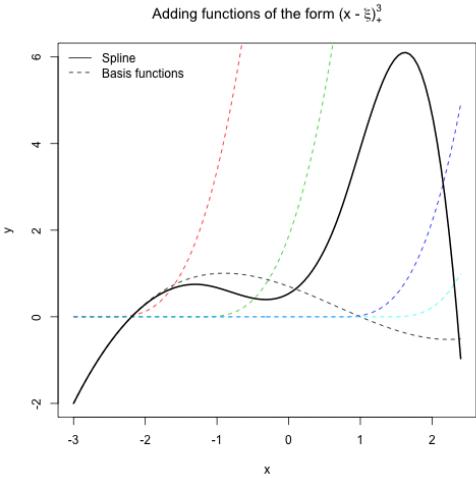
(b) Second region.



(c) Third region.



(d) Fourth region.



(e) Fifth region.

Figure 6.2: Cubic splines. The solid line is the global function while the dashed lines are the basis functions.

basis by imposing the boundary constraints.

Starting from the general continuous basis for four regions (four knots):

$$\begin{aligned}
 h_1(X) &= 1, & h_2(X) &= X, & h_3(X) &= X^2, & h_4(X) &= X^3, \\
 h_5(X) &= X - \xi_0, & h_6(X) &= (X - \xi_0)^2, & h_7(X) &= (X - \xi_0)^3 \\
 h_8(X) &= X - \xi_1, & h_9(X) &= (X - \xi_1)^2, & h_{10}(X) &= (X - \xi_1)^3 \\
 h_9(X) &= X - \xi_2, & h_{10}(X) &= (X - \xi_1)^2, & h_{11}(X) &= (X - \xi_2)^3
 \end{aligned} \tag{6.9}$$

Enforcing also continuity of the first and second derivatives at the knots we reduce the basis to:

$$\begin{aligned}
 h_1(X) &= 1, & h_2(X) &= X, & h_3(X) &= X^2, & h_4(X) &= X^3, \\
 h_5(X) &= (X - \xi_0)^3, & h_6(X) &= (X - \xi_1)^3, & h_7(X) &= (X - \xi_2)^3.
 \end{aligned} \tag{6.10}$$

Enforcing linearity beyond the boundaries, we eliminate  $h_3(X)$  and  $h_4(X)$ . We must also keep the cubic expression in the intermediate regions but somehow make the cubic part cancel out when reaching the fifth region since here it must be linear. We can add for each region in the interval  $[1, K - 2]$  the

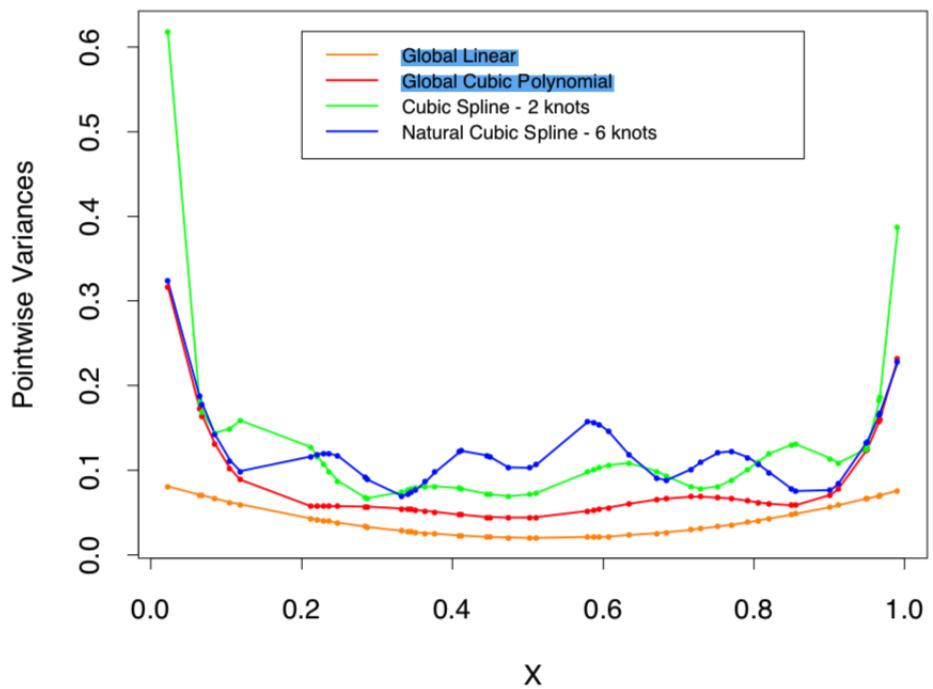


Figure 6.3:  $X$  consists of 50 points drawn randomly from  $U[0, 1]$  and an assumed error model of with constant variance. Both cubic splines have 6 degrees of freedom. The cubic spline has two knots at 0.33 and at 0.66 while the natural cubic spline has boundary knots at 0.1 and 0.9, and four interior knots uniformly spaced between them.

following basis function:

$$h_k(X) = d_k(X) - d_{K-1}(X)$$

where  $d_k(X) = \frac{(X - \xi_k)_+^3 - (X - \xi_K)_+^3}{\xi_K - \xi_k}$

(6.11)

In the first region we have:

$$\hat{f}_1(X) = \beta_0 + \beta_1 X$$
(6.12)

In the second region we have:

$$\begin{aligned} \hat{f}_2(X) &= \beta_0 + \beta_1 X + \beta_2 \frac{(X - \xi_0)^3}{\xi_2 - \xi_0} = \\ &= \beta_0 + \beta_1 X + \beta_2 \frac{X^3 - 3\xi_0 X^2 + 3\xi_0^2 X - \xi_0^3}{\xi_2 - \xi_0} = \\ &= \frac{\beta_2}{\xi_2 - \xi_0} X^3 - 3\beta_2 \frac{\xi_0}{\xi_2 - \xi_0} X^2 + (\beta_1 + 3\beta_2 \frac{\xi_0^2}{\xi_2 - \xi_0}) X + \beta_0 - \beta_2 \frac{\xi_0^3}{\xi_2 - \xi_0} \end{aligned}$$
(6.13)

In the third region we have:

$$\begin{aligned}
\hat{f}_3(X) &= \beta_0 + \beta_1 X + \beta_2 h_2(X) = \beta_0 + \beta_1 X + \beta_2 \left[ \frac{(X - \xi_0)^3}{\xi_2 - \xi_0} - \frac{(X - \xi_1)^3}{\xi_2 - \xi_1} \right] \\
&= \beta_0 + \beta_1 X + \beta_2 \left[ \frac{X^3 - 3\xi_0 X^2 + 3\xi_0^2 X - \xi_0^3}{\xi_2 - \xi_0} - \frac{X^3 - 3\xi_1 X^2 + 3\xi_1^2 X - \xi_1^3}{\xi_2 - \xi_1} \right] = \\
&= \beta_0 + \beta_1 X + \beta_2 \frac{(\xi_2 - \xi_1 - \xi_2 + \xi_0)X^3 - 3[\xi_0(\xi_2 - \xi_1) - \xi_1(\xi_2 - \xi_0)]X^2}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} + \\
&\quad + \frac{3[\xi_0^2(\xi_2 - \xi_1) - \xi_1^2(\xi_2 - \xi_0)]X - [(\xi_0^3(\xi_2 - \xi_1) - \xi_1^3(\xi_2 - \xi_0)]}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} = \\
&= \beta_0 + \beta_1 X + \beta_2 \frac{(-\xi_1 + \xi_0)X^3 - 3\xi_2(\xi_0 - \xi_1)X^2}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} + \\
&\quad + \frac{3[\xi_2(\xi_0 - \xi_1)(\xi_0 + \xi_1) - \xi_0\xi_1(\xi_0 - \xi_1)]X}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} + \\
&\quad - \frac{[\xi_2(\xi_0 - \xi_1)(\xi_0^2 - \xi_0\xi_1 + \xi_1^2) - \xi_0\xi_1(\xi_0 - \xi_1)(\xi_0 + \xi_1)]}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} = \\
&= \beta_0 + \beta_1 X - \beta_2(\xi_1 - \xi_0) \frac{X^3 - 3\xi_2 X^2}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} + \\
&\quad + \frac{3[\xi_2(\xi_0 + \xi_1) - \xi_0\xi_1]X - [\xi_2(\xi_0^2 - \xi_0\xi_1 + \xi_1^2) - \xi_0\xi_1(\xi_0 + \xi_1)]}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} = \\
&= -\beta_2 \frac{(\xi_1 - \xi_0)}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} X^3 + 3\beta_2 \frac{\xi_2(\xi_1 - \xi_0)}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} X^2 + \\
&\quad + (\beta_1 - 3\beta_2(\xi_1 - \xi_0)) \frac{\xi_2(\xi_0 + \xi_1) - \xi_0\xi_1}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} X + \\
&\quad + \beta_0 + \beta_2(\xi_1 - \xi_0) \frac{\xi_2(\xi_0^2 - \xi_0\xi_1 + \xi_1^2) - \xi_0\xi_1(\xi_0 + \xi_1)}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)}
\end{aligned} \tag{6.14}$$

In the fourth region:

$$\begin{aligned}
\hat{f}_3(X) &= \beta_0 + \beta_1 X + \beta_2 h_2(X) = \\
&= \beta_0 + \beta_1 X + \beta_2 \left[ \frac{(X - \xi_0)^3 - (X - \xi_2)^3}{\xi_2 - \xi_0} - \frac{(X - \xi_1)^3 - (X - \xi_2)^3}{\xi_2 - \xi_1} \right] \\
&= \beta_0 + \beta_1 X + \beta_2 \frac{X^3 - 3\xi_0 X^2 + 3\xi_0^2 X - \xi_0^3 - X^3 + 3\xi_2 X^2 - 3\xi_2^2 X + \xi_2^3}{\xi_2 - \xi_0} + \\
&\quad - \beta_2 \frac{X^3 - 3\xi_1 X^2 + 3\xi_1^2 X - \xi_1^3 - X^3 + 3\xi_2 X^2 - 3\xi_2^2 X + \xi_2^3}{\xi_2 - \xi_1} = \\
&= \beta_0 + \beta_1 X + \beta_2 \frac{3(\xi_2 - \xi_0)X^2 - 3(\xi_2^2 - \xi_0^2)X + \xi_2^3 - \xi_0^3}{\xi_2 - \xi_0} + \\
&\quad - \beta_2 \frac{3(\xi_2 - \xi_1)X^2 - 3(\xi_2^2 - \xi_1^2)X + \xi_2^3 - \xi_1^3}{\xi_2 - \xi_1} = \\
&= \beta_0 + \beta_1 X + \beta_2 \frac{\cancel{3(\xi_2 - \xi_1)(\xi_2 - \xi_0)X^2} - 3(\xi_2 - \xi_1)(\xi_2^2 - \xi_0^2)X + (\xi_2 - \xi_1)(\xi_2^3 - \xi_0^3)}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} + \\
&\quad - \beta_2 \frac{\cancel{3(\xi_2 - \xi_0)(\xi_2 - \xi_1)X^2} - 3(\xi_2 - \xi_0)(\xi_2^2 - \xi_1^2)X + (\xi_2 - \xi_0)(\xi_2^3 - \xi_1^3)}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} = \\
&= \beta_0 + \beta_1 X + \beta_2 \frac{-3(\xi_2 - \xi_1)(\xi_2^2 - \xi_0^2)X + (\xi_2 - \xi_1)(\xi_2^3 - \xi_0^3)}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} + \\
&\quad - \beta_2 \frac{-3(\xi_2 - \xi_0)(\xi_2^2 - \xi_1^2)X + (\xi_2 - \xi_0)(\xi_2^3 - \xi_1^3)}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} = \\
&= \beta_0 + \beta_1 X + \beta_2 \frac{3[-\xi_2(\xi_1^2 - \xi_0^2) + \xi_2^2(\xi_1 - \xi_0) + \xi_0 \xi_1(\xi_1 - \xi_0)]X +}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)} \\
&\quad - \frac{\xi_2(\xi_1^3 - \xi_0^3) - \xi_2^3(\xi_1 - \xi_0) - \xi_0 \xi_1(\xi_1 - \xi_0)}{(\xi_2 - \xi_0)(\xi_2 - \xi_1)}
\end{aligned} \tag{6.15}$$

Note that the fourth region is linear.

### 6.3 Smoothing splines

We can avoid knot selection by using a maximal set of knots, controlled by a regularization process. The problem is: *Among all functions  $f(x)$  with two continuous derivatives, find the one that minimizes the penalized residual sum*

of squares:

$$\text{RSS}(f, \lambda) = \sum_{i=1}^N [y_i - f(x_i)]^2 + \lambda \int f''(t) dt \quad (6.16)$$

The first term measures closeness to the data, while the second term penalizes curvature in the function. If  $\lambda = 0$   $f$  can be any function that interpolates the data so we can achieve smoothness. If  $\lambda = \infty$  simple least squares line fit, since no second derivative can be tolerated and we get a "rough" function. 6.16 has an explicit finite-dimensional unique minimizer which is a natural cubic spline with knots at the unique values of the  $x_i$ ,  $i = 1, \dots, N$ , so there are as many as  $N$  knots, hence  $N$  degrees of freedom. The penalty translates to a penalty on the spline coefficients, which are shrunk to the linear fit.

Being the solution a natural spline, we can write it as:

$$f(x) = \sum_{j=1}^N N_j(x) \theta_j \quad (6.17)$$

where  $N_j(x)$  are the  $N$ -dimensional set of basis functions for representing this family of natural splines:

$$\text{RSS}(\theta, \lambda) = (\mathbf{y} - \mathbf{N}\theta)^T (\mathbf{y} - \mathbf{N}\theta) + \lambda \theta^T \Sigma_N \theta \quad (6.18)$$

where  $N_{i,j} = N_j(x_i)$  and

$$\Sigma_{Nj,k} = \int N_j''(t) N_k''(t) dt$$

. The solution is :

$$\hat{\theta} = \left( \mathbf{N}^T \mathbf{N} + \lambda \Sigma_N \right)^{-1} \mathbf{N}^T \mathbf{y} = \mathbf{S}_\lambda \mathbf{y} \quad (6.19)$$

which is a generalized ridge regression.  $\mathbf{S}_\lambda$  is positive-definite, symmetric and  $\mathbf{S}_\lambda \mathbf{S}_\lambda \leq \mathbf{S}_\lambda$ . Since it is symmetric and positive-definite it has a real eigenvalue decomposition. Let us re-write  $\mathbf{S}_\lambda = (\mathbf{I} - \lambda \mathbf{K})^{-1}$ . The eigenvalue decomposition of  $\mathbf{S}_\lambda$  is:

$$\begin{aligned} \mathbf{S}_\lambda &= \sum_{k=1}^N \rho_k(\lambda) \mathbf{u}_k \mathbf{u}_k^T \\ \rho_k(\lambda) &= \frac{1}{1 + \lambda d_k} \end{aligned} \quad (6.20)$$

The degrees of freedom are  $df_\lambda = \text{Tr}(\mathbf{S}_\lambda)$ .

The eigenvectors are not affected by changes in  $\lambda$ , and hence the whole family of smoothing splines for a particular sequence of  $x$ , indexed by  $\lambda$  have the same eigenvectors.  $\mathbf{S}_\lambda \mathbf{y} = \sum_{k=1}^N \mathbf{u}_k \rho_k(\lambda) \langle \mathbf{u}_k, \mathbf{y} \rangle$ : the smoothing spline decomposes  $\mathbf{y}$  w.r.t. the complete basis  $\mathbf{u}_k$  and differently shrinking the contributions using  $\rho_k(\lambda)$ . So for example suppose  $\mathbf{B}_{xi}$  is a matrix of cubic-splines basis functions. Then the vector of fitted spline values is given by  $\hat{\mathbf{f}} = \mathbf{B}_\xi (\mathbf{B}_\xi^T \mathbf{B}_\xi)^{-1} \mathbf{B}_\xi^T \mathbf{y} = \mathbf{H}_\xi \mathbf{y}$ . In such a basis regression method the contributions are either left alone or shrunk to 0. The first two eigenvalues are always 1 and they correspond to the two-dimensional eigenspace of functions linear in  $x$  which are never shrunk. The eigenvalues  $\rho_k(\lambda) = 1/(1 + \lambda d_k)$  are an inverse function of the eigenvalues  $d_k$  of the penalty matrix  $\mathbf{K}$ , moderated by  $\lambda$ ;  $\lambda$  controls the rate at which the  $\rho_k(\lambda)$  decrease to zero.  $d_1 = d_2 = 0$  and again linear functions are not penalized.

## 6.4 Multidimensional splines

Suppose  $X \in \mathcal{R}^2$  and suppose we have two sets:  $h_{1,k}(X_1), k = 1, \dots, M_1$  for representing functions of coordinate  $X_1$ , and a set of  $M_2$  functions  $h_{2,k}(X_2)$  for coordinate  $X_2$ . Then the  $M_1 \times M_2$  dimensional tensor product basis defined by:

$$g_{j,k} = h_{1,j}(X_1)h_{2,k}(X_2), \quad j = 1, \dots, M_1, \quad k = 1, \dots, M_2 \quad (6.21)$$

can be used for representing a two-dimensional function:

$$g(X) = \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \theta_{jk} g_{jk}(X) \quad (6.22)$$

The coefficients can be fit with least squares. This can be generalized to  $d$  dimensions, but note that the dimension of the basis grows exponentially fast.

One-dimensional smoothing splines (via regularization) generalize to higher dimensions as well. Suppose we have pairs  $y_i, x_i$  with  $x_i \in \mathcal{R}^d$ , and we seek a  $d$ -dimensional regression function  $f(x)$ . The idea is to set up the problem:

$$\min_f \sum_{i=1}^N [y_i - f(x_i)]^2 + \lambda J[f] \quad (6.23)$$

where  $J$  is an appropriate penalty functional for stabilizing a function  $f$  in  $\mathcal{R}^d$ . For example:

$$J[f] = \int \int_{\mathcal{R}^2} \left[ \left( \frac{\partial^2 f(x)}{\partial x_1^2} \right)^2 + 2 \left( \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} \right)^2 + \left( \frac{\partial^2 f(x)}{\partial x_2^2} \right)^2 \right] dx_1 dx_2 \quad (6.24)$$

If  $\lambda \rightarrow 0$  the solution approaches an interpolating function, as  $\lambda$  the solution approaches the least squares plane. The solution has the form:

$$f(x) = \beta_0 + \beta^T x + \sum_{j=1}^N \alpha_j h_j(x) \quad (6.25)$$

Additive spline model can be represented in this formulation too: there exists a penalty  $J[f]$  that guarantees that the solution has the form  $f(X) = \alpha + f_1(X_1) + \dots + f_d(X_d)$  and that each of the functions  $f_j$  are univariate splines. In this case it is better to assume  $f$  is additive and impose an additional penalty and impose an additional penalty on each of the component functions:

$$J[f] = J[f_1 + f_2 + \dots + f_d] = \sum_{j=1}^d \int f_j''(t_j) dt_j \quad (6.26)$$

These are naturally extended to ANOVA spline decomposition:

$$f(X) = \alpha + \sum_j f_j(X_j) + \sum_{j < k} f_{jk}(X_j, X_k) + \dots \quad (6.27)$$

where each of the components are splines of the required dimension. There are many choices to be made:

- maximum order of interaction (the one above is up to order 2);
- which term to include
- the representation to use (regression splines with a small number of basis functions and their tensor product for interaction or a complete basis as in smoothing splines and include appropriate regularizers for each term in the expansion).

When the number of potential dimensions is large automatic methods are desirable (for example MARS and MART procedures).

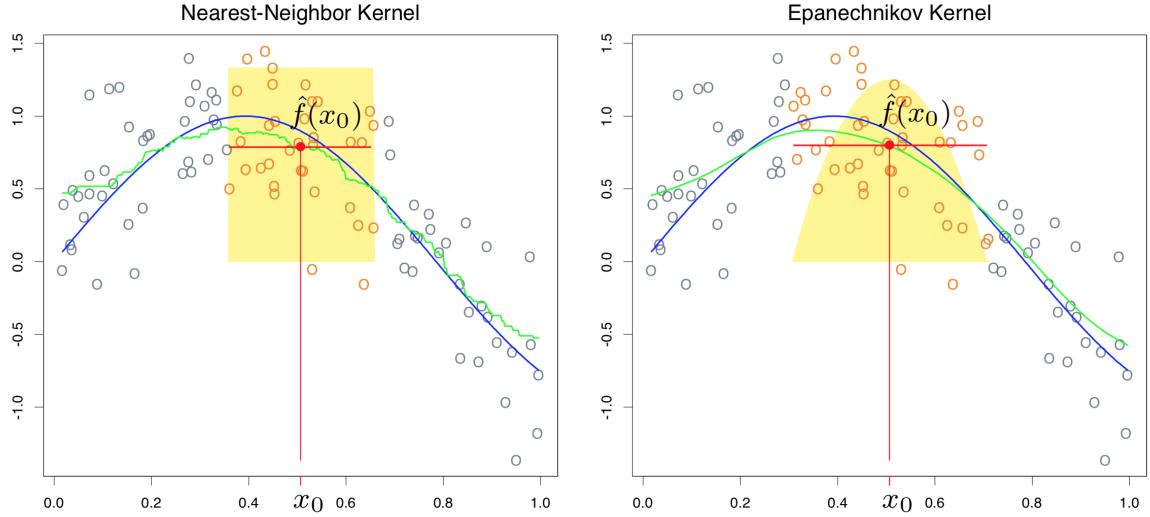


Figure 7.1: In green the fitting curves. On the left the one resulting from *k-nearest neighbourhood*, on the right the metric neighbourhood.

## 6.5 Wavelet smoothing

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# 7 Kernel smoothing methods

## 7.1 One-dimensional kernel smoothers

We have seen the *k-nearest neighbourhood* average as an estimate of the regression function  $E(Y|X = x)$ :

$$\hat{f} = \text{Ave}(y_i|x_i \in N_k(x)) \quad (7.1)$$

where  $N_k(x)$  is the set of  $k -$ points nearest to  $x$  in squared distance. An example of the resulting fitting curve is shown in green on the left of 7.1. The green curve is bumpy, since  $\hat{f}(x)$  is discontinuous in  $x$ . As we move  $x_0$  from left to right, the  $k$ -nearest neighborhood remains constant, until a point  $x_i$  to the right of  $x_0$  becomes closer than the furthest point  $x_{i'}$  in the neighbourhood to the left of  $x_0$ , at which time  $x_i$  replaces  $x_{i'}$ .

Rather than give all the points in the neighbourhood equal weights, we can assign weights that die off smoothly with distance from the target

point. The right panel in 7.1 shows an example of this, using the so-called Nadaraya–Watson kernel-weighted average:

$$\hat{f}(x) = \frac{\sum_{i=1}^N K_\lambda(x_0, x_i) y_i}{\sum_{i=1}^N K_\lambda(x_0, x_i)} \quad (7.2)$$

with the Epanechnikov quadratic kernel:

$$K_\lambda(x_0, x_i) = D\left(\frac{|x - x_0|}{\lambda}\right) = \begin{cases} \frac{3}{4} \left[1 - \left(\frac{|x - x_0|}{\lambda}\right)^2\right] & \text{if } \frac{|x - x_0|}{\lambda} \leq 1 \\ 0 & \text{otherwise} \end{cases} \quad (7.3)$$

Now the function is continuous. As we move the target from left to right, points enter the neighborhood initially with weight zero, and then their contribution slowly increases. Note that  $\lambda$  dictates the width of the window which is fixed. On the contrary, for the *k-nearest neighbourhood* the window size depends on the density since anyway k points must be considered. 7.2 shows other kernels. Another popular one is the tri-cube function:

$$D\left(\frac{|x - x_0|}{\lambda}\right) = \begin{cases} \left[1 - \left(\frac{|x - x_0|}{\lambda}\right)^3\right]^3 & \text{if } \frac{|x - x_0|}{\lambda} \leq 1 \\ 0 & \text{otherwise} \end{cases} \quad (7.4)$$

Both are compact functions. A common non-compact function is the Gaussian function.

Generalizing we can use a width function  $h_\lambda(x_0)$  that determines the width of the neighbourhood at  $x_0$  (previously we have used  $h_\lambda(x_0) = \lambda$ ).

There are a number of details to be clarified:

- the value of  $\lambda$  which selects the window size. Large values imply lower variance but higher bias;
- $h_\lambda(x_0)$  can be constant (i.e.,  $h_\lambda(x_0) = \lambda$ ) or variable. Constant values (**metric window widths**) keep the bias constant but the variance is inversely proportional to the local density. Nearest neighbourhood has opposite behaviour: the variance stays constant and the absolute bias varies inversely with local density.
- boundary issues: the metric neighbourhood tend to contain less points on the boundaries while the nearest-neighbourhood get wider.

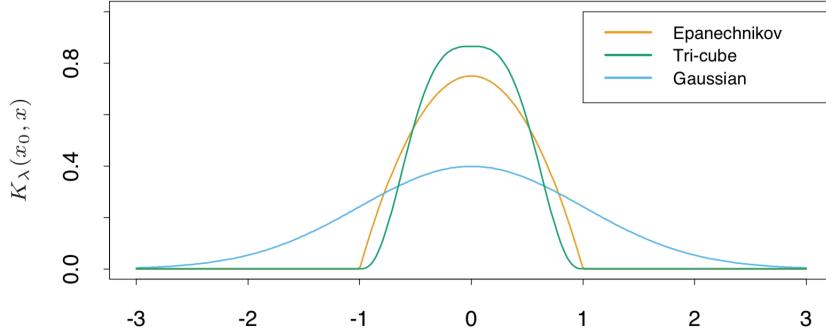


Figure 7.2: A comparison of three popular kernels for local smoothing. Each has been calibrated to integrate to 1. The tri-cube kernel is compact and has two continuous derivatives at the boundary of its support, while the Epanechnikov kernel has none. The Gaussian kernel is continuously differentiable, but has infinite support.

### 7.1.1 Local linear regression

Smooth kernel fit still has a problem close to the boundaries: because of the asymmetry in this region weighted averages can be badly biased (left in 7.3). By fitting straight lines rather than constants locally, we can remove this bias effect. Actually, this bias can be present in the interior of the domain as well, if the  $X$  values are not equally spaced. Locally weighted regression solves a separate weighted least squares problem at each target point  $x_0$ :

$$\min_{\alpha(x_0), \beta(x_0)} \sum_{i=1}^N K_\lambda(x_0, x_i) [y_i - \alpha(x_0) - \beta(x_0)x_i]^2 \quad (7.5)$$

and the estimate becomes:

$$\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0)x_0 \quad (7.6)$$

Notice that although we fit an entire linear model to the data in the region, we only use it to evaluate the fit at the single point  $x_0$ .

Define the vector-valued function  $b(x)^T = (1, x)$ . Let  $B$  be the  $N \times 2$  regression matrix with  $i$ -th row  $b(x_i)^T$ , and  $W(x_0)$  the  $N \times N$  diagonal matrix with  $i$ -th diagonal element  $K_\lambda(x_0, x_i)$ . Then

$$\hat{f}(x_0) = b(x_0)^T (B^T W(x_0) B)^{-1} B^T W(x_0) y = \sum_{i=1}^N l_i(x_0) y_i \quad (7.7)$$

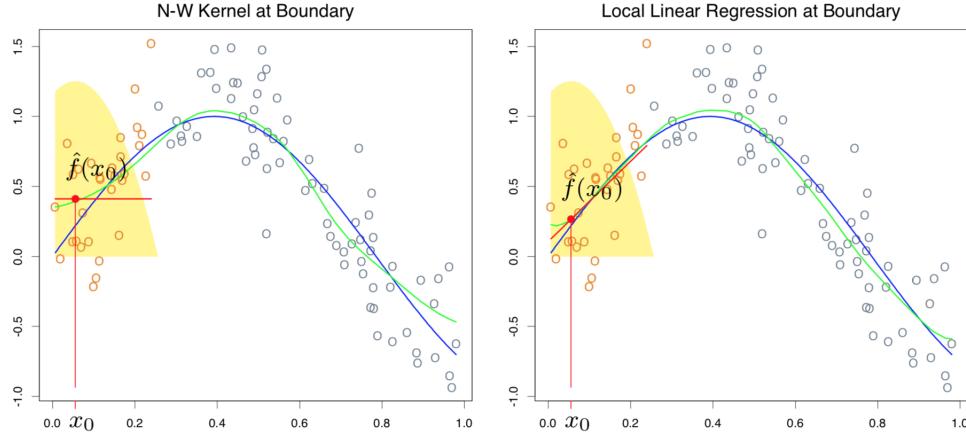


Figure 7.3: On the left it can be noticed the bias effect at the boundaries.

The weights  $l_i(x_0)$  combine the weighting kernel  $K_\lambda(x_0, \cdot)$  and the least squares operations and are referred to as the equivalent kernel. Local linear regression automatically modifies the kernel to correct the bias exactly to first order, a phenomenon dubbed as **automatic kernel carpentry**.

### 7.1.2 Local polynomial regression

We can fit local polynomial fits of any degree  $d$ :

$$\min_{\alpha(x_0), \beta_j(x_0), j=1, \dots, d} \sum_{i=1}^N K_\lambda(x_0, x_i) \left[ y_i - \alpha_0 - \sum_{j=1}^d \beta_j(x_0) x_i^j \right]^2 \quad (7.8)$$

$$\hat{f} = \hat{\alpha}(x_0) + \sum_{j=1}^d \hat{\beta}_j(x_0) x_0^j$$

Local linear fits tend to be biased in regions of curvature of the true function, a phenomenon referred to as **trimming the hills** and **filling the valleys**. Local quadratic regression is generally able to correct this bias. There is of course a price to be paid for this bias reduction, and that is increased variance. The fit in the right panel of 7.4 is slightly more wiggly, especially in the tails. Summarizing, local linear fits can help bias dramatically at the boundaries at a modest cost in variance. Local quadratic fits do little at the boundaries for bias, but increase the variance a lot. Local quadratic fits

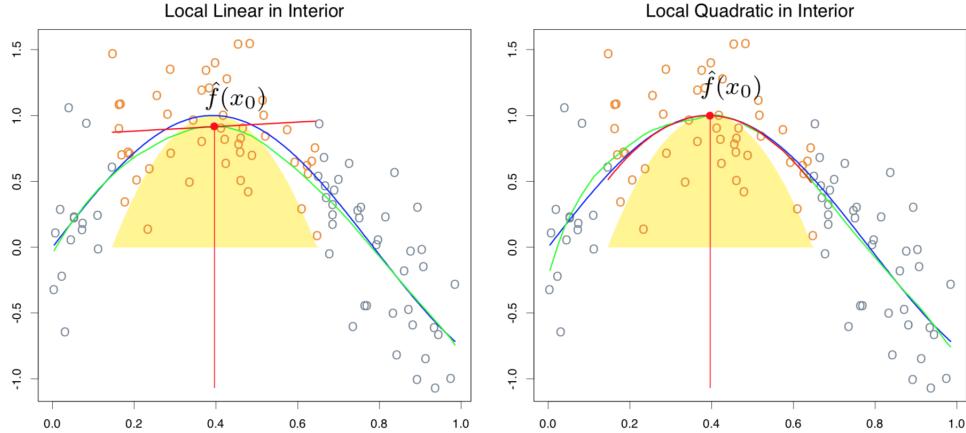


Figure 7.4: Local linear fits exhibit bias in regions of curvature of the true function. Local quadratic fits tend to eliminate this bias.

tend to be most helpful in reducing bias due to curvature in the interior of the domain. Asymptotic analysis suggest that local polynomials of odd degree dominate those of even degree. This is largely due to the fact that asymptotically the MSE is dominated by boundary effects.

## 7.2 Local regression in $\mathcal{R}^p$

Let  $b(X)$  be a vector of polynomial terms in  $X$  of maximum degree  $d$ . For example, with  $d = 1$  and  $p = 2$  we get  $b(X) = (1, X_1, X_2)$ ; with  $d = 2$  we get  $b(X) = (1, X_1, X_2, X_1^2, X_2^2, X_1 X_2)$ ; and trivially with  $d = 0$  we get  $b(X) = 1$ . At each  $x_0 \in \mathcal{R}^p$  solve:

$$\min_{\beta(x_0)} \sum_{i=1}^N K_\lambda(x_0, x_i) \left( y_i - b(x_i)^T \beta(x_0) \right)^2 \quad (7.9)$$

to produce the fit

$$\hat{f}(x_0) = b(x_0)^T \hat{\beta}(x_0) \quad (7.10)$$

While boundary effects are a problem in one-dimensional smoothing, they are a much bigger problem in two or higher dimensions, since the fraction of points on the boundary is larger. In fact, one of the manifestations of the curse of dimensionality is that the fraction of points close to the boundary

increases to one as the dimension grows. Directly modifying the kernel to accommodate two-dimensional boundaries becomes very messy, especially for irregular boundaries. Directly modifying the kernel to accommodate two-dimensional boundaries becomes very messy, especially for irregular boundaries. Local regression becomes less useful in dimensions much larger than 2.

For high dimensionality it is impossible to simultaneously maintain localness (i.e., low bias) and a sizable sample in the neighbourhood (low variance) as dimensions increase, without the total sample size increasing exponentially with  $p$ .

### 7.3 Structured local regression models in $\mathcal{R}^p$

When the dimension to sample-size ratio is unfavorable, local regression does not help us much, unless we are willing to make some structural assumptions about the model.

#### 7.3.1 Structured kernels

The default spherical kernel gives equal weight to each coordinate and we can standardize the variables to unit deviation.

Another way is to use a positive definite matrix  $A$  to weigh the different coordinates:

$$K_\lambda(x_0, x) = D \left( \frac{(x - x_0)^T A (x - x_0)}{\lambda} \right) \quad (7.11)$$

Entire coordinates or directions can be downgraded or omitted by imposing appropriate restrictions on  $A$ . For example, if  $A$  is diagonal, then we can increase or decrease the influence of individual predictors  $X_j$  by increasing or decreasing  $A_{jj}$ .

#### 7.3.2 Structured regression function

We are trying to fit a regression function  $E[Y|X] = f(X_1, X_2, \dots, X_p)$  in CMcalRP in which every level of interaction is potentially present. It is natural to consider analysis-of-variance (ANOVA) decompositions of the form

$$f(X_1, X_2, \dots, X_p) = \alpha + \sum_j g_j(X_j) + \sum_{k < l} g_{kl}(X_k, X_l) + \dots \quad (7.12)$$

and then introduce structure by eliminating the higher-order terms. Additive models assume only main effect terms:  $f(X) = \alpha + \sum_{j=1}^p g_j(X_j)$ , second order models will have terms with interactions of order at most two and so on. The important detail is that at any stage, one-dimensional local regression is all that is needed. The same ideas can be used to fit low-dimensional ANOVA decompositions.

## 7.4 Local likelihood and other models

Any parametric model can be made local.

For example we can use likelihood local to  $x_0$ , with the parameters  $\theta(x_0) = x_0^T \beta(x_0)$ :

$$l(\beta(x_0)) = \sum_{i=1}^N K_\lambda(x_0, x_i) l(y_i, x_i^T \beta(x_0)) \quad (7.13)$$

Also time-series can be made local by fitting by local least squares with a kernel in order to vary according to the short-term history of the series.

### 7.4.1 Local multiclassifier linear logistic regression

Consider categorical responses  $g_i \in 1, 2, \dots, J$ . The global linear model is:

$$\Pr(G = j | X = x) = \frac{e^{\beta_{j0} + \beta_j^T x}}{1 + \sum_{k=1}^{J-1} e^{\beta_{k0} + \beta_k^T x}}$$

The local log-likelihood for the class  $J$  can be written as:

$$\begin{aligned} & \sum_{i=1}^N K_\lambda(x_0, x_i) \left\{ \beta_{gi0}(x_0) + \beta_{gi}(x_0)^T (x_i - x_0) + \right. \\ & \left. - \log \left[ 1 + \sum_{k=1}^{J-1} e^{\beta_{k0}(x_0) + \beta_k(x_0)^T (x_i - x_0)} \right] \right\} \end{aligned} \quad (7.14)$$

Notice that  $\beta_{J0} = \beta_J = 0$  i.e., the last class is taken as reference. Also, we have centred the local regression at  $x_0$ , so that the fitted posterior probabilities at  $x_0$  are simply:

$$\hat{\Pr}(G = j, X = x_0) = \frac{e^{\hat{\beta}_{j0}(x_0)}}{1 + \sum_{k=1}^{J-1} e^{\hat{\beta}_{k0}(x_0)}} \quad (7.15)$$

## 7.5 Kernel density classification

One can use nonparametric density estimates for classification in a straightforward fashion using Bayes' theorem:

$$\hat{P}r(G = k | X = x_0) = \frac{\hat{\pi}_k \hat{f}_k(x_0)}{\sum_{j=1}^J \hat{\pi}_k \hat{f}_j(x_0)} \quad (7.16)$$

with  $\hat{f}_j$  being a fitted nonparametric density estimates for each class separately.

## 7.6 Naive-Bayes classifier

It assumes that given a class  $G = j$ , the features  $X_k$  are independent:

$$f_j(X) = \prod_{k=1}^p f_{jk}(X_k) \quad (7.17)$$

While this assumption is generally not true, it does simplify the estimation dramatically since  $f_{jk}$  can be estimated separately using one dimensional kernel density estimates. Despite these rather optimistic assumptions, Naive-Bayes classifiers often outperform far more sophisticated alternatives. The reasons are that although the individual class density estimates may be biased, this bias might not hurt the posterior probabilities as much, especially near the decision regions. In fact, the problem may be able to withstand considerable bias for the savings in variance such a "naive" assumption earns.

## 7.7 Radial basis functions

Radial basis functions combine the idea of basis methods and kernel functions by treating  $K_\lambda(\xi, x)$  as a basis function:

$$f(x) = \sum_{j=1}^M K_{\lambda_j}(\xi_j, x) \beta_j = \sum_{j=1}^M D\left(\frac{\|x - \xi_j\|}{\lambda_j}\right) \beta_j \quad (7.18)$$

A popular choice for  $D$  is the standard Gaussian density function. There are several methods to estimate the parameters, among which one of the

most common is the least squares. We can optimize the sum-of-squares with respect to all parameters:

$$\min_{\{\lambda_j, \xi_j, \beta_j\}_1^M} \sum_{i=1}^N \left( y_i - \beta_0 - \sum_{j=1}^M \beta_j e^{-\frac{(x_i - \xi_j)^T(x_i - \xi_j)}{\lambda_j^2}} \right)^2 \quad (7.19)$$

This model is referred to as RBF network, with  $\xi_j$  and  $\lambda_j$  playing the role of weights. This criterion is non-convex with multiple local minima.

Another way is to estimate  $\{\lambda_j, \xi_j\}$  separately from  $\beta_j$ . Often, the kernel parameters  $\lambda_j$  and  $\xi_j$  are chosen in an unsupervised way using the  $X$  distribution alone. One of the method is to fit a Gaussian mixture density model to the training  $x_i$ , which provides both the centres  $\xi_j$  and the scales  $\lambda_j$ . Other approaches use cluster methods to locate  $\xi_j$  and treat  $\lambda_j = \lambda$  as a hyper-parameter.

Using a constant  $\lambda$  might create holes-regions (regions that are not fitted by any gaussian) where no kernels has appreciable support. Renormalized radial basis functions solve this problem:

$$h_j(x) = \frac{D\left(\frac{\|x - \xi_j\|}{\lambda}\right)}{\sum_{k=1}^M D\left(\frac{\|x - \xi_k\|}{\lambda}\right)} \quad (7.20)$$

## 7.8 Mixture Models for Density Estimation and Classification

The mixture model can be viewed as a kind of kernel method:

$$f(x) = \sum_{m=1}^M \alpha_m \phi(x, \mu_m, \Sigma_m) \quad (7.21)$$

$$\sum_m \alpha_m = 1$$

It is possible to use any density instead of the Gaussian densities.

The parameters are usually fit by maximum likelihood, using the EM algorithm. If the covariance matrix is force to be scalar  $\Sigma_m = \sigma_m I$ , then 7.21 has the form of a radial basis expansion. If  $\sigma_m = \sigma > 0$  and  $M \uparrow$

## 8 Model assessment and selection

Take a look also at this: <https://machinelearningmastery.com/probabilistic-model-selection-measures/>

**Definition 8.1. Training error:** it is the average loss over the training samples:

$$\bar{e}_{rr} = \frac{1}{N} \sum_{i=1}^N L(y_i, \hat{f}(x_i)) \quad (8.1)$$

For categorical variables it is:

$$\bar{e}_{rr} = -\frac{2}{N} \sum_{i=1}^N \log \hat{p}_k(x_i) \quad (8.2)$$

The "–2" in the definition makes the log-likelihood loss for the Gaussian distribution match squared-error loss.

**Definition 8.2. Test error:** with the term *test error* or *generalization error* we indicate the prediction error over an independent test sample different from the one used for the training and it is indicated as

$$Err_\tau [L(Y, \hat{f}(X)|\tau)] \quad (8.3)$$

where  $\tau$  indicates the training set and  $X$  and  $Y$  are drawn randomly from their joint distribution.

**Definition 8.3. Expected prediction error:** or **expected test error** is the expectation of the test.

$$Err = E [L(Y, \hat{f}(X))] = E [Err_\tau] \quad (8.4)$$

8.1 shows the prediction errors of the same type of model trained with different training sets in light red and their expectation (average) in dark red.

To judge the prediction capability of a model we need to estimate  $Err_\tau$ . As the model becomes more and more complex, it uses the training data more and is able to adapt to more complicated underlying structures. Hence there is a decrease in bias but an increase in variance. There is some intermediate

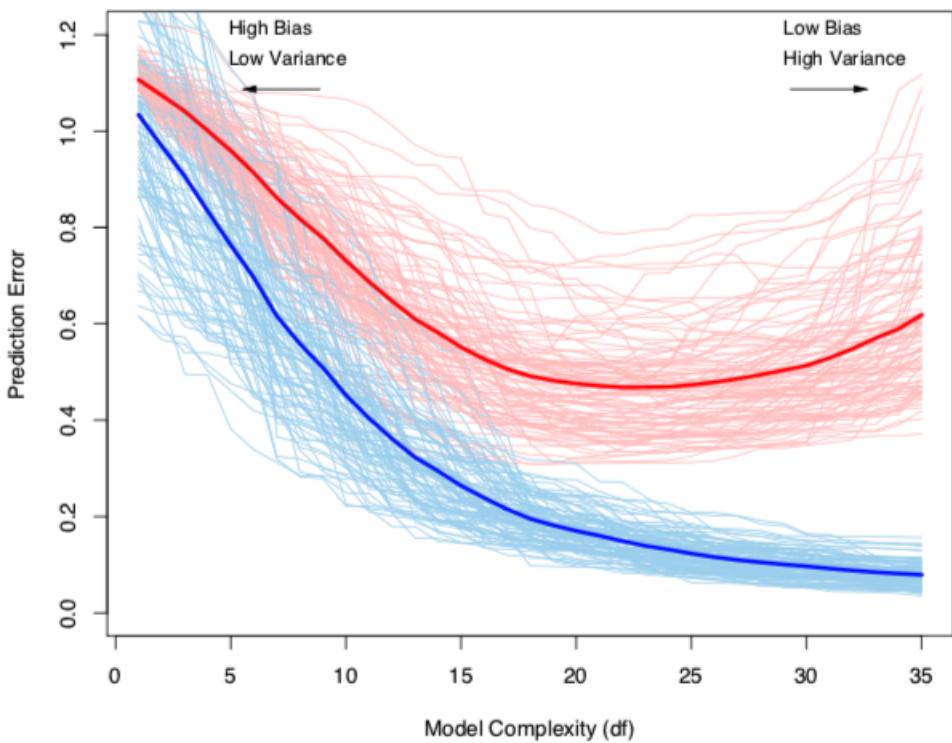


Figure 8.1: Behaviour of test sample and training sample error as the model complexity is varied. The light blue curves show the training error  $\bar{e}_{rr}$ , while the light red curves show the conditional test error  $Err_T$  for 100 training sets of size 50 each, as the model complexity is increased. The solid curves show the expected test error  $Err$  and the expected training error  $E[\bar{e}_{rr}]$ .

model complexity that gives minimum expected test error. The training error is not reliable because it always decreases with the model complexity and with too much complexity it loses the capability to generalize.

The same holds for categorical variables (introduced in 8.1). Typical loss functions are:

$$\begin{aligned} L(G, \hat{G}) &= I(G \neq \hat{G}(X)) \quad \text{0-1 loss,} \\ L(G, \hat{p}(X)) &= -2 \sum_{k=1}^K I(G = k) \log \hat{p}_k(X) \quad -2 \times \text{log-likelihood,} \end{aligned} \tag{8.5}$$

where the quantity  $-2 \times \text{log-likelihood}$  is generally referred as deviance. The "−2", as already said, in the definition makes the log-likelihood loss for the Gaussian distribution match squared-error loss. A number of methods for estimating the expected test error for a model exists. Typically our model will have a tuning parameter or parameters  $\alpha$  and so we can write our predictions  $\hat{a}(x)_\alpha$ . The tuning parameter varies the complexity of our model, and we wish to find the value of  $\alpha$  that minimizes error, that is, produces the minimum of the average test error curve. There are two goals that one might want to achieve:

**Definition 8.4. model selection:** estimating the performance of different models in order to choose the best one.

**Definition 8.5. model assessment:** having chosen a final model, estimate its prediction error on new data.

If we are in a data-rich situation, the best approach for both problems is to randomly divide the dataset into three parts: a training set, a validation set, and a test set. The training set is used to fit the models; the validation set is used to estimate prediction error for model selection; the test set is used for assessment of the generalization error of the final chosen model. Ideally, the test set should be kept in a "vault", and be brought out only at the end of the data analysis. It is difficult to give a general rule on how to choose the number of observations in each of the three parts, as this depends on the signal-to-noise ratio in the data and the training sample size. A typical split might be 50% for training, and 25% each for validation and testing.

The following methods allows to work in a situation with insufficient data. The methods can be distinguished in analytical (AIC, BIC, MDL, SRM) or by efficiently sample re-use (cross-validation and boot-strap). Typically the

more complex we make the model  $f$ , the lower the (squared) bias but the higher the variance.

## 8.1 Optimism of the training error rate

Given a training set  $\tau$  the generalization error of a model is:

$$\text{Err}_\tau = \mathbf{E}_{X^0, Y^0} [L(Y^0, \hat{f}(X^0)) | \tau] \quad (8.6)$$

where the point  $(X^0, Y^0)$  is a new test data point. Averaging over training sets  $\tau$  (i.e., averaging over the same type of models  $\hat{f}$  but trained with different trainsets belonging to the same distribution):

$$\text{Err} = \mathbf{E}_\tau \mathbf{E}_{X^0, Y^0} [L(Y^0, \hat{f}(X^0)) | \tau] \quad (8.7)$$

The training error  $\bar{\text{err}} = \frac{1}{N} \sum_{i=1}^N L(y_i, \hat{f}(x_i))$  will be less than the true error, because the same data is being used to fit the method and assess its error. A fitting method typically adapts to the training data, and hence the apparent or training error  $\bar{\text{err}}$  will be an overly optimistic estimate of the generalization error  $\text{Err}_\tau$ , which can be thought as *extra-sample error*.

The nature of the optimism in the training error can be explained considering the *in-sample error*:

$$\text{Err}_{in} = \frac{1}{N} \sum_{i=1}^N \mathbf{E}_{Y^0} [L(Y_i^0, \hat{f}(x_i)) | \tau] \quad (8.8)$$

To explain it better consider the same input points  $x_i$ ,  $i = 1, \dots, N$ . In the training set for these points we got a given set of values, while on new data we get a slightly different values  $Y^0$  due to the random process involved (for example the noise considering the additive model). The model  $\hat{f}$  have been trained using the training set, so for its prediction for those points will be close to the values seen in the training set (influenced by randomness) and it cannot foresee the non-deterministic part in the new samples. We define the optimism as the difference between the real  $\text{Err}_{in}$  and the training error:

$$op \equiv \text{Err}_{in} - \bar{\text{err}} \quad (8.9)$$

and this is typically positive since the second term is generally biased downward. Averaging the optimism:

$$\omega = \mathbf{E}_y(\text{op}) \quad (8.10)$$

where the notation  $\mathbf{E}_y$  has been used instead of  $\mathbf{E}_\tau$  because the predictors (the inputs) are fixed, while the outputs vary.

For squared error, 0-1 loss functions and other loss functions one can show:

$$\omega = \frac{2}{N} \sum_{i=1}^N \text{Cov}(\hat{y}_i, y_i) \quad (8.11)$$

Thus the amount by which err underestimates the true error depends on how strongly  $y_i$  affects its own prediction. The harder we fit the data, the greater the covariance will be, thereby increasing the optimism. We have the relationship:

$$\mathbf{E}_y(\text{Err}_{\text{in}}) = \mathbf{E}_y(\bar{\text{err}}) + \frac{2}{N} \sum_{i=1}^N \text{Cov}(\hat{y}_i, y_i) \quad (8.12)$$

This expression simplifies if  $\hat{y}_i$  is obtained by a linear fit with  $d$  inputs or basis functions. For example for the additive model  $Y = f(X) + \epsilon$ :

$$\sum_{i=1}^N \text{Cov}(\hat{y}_i, y_i) = d\sigma_\epsilon^2 \quad (8.13)$$

and so

$$\mathbf{E}_y(\text{Err}_{\text{in}}) = \mathbf{E}_y(\bar{\text{err}}) + \frac{2d}{N} \sigma_\epsilon^2 \quad (8.14)$$

We can use these expressions to select the effective number of parameters. The optimism increases with the number  $d$  of inputs or basis functions we use, but decreases as the training sample size increases

An obvious way to estimate prediction error is to estimate the optimism and then add it to the training error. The methods such as Cp, AIC, BIC and others work in this way, for a special class of estimates that are linear in their parameters. In contrast, cross-validation and bootstrap methods are direct estimates of the extra-sample error. These general tools can be used with any loss function, and with nonlinear, adaptive fitting techniques. In-sample error is not usually of direct interest since future values of the features

are not likely to coincide with their training set values. But for comparison between models, in-sample error is convenient and often leads to effective model selection. The reason is that the relative (rather than absolute) size of the error is what matters.

## 8.2 $C_p$ metric

One can estimate the in-sample error as

$$\hat{E}\text{rr} = e\bar{r}r + \hat{\omega} \quad (8.15)$$

where  $\hat{\omega}$  is an estimate of the average optimism. Using 8.14:

$$C_p = e\bar{r}r + \frac{2d}{N}\hat{\sigma}_\epsilon^2 \quad (8.16)$$

where  $\hat{\sigma}_\epsilon^2$  is an estimate of the noise variance.

The model with lowest  $C_p$  should be selected.

## 8.3 Akaike Information Criterion

Suppose we have models  $\mathcal{M}_1, \dots, \mathcal{M}_k$  where each model is a set of densities:

$$\mathcal{M}_j = \{p(y; \theta_j) : \theta_j \in \Theta_j\}. \quad (8.17)$$

and we have data  $Y_1, \dots, Y_n$  drawn from an unknown density  $f$  that we do not know if it is in any of the models. Let  $\hat{\theta}_j$  be the Maximum Likelihood estimation from the model  $j$ . Using this we can estimate  $f$  with  $\hat{p}_j(y) = p(y; \hat{\theta}_j)$ . The quality of  $\hat{p}_j(y)$  (i.e., its distance from  $f$ ) can be measured by the **Kullback-Leibler distance**:

$$\begin{aligned} K(p, \hat{p}_j) &= \int p(y) \log \frac{p(y)}{\hat{p}_j(y)} dy = \\ &= \int p(y) \log p(y) dy - \int p(y) \log \hat{p}_j(y) dy \end{aligned} \quad (8.18)$$

We want to minimize this distance. The first term is constant while we can act on  $\hat{p}_j(y)$ . Since it is a probability (i.e.  $\hat{p}_j(y)$  is at most one, minimizing the distance is equivalent to maximizing the second term:

$$K_j = \int p(y) \log \hat{p}_j(y) dy \quad (8.19)$$

Intuitively one estimate of  $K_j$  might be:

$$\bar{K}_j = \frac{1}{N} \sum_{i=1}^N \log p_j(Y_i, \hat{\theta}_j) = \frac{\ell_j(\hat{\theta}_j)}{N} \quad (8.20)$$

i.e., assuming a uniform distribution. This estimation is very biased because data are being used twice: once for the MLE and the second one to calculate the integral. So we have  $\bar{K}_j \neq K_j$ . We want to find such difference.

Let us drop the index  $j$  (i.e., we are considering just one model and not a set) and just use  $K$  and  $\bar{K}$ . Let  $\theta_0$  be the parameters that minimize  $K(f, p(\cdot, \theta))$ . So  $p(y, \theta_0)$  is the closest density in the model to the true density. Let  $\ell(y, \theta) = \log p(y, \theta)$  and let us define the **score** as:

$$s(y, \theta) = \frac{\partial \log p(y, \theta)}{\partial \theta} \quad (8.21)$$

and let  $H(y, \theta)$  be the matrix of second derivatives. Let

$$Z_N = \sqrt{N} (\hat{\theta} - \theta_0) \quad (8.22)$$

and recall (?) that :

$$Z_N \rightarrow \mathcal{N}(0, J^{-1} V J^{-1}) \quad (8.23)$$

where

$$\begin{aligned} J &= -\mathbf{E}[H(Y, \theta_0)] \\ V &= \text{Var}(s(Y, \theta_0)) \end{aligned} \quad (8.24)$$

Let

$$S_N = \frac{1}{N} \sum_{i=1}^N s(Y_i, \theta_0) \quad (8.25)$$

By the **Central Limit Theorem**, and recalling that  $\theta_0$  is the value that minimizes  $K$  (if it is a convex function then for this value the score is 0 i.e., 0 mean):

$$\sqrt{N} S_N \rightarrow \mathcal{N}(0, V) \quad (8.26)$$

since

$$\begin{aligned}
\text{Var} [\sqrt{N}S_n] &= E \left[ (\sqrt{N}S_n - \mu_{S_n})^2 \right] = \\
&= N E \left[ \left( \frac{1}{N} \sum_{i=1}^N s(Y_i, \theta_0) \right)^2 \right] = \frac{1}{N} E \left[ \left( \sum_{i=1}^N s(Y_i, \theta_0) \right)^2 \right] = \\
&= \frac{1}{N} \left( \sum_{i=1}^N E[s(Y_i, \theta_0)]^2 \right) = \frac{1}{N} NV = V
\end{aligned} \tag{8.27}$$

Now  $J$  is a scalar, considering the distribution  $JZ_N$  where  $Z_N \sim \mathcal{N}(0, J^{-1}VJ^{-1})$ , the result is still a distribution with 0. For the variance let us use the property:

$$\begin{aligned}
\text{Var}[JZ_N] &= J(J^{-1}VJ^{-1})J^T = V \\
\Rightarrow JZ_N &\sim \mathcal{N}(0, V)
\end{aligned} \tag{8.28}$$

By using **Taylor series expansion**:

$$K \approx \int p(y) \left( \log p(y, \theta_0) + \cancel{\left( \hat{\theta} - \theta_0 \right)^T s(y, \theta_0)} + \frac{1}{2} \left( \hat{\theta} - \theta_0 \right)^T H(y, \theta_0) \left( \hat{\theta} - \theta_0 \right) \right) dy \tag{8.29}$$

The second term  $\cancel{\left( \hat{\theta} - \theta_0 \right)^T s(y, \theta_0)}$  is 0 because the score has 0 mean. Defining

$$K_0 = \int p(y) \log p(y, \theta_0) dy \tag{8.30}$$

we have:

$$\begin{aligned}
K &\approx K_0 + \frac{1}{\sqrt{N}} Z_N^T \int H(y, \theta_0) p(y) dy \frac{1}{\sqrt{N}} Z_N = \\
&= K_0 + \frac{1}{\sqrt{N}} Z_N^T \int H(y, \theta_0) p(y) dy \frac{1}{\sqrt{N}} Z_N = k_0 - \frac{1}{2N} Z_N^T J Z_N
\end{aligned} \tag{8.31}$$

Now applying the **Taylor series expansion** to  $\hat{K}$ :

$$\bar{K} \approx \frac{1}{N} \sum_{i=1}^N \left( \ell(Y_i, \theta_0) + \left( \hat{\theta} - \theta_0 \right)^T s(Y_i, \theta_0) \right) + \frac{1}{2} \left( \hat{\theta} - \theta_0 \right)^T H(Y_i, \theta_0) \left( \hat{\theta} - \theta_0 \right) \tag{8.32}$$

Defining

$$\begin{aligned} A_N &= \frac{1}{N} \sum_{i=1}^N \ell(Y_i, \theta_0) - K_0 = \frac{1}{N} \sum_{i=1}^N (\ell(Y_i, \theta_0) - K_0) \\ J_N &= -\frac{1}{N} \sum_{i=1}^N H(Y_i, \theta_0) - \xrightarrow{P} J \end{aligned} \quad (8.33)$$

we have

$$\begin{aligned} \bar{K} &\approx K_0 + A_N + (\hat{\theta} - \theta_0) S_N - \frac{1}{2N} Z_N^T J_N Z_N \approx \\ &\approx K_0 + A_N + \frac{Z_N^T}{N} \sqrt{N} J^{-1} J S_N - \frac{1}{2N} Z_N^T J Z_N = \\ &= K_0 + A_N + \frac{Z_N^T J Z_N}{N} - \frac{1}{2N} Z_N^T J Z_N \end{aligned} \quad (8.34)$$

where 8.28 has been used again ( $J^{-1} S_N \rightarrow J^{-1} \mathcal{N}(0, V) = \mathcal{N}(0, J^{-1} V J^{-1}) = Z_N$ ). We need another property. Let  $\epsilon$  be a random vector with mean  $\mu$  and variance  $\Sigma$  and let

$$Q = \epsilon^T A \epsilon \quad (8.35)$$

with  $Q$  called a quadratic form. Then

$$E[Q] = \text{trace}(A\Sigma) + \mu^T A \mu \quad (8.36)$$

Now taking the difference:

$$\begin{aligned} E[\hat{K} - K] &= E[A_N] + E\left[\frac{Z_N^T J Z_N}{N}\right] = 0 + \frac{\text{trace}(J J^{-1} V J^{-1})}{N} = \\ &= \frac{\text{trace}(J^{-1} V J^{-1} J)}{N} = \frac{\text{trace}(J^{-1} V)}{N} \end{aligned} \quad (8.37)$$

If the model is correct then  $J^{-1} = V$  so that  $\text{trace}(J^{-1} V) = \text{trace}(I) = d$ :

$$K \approx \hat{K} = \bar{K} - \frac{d}{N} \quad (8.38)$$

So the bias is approximately  $\frac{d}{N}$ . Considering the model  $j$ :

$$\begin{aligned} \hat{K}_j &= \bar{K}_j - \frac{d_j}{N} \\ \text{AIC}(j) &= 2N\hat{K}_j = \ell_j(\hat{\theta}_j) - 2d_j \end{aligned} \quad (8.39)$$

Maximizing  $\hat{K}_j$  is the same as maximising AIC(j). Constants are not important in the maximization process. With this representation we choose the model with the highest AIC. Other books use the following representation:

$$AIC(j) = -\frac{2}{N} \ell_j(\hat{\theta}_j) + 2 \frac{d_j}{N} \quad (8.40)$$

and with this representation the best model is the one that minimizes the AIC, since the signs have been inverted.

For the Gaussian model, with variance  $\sigma_\epsilon^2 = \hat{\sigma}_\epsilon^2$ , the AIC statistic is equivalent to  $C_p$ .

For non-linear and other complex models we replace d with a measure of the model complexity. Given a set of models  $f_\alpha$ ,  $\bar{err}(\alpha)$  is the training error and  $d(\alpha)$  the number of parameters:

$$AIC(\alpha) = \bar{err}(\alpha) + 2 \frac{d\alpha}{N} \hat{\sigma}_\epsilon^2 \quad (8.41)$$

## 8.4 Effective number of parameters

A linear fitting method (linear regression, derived basis sets and smoothing methods with quadratic shrinkage such as ridge regression and cubic smoothing splines) have the form:

$$\hat{\mathbf{y}} = \mathbf{S}\mathbf{y} \quad (8.42)$$

where  $\mathbf{S}$  is a  $N \times N$  matrix. The effective number of parameters is defined as:

$$df(\mathbf{S}) = \text{trace}(\mathbf{S}) = M \quad (8.43)$$

since  $\mathbf{S}$  is an orthogonal projection matrix onto a basis set spanned by M features. Then instead of d we use  $\text{trace}(\mathbf{S})$ .

For models like NN in which we minimize an error function with weight decay penalty (regularization)  $\alpha \sum_m w_m^2$ , the effective number of parameters has the form:

$$df(\alpha) = \sum_{m=1}^M \frac{\theta_m}{\theta_m + \alpha} \quad (8.44)$$

where  $\theta_m$  are the eigenvalues of the Hessian matrix  $\partial R(\omega)/\partial \omega \partial \omega^T$ .

## 8.5 Bayesian Information Criterion

Known also as *Schwarz Criterion*, it is equivalent to the MDL. We choose  $j$  to maximize

$$BIC(j) = \ell_j(\hat{\theta}_j) - \frac{d_j}{2} \log n \quad (8.45)$$

It is similar to the AIC but it has a stronger penalization and tends to choose simpler models.

Using priors  $\pi_j(\theta_j)$  on the parameters  $\theta_j$  and a probability  $p_j$  indicating the probability that  $\mathcal{M}_j$  is the true model, by Bayesian theory, indicating with  $\mathbf{Z}$  the training set, we have:

$$P(\mathcal{M}_j | \mathbf{Z}) \propto p(\mathbf{Z} | \mathcal{M}_j) p_j \quad (8.46)$$

Furthermore

$$\begin{aligned} p(\mathbf{Z} | \mathcal{M}_j) &= \int p(\mathbf{Z} | \mathcal{M}_j, \theta_j) \pi_j(\theta_j) d\theta_j = \\ &= \int L(\theta_j) \pi_j(\theta_j) d\theta_j \end{aligned} \quad (8.47)$$

So equivalently we choose  $j$  to maximize:

$$\log \int L(\theta_j) \pi_j(\theta_j) d\theta_j + \log p_j \quad (8.48)$$

Using Taylor expansion:

$$\begin{aligned} \log \int L(\theta_j) \pi_j(\theta_j) d\theta_j + \log p_j &\approx \ell_j(\hat{\theta}_j) - \frac{d_j}{2} \log n \\ \Rightarrow BIC(j) &= \ell_j(\hat{\theta}_j) - \frac{d_j}{2} \log n \end{aligned} \quad (8.49)$$

The prior has been ignored because it can be shown that the terms involving the prior are lower orders than the ones appearing in 8.49. Again in some books the signs are inverted.

**The difference from AIC and Cross-Validation** is that BIC assumes that one of the models is true and that we are trying to find the model most likely to be true in a Bayesian sense. AIC and Cross-Validation tries to find the model that predicts the best.

Under the Gaussian model, assuming the variance  $\sigma_\epsilon^2$  is known, with a squared error loss:

$$\begin{aligned} \bar{e\text{rr}} &= \sum_i \left( y_i - \hat{f}(x_i) \right)^2 \\ 2\ell_j(\hat{\theta}_j) &= -N \frac{\bar{e\text{rr}}}{\sigma_\epsilon^2} \\ \text{BIC}(j) &= -\frac{N}{2\sigma_\epsilon^2} \bar{e\text{rr}} - \frac{d_j}{2} \log n = \frac{N}{2\sigma_\epsilon^2} \left[ \frac{d_j}{N} \sigma_\epsilon^2 \log N - \bar{e\text{rr}} \right] \end{aligned} \quad (8.50)$$

Hence BIC is proportional to AIC with the factor 2 replaced by  $\log N$ .

## 8.6 Minimum Description Length

The minimum description length (MDL) principle is a formalization of Occam's razor in which the best hypothesis (a model and its parameters) for a given set of data is the one that leads to the best compression of the data. The Minimum Description Length is the minimum number of bits, or the minimum of the sum of the number of bits required to represent the data and the model. . . .

## 8.7 Cross-Validation

It is the simplest and most widely used widely used method for estimating prediction error is cross-validation. This method directly estimates the expected extra-sample error. It consists of dividing data set in parts: a training set and using an independent test sample from the joint distribution. So one set is used for training and the other to avoid overfitting (to validate the model).

### 8.7.1 K-fold cross-validation

K-fold cross-validation uses part of the available data to fit the model, and a different part to test it. For the  $k$ -th part, we fit the model using the other  $K - 1$  parts for training and we calculate the prediction error of the fitted model on the  $k$ -th part. We do this for all  $k = 1, \dots, K$ , fitting the model resulting from the previous step using the new partition of data. Typical choices of  $K$  are 5 or 10.  $K = N$  case is known as live-one-out

cross-validation. The higher value of  $K$  leads to less biased model (but large variance might lead to overfit), whereas the lower value of  $K$  is similar to the train-test split approach we saw before.

## 8.8 Bootstrap Methods

The general idea is to randomly draw datasets with replacement from training data. Samples are constructed by drawing observations from a large data sample one at a time and returning them to the data sample after they have been chosen. This allows a given observation to be included in a given small sample more than once. This approach to sampling is called sampling with replacement. This is done  $B$  times, producing  $B$  datasets.

For the process we need to decide the number of bootstrap samples and a sample size. Then for each bootstrap sample, we refit the model to each of the bootstrap datasets and examine the behaviour of the fits over the  $B$  replications.

[From wiki:] As an example, assume we are interested in the average (or mean) height of people worldwide. We cannot measure all the people in the global population, so instead we sample only a tiny part of it, and measure that. Assume the sample is of size  $N$ ; that is, we measure the heights of  $N$  individuals. From that single sample, only one estimate of the mean can be obtained. In order to reason about the population, we need some sense of the variability of the mean that we have computed. The simplest bootstrap method involves taking the original data set of  $N$  heights, and, using a computer, sampling from it to form a new sample (called a 'resample' or bootstrap sample) that is also of size  $N$ . The bootstrap sample is taken from the original by using sampling with replacement (e.g. we might 'resample' 5 times from [1,2,3,4,5] and get [2,5,4,4,1]), so, assuming  $N$  is sufficiently large, for all practical purposes there is virtually zero probability that it will be identical to the original "real" sample. This process is repeated a large number of times (typically 1,000 or 10,000 times), and for each of these bootstrap samples we compute its mean (each of these are called bootstrap estimates). We now can create a histogram of bootstrap means. This histogram provides an estimate of the shape of the distribution of the sample mean from which we can answer questions about how much the mean varies across samples.

## 9 Additive models

A linear model has the form  $\alpha + f_1(X_1) + f_2(X_2) + f_3(X_3) + \dots$ , where  $X$  are the predictors.

### 9.1 Tree based methods

Tree-based methods partition the feature space into a set of rectangles, and then fit a simple model (like a constant) in each one.

We restrict attention to recursive binary partitions. We first split the space into two regions, and model the response by the mean of  $Y$  in each region. We choose the variable and split-point to achieve the best fit. Then one or both of these regions are split into two more regions, and this process is continued, until some stopping rule is applied.

For example we first split at  $X_1 = t_1$ . Then the region  $X_1 \leq t_1$  is split at  $X_2 = t_2$  and the region  $X_1 > t_1$  is split at  $X_1 = t_3$  and so on. To each sub-region we assign a constant as output:

$$\hat{f}(X) = \sum_{m=1}^M c_m I\{\mathbf{x} \in \mathcal{R}_m\} \quad (9.1)$$

An advantage of this representation is its interpretability. When more than 2 inputs are involved, it is difficult to represent the partition of the input space.

#### 9.1.1 Regression Trees

The algorithm needs to decide automatically the splitting variables and points. We can start defining the values of the constant of each region:

$$\hat{c}_m = \text{ave}(y_i | x_i \in C \cap R_m) \quad (9.2)$$

Now finding the best binary partition in terms of minimum sum of squares is generally computationally infeasible. Hence we proceed with a greedy algorithm. Consider a splitting variable  $j$  and split point  $s$  and define the pair of half-planes:

$$R_1(j, s) = \{X | X_j \leq s\}, \quad R_2(j, s) = \{X | X_j > s\} \quad (9.3)$$

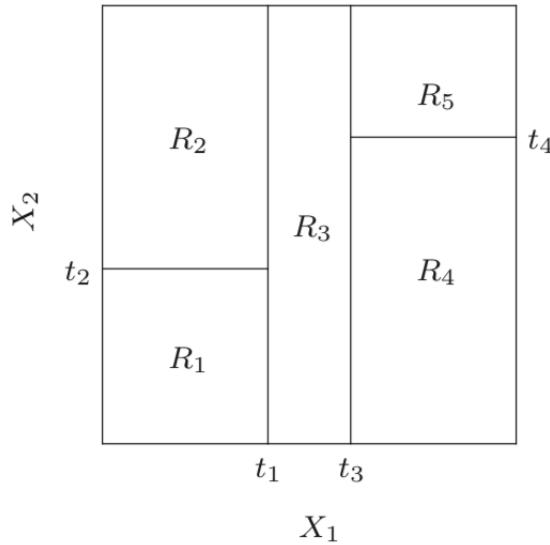


Figure 9.1: 2D-input space binary tree partition.

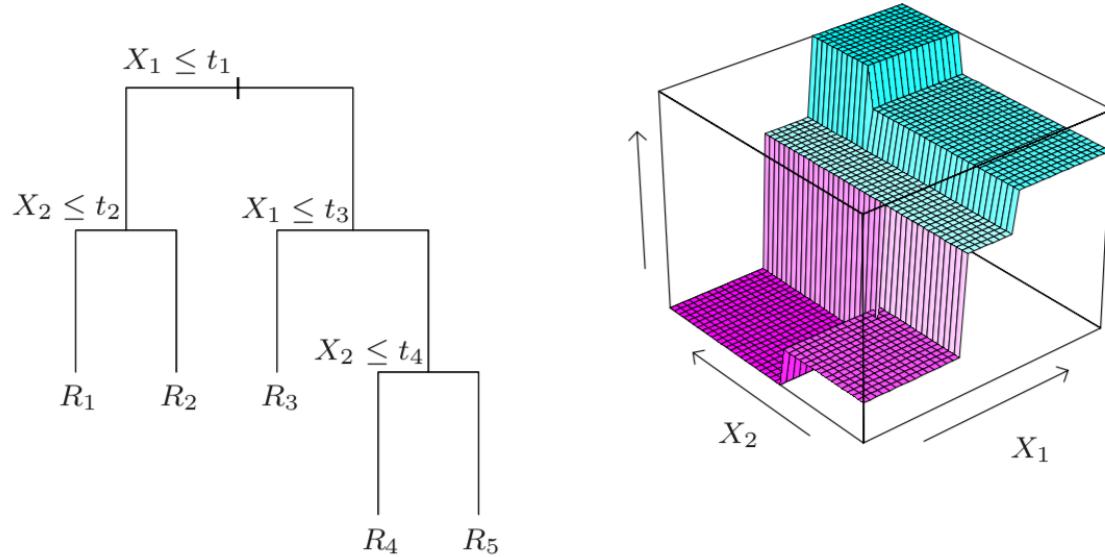


Figure 9.2: Another representation of the binary tree on the left. On the right the 3D resulting shape of the function.

Then we seek the splitting variable  $j$  and split point  $s$  that solve:

$$\begin{aligned} \min_{j,s} & \left[ \min_{c_1} \sum_{x_i \in \mathcal{R}_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in \mathcal{R}_2(j,s)} (y_i - c_2)^2 \right] \\ & \hat{c}_1 = \text{ave}(y_i | x_i \in \mathcal{R}_1(j,s)) \\ & \hat{c}_2 = \text{ave}(y_i | x_i \in \mathcal{R}_2(j,s)) \end{aligned} \quad (9.4)$$

For each splitting variable, the determination of the split point  $s$  can be done very quickly and hence by scanning through all of the inputs, determination of the best pair  $(j, s)$  is feasible. Having found the best split, we partition the data into the two resulting regions and repeat the splitting process on each of the two regions. Then this process is repeated on all of the resulting regions.

Tree size is a tuning parameter governing the model's complexity, and the optimal tree size should be adaptively chosen from the data. One approach would be to split tree nodes only if the decrease in sum-of-squares due to the split exceeds some threshold. This strategy is too short-sighted, however, since a seemingly worthless split might lead to a very good split below it. The preferred strategy is to grow a large tree  $T_0$ , stopping the splitting process only when some minimum node size (say 5) is reached. Then this large tree is pruned using **cost-complexity pruning**.

The **cost-complexity pruning** is the following. We define a subtree  $T$  of  $T_0$  obtained by collapsing any number of its internal nodes. We index the terminal nodes by  $m$ . let  $|T|$  denote the number of terminal nodes in  $T$  and

$$\begin{aligned} N_m &= \#\{x_i \in \mathcal{R}_m\} \\ \hat{c}_m &= \frac{1}{N_m} \sum_{x_i \in \mathcal{R}_m} y_i \end{aligned} \quad (9.5)$$

$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2$$

We define the cost complexity criterion:

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha |T| \quad (9.6)$$

The idea is to find for each  $\alpha$  the subtree  $T_\alpha$  of  $T_0$  to minimize such a function. For each  $\alpha$  there is a unique smallest subtree  $T_\alpha$  that minimizes  $C_\alpha(T)$ . To find  $T_\alpha$  we use the **weakest link pruning**: we collapse the internal node that produces the smallest per-node increase and we continue until we produce the single-node (root) tree. So we have a sequence of subtrees that must contain  $T_\alpha$ . We choose  $\alpha$  to minimize the cross-validated sum of squares, obtaining the tree  $T_\alpha$ .

## 9.2 Classification trees

The procedure is very similar. In a node  $m$  representing the region  $R_m$  with  $N_m$  observations, let

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{\mathbf{x}_i \in R_m} I(y_i = k) \quad (9.7)$$

We classify the observations in node  $m$  to class

$$k(m) = \operatorname{argmax}_k \hat{p}_{mk}, \quad (9.8)$$

the majority class in node  $m$ . Different measures  $Q_m(T)$  of node impurity exist

$$\begin{aligned} \text{Misclassification error} & \quad \frac{1}{N_m} \sum_{i \in CM \cap R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{km} \\ \text{Gini index} & \quad \sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^K \hat{p}_{mk} (1 - \hat{p}_{mk}) \\ \text{Cross-entropy or deviance} & \quad - \sum_{k=1}^K \hat{p}_{mk} \log \hat{p}_{mk} \end{aligned} \quad (9.9)$$

These trees are referred as CART (classification and regression trees).

### 9.2.1 Linear Combination splits

Rather than using splits of the type  $X_j \leq s$  we can use splits of the type  $\sum a_j X_j \leq s$ . The weights  $a_j$  and split point  $s$  are optimized to minimize the relevant criterion such as the Gini index.

### 9.2.2 Limitations of trees

One major problem of trees is **the instability (i.e., high variance)**. A small change in the data can result in a very different series of splits, making interpretation somewhat precarious. The major reason is the hierarchical nature of the process: the effect of an error in the top split is propagated down to all the next splits. The problem can be attenuated but not completely solved.

Another problem of trees is the **lack of smoothness**. This is not a problem in classification but it is in regression.

Also they are not good at capturing additive structures, such as  $Y = c_1(X_1 < t_1) + c_2(X_2 < t_2) + \epsilon$  where the noise is 0 mean. Then a binary tree might make its first split on  $X_1$  near  $t_1$ . At the next level down it would have to split both nodes  $X_2$  at  $t_2$  in order to capture the additive structure. This is achieved with sufficient data, but it is a fragile mechanism and can fail in case of many additive effects.

## 9.3 Patient rule induction method (PRIM)

Also PRIM finds boxes in the feature space, but it seeks boxes in which the response average is high. Hence it looks for maxima in the target function, an exercise known as bump hunting. The main box construction method in PRIM works starting with a box containing all of the data. The box is compressed along one face by a small amount, and peeling off a constant portion of data denoted by  $\alpha$ . Typically  $\alpha$  is 0.05 and 0.1 of the remaining points at each stage. The face chosen for compression is the one resulting in the largest box mean, after the compression is performed. Then the process is repeated, stopping when the current box contains some minimum number of data points.

After the top-down sequence is computed, PRIM reverses the process, expanding along any edge, if such an expansion increases the box mean. This is called pasting. The result of these steps is a sequence of boxes, with different numbers of observation in each box. Cross-validation, combined with the judgement of the data analyst, is used to choose the optimal box size. Denote by  $B_1$  the points in this first box. These points are now removed from the training set and we repeat the two processes (top-down peeling and bottom-up pasting) several times, obtaining for each iteration a new box  $B_i$ .

Each box is defined by a set of rules involving a subset of predictors such as:

$$(a_1 \leq X_1 \leq b_1) \quad (b_1 \leq X_3 \leq b_2) \quad (9.10)$$

PRIM can handle a categorical predictor by considering all partitions of the predictor, as in CART. Missing values are also handled in a manner similar to CART. PRIM is designed for regression

- 
- 
- Start with all of the training data, and a maximal box containing all of the data;
  - Consider shrinking the box by compressing one face, so as to peel off the proportion  $\alpha$  of observations having either the highest values of a predictor  $X_j$  or the lowest. Choose the peeling that produces the highest response mean in the remaining box;
  - Repeat step 2 until some minimal number of observations (say 10) remain in the box;
  - Expand the box along any face, as long as the resulting box mean increases;
  - Steps 1-4 give a sequence of boxes, with different numbers of observations in each box. Use cross-validation to choose a member of the sequence. Call the box  $B_1$ .
  - Remove the data in the box  $B_1$  from the dataset and repeat steps 2-5 to obtain a second box. and continue to get as many boxes as desired.
- 

PRIM is designed for binary regression. There is no simple way to deal with  $k > 2$  classes simultaneously: it is possible to run PRIM separately for each class versus a baseline class. In any case, the ability of PRIM to be more patient should help the top-down greedy algorithm find a better solution.

## 9.4 Multivariate Adaptive Regression Splines (MARS)

It is a procedure well-suited for high-dimensional problems. MARS uses expansions in piecewise linear basis functions of the form  $(x-t)_+$  and  $(t-x)_+$ .

Each function is piecewise linear, with a knot at the value  $t_1$ . We call the two functions a **reflected pair**. The idea is to form reflected pairs for each input  $X_j$  with knots at each observed value  $x_{ij}$  of that input. If all of the input values are distinct, there are  $2N_p$  basis functions altogether.

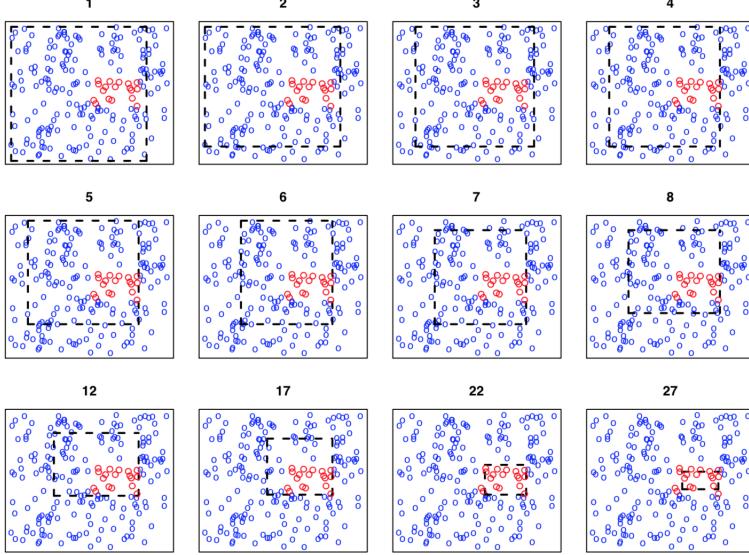


Figure 9.3: Steps in PRIM.

The model-building strategy is like a forward stepwise linear regression, but instead of using the original inputs, we are allowed to use functions from the set  $\mathcal{C}$  and their products:

$$\mathcal{C} = \{(X_j - t)_+, (t - X_j)_+\}_{t \in \{x_{1j}, \dots, x_{Nj}\}, j=1, \dots, p} \quad (9.11)$$

Thus the model has the form:

$$f(X) = \beta_0 + \sum_{m=1}^M \beta_m h_m(X) \quad (9.12)$$

where each  $h_m(X)$  is a function in  $\mathcal{C}$  or a product of two or more such functions. Given the choice for  $h_m(X)$ , the coefficients are estimated with the residual sum of squares. We start with only a constant  $h_0(X) = 1$  and all the functions are candidate functions. At each step we consider as a new basis function pair all products of a function  $h_m$  in the model set  $\mathcal{M}$  with one of the reflected pairs in  $\mathcal{C}$ . We add to the model  $\mathcal{M}$  the term of the form:

$$\hat{\beta}_{M+1} h_\ell(X)(X_j - t)_+ + \hat{\beta}_{M+2} h_\ell(X)(t - X_j)_+, h_\ell \in \mathcal{M} \quad (9.13)$$

that produces the largest decrease in training error. For example, at the first stage we consider adding to the model a function of the form:  $\hat{\beta}_1(X_2 - x_{72})_+$

$\hat{\beta}_2(x_{72} - X_2)_+$ . Then this pair of basis functions is added to the set  $\mathcal{M}$  and at the next stage we consider including a pair of products in the form:

$$h_m(X)(X_j - t)_+ \quad \text{and} \quad h_m(X)(t - X_j)_+, t \in \{x_{ij}\} \quad (9.14)$$

where for  $h_m$  we have the choices:

$$\begin{aligned} h_0(X) &= 1 \\ h_1(X) &= (X_2 - x_{72})_+, \quad \text{or} \\ h_2(X) &= (x_{72} - X_2)_+ \end{aligned} \quad (9.15)$$

At the end of this process we have a large model. This model typically overfits the data, and so a backward deletion procedure is applied. The term whose removal causes the smallest increase in residual squared error is deleted from the model at each stage, producing an estimated best model  $\hat{f}_\lambda$  of each size (number of terms)  $\lambda$ . One could use cross-validation to estimate the optimal value of  $\lambda$ , but for computational savings the MARS procedure instead uses generalized cross-validation:

$$GCV(\lambda) = \frac{\sum_{i=1}^N (y_i - \hat{f}_\lambda(x_i))^2}{(1 - \frac{M(\lambda)}{N})^2} \quad (9.16)$$

The value  $M(\lambda)$  is the effective number of parameters in the model: this accounts both for the number of terms in the models, plus the number of parameters used in selecting the optimal positions of the knots.

Some mathematical and simulation results suggest that one should pay a price of three parameters for selecting a knot in a piecewise linear regression. Thus if there are  $r$  linearly independent basis functions in the model, and  $K$  knots were selected in the forward process, the formula is  $M(\lambda) = r + cK$ , where  $c = 3$ .

The MARS method and algorithm can be extended to handle classification problems. Several strategies have been suggested. For two classes, one can code the output as 0/1 and treat the problem as a regression; we did this for the spam example. For more than two classes, one can use the indicator response approach. One codes the  $K$  response classes via 0/1 indicator variables, and then performs a multi-response MARS regression. There are, however, potential masking problems with this approach.

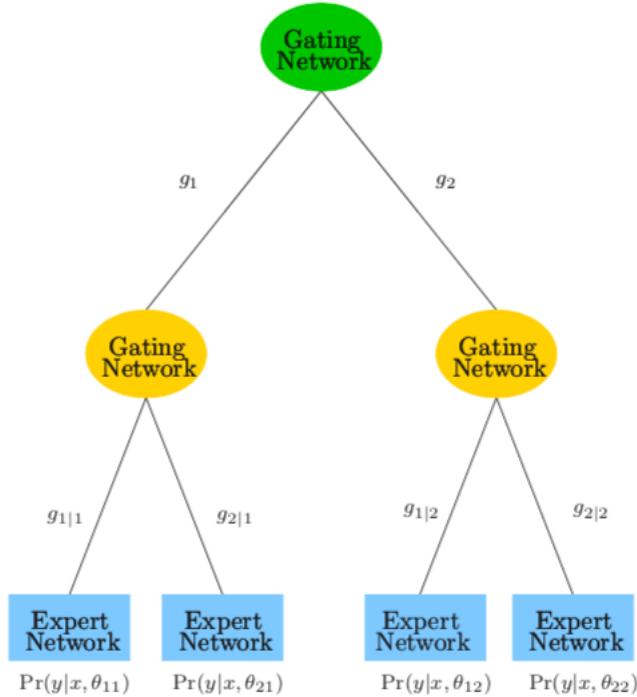


Figure 9.4: A two-level HME model.

## 9.5 Hierarchical Mixture of Experts

This can be viewed as a variant of tree-based methods. The main difference is that the tree splits are not hard decisions but rather soft probabilistic ones. At each node an observation goes left or right with probabilities depending on its input values. In an HME, a linear (or logistic regression) model is fit in each terminal node, instead of a constant as in CART (the split can be multiway, not only binary).

The terminal nodes are called **experts**, and the non-terminal nodes are called **gating networks**. The idea is that each expert provides an opinion (prediction) about the response, and these are combined together by the gating networks. The model is formally a mixture model, and the two-level model in the figure can be extended to multiple levels, hence the name hierarchical mixtures of experts.

### 9.5.1 How HME works

Consider the data  $(x_i, y_i)$ ,  $i = 1, \dots, N$  either for regression or classification problem. The **top-gating** network has the output:

$$g_j(\mathbf{x}, \gamma_j) = \frac{e^{\gamma_j^T \mathbf{x}}}{\sum_{k=1}^K e^{\gamma_k^T \mathbf{x}}}, \quad j = 1, \dots, K \quad (9.17)$$

where  $\gamma_j$  is a vector of unknown parameters. Each  $g_j$  is the probability of assigning an observation with feature vector  $\mathbf{x}$  to the  $j$ -th branch (soft K-way split). At second level the **gating networks** have similar form:

$$g_{\ell|j}(\mathbf{x}, \gamma_{j|\ell}) = \frac{e^{\gamma_{j|\ell}^T \mathbf{x}}}{\sum_{k=1}^K e^{\gamma_{j|k}^T \mathbf{x}}}, \quad \ell = 1, \dots, L \quad (9.18)$$

This is the probability of assignment to the  $\ell$ -th branch, given assignment to the  $j$ -th branch at the level above. At each expert (terminal node), we have a model for the response variable of the form:

$$Y \sim \Pr(y|\mathbf{x}, \theta_{j\ell}) \quad (9.19)$$

which is different according to the type of problem. For **regression** the Gaussian linear model is used with  $\theta_{j\ell} = (\beta_{j\ell}, \sigma_{jl}^2)$ :

$$Y = \beta_{j\ell}^T \mathbf{x} + \text{epsilon}, \quad \mathcal{N} \sim (0, \sigma_{jl}^2). \quad (9.20)$$

For **classification** the linear logistic regression is used:

$$\Pr(Y = 1|\mathbf{x}, \theta_{j\ell}) = \frac{1}{1 + e^{-\theta_{j\ell}^T \mathbf{x}}} \quad (9.21)$$

Denoting with  $\Phi = \{\gamma_j, \gamma_{j\ell}, \theta_{j\ell}\}$  the collections of all parameters, the total probability that  $Y = y$  is:

$$\Pr(y|\mathbf{x}, \Phi) = \sum_{k=1}^K g_j(\mathbf{x}, \gamma_j) \sum_{\ell=1}^L g_{\ell|j}(\mathbf{x}, \gamma_{j|\ell}) \Pr(y|\mathbf{x}, \theta_{j\ell}) \quad (9.22)$$

To estimate the parameters we maximize the log-likelihood of the data over  $\Phi$ . The most convenient method is the EM algorithm.

## 9.6 Missing data

The usual approach is to fill-in missing values. Roughly speaking, data are missing at random if the mechanism resulting in its omission is independent of its (unobserved) value. A more precise definition is given in Little and Rubin (2002). Suppose  $y$  is the response vector and  $X$  is the  $N \times p$  matrix of inputs (some of which are missing). Denote by  $X_{\text{obs}}$  the observed entries in  $X$  and let  $\mathbf{Z} = (y, X)$ ,  $\mathbf{Z}_{\text{obs}} = (y, X_{\text{obs}})$ . Finally, if  $\mathbf{R}$  is an indicator matrix with  $ij$ -th entry 1 if  $x_{ij}$  is missing and zero otherwise, then the data is said to be missing at random (MAR) if the distribution of  $\mathbf{R}$  depends on the data  $\mathbf{Z}$  only through  $Z_{\text{obs}}$ :

$$\Pr(\mathbf{R}|\mathbf{Z}, \theta) = \Pr(\mathbf{R}|\mathbf{Z}_{\text{obs}}, \theta) \quad (9.23)$$

Data are said to be **missing completely at random (MCAR)** if the distribution  $\mathbf{R}$  does not depend on the observed or missing data:

$$\Pr(\mathbf{R}|\mathbf{Z}, \theta) = \Pr(\mathbf{R}|\theta) \quad (9.24)$$

For example, if a patient's measurement was not taken because the doctor felt he was too sick, that observation would not be MAR or MCAR.

Assuming the features are missing completely at random, there are a number of ways of proceeding:

1. Discard observations with any missing values.
2. Rely on the learning algorithm to deal with missing values in its training phase.
3. Impute all missing values before training.

Approach 1 can be used if the relative amount of missing data is small, but otherwise should be avoided. Regarding 2, CART is one learning algorithm that deals effectively with missing values, through surrogate splits. MARS and PRIM use similar approaches. In generalized additive modeling, all observations missing for a given input feature are omitted when the partial residuals are smoothed against that feature in the backfitting algorithm, and their fitted values are set to zero. Since the fitted curves have mean zero (when the model includes an intercept), this amounts to assigning the average fitted value to the missing observations. For most learning methods,

the imputation approach 3 is necessary. The simplest tactic is to impute the missing value with the mean or median of the non-missing values for that feature.

If the features have at least some moderate degree of dependence, one can do better by estimating a predictive model for each feature given the other features and then imputing each missing value by its prediction from the model, distinctly from the method used to predict  $y$  from  $\mathbf{x}$ .

## 10 Boosting and Additive Trees

### 10.1 Boosting methods

It was originally designed for classification problems but it can profitably be extended to regression as well. The motivation for boosting was a procedure that combines the outputs of many "weak" classifiers to produce a powerful "committee".

A weak classifier is one whose error rate is only slightly better than random guessing. The purpose of boosting is to sequentially apply the weak classification algorithm to repeatedly modified versions of the data, thereby producing a sequence of weak classifiers  $G(x)$ ,  $m = 1, \dots, M$ . Consider a two-class problem with the output variable coded as  $Y \in \{-1, 1\}$ . Given a vector of predictors  $\mathbf{X}$ , a classifier  $G(X)$  produces a prediction taking one of the two values  $\{-1, 1\}$ . The predictions from all of them are then combined to through a weighted majority of vote to produce the final prediction:

$$G(x) = \text{sign} \left( \sum_{i=1}^M \alpha_i G_i(x) \right) \quad (10.1)$$

This is the **AdaBoost** procedure. Here  $\alpha_1, \dots, \alpha_M$  are computed by the boosting algorithm and weight the single contribution. The data modifications at each boosting step consist of applying weights  $w_1, \dots, w_N$  to each of the training observations. Initially all the weights are  $1/N$ . For successive iterations, the observation weights are individually modified and the classification algorithm is reapplied to the weighted observations. At step  $m$  the observations that were misclassified by the classifier  $G_{m-1}(x)$  have their weights increased, whereas the weights are decreased for those that were

classified correctly. Thus as iterations proceed, observations that are difficult to classify correctly receive ever-increasing influence. Each successive classifier is thereby forced to concentrate on those training observations that are missed by previous ones in the sequence.

The **AdaBoost.M1** algorithm, aka **Discrete Adaboost**, is shown in 1. If the base classifier instead returns a real-valued prediction (e.g., a probability mapped to the interval  $[-1, 1]$ ), AdaBoost can be modified appropriately and becomes **Real Adaboost**. The power of AdaBoost to dramatically

---

**Algorithm 1:** AdaBoost.M1 algorithm.

---

```
wi = 1/N, i = 1, … , N
for (m = 1 : M) do
    Fit a classifier Gm(x) to training data using wi;
    Compute the training error
    errm =  $\frac{\sum_{i=1}^N w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^N w_i}$ ; (10.2)
    Compute  $\alpha_m = \log \frac{1 - err_m}{err_m}$ ;
    wi  $\leftarrow w_i e^{\alpha_m I(y_i \neq G_m(x_i))}$ , i = 1, … , N;
    return G(x) = sign( $\sum_{i=1}^M \alpha_m G_m(x)$ )
```

---

increase the performance of even a very weak classifier.

## 10.2 Boosting fits an additive model

Boosting is a way of fitting an additive expansion in a set of basis-functions where the basis functions are the individual classifiers. The basis function expansion takes the form:

$$f(x) = \sum_{m=1}^M \beta_m b(x, \gamma_m) \quad (10.3)$$

Typically these models are fit by minimizing a loss function averaged over the training data, such as the squared error or a likelihood-based loss function:

$$\min_{\{\beta_m, \gamma_m\}_1^M} \sum_{i=1}^N L\left(y_i, \sum_{m=1}^M \beta_m b(x_i, \gamma_m)\right) \quad (10.4)$$

This is sometimes computationally infeasible and it is approximated by:

$$\min_{\{\beta_m, \gamma_m\}_1^M} \sum_{i=1}^N L(y_i, \beta b(x_i, \gamma)) \quad (10.5)$$

### 10.3 Forward Stagewise Additive Modeling

Forward stagewise modelling approximates the solution of 10.4 by sequentially adding new basis functions to the expansion without adjusting the parameters and coefficients of those that have already been added. At each iteration  $m$  one solves for the optimal basis function  $b(x, \gamma_m)$  and corresponding coefficient  $\beta_m$  to add the current expansion  $f_{m-1}(x)$ . This produces  $f_m(x)$  and the process is repeated. For squared error loss one has:

$$\begin{aligned} L(y_i, f_{m-1}(x_i) + \beta b(x_i, \gamma)) &= (y_i - f_{m-1}(x_i) - f_{m-1}(x_i) - \beta b(x_i, \gamma))^2 = \\ &= (r_i - \beta b(x_i, \gamma))^2 \end{aligned} \quad (10.6)$$

The term that best fits the residual is added to the expansion at each step.

Stagewise additive modelling is equivalent to AdaBoost.M1 using the exponential loss-function:

$$L(y, f(x)) = \exp(-yf(x)) \quad (10.7)$$

The principal attraction of exponential loss in the context of additive modeling is computational; it leads to the simple modular reweighting AdaBoost algorithm.

## 11 Procedure for datamining

In data mining applications, usually only a small fraction of the large number of predictor variables that have been included in the analysis are actually relevant to prediction. Also, unlike many applications such as pattern recognition, there is seldom reliable domain knowledge to help create especially

relevant features and/or filter out the irrelevant ones, the inclusion of which dramatically degrades the performance of many methods. In addition, data mining applications generally require interpretable models. It is not enough to simply produce predictions. It is also desirable to have information providing qualitative understanding of the relationship between joint values of the input variables and the resulting predicted response value. Thus, black box methods such as neural networks, which can be quite useful in purely predictive settings such as pattern recognition, are far less useful for data mining.

An "off-the-shelf" method is one that can be directly applied to the data without requiring a great deal of time-consuming data preprocessing or careful tuning of the learning procedure. Decision trees come closest to meeting the requirements for serving as an off-the-shelf procedure for data mining. They are relatively fast to construct and they produce interpretable models (if the trees are small). They naturally incorporate mixtures of numeric and categorical predictor variables and missing values. They are invariant under (strictly monotone) transformations of the individual predictors. As a result, scaling and/or more general transformations are not an issue, and they are immune to the effects of predictor outliers. They perform internal feature selection as an integral part of the procedure. They are thereby resistant, if not completely immune, to the inclusion of many irrelevant predictor variables. These properties of decision trees are largely the reason that they have emerged as the most popular learning method for data mining. Trees have one aspect that prevents them from being the ideal tool for predictive learning, namely inaccuracy. They seldom provide predictive accuracy comparable to the best that can be achieved with the data at hand.

## 11.1 Boosting trees

The boosted tree model is a sum of trees induced in a forward stagewise manner:

$$f_M(x) = \sum_{m=1}^M T(x, \Theta_m) \quad (11.1)$$

$$T(x, \Theta_m) = \sum_{j=1}^J \gamma_j I(x \in R_j)$$

where  $\Theta_m$  is the vector of parameters. Considering a single tree, the parameters are found by minimizing the empirical risk:

$$\hat{\Theta} = \arg \min_{\Theta} \sum_{j=1}^J \sum_{x_i \in R_j} L(y_i, \gamma_j) \quad (11.2)$$

Due to the combinatorial problem, we usually settle for suboptimal solutions, dividing the problem into two parts:

- **Finding  $\gamma_j$  given  $R_j$ :** this is typically trivial and often  $\hat{\gamma}_j = \bar{y}_j$ , the mean of  $y_i$  falling in region  $R_j$ .
- **Finding  $R_j$ :** this is the difficult part. A typical strategy is to use a greedy top-down recursive partitioning algorithm to find  $R_j$ .

The boosted tree is induced in a forward stagewise manner. At each step one must solve:

$$\hat{\Theta}_m = \arg \min_{\Theta_m} \sum_{i=1}^N L(y_i, f_{m-1}(x_i) + T(x_i, \Theta_m)) \quad (11.3)$$

for the region set and constants  $\Theta_m = \{R_{jm}, \gamma_{jm}\}_1^{J_m}$  for the next tree, given the current model  $f_{m-1}(x)$ . Given  $R_{jm}$ , finding the optimal constants  $\gamma_{jm}$  in each region is typically straightforward:

$$\hat{\gamma}_{jm} = \arg \min_{\gamma_{jm}} \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \gamma_{jm}) \quad (11.4)$$

Finding the regions is more difficult, and even more difficult than for a single tree.

Defining the loss function as

$$L(f) = \sum_{i=1}^N L(y_i, f(x_i)) \quad (11.5)$$

where  $f$  is a sum of trees. So,  $\hat{f} = \arg \min_f L(f)$ ,  $f = \{f(x_1), f(x_2), \dots, f(x_N)\}$ .

Numerical procedures exist to find  $\hat{f}$  as a sum of component vectors:

$$f_M = \sum_{m=0}^M h_m, \quad h_m \in CMcalR^N \quad (11.6)$$

with  $\mathbf{f}_0 = \mathbf{h}_0$  is an initial guess.

One optimization is the **Steepest descent**:  $\mathbf{h}_m = -\rho_m \mathbf{g}_m$ ,  $\mathbf{g}$  being the gradient of  $L(f)$  evaluated at  $\mathbf{f}_{m-1}$ .

Another way is the **Gradient Boosting**. The gradient is trivial to calculate for any differentiable loss function but it is defined only at the training data points  $x_i$  whereas the ultimate goal is to generalize it to new data not in the training set.

A possible resolution to this dilemma is to induce a tree  $T(x, \Theta_m)$  at the  $m$ -th iteration whose predictions  $t_m$  are as close as possible to the negative gradient. Using squared error loss to measure closeness:

$$\tilde{\Theta}_m = \arg \min_{\Theta} \sum_{i=1}^N (-g_{im} - T(x_i, \Theta))^2 \quad (11.7)$$

The algorithm for classification is similar. Two basic tuning parameters are

---

**Algorithm 2:** Gradient Tree Boosting algorirthm.

---

```

 $f_0 \leftarrow \arg \min_{\gamma} \sum_{i=1}^N L(y_i, \gamma);$ 
for ( $m = 1 : M$ ) do
  for ( $i = 1 : N$ ) do
     $r_{im} = \left[ \frac{\partial L(y_i, f(x_i))}{\partial f(x_i)} \right]_{f=f_{m-1}};$ 
    Fit a regression tree to the targets  $r_{im}$  giving terminal regions
     $R_{jm}, j = 1, \dots, J_m;$ 
    for ( $i = 1 : J_m$ ) do
       $\gamma_{jm} = \arg \min_{\gamma} \sum_{x_j \in R_{jm}} L(y_i, f_{m-1}(x_i) + \gamma);$ 
     $f_m(x) \leftarrow f_{m-1} + \sum_{j=1}^{J_m} L(y_i, f_{m-1}(x_i) + \gamma);$ 
  return  $\hat{f} = f_M(x)$ 

```

---

the number of iterations  $M$  and the sizes of each of the constituent trees  $J_m, m = 1, 2, \dots, M$ .

## 11.2 Right-sized Trees for boosting

[skipped, at least for now]

## 11.3 Regularization

Besides the size of the constituent trees,  $J$ , the other meta-parameter of gradient boosting is the number of boosting iterations  $M$ . Each iteration usually reduces the training risk  $L(f_M)$ , so that for  $M$  large enough this risk can be made arbitrarily small. However, fitting the training data too well can lead to overfitting, which degrades the risk on future predictions. Thus, there is an optimal number  $M^*$  minimizing future risk that is application dependent. A convenient way to estimate  $M^*$  is to monitor prediction risk as a function of  $M$  on a validation sample. The value of  $M$  that minimizes this risk is taken to be an estimate of  $M^*$ .

### 11.3.1 Shrinkage

Controlling the value of  $M$  is not the only possible regularization strategy. Shrinkage techniques can be employed as well. The simplest implementation of shrinkage in this case is to scale the contribution of each tree by a factor  $0 < \nu < 1$  when it is added to the current approximation:

$$f_m(x) = f_{m-1}(x) + \nu \sum_{j=1}^J \gamma_{jm} I(x \in R_{jm}). \quad (11.8)$$

Smaller values of  $\nu$  (more shrinkage) result in larger training risk for the same number of iterations  $M$ . Empirically it has been found (Friedman, 2001) that smaller values of  $\nu$  favor better test error, and require correspondingly larger values of  $M$ . The best strategy appears to be to set  $\nu$  to be very small ( $\nu < 0.1$ ) and then choose  $M$  by early stopping, however more iterations are needed so the computational cost is higher.

## 12 Support Vector Machines and Flexible Discriminants

We have seen **Optimal separating hyperplanes** in 5.11. Here we will see the case for non-separable classes, where the classes overlap.

## 12.1 Support Vector Classifier

With  $N$  pairs  $(x_i, y_i) \in \mathcal{R}^p$  and  $y_i \in \{-1, 1\}$ , define a hyperplane:

$$\{x : f(c) = x^T \beta + \beta_0 = 0\} \quad (12.1)$$

where  $|\beta| = 1$  is a unit vector. A classification rule induced by  $f(x)$  is:

$$G(x) = \text{sign}[x^T \beta + \beta_0] \quad (12.2)$$

When the classes are separable, we can find a function  $f(x) = x^T \beta + \beta_0$  with  $y_i f(x_i) > 0, \forall i$ . Hence, we are able to find the hyperplane creating the biggest margin between training points belonging to the two different classes:

$$\begin{aligned} & \max_{\beta, \beta_0, |\beta|=1} M \\ & \text{subject to } y_i(x_i^T \beta + \beta_0) \geq M, \quad i = 1, \dots, N \end{aligned} \quad (12.3)$$

or equivalently:

$$\begin{aligned} & \min_{\beta, \beta_0} |\beta| \\ & \text{subject to } y_i(x_i^T \beta + \beta_0) \geq 1, \quad i = 1, \dots, N \end{aligned} \quad (12.4)$$

$M$  is the distance from the hyperplane to the wither side and it is called **margin**. This is a convex optimization problem.

**Suppose now that the classes overlap in the feature space.** We can still maximize  $M$  allowing some points to be on the wrong side. We define a slack variable  $\xi = (\xi_1, \xi_2, \dots, \xi_N)$ . There are two ways to modify the constraint:

$$\begin{aligned} & y_i(x_i^T \beta + \beta_0) \geq M - \xi_i \\ & \text{or } y_i(x_i^T \beta + \beta_0) \geq M(1 - \xi_i) \\ & \forall i, \xi_i \geq 0, \sum_{i=1}^N \xi_i \leq \text{constant.} \end{aligned} \quad (12.5)$$

The two choices lead to different solutions. The first choice is more natural since it measures overlap in actual distance from the margin. The second choice measures the overlap in relative distance, which changes the width of the margin  $M$ . However, the first choice leads to a nonconvex optimization, while the second results to the standard support vector classifier.

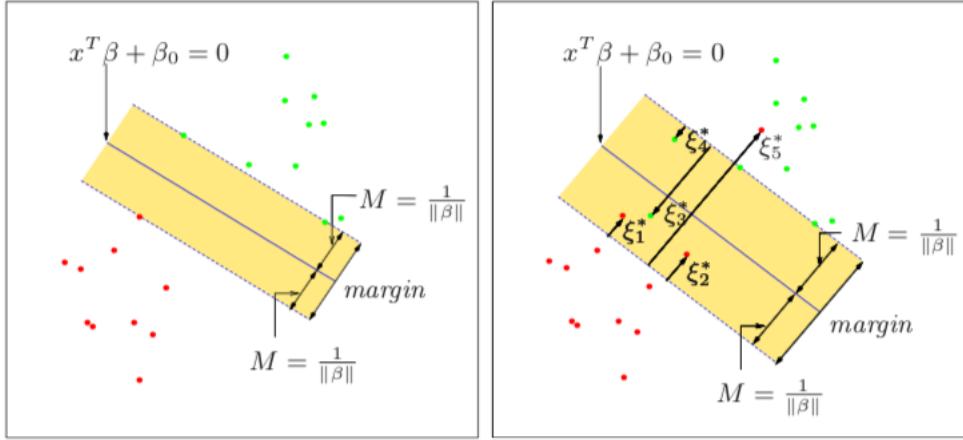


Figure 12.1: Separable and non separable support vector classifiers.

The value  $\xi_i$  is the proportional amount by which the prediction  $f(x_i) = x_i^T \beta + \beta_0$  is on the wrong side of the margin. Hence by up-bounding the sum  $\sum \xi_i$  we limit the total proportional amount by which predictions fall on the wrong side. Misclassifications occur when  $\xi_i > 1$ . So using a constant  $K$  one bounds the total number of misclassifications to  $K$ . Again, we can drop the norm constraint on  $\beta$ :

$$M = \frac{1}{\|\beta\|}$$

subject to  $y_i(x_i^T \beta + \beta_0) \geq 1 - \xi_i \quad \forall i$

and subject to  $\xi_i \geq 0, \sum_i \xi_i \leq \text{constant}$

(12.6)

The misclassified points are on the wrong side for an amount  $\xi^* = M\xi$  while the correctly classified points have  $\xi^* = 0$ . One sees that points inside their class boundary do not play a big role in shaping the boundary. This seems like an attractive property, and one that differentiates it from linear discriminant analysis (5.2). In LDA, the decision boundary is determined by the covariance of the class distributions and the positions of the class centroids. Logistic regression is more similar to the support vector classifier in this regard.

### 12.1.1 Computing the support vector classifier

The problem 12.6 is quadratic with linear inequality constraints, hence it is a convex optimization problem. We describe a quadratic programming solution using Lagrange multipliers. Computationally it is convenient to re-express 12.6 in the equivalent form:

$$\begin{aligned} \min_{\beta, \beta_0} & \frac{1}{2} |\beta|^2 + C \sum_{i=1}^N \xi_i \\ \text{subject to} & \xi \geq 0, y_i(x_i^T \beta + \beta_0) \geq 1 - \xi_i, \forall i \end{aligned} \quad (12.7)$$

where  $C$  replaces the constant. The separable case corresponds to  $C = \infty$ .

The Lagrange primal function is

$$L_P = \frac{1}{2} |\beta|^2 + C \sum_{i=1}^N \xi_i - \sum_{i=1}^N \alpha_i \left[ y_i (x_i^T \beta + \beta_0) - (1 - \xi_i) \right] - \sum_{i=1}^N \mu_i \xi_i \quad (12.8)$$

which we minimize w.r.t.  $\beta, \beta_0, \xi$ . Setting the respective derivatives to 0:

$$\begin{aligned} \beta &= \sum_{i=1}^N \alpha_i y_i x_i, \\ 0 &= \sum_{i=1}^N \alpha_i y_i \\ \alpha_i &= C - \mu_i \quad \forall i \\ \text{constrained to} & \quad \alpha_i, \mu_i, \xi_i \geq 0 \quad \forall i \end{aligned} \quad (12.9)$$

Substituting in 12.8, we obtain the Lagrangian (Wolfe) dual objective func-

tion:

$$\begin{aligned}
L_D &= \frac{1}{2} \beta^T \beta + \sum_{i=1}^N [(\mathbf{C} - \mu_i) \xi_i] - \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \beta - \sum_{i=1}^N \alpha_i y_i \beta_0 + \\
&\quad + \sum_{i=1}^N \alpha_i - \sum_{i=1}^N \alpha_i \xi_i = \\
&= \frac{1}{2} \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \cdot \sum_{j=1}^N \alpha_j y_j \mathbf{x}_j + \cancel{\sum_{i=1}^N \alpha_i \xi_i} - \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \beta - \sum_{i=1}^N \alpha_i y_i \beta_0 + \\
&\quad + \sum_{i=1}^N \alpha_i - \cancel{\sum_{i=1}^N \alpha_i \xi_i} = \\
&= \frac{1}{2} \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \cdot \sum_{j=1}^N \alpha_j y_j \mathbf{x}_j - \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \beta - \beta_0 \sum_{i=1}^N \alpha_i y_i + \sum_{i=1}^N \alpha_i = \\
&= \frac{1}{2} \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \cdot \sum_{j=1}^N \alpha_j y_j \mathbf{x}_j - \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \sum_{j=1}^N \alpha_j y_j \mathbf{x}_j + \sum_{i=1}^N \alpha_i = \\
&= \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \sum_{j=1}^N \alpha_j y_j \mathbf{x}_j = \\
&= \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i y_i \alpha_j y_j \mathbf{x}_i^T \mathbf{x}_j
\end{aligned} \tag{12.10}$$

where we used the properties that  $\alpha_i, y_i$  are scalar and that  $\beta, \beta_0$  can be taken out. Notice that  $\beta^T \beta = \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^T \sum_{j=1}^N \alpha_j y_j \mathbf{x}_j = \sum_{i=1}^N \sum_{j=1}^N \alpha_i y_i \alpha_j y_j \mathbf{x}_i^T \mathbf{x}_j \neq \sum_{i=1}^N (\alpha_i y_i)^2 \mathbf{x}_i^T \mathbf{x}_i$ . In fact consider for example:  $\beta = c_1 \mathbf{x}_1 + c_2 \mathbf{x}_2$  with  $\mathbf{x}_i = [x_{1i}, x_{2i}]^T$ .  $\beta = [c_1 x_{11} + c_2 x_{12}, c_1 x_{21} + c_2 x_{22}]^T$  and  $\beta^T \beta = (c_1 x_{11} + c_2 x_{12})^2 + (c_1 x_{21} + c_2 x_{22})^2$ , so we are missing some cross-products. The Lagrangian (Wolfe) dual objective function gives a lower bound on the objective function for any feasible point. We maximize  $L_D$  subject to  $0 \leq \alpha_i \leq C$  and  $\sum_{i=1}^N \alpha_i y_i$ . In addition to the derivatives, the **Karush-kuhn-Tucker** con-

ditions include constraints:

$$\begin{aligned} \alpha_i [y_i (x_i^T \beta + \beta_0) - (1 - \xi_i)] &= 0 \\ \mu_i \xi_i &= 0 \\ y_i (x_i^T \beta + \beta_0) - (1 - \xi_i) &\geq 0 \end{aligned} \tag{12.11}$$

for  $i = 1, \dots, N$ . These constraints and the ones originating from the derivatives uniquely characterize the primal and dual problem.

From  $\beta = \sum_{i=1}^N \alpha_i y_i x_i$ , we can see:

$$\hat{\beta} = \sum_{i=1}^N \hat{\alpha}_i y_i x_i \tag{12.12}$$

with  $\hat{\alpha}_i \neq 0$  only for those observations  $i$  for which the constraints in the last equation of 12.11 are exactly met. These observations are called **support vectors**, since  $\hat{\beta}$  is represented in terms of them alone. Among these support points, some will lie on the edge of the margin ( $\hat{\xi}_i = 0$ ) and hence will be characterized by  $0 < \hat{\alpha}_i < C$ : the remainder ( $\hat{\xi}_i > 0$ ) have  $\hat{\alpha}_i = C$ . We can see that any of these margin points ( $0 < \hat{\alpha}_i, \hat{\xi}_i = 0$ ), can be used to solve for  $\beta_0$ , and we typically use an average of all the solutions for numerical stability. Maximizing the dual is a simpler convex quadratic programming problem than the primal and can be solved with standard techniques such (Murray et. al, 1981).

Points on the wrong side of the boundary are support vectors. In addition, points on the correct side of the boundary but close to it (in the margin), are also support vectors.

Given the solutions  $\hat{\beta}, \hat{\beta}_0$ , the decision function can be written as:

$$\hat{G}(x) = \text{sign}(\hat{f}(x)) = \text{sign}(x^T \hat{\beta} + \beta_0) \tag{12.13}$$

The tuning parameter of this procedure is the cost parameter  $C$ . The optimal value for  $C$  can be estimated by cross-validation.

## 12.2 Support vector machines and Kernels

We can make the procedure more flexible by enlarging the feature space using basis expansions such as polynomials or splines. Generally linear boundaries in the enlarged space achieve better training-class separation, and translate to nonlinear boundaries in the original space.

### 12.2.1 Computing SVM for classification

The Lagrange dual function has the form:

$$L_D = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i y_i \alpha_j y_j \langle h(x_i), h(x_j) \rangle \quad (12.14)$$

So  $f(x)$  can be written as

$$f(x) = h(x)^T \beta + \beta_0 = \sum_{i=1}^N \alpha_i y_i \langle h(x), h(x_i) \rangle + \beta_0 \quad (12.15)$$

As before, given  $\alpha_i, \beta_0$  can be determined by solving  $y_i f(x_i) = 1$  for any (or all)  $x_i$  for which  $0 < \alpha_i < C$ . So  $h(x_0)$  is involved only in terms of its inner product: **we do not need to specify the transformation but only the knowledge of the kernel function is required**:

$$K(x, x') = \langle h(x), h(x') \rangle \quad (12.16)$$

$K$  should be symmetric positive (semi-) definite. Possible popular choices are:

$$\begin{aligned} \text{dth-Degree polynomial: } K(x, x') &= (1 + \langle x, x' \rangle)^d \\ \text{Radial basis: } K(x, x') &= e^{-\gamma|x-x'|^2} \\ \text{Neural Network: } K(x, x') &= \tanh(k_1 \langle x, x' \rangle + k_2) \end{aligned} \quad (12.17)$$

## 12.3 SVM for Regression

SVM can be adapted for regression. The linear regression model is in the form

$$f(x) = x^T \beta + \beta_0 \quad (12.18)$$

and then handle non-linear generalizations. To estimate  $\beta$  we consider minimization of:

$$\begin{aligned} H(\beta, \beta_0) &= \sum_{i=1}^N V(y_i - f(x_i)) + \frac{\lambda}{2} |\beta|^2 \\ V_\epsilon &= \begin{cases} 0 & \text{if } |r| < 1 \\ |r| - \epsilon & \text{otherwise} \end{cases} \end{aligned} \quad (12.19)$$

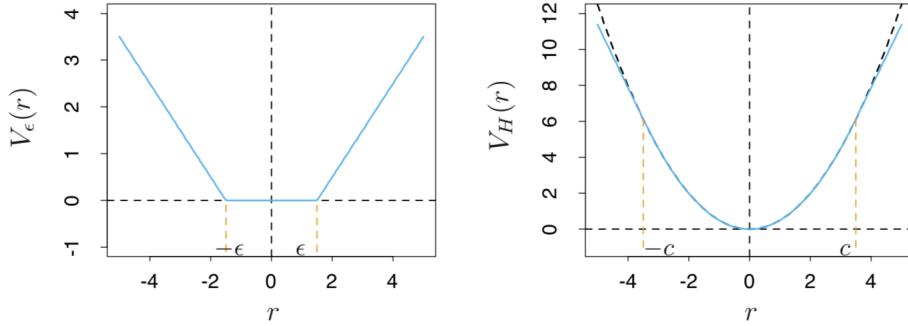


Figure 12.2: The left panel shows the  $\epsilon$ -insensitive error function used by the support vector regression machine. The right panel shows the error function used in Huber's robust regression (blue curve) used in statistics. Beyond  $|c|$ , the function changes from quadratic to linear reducing the contribution of outliers.

This is an " " $\epsilon$ -insensitive" error measure, ignoring errors of size less than  $\epsilon$  (left panel of 12.2). There is a rough analogy with the support vector classification setup, where points on the correct side of the decision boundary and far away from it, are ignored in the optimization. In regression, these "low error" points are the ones with small residuals.

The support vector error measure has linear tails (beyond  $\epsilon$ ), but in addition it flattens the contributions of those cases with small residuals.

If  $\hat{\beta}, \hat{\beta}_0$  are the minimizers of  $H$ , the solution function can be shown to have the form:

$$\begin{aligned}\hat{\beta} &= \sum_{i=1}^N (\hat{\alpha}_i^* - \hat{\alpha}_i) x_i \\ \hat{f}(x) &= \sum_{i=1}^N (\hat{\alpha}_i^* - \hat{\alpha}_i) \langle x, x_i \rangle + \beta_0\end{aligned}\tag{12.20}$$

where  $\hat{\alpha}_i^*, \hat{\alpha}_i$  are positive and solve the quadratic problem:

$$\begin{aligned} & \min_{\alpha_i, \alpha_i^*} \epsilon \sum_{i=1}^N (\alpha_i^* + \alpha_i) - \sum_{i=1}^N y_i (\alpha_i^* - \alpha_i) + \frac{1}{2} \sum_{i,j=1}^N (\alpha_i^* - \alpha_i)(\alpha_j^* - \alpha_j) \langle x_i, x_j \rangle \\ & \text{subject to } \begin{cases} 0 \leq \alpha_i, \alpha_i^* \leq \frac{1}{\lambda} \\ \sum_{i=1}^N (\alpha_i^* - \alpha_i) = 0 \\ \alpha_i, \alpha_i^* = 0 \end{cases} \end{aligned} \quad (12.21)$$

Due to the nature of these constraints, typically only a subset of the solution values  $(\hat{\alpha}_i^* - \hat{\alpha}_i)$  are nonzero, and the associated data values are called the support vectors. There are two parameters:  $\epsilon$  is a parameter of the loss function.  $\lambda$  is a regularization parameter and can be estimated by cross validation.

**The SVM can be extended to multiclass problems** by solving many two-class problems. A classifier is built for each pair of classes and the final classifier is the one that dominates the most.

## 12.4 Generalized LDA

LDA is a simple prototype classifier which classifies points closest to the centroid. LDA is the estimated Bayes classifier if the observations are multivariate Gaussian in each class, with common covariance matrix, which is very unlikely. LDA has linear boundaries and provides natural low-dimensional views of data. Despite these properties, it fails in a number of situations. One is when more flexibility at for the boundaries is required; in this case QDA works. It does not work well neither with too many correlated predictors, for example in case of digitalized analogue signals and images, since in this case it uses too many parameters. Finally, LDA assumes a single centroid (prototype) per class (and a common covariance matrix) to describe the spread of the data in each class. Sometimes several centroids are more appropriate.

Three alternatives exist to these three situations:

- **recast the LDA problem as a linear regression problem**, which in turn can be converted to a non-parametric form of regression, achieving more flexibility. These are called **FDA**. The regression procedures can be seen to identify an enlarged set of predictors via basis expansions. FDA amounts to LDA in this enlarged space.

- When there are too many predictors, we do not want to expand the set. The second idea is to fit LDA but penalize its coefficients to be smooth or otherwise coherent in the spatial domain, such as an image. This is called **Penalized Discriminant Analysis (PDA)**.
- **Model each class by a mixture of two or more Gaussians with different centroids sharing the same covariance matrix.** This allows for more complex decision boundaries and allows for subspace reduction. This is called **Mixture Discriminant Analysis (MDA)**.

#### 12.4.1 Flexible Discriminant Analysis (FDA)

This technique performs LDA using linear-regression on derived responses. Assume we have observations with a quantitative response  $G$  falling into one of  $K$  classes. Suppose  $\theta : \mathcal{G} \rightarrow \mathcal{R}^1$  is a function that assigns scores to the classes such that the transformed class labels are optimally predicted by linear regression, producing the derived responses. Then, having as training examples  $(g_i, x_i)$ , we solve:

$$\min_{\theta, \beta} \sum_{i=1}^N (\theta(g_i) - x_i^T \beta)^2 \quad (12.22)$$

with restrictions on  $\theta$  to avoid trivial solutions (mean zero and unit variance over the training data).

More generally, we can find up to  $L \leq K - 1$  sets of independent scorings for the class labels,  $\theta_1, \theta_2, \dots, \theta_L$ , and  $L$  corresponding linear maps  $\eta_l(X) = X^T \beta_l, l = 1, \dots, L$ , chosen to be optimal for multiple regression in  $\mathcal{R}^p$ . So the mapping function for one class does not to be the same for the others.

The scores  $\theta_l(g)$  and maps  $\beta_l$  are chosen to minimize the average squared residual:

$$ASR = \frac{1}{N} \sum_{l=1}^L \left[ (\theta_l(g_i) - x_i^T \beta_k)^2 \right] \quad (12.23)$$

The set of scores are assumed to be mutually orthogonal and normalized with respect to an appropriate inner product to prevent trivial zero solutions.

The Mahalanobis distance of a test point  $x$  to the  $k$ -th class centroid  $\hat{\mu}_k$  is given by:

$$\delta_j(x, \hat{\mu}_k) = \sum_{\ell=1}^{K-1} w_\ell \left( \hat{\eta}_\ell(x) - \eta_\ell^{-k}(x) \right) + D(x) \quad (12.24)$$

where  $\eta_\ell^{-k}(x)$  is the mean of  $\hat{\eta}_\ell(x)$  in the  $k$ -th class, and  $D(x)$  does not depend on  $k$  and  $w_l$  are defined in terms of the mean squared residual  $r_\ell^2$  for the  $\ell$ th optimally scored fit:

$$w_\ell = \frac{1}{r_\ell^2(1-r_\ell^2)} \quad (12.25)$$

To summarize, LDA can be performed by a sequence of linear regressions, followed by classification to the closest class centroid in the space of fits.

The power is that we can replace the linear regression with more flexible non-parametric fits, achieving a more flexible classifier. We can use generalized additive fits, spline functions, MARS and others. In this more general form the regression problems are defined by the criterion:

$$\text{ASR}\left(\{\theta_\ell, \eta_\ell\}_{\ell=1}^L\right) = \frac{1}{N} \sum_{\ell=1}^L \left[ \sum_{i=1}^N (\theta_\ell(g_i) - \eta_\ell(x_i))^2 + \lambda J(\eta_\ell) \right] \quad (12.26)$$

where  $J$  is a regularizer appropriate for some forms of nonparametric regression.

The computations of FDA coordinates can be simplified in cases when the nonparametric procedure can be represented as a linear operator  $S_\lambda$ , that is  $\hat{y} = S_\lambda y$ . Additive splines have this property if the smoothing parameters are fixed, as well as MARS when the basis functions are selected. The subscript  $\lambda$  denotes the entire set of smoothing parameters. If  $S_\lambda = H_X$ , the linear regression projection operator, then we are back to LDA.

We create  $N \times K$  *indicator response matrix*  $\mathbf{Y}$  from the response  $g_i$ , such that  $y_{ik} = 1$  if  $g_i = k$ , 0 otherwise. Each row in  $\mathbb{Y}$  has only one 1. The steps are the following:

1. **Multivariate nonparametric regression:** fit a multiresponse, adaptive nonparametric regression of  $\mathbf{Y}$  on  $\mathbf{X}$ , giving the fitted values  $\hat{\mathbf{Y}}$ . Let  $S_\lambda$  be the linear operator that fits the final chosen model and  $\eta^*(x)$  be the vector of fitted regression functions .
2. **Optimal scores:** compute the eigen-decomposition of  $\mathbf{Y}^T \hat{\mathbf{Y}} = \mathbf{Y}^T S_\lambda \mathbf{Y}$  where the eigenvectors  $\Phi$  are normalized:  $\Phi^T D_\pi \Phi^T$ . here  $D_\pi = \mathbf{Y}^T \mathbf{Y} / N$  is a diagonal matrix of the estimated class prior probabilities.
3. **Update** the model from step 1 using the optimal scores  $\eta(x) = \Phi^T \eta^*(x)$ .

### 12.4.2 Penalized discriminant analysis

Although FDA is motivated by generalizing optimal scoring, it can also be viewed directly as a form of regularized discriminant analysis. Suppose the regression procedure used in FDA amounts to a linear regression onto a basis expansion  $h(X)$ , with a quadratic penalty on the coefficients:

$$\text{ASR}\left(\{\theta_\ell, \beta_\ell\}_{\ell=1}^L\right) = \frac{1}{N} \sum_{\ell=1}^L \left[ \sum_{i=1}^N \left( \theta_\ell(g_i) - h^T(x_i)\beta_\ell \right)^2 + \lambda \beta_\ell^T \Omega \beta_\ell \right] \quad (12.27)$$

The choice of  $\Omega$  depends on the problem. if  $\eta_\ell(x) = h(x)\beta_\ell$  is an expansion on spline basis functions,  $\Omega$  might constrain  $\eta_\ell$  to be smooth over  $\mathcal{R}^p$ . In the case of additive splines, there are  $N$  spline basis functions for each coordinate, resulting in a total of  $N_p$  basis functions in  $h(x)$ ;  $\Omega$  in this case is  $N_p \times N_p$  and block diagonal.

The steps in FDA can then be viewed as a generalized form of LDA, which we call penalized discriminant analysis, or PDA:

- Enlarge the set of predictors  $X$  via a basis expansion  $h(X)$ .
- Use (penalized) LDA in the enlarged space where the Mahalanobis distance is given by:

$$D(x, \mu) = (h(x) - h(\mu))^T (\Sigma_W + \lambda \Sigma)^{-1} (h(x) - h(\mu)) \quad (12.28)$$

where  $\Sigma_W$  is the within-class covariance matrix of the derived variables  $h(x_i)$ .

- Decompose the classification subspace using a penalized metric:

$$\max u^T \Sigma_{\text{Bet}} u \quad \text{subject to} \quad u^T (\Sigma_W + \lambda \Sigma) u = 1 \quad (12.29)$$

For some classes of problems, the first step, involving the basis expansion, is not needed; we already have far too many (correlated) predictors. An example is when the objects are digitalized analogue signals. Neighboring pixel values will tend to be correlated, being often almost the same. This implies that the pair of corresponding LDA coefficients for these pixels can be wildly different and opposite in sign, and thus cancel when applied to similar pixel values. Positively correlated predictors lead to noisy, negatively

correlated coefficient estimates, and this noise results in unwanted sampling variance. A reasonable strategy is to regularize the coefficients to be smooth over the spatial domain, as with images. This is what PDA does. The computations proceed just as for FDA, except that an appropriate penalized regression method is used.

### 12.4.3 Mixture Discriminant Analysis

Linear discriminant analysis can be viewed as a prototype classifier. Each class is represented by its centroid, and we classify to the closest using an appropriate metric. In many situations a single prototype is not sufficient to represent inhomogeneous classes and mixture models are more appropriate.

A Gaussian mixture model for the  $k$ -th class has density:

$$P(X|G=k) = \sum_{r=1}^{R_k} \pi_{kr} \phi(X, \mu_{kr}, \Sigma) \quad (12.30)$$

where the **mixing proportions**  $\pi_{kr}$  sum to one. The class posterior probabilities are given by

$$P(G=k|X=x) = \frac{\sum_{r=1}^{R_k} \pi_{kr} \phi(x, \mu_{kr}, \Sigma) \Pi_k}{\sum_{\ell=1}^K \sum_{r=1}^{R_\ell} \pi_{\ell r} \phi(x, \mu_{\ell r}, \Sigma) \Pi_\ell} \quad (12.31)$$

where  $\Pi_k$  are the class priors.

As in LDA we estimate the parameters by MLE, using the joint log-likelihood based on  $P(G, X)$ :

$$\sum_{k=1}^K \sum_{g_i=k} \log \left[ \sum_{r=1}^{R_k} \pi_{kr} \phi(x_i, \mu_{kr}, \Sigma) \Pi_k \right] \quad (12.32)$$

The sum within the log makes this a rather messy optimization problem if tackled directly. The classical and natural method for computing the maximum-likelihood estimates (MLEs) for mixture distributions is the EM algorithm. EM alternates between the two steps:

- **E-step** Given the current parameters, compute the **responsability** of subclass  $c_{kr}$  within class  $k$  for each of the class- $k$  observations ( $g_i = k$ ):

$$W(c_{kr}|x_i, g_i) = \frac{\pi_{kr} \phi(x_i, \mu_{kr}, \Sigma)}{\sum_{\ell=1}^{R_k} \pi_{k\ell} \phi(x_i, \mu_{k\ell}, \Sigma)} \quad (12.33)$$

- **M-step:** compute the weighted MLEs for the parameters of each of the component Gaussians within each of the classes, using the weights from the E-step.

In the E-step, the algorithm apportions the unit weight of an observation in class  $k$  to the various subclasses assigned to that class. If it is close to the centroid of a particular subclass, and far from the others, it will receive a mass close to one for that subclass. On the other hand, observations halfway between two subclasses will get approximately equal weight for both.

In the M-step, an observation in class  $k$  is used  $R_k$  times, to estimate the parameters in each of the  $R_k$  component densities, with a different weight for each.

## 13 Prototype methods and Nearest-Neighbours

There exist model-free methods for classification and pattern recognition. Because they are highly unstructured, they typically are not useful for understanding the nature of the relationship between the features and class outcome but they work more in a black-box manner.

**Prototype methods** represent points in a feature space. Each prototype has an associated class label and classification of a point is made to the class of the closest prototype, generally in terms of Euclidean distance in a feature space, after each feature has been standardized (0-mean, unit variance).

### 13.1 K-means clustering

It is a method to find clusters and cluster centres in a set of unlabeled data. Once chooses the desired number of cluster centres,  $R$ , and the K-means procedure iteratively moves the centres to minimize the total within cluster variance ( $K$  is the number of classes,  $R$  of clusters).

Given an initial set of centres, the algorithm alternates two steps:

- for each centre we identify the subset of training points (its cluster) that is closer to it than any other center;
- the means of each feature for the data points in each cluster are computed and this mean vector becomes the new centre for that cluster.

These steps are iterated until convergence. Typically the initial  $R$  centres are randomly chosen from the training set.

To use K-means clustering for classification of labeled data, the steps are:

- apply K-means clustering to the training data in each class separately, using  $R$  prototypes;
- assign a class label to each of the  $K \times R$  prototypes;
- classify a new feature  $x$  to the class of the closest prototype.

Prototypes near the class boundaries might lead to misclassification errors for points near these boundaries. This results from the fact that for each class, the other classes do not have a say in the positioning of the prototypes for that class.

## 13.2 Learning Vector Quantization

LVQ places prototypes in strategical position w.r.t. decision boundaries. It is an online algorithm: observations are processed one at a time.

The idea is that the training points attract prototypes of the correct class, and repel other prototypes. When the iterations settle down, prototypes should be close to the training points in their class. The learning rate  $\alpha$  is decreased to zero with each iteration. The prototypes tend to move away from the decision boundaries, and away from prototypes of competing classes. A drawback is that they are defined by algorithms, rather than optimization of some fixed criteria; this makes it difficult to understand their properties.

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**Algorithm 3:** Learning Vector Quantization

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Chose R initial prototypes for each class:  $m_1(k), \dots, m_R(k)$ ,  
 $k = 1, \dots, K$ , for example by sampling R training points at random  
from each class;  
Sample a training point  $(x_i, g_i)$  randomly and let  $(j, k)$  index the  
closest prototype  $m_j(k)$  to  $x_i$ ;  
**if**  $g_i = k$  **then**  
     $m_j(k) \leftarrow m_j(k) + \epsilon(x_i - m_j(k))$ : move the prototype towards the  
    the training point;  
**else**  
     $m_j(k) \leftarrow m_j(k) - \epsilon(x_i - m_j(k))$ : move the prototype away from the  
    training point;  
**end**  
Repeat step 2, decreasing the learning rate  $\epsilon$  with each iteration  
towards 0.

---

### 13.3 Gaussian Mixtures

Each cluster is described in terms of a Gaussian density with mean and covariance matrix. The two steps of the alternating EM algorithm are very similar to the two steps in K-means:

- In the E-step, each observation is assigned a responsibility or weight for each cluster, based on the likelihood of each of the corresponding Gaussians. Observations close to the center of a cluster will most likely get weight 1 for that cluster, and weight 0 for every other cluster. Observations half-way between two clusters divide their weight accordingly.
- In the M-step, each observation contributes to the weighted means (and covariances) for every cluster.

The Gaussian mixture model is often referred to as a soft clustering method, while K-means is hard. When Gaussian mixture models are used to represent the feature density in each class, it produces smooth posterior probabilities while the classification rule is  $\hat{G}(x) = \arg \max_k \hat{p}_k(x)$ .

Although the decision boundaries are roughly similar, those for the mixture model are smoother (although the prototypes are in approximately the same positions).

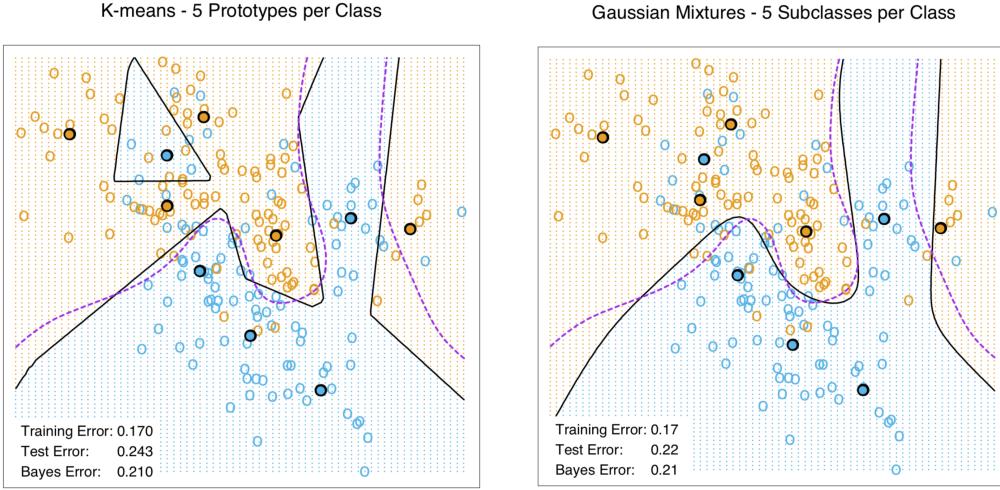


Figure 13.1: Comparison between k-means and Gaussian Mixture model with the same prototypes.

### 13.4 K-nearest neighbour classifier

These classifiers are memory-based, and require no model to be fit. Given a query point  $x_0$ , we find the  $k$  training points  $x(r), r = 1, \dots, k$  closest in distance to  $x_0$ , and then classify using majority vote among the  $k$ -neighbors. Ties are broken at random. Typically we first standardize each of the features to have mean zero and variance 1, since it is possible that they are measured in different units. Because it uses only the training point closest to the query point, the bias of the 1-nearest-neighbor estimate is often low, but the variance is high.

### 13.5 Adaptive Nearest Neighbour

Implicit in near-neighbor classification is the assumption that the class probabilities are roughly constant in the neighborhood, and hence simple averages give good estimates. However, in the example of 13.2 the class probabilities vary only in the horizontal direction. If we knew this, we would stretch the neighborhood in the vertical direction, as shown by the tall rectangular region. This will reduce the bias of our estimate and leave the variance the same.

### 5-Nearest Neighborhoods

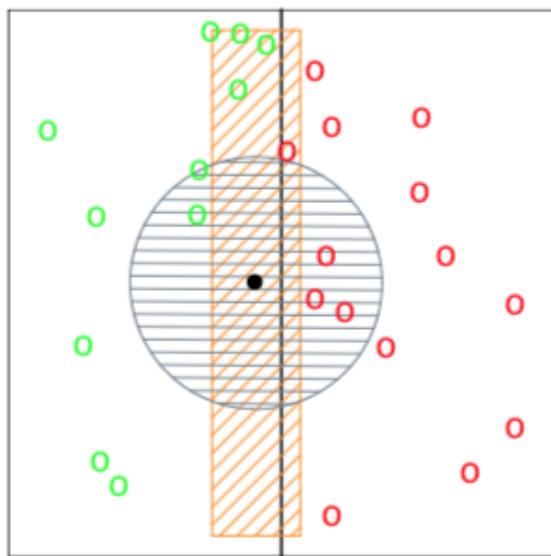


Figure 13.2: The points are uniform in the cube, with the vertical line separating class red and green. The vertical strip denotes the 5-nearest-neighbor region using only the horizontal coordinate to find the nearest-neighbors for the target point (solid dot). The sphere shows the 5-nearest-neighbor region using both coordinates, and we see in this case it has extended into the class-red region (and is dominated by the wrong class in this instance).

This suggests the idea of adapting metrics, so that the resulting neighbourhood stretch out in directions for which the class probabilities do not change much. One of these methods is the **Discriminant Adaptive Nearest-Neighbourhood (DANN)**. At each query point a neighborhood of say 50 points is formed, and the class distribution among the points is used to decide how to deform the neighborhood—that is, to adapt the metric. The adapted metric is then used in a nearest-neighbor rule at the query point. Thus at each query point a potentially different metric is used.

The DANN metric at a query  $x_0$  is defined by:

$$\begin{aligned}
 D(x, x_0) &= (x - x_0)^T \Sigma (x - x_0) \\
 \Sigma &= \mathbf{W}^{-\frac{1}{2}} \left[ \mathbf{W}^{-\frac{1}{2}} \mathbf{B} \mathbf{W}^{-\frac{1}{2}} + \epsilon \mathbf{I} \right] \mathbf{W}^{-\frac{1}{2}} = \\
 &= \mathbf{W}^{-\frac{1}{2}} [\mathbf{B}^* + \epsilon \mathbf{I}] \mathbf{W}^{-\frac{1}{2}} \\
 \mathbf{W} &= \sum_{k=1}^K \pi_k \mathbf{W}_k \\
 \mathbf{B} &= \sum_{k=1}^K \pi_k (\bar{x}_k - \bar{x})(\bar{x}_k - \bar{x})^T
 \end{aligned} \tag{13.1}$$

$\mathbf{W}$  is the pooled within-class covariance matrix and  $\mathbf{B}$  is the between class covariance matrix, both computed with the  $K$  nearest neighbours around  $x_0$ . The formula first spheres the data with respect to  $\mathbf{W}$  and then stretches the neighbourhood in the zero-eigenvalue directions of  $\mathbf{B}^*$ . This makes sense, since locally the observed class means do not differ in these directions. The  $\epsilon$  parameter rounds the neighborhood, from an infinite strip to an ellipsoid, to avoid using points far away from the query point. The value of  $\epsilon = 1$  seems to work well in general.

13.3 shows the resulting neighborhoods for a problem where the classes form two concentric circles. Notice how the neighborhoods stretch out orthogonally to the decision boundaries when both classes are present in the neighborhood. In the pure regions with only one class, the neighborhoods remain circular: in these cases the between matrix  $\mathbf{B} = 0$ , and the  $\Sigma$  is the identity matrix.

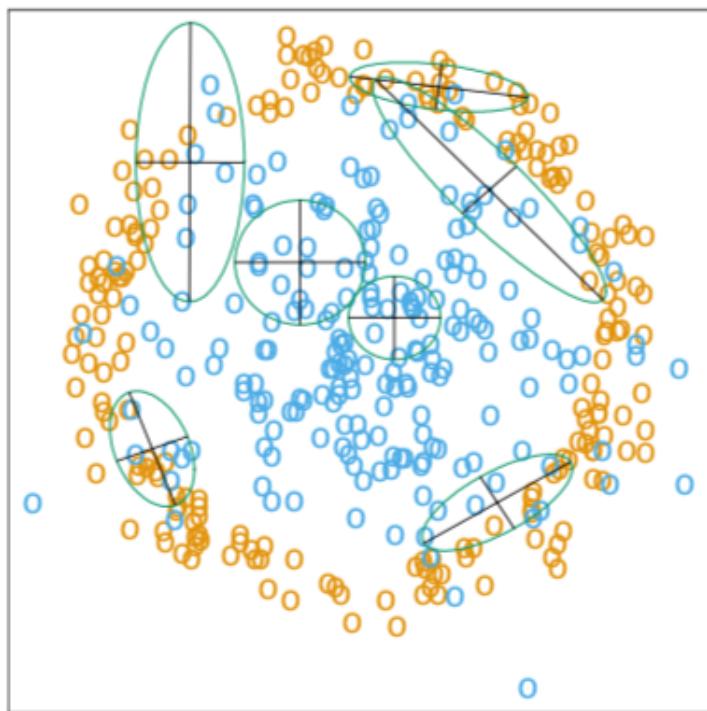


Figure 13.3: Neighborhoods found by the DANN procedure, at various query points (centers of the crosses). There are two classes in the data, with one class surrounding the other. 50 nearest-neighbors were used to estimate the local metrics. Shown are the resulting metrics used to form 15-nearest-neighborhoods.

### 13.5.1 Global Dimension Reduction for Nearest Neighbours

The discriminant-adaptive nearest-neighbor method carries out local dimension reduction, that is, dimension reduction separately at each query point. In many problems we can also benefit from global dimension reduction, that is, apply a nearest-neighbor rule in some optimally chosen subspace of the original feature space.

At each training point  $x_i$ , the between-centroids sum of squares matrix  $B_i$  is computed, and then these matrices are averaged over all training points:

$$\bar{B} = \frac{1}{N} \sum_{i=1}^N B_i \quad (13.2)$$

Let  $e_1, \dots, e_p$  be the eigenvectors of the matrix  $B$  decreasingly ordered. These eigenvectors span the optimal subspaces for global subspace reduction. The rank- $L$  approximation to  $\bar{B}$  is:

$$\bar{B}_L = \sum_{\ell=1}^L \theta_\ell e_\ell e_\ell^T \quad (13.3)$$

and it solves the least squares problem

$$\min_{\text{rank}(M)=L} \sum_{i=1}^N \text{trace} [(B_i - M)^2] \quad (13.4)$$

$B_i$  contains information on the local discriminant subspace and the strength of discriminant in that subspace, it can be seen as a way of finding the best approximating subspace of dimension  $L$  to a series of  $N$  subspaces by weighted least squares.

For example, when some eigenvalues turn out to be large (having eigenvectors nearly spanning the interesting subspace), and the remaining six are near zero, we project the data into the leading four-dimensional subspace, and then carry out nearest neighbour classification.

### 13.5.2 Computational considerations

One drawback of nearest-neighbour is the computational load, both in finding the neighbours and storing the entire training set.

Reducing the storage requirements is difficult, and various editing and condensing procedures have been proposed. The idea is to isolate a subset of the training set that suffices for nearest-neighbour predictions, and throw away the remaining training data. Intuitively, it seems important to keep the training points that are near the decision boundaries and on the correct side of those boundaries, while some points far from the boundaries could be discarded. The multi-edit algorithm of Devijver and Kittler (1982) divides the data cyclically into training and test sets, computing a nearest neighbour rule on the training set and deleting test points that are misclassified. The idea is to keep homogeneous clusters of training observations.

The condensing procedure of Hart (1968) goes further, trying to keep only important exterior points of these clusters. Starting with a single randomly chosen observation as the training set, each additional data item is processed one at a time, adding it to the training set only if it is misclassified by a nearest-neighbour rule computed on the current training set.

## 14 Unsupervised learning

In unsupervised learning one is given  $N$  observations  $x_1, x_N$  of a random  $p$ -vector  $X$  having joint density  $\Pr(X)$ . The goal is to directly infer the properties of this probability density without the help of a supervisor providing correct answers or degree of error.

The dimension of  $X$  is sometimes much higher than in supervised learning, and the properties of interest are often more complicated than simple location estimates. These factors are somewhat mitigated by the fact that  $X$  represents all of the variables under consideration; one is not required to infer how the properties of  $\Pr(X)$  change, conditioned on the changing values of another set of variables.

In the context of unsupervised learning, there is no such direct measure of success. It is difficult to ascertain the validity of inferences drawn from the output of most unsupervised learning algorithms. One must resort to heuristic arguments not only for motivating the algorithms, as is often the case in supervised learning as well, but also for judgements as to the quality of the results.

## 14.1 Association rule

The goal is to find joint values of the variables  $X = (X_1, X_2, \dots, X_p)$  that appear most frequently in the data base. It is mostly applied to binary-valued data  $X_j = \{0, 1\}$ , where it is referred to as **Market basket analysis**. In this context the observations are sales transactions, such as those occurring at the checkout counter of a store. The variables represent all of the items sold in the store. For observation  $i$ , each variable  $X_j$  is assigned 1 if the item is purchased, 0 otherwise.

More generally, the basic goal of association rule analysis is to find a collection of prototype  $X$ -values  $v_1, \dots, v_L$  for the feature vector  $X$ , such that the probability density  $\Pr(v_l)$  evaluated at each of those values is relatively large. This basically means find any kind of pattern that tells us how things go together. In this way the problem can be seen as **mode finding** or **bump hunting**.

A natural estimation of  $\Pr(v_l)$  is the number of occurrences for which  $X = v_l$ . With a large number of variables however, such observations will be too few to be reliable. The problem can be restated in another way.

Instead of seeking the values  $x$  where  $\Pr(x)$  is large, one seeks region of the  $X$ -space with high probability content relative to their size or support.

**Definition 14.1. Support** The support  $S_j$  of a variable  $j$  is the set of all possible values for the variable.

Let  $S_j$  represent the set of all possible values of the  $j$ -th variable (its support) and let  $s_j \subseteq S_j$  be a subset of these values. The modified goal can be stated as attempting to find subsets of variable values  $s_1, \dots, s_p$  such that the probability of each of the variables is simultaneously assuming a value within its respective subset

$$\Pr \left[ \bigcap_{j=1}^p (X_j \in s_j) \right] \quad (14.1)$$

is relatively large.  $\bigcap_{j=1}^p (X_j \in s_j)$  is the intersection of subsets and it is called **conjunctive rule**.

### 14.1.1 Market basket analysis

For commercial databases  $p \sim 10^4$ ,  $N \sim 10^8$ . In this cases many existing algorithm are not feasible and market basket analysis is applied.

Some simplifications are required: either  $s_j$  consists of a single value of  $X_j$  ( $s_j = v_{0j}$ ), or it consists of the entire set of values of  $X_j$  ( $s_j = S_j$ ). So this simplifies to the problem of identifying the subset for which  $s_j$  is a single value and this set is named  $\mathcal{J} \subset \{1, \dots, p\}$  and for each element in this subset find the corresponding value  $v_{0j}$  such that:

$$\Pr \left[ \bigcap_{j \in \mathcal{J}} (X_j = v_{0j}) \right] \quad (14.2)$$

is large.

One can apply the technique of dummy variables to turn 14.4 into a problem involving only binary-valued variables. Here we assume that the support  $S_j$  is finite for each variable  $X_j$ . Specifically, a new set of variables  $Z_1, \dots, Z_K$  is created, one such variable for each of the values  $v_{lj}$  attainable by each of the original variables  $X_1, \dots, X_p$ . The number of dummy variables  $K$  is

$$K = \sum_{j=1}^p |\mathcal{S}_j| \quad (14.3)$$

where  $|\mathcal{S}_j|$  is the number of distinct values attainable by  $X_j$ . Each dummy variable is assigned the value  $Z_k = 1$  (with  $Z_k$  being associated to  $v_{lj}$ ), if the variable with which it is associated takes on the corresponding value to which  $Z_k$  is assigned (i.e.,  $Z_k$  is associated with  $v_{lj}$ ;  $Z_k = 1$  if  $X_j = v_{lj}$ ), and  $Z_k = 0$  otherwise. This corresponds to find a subset of integers  $\mathcal{K} \subset \{1, \dots, K\}$  such that:

$$\Pr \left[ \bigcap_{k \in \mathcal{K}} (Z_k = 1) \right] = \Pr \left[ \prod_{k \in \mathcal{K}} Z_k = 1 \right] \quad (14.4)$$

is large.

This is the standard formulation of the market basket problem. The set  $K$  is called an **item set**. The number of variables  $Z_k$  in the item set is called its "size" (note that the size is no bigger than  $p$ ).

The estimated value of the previous expression is taken to be the fraction of observations in the database for which the conjunction is true:

$$\hat{\Pr} \left[ \bigcap_{k \in \mathcal{K}} (Z_k = 1) \right] = \frac{1}{N} \sum_{i=1}^N \prod_{k \in \mathcal{K}} z_{ik} \quad (14.5)$$

where  $z_{ik}$  is the value of  $Z_k$  in the  $i$ -th case. This is called support or prevalence  $T(\mathcal{K})$  if the item-set  $\mathcal{K}$ .

In association rule, a lower support bound  $t$  is specified and one seeks all sets  $\mathcal{K}_l$  that can be formed from the variables  $Z_k$  with support in the data base greater than this lower bound  $t$ .

#### 14.1.2 Apriori algorithm

For a given support threshold  $t$  The cardinality  $|\{\mathcal{K}|T(\mathcal{K})\}|$  is relatively small. Any item set consisting of a subset of the items  $\mathcal{K}$  must have support greater than or equal to that of  $\mathcal{K}$ :  $\mathcal{L} \subseteq \mathcal{K} \Rightarrow T(\mathcal{L}) \geq T(\mathcal{K})$ .

The first pass over the data computes the support of all single-item sets. Those whose support is less than the threshold are discarded. The second pass computes the support of all item sets of size two that can be formed from pairs of the single items surviving the first pass. Each successive pass over the data considers only those item sets that can be formed by combining those that survived the previous pass with those retained from the first pass. Passes over the data continue until all candidate rules from the previous pass have support less than the specified threshold.

The items  $Z_k$ ,  $k \in K$ , are partitioned into two disjoint subsets,  $A \cup B = K$ , and written  $A \Rightarrow B$ .  $A$  is called antecedent and  $B$  consequent.

Association rules are defined to have several properties based on the prevalence of the antecedent and consequent item sets in the data base. The support of the rule  $T(A \Rightarrow B)$  is the fraction of observations in the union of the antecedent and consequent, which is just the support of the item set  $K$  from which they were derived. It can be viewed as an estimate of the probability of simultaneously observing both item sets  $\Pr(A \text{and } B)$  in a randomly selected market basket. The "confidence" or "predictability"  $C(A \Rightarrow B)$  of the rule is its support divided by the support of the antecedent:

$$C(A \Rightarrow B) = \frac{T(A \Rightarrow B)}{T(A)} \quad (14.6)$$

which can be viewed as an estimate  $\text{Pr}(A|B)$ .

The "expected confidence" is defined as the support of the consequent  $T(B)$ , which is an estimate of the unconditional probability  $\text{Pr}(B)$ . Finally, the "lift" of the rule is defined as the confidence divided by the expected confidence:

$$L(A \Rightarrow B) = \frac{C(A \Rightarrow B)}{T(B)} \quad (14.7)$$

This is an estimate of the association measure  $\text{Pr}(A \text{ and } B)/\text{Pr}(A)\text{Pr}(B)$ .

Suppose the item set  $K = \{\text{peanutbutter}, \text{jelly}, \text{bread}\}$  and consider the rule  $\{\text{peanutbutter}, \text{jelly}\} \Rightarrow \{\text{bread}\}$ . A support value of 0.03 for this rule means that peanut butter, jelly, and bread appeared together in 3% of the market baskets. A confidence of 0.82 for this rule implies that when peanut butter and jelly were purchased, 82% of the time bread was also purchased. If bread appeared in 43% of all market baskets then the rule  $\{\text{peanutbutter}, \text{jelly}\} \Rightarrow \{\text{bread}\}$  would have a lift of 1.95.

A confidence threshold  $c$  is set, and all rules that can be formed from those item sets with confidence greater than this value:

$$\{A \Rightarrow B | C(A \Rightarrow B) > c\} \quad (14.8)$$

The output of the entire analysis is a collection of association rules (14.7) that satisfy the constraints:

$$T(A \Rightarrow B) > t \quad \text{and} \quad C(A \Rightarrow B) > c \quad (14.9)$$

## 14.2 Generalized association rule

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## 14.3 Cluster Analysis

The goal is grouping or segmenting a collection of objects into subsets or "clusters", such that those within each cluster are more closely related to one another than objects assigned to different clusters. Objects can be described by a set of measurements, or by relations to other objects. In addition, the goal is sometimes to arrange the clusters into a natural hierarchy. This involves successively grouping the clusters themselves.

A clustering method attempts to group the objects based on the definition of similarity supplied to it.

K-means clustering starts with guesses for the three cluster centers. Then it alternates the following steps until convergence:

- for each data point, the closest cluster center (in Euclidean distance) is identified;
- each cluster center is replaced by the coordinate-wise average of all data points that are closest to it.

This is a top-down procedure.

#### 14.3.1 Proximity Matrices and dissimilarities

In social science experiments, participants are asked to judge by how much certain objects differ from one another. Dissimilarities can then be computed by averaging over the collection of such judgements.

This type of data can be represented by an  $N \times N$  matrix  $D$ , where  $N$  is the number of objects, and each element  $d_{ii'}$  records the proximity between the  $i$ -th and  $i'$ -th objects. Most algorithms use  $d_{ii} = 0$  and non negative weights.

Some algorithms require a dissimilarity matrix. Given  $d_j(x_{ij}, x_{i'j})$  a dissimilarity between values of the  $j$ -the attribute, we define the dissimilarity between objects  $i$  and  $i'$  as:

$$D(x_i, x_{i'}) = \sum_{j=1}^p d_j(x_{ij}, x_{i'j}) \quad (14.10)$$

Most likely  $d_j$  is the squared distance. For quantitative variables other common choice are the absolute error or correlation:

$$\rho(x_i, x_{i'}) = \frac{\sum_j (x_{ij} - \bar{x}_i)(x_{i'j} - \bar{x}_i)}{\sqrt{\sum_j (x_{ij} - \bar{x}_i)^2 (x_{i'j} - \bar{x}_i)^2}} \quad (14.11)$$

**Ordinal variables** are often represented as contiguous integers. Examples are academic grades (A, B, C, D, E, F), degree of preference and so on.

**Categorical or nominal variables** one can build a symmetric matrix with  $M$  values s.t.  $L_{ij} = L_{ji} \geq 0$  and  $L_{ii} = 0$ . A popular choice is  $L_{ii} = 0$ .

To calculate **dissimilarity between objects** generally a weighted average is used:

$$D(x_i, x_{i'}) = \sum_{j=1}^p w_j d_j(x_{ij}, x_{i'j}) \quad (14.12)$$

Let us define the average dissimilarity on the j-th attribute as:

$$\bar{d}_j = \frac{1}{N^2} \sum_{i=1}^N \sum_{i'=1}^N d_j(x_{ij}, x_{i'j}) \quad (14.13)$$

We might define  $w_j \sim \frac{1}{d_j}$  would give all attributes equal influence in characterizing overall dissimilarity between objects. In general, setting  $w_j = \frac{1}{d_j}$  for all attributes, irrespective of type, will cause each one of them to equally influence the overall dissimilarity between pairs of objects. However, if the goal is to segment the data into groups of similar objects, all attributes may not contribute equally to the (problem-dependent) notion of dissimilarity between objects.

### 14.3.2 Combinatorial Algorithms

Combinatorial algorithms work directly on the observed data with no direct reference to an underlying probability model. They assign each observation to a group or cluster without regard to a probability model describing the data. Each observation is uniquely labeled by an integer  $i \in \{1, \dots, N\}$ .

A prespecified number of clusters  $K < N$  is assumed. Each observation is assigned to one and only one cluster. Given the dissimilarities between every pair of observations we want to assign each point to a cluster by the algorithm outputting a value corresponding to the cluster.

One approach is to directly specify a mathematical loss function and attempt to minimize it through some combinatorial optimization algorithm. Since the goal is to assign close points to the same cluster, a natural loss (or "energy") function would be:

$$W(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(i')=k} d(x_i, x_{i'}) \quad (14.14)$$

where  $C(i) = k$  is an encoder assigning someway the point  $i$  to the class  $k$ . This criterion characterizes the extent to which observations assigned to the same cluster tend to be close to one another.

$W(C)$  is referred to as **within-cluster point scatter** while

$$B(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(i') \neq k} d(x_i, x_{i'}) \quad (14.15)$$

as the **between-cluster point scatter** and

$$T = \frac{1}{2} \sum_{i=1}^N \sum_{i'=1}^N d_{ii'} = W(C) + B(C) = \text{const} \quad (14.16)$$

is the **total point scatter** which is a constant given the data.  $B(C)$  tends to be large when observations assigned to different clusters are far apart. So we have  $W(C) = T - B(C)$  minimizing  $W(C)$  is equivalent to maximizing  $B(C)$ .

Such optimization by complete enumeration is feasible only for very small data sets. The number of distinct assignments is

$$S(N, K) = \frac{1}{K!} \sum_{k=1}^K (-1)^{K-k} \binom{K}{k} k^N \quad (14.17)$$

For example,  $S(10, 4) = 34105$  which is still feasible, but  $S(19, 4) \approx 10^{10}$ . For this reason, practical clustering algorithms are able to examine only a very small fraction of all possible encoders  $k = C(i)$ . The goal is to identify a small subset that is likely to contain the optimal one, or at least a good suboptimal partition. Such feasible strategies are based on iterative greedy descent.

### 14.3.3 K-means

The K-means algorithm is one of the most popular iterative descent clustering methods. It is intended for situations in which all variables are of the quantitative type, and squared Euclidean distance. The within-point scatter

can be written as:

$$W(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(i')=k} |x_i - x_{i'}|^2 = \sum_{k=1}^K N_k \sum_{C(i)=k} |x_i - \bar{x}_k|^2$$

$$N_k = \sum_{i=1}^N I(C(i) = k)$$
(14.18)

where  $\bar{x}_k$  is the mean vector associated with the  $k$ th-cluster. So the  $N$  observations are assigned in a way such that within each cluster the average dissimilarity of the observations from the cluster mean is minimized.

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#### **Algorithm 4:** K-means algorithm

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For a given cluster assignment  $C$ , the total cluster variance is minimized w.r.t.  $m_1, \dots, m_K$ , yielding the means of the currently assigned clusters;

Given a current set of means the total cluster variance is minimized by assigning each observation to the closest cluster mean:

$$C(i) = \arg \min_{1 \leq k \leq K} |x_i - m_k|^2;$$

Iterate the previous steps until assignment do not change.

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#### 14.3.4 Gaussian Mixtures as Soft K-means Clustering

The K-means clustering procedure is closely related to the EM algorithm for estimating a certain Gaussian mixture model. The E-step of the EM algorithm assigns "responsibilities" for each data point based in its relative density under each mixture component, while the M-step recomputes the component density parameters based on the current responsibilities. Suppose we specify  $K$  mixture components, each with a Gaussian density having scalar covariance matrix  $\sigma^2 \mathbf{I}$ . Then the relative density under each mixture component is a monotone function of the Euclidean distance between the data point and the mixture center. Hence in this setup EM is a "soft" version of K-means clustering, making probabilistic (rather than deterministic) assignments of points to cluster centres. With  $\sigma^2 \rightarrow 0$  the models coincide.

## 14.4 Vector quantization

Used in image processing to compress images at a cost of loss in quality. VQ breaks the image into small blocks of pixels  $2 \times 2$  for example. Suppose the image is  $1024 \times 1024$  pixels, then we get  $512 \times 512$  blocks of four pixels, i.e. a vector in  $\mathcal{R}^4$ . A k-means clustering algorithm is run in this space. Each block is approximated with its closest cluster, known as codeword. The bigger K the less lossy is the compression, and it is big enough we can achieve a lossless compression. The clustering process is called the encoding step, and the collection of centroids is called the codebook. To name and identify the codebook entries approximating the blocks will require  $\log_2(K)$  bits per block. We also need to supply the codebook itself, which is  $K \times 4$  real numbers.

### 14.4.1 K-medoids

Squared Euclidean distance places the highest influence on the largest distances. This causes the procedure to lack robustness against outliers that produce very large distances. In the most common form, centres for each cluster are restricted to be one of the observations assigned to the cluster. This algorithm assumes attribute data, but the approach can also be applied to data described only by proximity matrices.

### 14.4.2 Number of cluster

Suggestions range from simple random selection to a deliberate strategy based on forward stepwise assignment. At each step a new center  $i_k$  is chosen to minimize the given criterion, given the centres  $i_1, \dots, i_{k-1}$  chosen at the previous steps. This continues for K steps, thereby producing K initial centres with which to begin the optimization algorithm.

For data segmentation K is usually defined as part of the problem. For example, a company may employ K sales people, and the goal is to partition a customer database into K segments, one for each sales person, such that the customers assigned to each one are as similar as possible.

In other cases it must be estimated typically by examining the within-cluster dissimilarity  $W_K$  as a function of the number of clusters K. Separate solutions are obtained for  $K \in \{1, \dots, K_{\max}\}$ . Generally  $W_k$  decreases with increasing K, even when the criterion is evaluated on an independent test set.

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**Algorithm 5:** K-medoids

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For a given cluster assignment  $C$  find the observation in the cluster minimizing total distance to other points in that cluster:

$$i_k^* = \arg \min_{\{i: C(i)=k\}} \sum_{C(i')=k} D(x_i, x_{i'}) \quad (14.19)$$

Then  $m_k = x_{i_k^*}$ ,  $k = 1, \dots, K$  are the current estimates of the cluster centres;

Given a current set of clusters centres  $\{m_1, \dots, m_K\}$  minimize the total error by assigning each observation to the closest current cluster centre:

$$C(i) = \arg \min_{1 \leq k \leq K} D(x_i, m_k) \quad (14.20)$$

;

Iterate the previous steps until the assignment do not change.

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#### 14.4.3 Hierarchical clustering

Hierarchical clustering methods require the user to specify a measure of dissimilarity between (disjoint) groups of observations, based on the pairwise dissimilarities among the observations in the two groups. They produce hierarchical representations in which the clusters at each level of the hierarchy are created by merging clusters at the next lower level. At the lowest level, each cluster contains a single observation. At the highest level there is only one cluster containing all of the data.

Strategies for hierarchical clustering divide into two basic paradigms: agglomerative (bottom-up, ) and divisive (top-down).

In agglomerative methods, the pair chosen for merging consist of the two groups with the smallest intergroup dissimilarity. For divisive-methods, the split is chosen to produce two new groups with the largest between-group dissimilarity. With both paradigms there are  $N - 1$  levels in the hierarchy.

Recursive binary splitting/agglomeration can be represented by a rooted binary tree.

#### 14.4.4 Agglomerative clustering

Agglomerative clustering algorithms begin with every observation representing a singleton cluster. At each of the  $N - 1$  steps the closest two (least dissimilar) clusters are merged into a single cluster, producing one less cluster at the next higher level. Therefore, a measure of dissimilarity between two clusters (groups of observations) must be defined.

Given two groups  $G$  and  $H$  and two observations  $i \in G, i' \in H$  the pairwise observation dissimilarity between these two points is  $d_{ii'}$ . The dissimilarity bbtw  $G$  and  $H$  is computed from the set of all dissimilarities.

**Single linkage** agglomerative clustering takes the intergroup dissimilarity to be that of the closest (least dissimilar) pair:

$$D_{SL} = \min_{i \in G, i' \in H} d_{ii'} \quad (14.21)$$

This is often called **nearest neighbour technique**. **Complete linkage** agglomerative clustering takes the intergroup dissimilarity to be that of the furthest pair (most dissimilar pair):

$$d_{CL}(G, H) = \max_{i \in G, i' \in H} d_{ii'} \quad (14.22)$$

**Group average** clustering uses the average:

$$d_{GA} = \frac{1}{N_G N_H} \sum_{i \in G} \sum_{i' \in H} \quad (14.23)$$

where  $N$  are the num. observations in each group. If the data dissimilarities exhibit a strong clustering tendency, with each of the clusters being compact and well separated from others, then all three methods produce similar results.

Single linkage only requires that a single dissimilarity be small for two groups to be considered close together, irrespective of the other observation dissimilarities between the groups. It will therefore have a tendency to combine, at relatively low thresholds, observations linked by a series of close intermediate observations. This phenomenon, referred to as **chaining**, is often considered a defect of the method.

Complete linkage represents the opposite extreme. Two groups  $G$  and  $H$  are considered close only if all of the observations in their union are relatively similar. It will tend to produce compact clusters with small diameters.

However, it can produce clusters that violate the "closeness" property. That is, observations assigned to a cluster can be much closer to members of other clusters than they are to some members of their own cluster. Group average clustering represents a compromise between the two extremes of single and complete linkage. It attempts to produce relatively compact clusters that are relatively far apart. However, its results depend on the numerical scale on which the observation dissimilarities are measured.

#### 14.4.5 Divisive clustering

The divisive paradigm can be employed by recursively applying any of the combinatorial methods such as K-means or K-medoids , with  $K = 2$ , to perform the splits at each iteration.

A better approach is by Smith et. al(1965). It begins by placing all observations in a single cluster G. It then chooses that observation whose average dissimilarity from all the other observations is largest. This observation forms the first member of a second cluster H. At each successive step that observation in G whose average distance from those in H, minus that for the remaining observations in G is largest, is transferred to H. This continues until the corresponding difference in averages becomes negative. That is, there are no longer any observations in G that are, on average, closer to those in H.

#### 14.4.6 Self-organizing maps

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### 14.5 Principal components, curves and surfaces

The principal components of a set of data in  $\mathcal{R}^p$  provide a sequence of best linear approximations to that data, of all ranks  $q \leq p$ . Given the observations  $x_1, \dots, x_N$ , the linear approximation is:

$$f(\lambda) = \mu + \mathbf{V}_q \lambda \quad (14.24)$$

where  $\mathbf{V}_q$  is a  $p \times q$  matrix with  $q$  orthogonal unit vectors as columns,  $\lambda$  a  $q$  vector of parameters and  $\mu$  a location vector in  $\mathcal{R}^p$ . This is  $p$  hyperplane.

Fitting such a model corresponds to minimize the reconstruction error:

$$\min_{\mu, \{\lambda_i\}, \mathbf{V}_q} \sum_{i=1}^N \|x_i - \mu - \mathbf{V}_q \lambda_i u\|^2 \quad (14.25)$$

We can partially optimize to obtain:

$$\begin{aligned} \hat{\mu} &= \bar{x} \\ \hat{\lambda}_i &= \mathbf{V}_q^T (x_i - \bar{x}) \end{aligned} \quad (14.26)$$

so we must find the matrix  $\mathbf{V}_q$ :

$$\min_{\mathbf{V}_q} \sum_{i=1}^N \|(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})\|^2 \quad (14.27)$$

For convenience we assume  $\bar{x} = 0$ , if not true then one replaces with  $\tilde{x}_i = x_i - \bar{x}$ . The matrix

$$\mathbf{H}_q = \mathbf{V}_q \mathbf{V}_q^T \quad (14.28)$$

is a projection matrix so that each point  $x_i$  is mapped onto its rank-q reconstruction  $\mathbf{H}_q x_i$ , the orthogonal projection of  $x_i$  spanned by the columns  $\mathbf{V}_q$ .

Consider the matrix  $\mathbf{X} = (x_1^T, \dots, x_N^T)$  of the observations and perform the singular value decomposition:

$$\mathbf{X} = \mathbf{U} \mathbf{D} \mathbf{V}^T \quad (14.29)$$

$\mathbf{U}$  is a  $N \times p$  orthogonal matrix  $\mathbf{U}^T \mathbf{U} = \mathbf{I}_p$  whose columns  $u_j$  are called **left singular vectors**.  $\mathbf{V}$  is a  $p \times p$  orthogonal matrix ( $\mathbf{V}^T \mathbf{V} = \mathbf{I}_p$ ) with columns  $v_j$  called the **right singular vectors**.  $\mathbf{D}$  is a diagonal  $p \times p$  matrix with  $d_1 \geq d_2 \geq \dots \geq d_p \geq 0$  known as **singular values**.

For each rank  $q$ , (i.e., the chosen dimensionality on which the observations are projected), the solution  $\mathbf{V}_q$ , consists of the first  $q$  columns of  $\mathbf{V}$ . The columns  $\mathbf{U} \mathbf{D}$  are called the **principal components** of  $\mathbf{X}$ . The  $N$  optimal  $\hat{\lambda}_i$  are given by the first  $q$  principal components (the  $N$  rows of the  $N \times q$  matrix  $\mathbf{U}_q \mathbf{D}_q$ ).

14.1 shows the one-dimensional principal component line in a  $\mathcal{R}^2$  input space ( $p = 2$ ,  $q = 1$ ). For each observation point  $x_i$  there is a closest point on the line given by  $u_{i1} d_1 v_1$  where  $v_1$  is the direction of the line ( $v_1$  is  $p = 2$  dimensional vector).  $\hat{\lambda}_1 = d_{i1} d_1$  measures distance along the line from the origin.

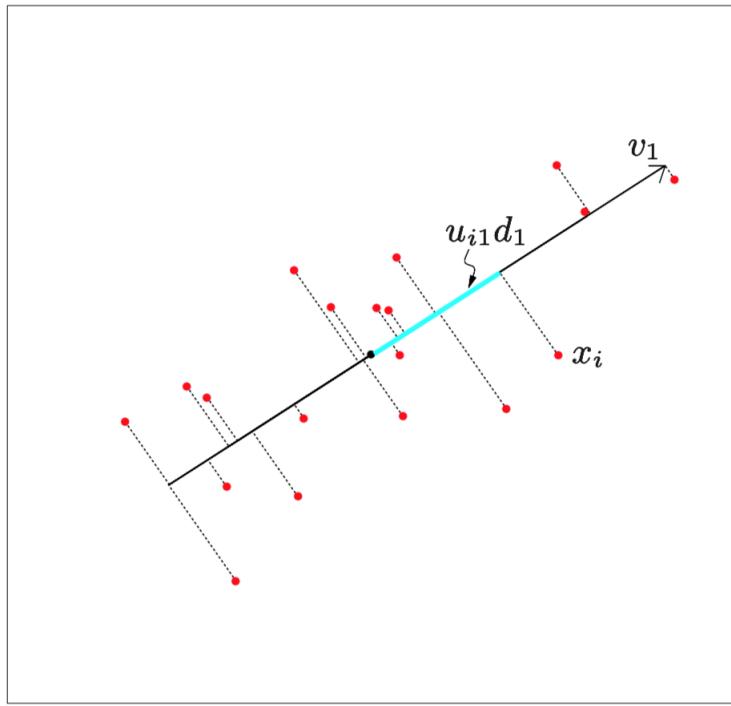


Figure 14.1: Example of SVD mapping of data from a  $\mathcal{R}^2$  space (i.e., a plane) onto a line  $\mathcal{R}$

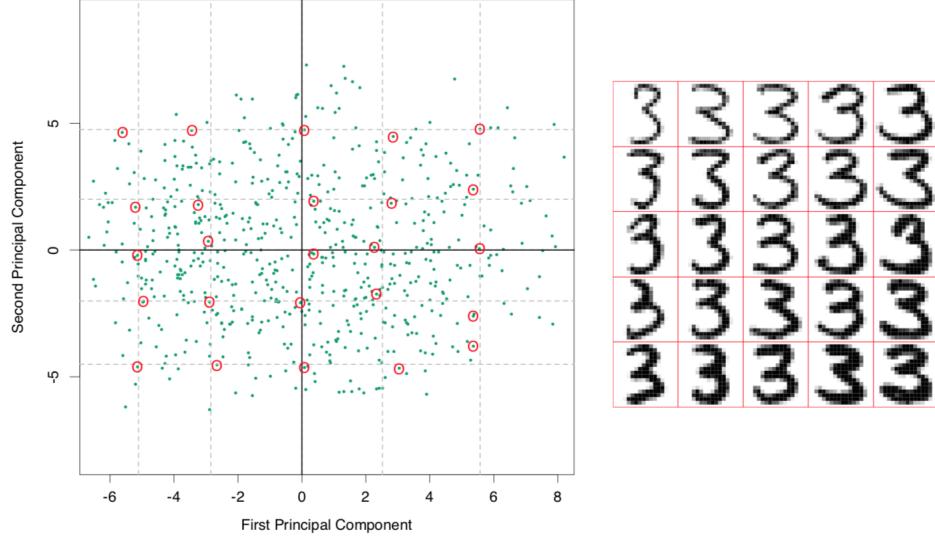


Figure 14.2: 2 Principal components analysis applied on the 3 hand-written digits.

#### 14.5.1 Applications

Principal components are a useful tool for dimension reduction and compression, for example for hand-written digits. If the inputs are  $16 \times 16$  images, inputs rely in a  $\mathcal{R}^{256}$  space.

Consider PCA on hand-written digits of a single number, for example a 3, and perform two principal components analysis  $u_{i1}d_1$  and  $u_{i2}d_2$  of each observation and calculate the quantiles 5%, 25%, 50%, 75%, 95% indicated by the grid in 14.2. Red circles indicate those images close to the vertices of the grid where distance is in terms of the projected coordinates (but some weight is given to the components in the orthogonal space (?)). On the right of 14.2 the images corresponding to the red circles are shown and this allows to visualize the nature of the first two PC.  $v_1$ , the horizontal direction, mainly accounts for the length of lower "tail" of the "3",  $v_2$  the vertical axis accounts for character thickness. The parametrized model is:

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2 \quad (14.30)$$

that in terms of images is something like the one in 14.3.

Although there are approximately 256 principal components,

$$= \boxed{3} + \lambda_1 \cdot \boxed{3} + \lambda_2 \cdot \boxed{3}.$$

Figure 14.3: Equivalence of the non-parametric model using image representation.

50 account for 90% of the variation in the threes, 12 account for 63%.

A relatively small subset of the principal components serve as excellent lower-dimensional features for representing the high-dimensional data.

The same technique, with some further calculations, can be applied to digital signature.