Lecture 1

Regression

- The task of finding the relationship *(mathematical function)* between one or more numerical inputs *(independent variables)* and one or more numerical outputs *(dependent variables)*

- Curve fitting

    - Given a set of points, try ot learn a function to describe them
    - Given a value x, we can predict the corresponding value y
    - Not just for straight line fitting

Simple example

Let us consider a simple *linear* example with 1 independent variable, x & 1 dependent variable, y

(1)

$$D = {(x_1,y_1),...,(x_n,y_n)} = {(x_i,y_i)}_{i=1}^N$$

Model the relationship between x and y with the function $f(\textbf{w},x)$, s.t $y_i \approx f(\textbf{w},x_i)$ Measurements of y, subject ot noise are defined by,

(2)

$$y_i = f(\textbf{w},w) + \epsilon$$

Where ϵ is a random number drawn from some continuous probability density function. Goal is to find some $\textbf{w}$ that solves, or provides the best approximation to the above equation.

First, let us approach this as a optimisation problem in which the objective is to find the value of **w** (denoted **w***) that minimises some *loss* or objective function $L(\textbf{w})$

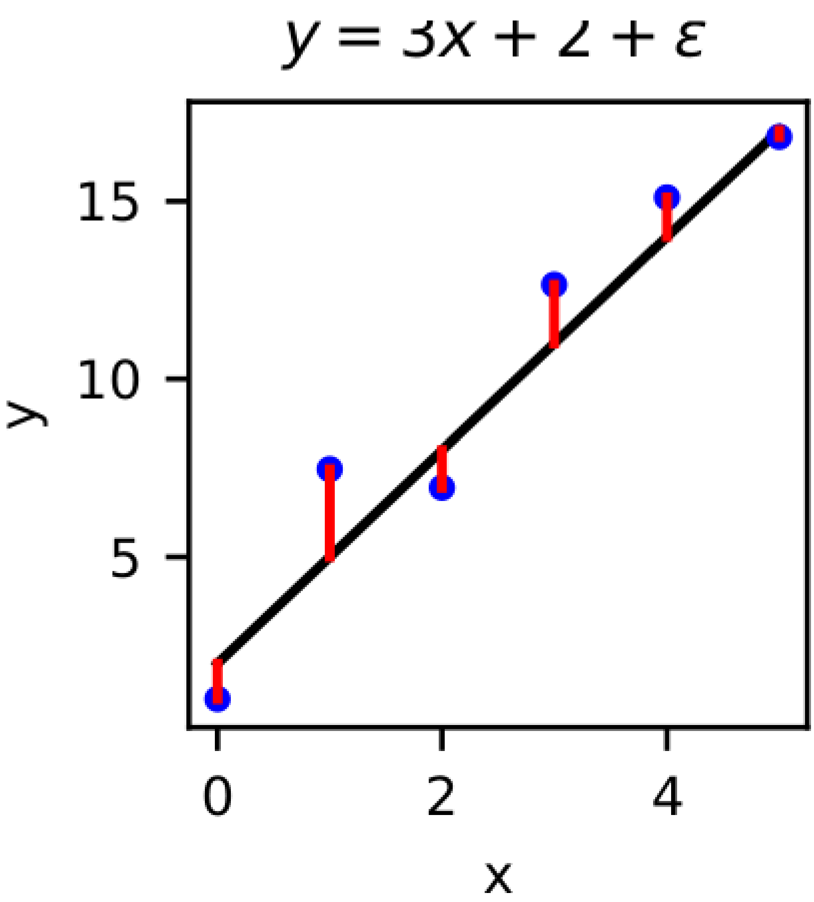
(3)

$$\textbf{w}* = \argmin_w L(\textbf{w}) $$

Intuitively, $L(\textbf{w})$ should be designed to capture the difference between the data and the predictions of the model, and seek to minimise this. One common choice for $L(\textbf{w})$ is *least-squares error*. Given our dataset D and modelling function $f(\textbf{w},x)$, we construct $\forall d \in D$ a residual error defined as:

(4)

$$ r_i(\textbf{w}) = y_i - f(\textbf{w}, x_i)$$



The least squares error *(LSE)* loss function is defined in terms of residuals as:

(5)

$$ L_{LSE}(\textbf{w}) = \sum_{i=1}^N r_i^2 = \textbf{r}^T\textbf{r} $$

It is important to note that the above definition implicitly has no upper bound but is restricted to being strictly posive, thus, allowing us to find a minimum value.

(6)

$$\textbf{w}^* = \argmin_\textbf{w} L_{LSE}(\textbf{w})$$

Optimisation is a very difficult problem to solve and so, for now, we resitct ourselves to a specifically *linear* case.

N.B. when we say *linear* we do not reference the problem being of the form "$y = mx + c$" but instead that our problem is linear in it's *unknown parameters*

Linear models take the form:

(7)

$$f(\textbf{w},x) = w_0\phi_0(x) + \cdots + w_{M-1}\phi_{M-1}(x) = \sum_{i=0}^{M-1} w_i\phi_i(x)$$

Our function is a *linear combination* of a set of *basis functions*, ${\phi_i(x) }*{i=0}^{M-1}$ weighted by our free parameters ${w_i}*{i=0}^{M-1}$.

A common choice of basis function is the polynomials ${x^i}_{i=0}^{M-1}$

For a finite set of data points D we can re-write the equation for $f(\textbf{w},x)$ in matrix form by defining a matrix **Φ** with components $\Phi_{ij} = \phi_j(x_i)$ which yields the equation:

(8)

$$f(w) = \Phi w$$

Where the variable x is swallowed by the construction of **Φ** in **f**

Example Φ Construction

For a simple quadratic model $f(\textbf{w},x) = w_0 + w_1x+ w_2x^2$ with basis functions ${x^0,x^1,x^2} = {1,x,x^2}$, we construct:

(9)

$$\boldsymbol{\Phi} = \begin{pmatrix} 1 & x_1 & x_1^2 \ 1 & x_2 & x_2^2 \ \vdots & \vdots & \vdots \ 1 & x_N & x_N^2 \end{pmatrix}$$

We can now begin to solve our equation here. The residuals defined here can be written as:

(10)

$$r = y - \Phi w$$

And our loss function, becomes:

(11)

$$L_{LSE}(\textbf{w}) = (\textbf{y}-\boldsymbol{\Phi}\textbf{w})^T(\textbf{y}-\boldsymbol{\Phi}\textbf{w})$$

As we have observed, L_{LSE} has no upper bound but does have a lower bound. To minimise L_{LSE} we find the point at which $L_{LSE}' = 0$ where L_{LSE}' is it's first derivative with respect to it's free parameters.

If we differentiate L_{LSE} with respect to $\textbf{w}$ we get:

(12)

$$\frac{\delta L_{LSE}(\textbf{w})}{\delta \textbf{w}} = -2 \boldsymbol{\Phi}^T(\textbf{y} - \boldsymbol{\Phi}\textbf{w})$$

For a proof of this, see Iain Style's Notes

Setting this result to 0 we obtain:

(13)

$$\boldsymbol{\Phi}^Ty - \boldsymbol{\Phi}^T\boldsymbol{\Phi}\textbf{w}^*=0$$

This is known as the **normal equations** and are a set of simultaneous linear equations which we can solve for $\textbf{w}^*$

These notes were heavily influenced by those of Dr. Iain Styles, University of Birmingham, School of Computer Science