

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 to 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)

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

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

(2)

$$y_i = f(\mathbf{w}, x_i) + \epsilon_i$$

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

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

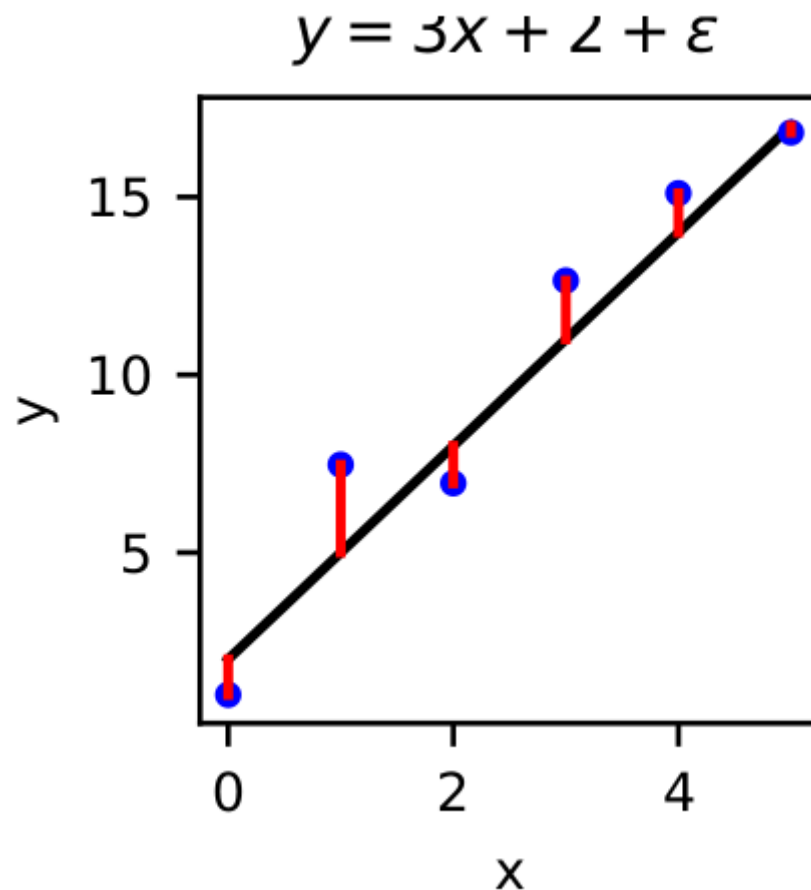
(3)

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} L(\mathbf{w})$$

Intuitively, $L(\mathbf{w})$ 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 $L(\mathbf{w})$ is *least-squares error*. Given our dataset D and modelling function $f(\mathbf{w}, x)$, we construct $\forall d \in D$ a residual error defined as:

(4)

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



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

(5)

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

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

(6)

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} L_{\text{LSE}}(\mathbf{w})$$

Optimisation is a very difficult problem to solve and so, for now, we restrict 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 its *unknown parameters*

Linear models take the form:

(7)

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

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 $f(\mathbf{w}, x)$ in matrix form by defining a matrix Φ with components $\Phi_{ij} = \phi_j(x_i)$ which yields the equation:

(8)

$$\mathbf{f}(\mathbf{w}) = \Phi \mathbf{w}$$

Where the variable x is swallowed by the construction of Φ in \mathbf{f}

Example Φ Construction

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

(9)

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

We can now begin to solve our [equation here](#). The residuals [defined here](#) can be written as:

(10)

$$\mathbf{r} = \mathbf{y} - \Phi \mathbf{w}$$

And our [loss function](#), becomes:

(11)

$$L_{\text{LSE}}(\mathbf{w}) = (\mathbf{y} - \Phi \mathbf{w})^T (\mathbf{y} - \Phi \mathbf{w})$$

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 $L_{\text{LSE}}' = 0$ where L_{LSE}' is it's first derivative with respect to it's free parameters.

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

(12)

$$\frac{\partial L_{\text{LSE}}(\mathbf{w})}{\partial \mathbf{w}} = -2 \Phi^T (\mathbf{y} - \Phi \mathbf{w})$$

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

Setting this result to 0 we obtain:

(13)

$$\mathbf{\Phi}^T \mathbf{y} - \mathbf{\Phi}^T \mathbf{\Phi} \mathbf{w} = 0$$

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

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