Linear Regression

Linear Regression with One Variable

Linear regression is a supervised learning algorithm which aims to model the linear relationship between the continuous dependent variable and independent variable.

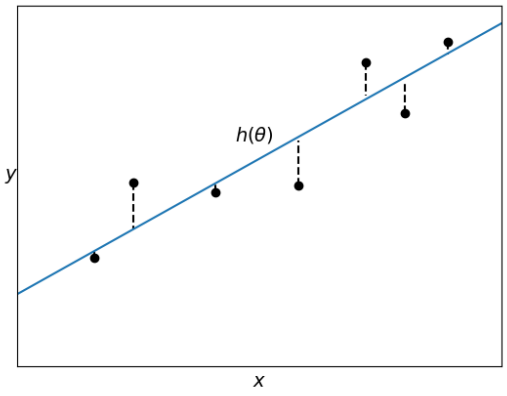


Figure 1: The line $h_\theta(x)$ represents a possible hypothesis function of the linear regression model for this two-dimensional dataset. The dotted lines between the hypothesis function and the samples represent the differences between the actual values (y-coordinate) and the values predicted by the hypothesis function. This can be interpreted as the error in the prediction of a sample value.

The univariate linear regression hypothesis function is

$$h_\theta(x) = \theta_0 + \theta_1 x \tag{1}$$

This can be represented as a line in the xy-plane which intercepts the y-axis at θ_0 and has the gradient θ_1.

The goal in linear regression is to choose the hypothesis function that produces the best fit to the data. This will allow us to make accurate predictions on future samples. In Figure 1 we can see that there are an infinite number of lines with different values of the parameters θ_0 and θ_1 that can be fit to the data, so how do we identify the one that produces the best fit?

We begin with introducing the notation x^i which denotes the feature of the i^{th} training sample. Likewise y^i denotes the y value of the i^{th} training sample.

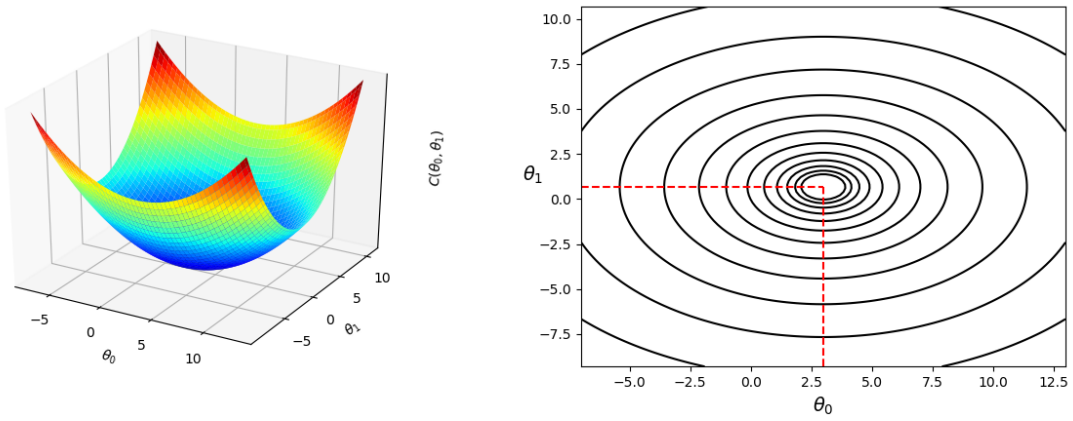
The error between the actual y value of a sample and the predicted value of the sample, $h_\theta(x^i)$, is given by $h_\theta(x^i) - y^i$.

To find the optimal parameters θ_0 and θ_1 we introduce the cost function

$$C(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} [h_\theta(x^i) - y^i]^2 \tag{2}$$

This is the sum of the squared errors for all m samples, divided by twice the number of samples, and is equal to the mean squared error (MSE) multiplied by a factor of $1/2$ (we will see why we have this factor later).

The optimal regression line for the data will be the one that produces the smallest errors between the $h_\theta(x^i)$ and the y^i. We can clearly see that this corresponds to minimising the cost function $C(\theta_0, \theta_1)$.



(a) Cost function surface plot.

(b) Contour plot of the same cost function.

Figure 2: (a) and (b) represent visualisations of the same cost function for some dataset in three and two dimensions, respectively. The minimum of the cost function is located where the dotted lines meet in (b).

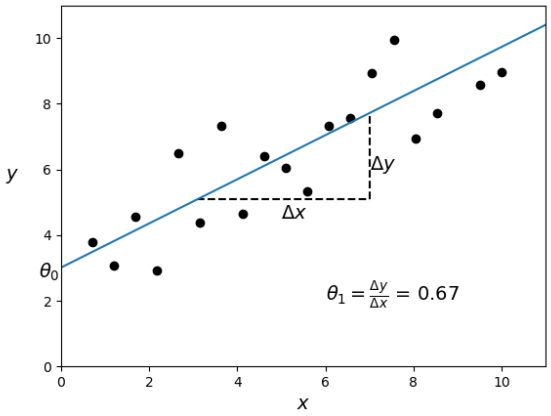


Figure 3: The linear regression model associated with the cost function depicted in Figure 2. Note that the parameters of θ_0 and θ_1 required for the best fit of the hypothesis function (represented by the blue line) to the data correspond to the cost function minimum (Figure 2(b)).

As a function of two variables, θ_0 and θ_1, the cost function represents a two-dimensional surface. It can be shown (see Appendix) that the MSE is always convex in linear regression, and therefore has a global minimum. The cost function, being just the MSE multiplied by a factor, also has these properties. The values of θ_0 and θ_1 at this minimum are the values that produce the hypothesis function with the best fit to the data.

Gradient Descent

So far we have determined that the values of θ_0 and θ_1 that result in an optimal fit of the hypothesis function to the data correspond to the location of the cost function minimum. One of the most common methods for minimising the cost function is gradient descent; the idea being to descend the convex surface of the cost function until the minimum is reached. Repeated steps are taken in the direction opposite to the gradient at the current point, which is the direction of steepest descent.

The gradient vector is given by

$$\boldsymbol{\nabla} C = \begin{pmatrix} \frac{\partial C}{\partial \theta_0} \\ \frac{\partial C}{\partial \theta_1} \end{pmatrix} \tag{3}$$

Starting at the value θ_j we apply the step

$$\theta_j \to \theta_j - \alpha \frac{\partial}{\partial \theta_j}[C(\theta_0, \theta_1)], \quad j = 0, 1 \tag{4}$$

where α is known as the learning rate and determines the size of the step taken. To descend the cost function in the direction opposite to that of the gradient, this step must be implemented simultaneously for θ_0 and θ_1.

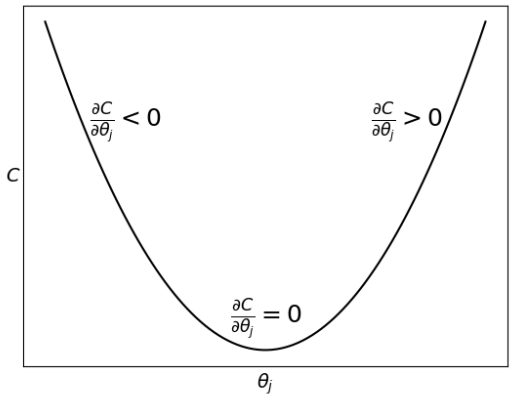


Figure 4: For values of θ_j smaller than the value at the minimum, the rate of change of the cost function with respect to θ_j is negative. For values of θ_j larger than than the value at the minimum, the rate of change is positive, and at the minimum it is equal to zero.

At θ_j, we subtract the partial derivative $\partial C/\partial \theta_j$ (multiplied by α). If the minimum occurs at a value smaller than θ_j then we know from the convex shape of the cost function that $\partial C/\partial \theta_j > 0$ (Figure 4). From equation (4) we can see that this will result in θ_j being reassigned to a smaller value ready for the next iterative step. Conversely, if the minimum occurs at a value larger than θ_j, then $\partial C/\partial \theta_j < 0$, and θ_j will be reassigned to a larger value. Finally, when we are at the minimum, $\partial C/\partial \theta_j = 0$, and no changes are made to θ_j, i.e., gradient descent stops.

Now let's compute the partial derivatives of C:

$$\frac{\partial C}{\partial \theta_0} = \frac{1}{2m}\frac{\partial}{\partial \theta_0}\sum_{i=1}^{m}(\theta_0 + \theta_1 x^i - y^i)^2 = \frac{2}{2m}\sum_{i=1}^{m}(\theta_0 + \theta_1 x^i - y^i) = \frac{1}{m}\sum_{i=1}^{m}[h_\theta(x^i) - y^i] \tag{5}$$

$$\frac{\partial C}{\partial \theta_1} = \frac{1}{2m}\frac{\partial}{\partial \theta_1}\sum_{i=1}^{m}(\theta_0 + \theta_1 x^i - y^i)^2 = \frac{2}{2m}\sum_{i=1}^{m}(\theta_0 + \theta_1 x^i - y^i)x^i = \frac{1}{m}\sum_{i=1}^{m}[h_\theta(x^i) - y^i]x^i \tag{6}$$

It becomes apparent why the MSE was multiplied by 1/2 for the cost function; it cancels out the factor of 2 obtained in the differentation.

Using equations (4), (5), and (6) the gradient descent algorithm becomes

$$\theta_0 \to \theta_0 - \frac{\alpha}{m}\sum_{i=1}^{m}[h_\theta(x^i) - y^i], \qquad \theta_1 \to \theta_1 - \frac{\alpha}{m}\sum_{i=1}^{m}[h_\theta(x^i) - y^i]x^i \tag{7}$$

Multivariable Linear Regression

If we want to model the linear relationship between a dependent variable and more than one independent variables we employ the hypothesis function

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + ... + \theta_n x_n \tag{8}$$

If we define $x_0 = 1$, then we can write

$$h_\theta(x) = \sum_{i=0}^{n} \theta_i x_i = \boldsymbol{\Theta}^T \boldsymbol{X} \tag{9}$$

where

$$\boldsymbol{\Theta} = \begin{pmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{pmatrix}, \qquad \boldsymbol{X} = \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \tag{10}$$

This is the equation of an n-dimensional hyperplane.

The multivariable linear regression cost function takes the same form as in the single variable case

$$C(\theta_0, \theta_1, ..., \theta_n) = \frac{1}{2m} \sum_{i=1}^{m} [h_\theta(x^i) - y^i]^2 \tag{11}$$

To find the best hypothesis for the data we again look to minimise the errors between the $h_\theta(x^i)$ and the y^i, which is equivalent to minimising the cost function. The values of the θ_i obtained will define the hyperplane that is the optimal hypothesis function.

The partial derivatives of C are

$$\frac{\partial C}{\partial \theta_0} = \frac{1}{m} \sum_{i=1}^{m} [h_\theta(x^i) - y^i] \tag{12}$$

and

$$\frac{\partial C}{\partial \theta_j} = \frac{1}{m} \sum_{i=1}^{m} [h_\theta(x^i) - y^i] {x_j}^i, \qquad for \;\; j = 1, 2, ..., n \tag{13}$$

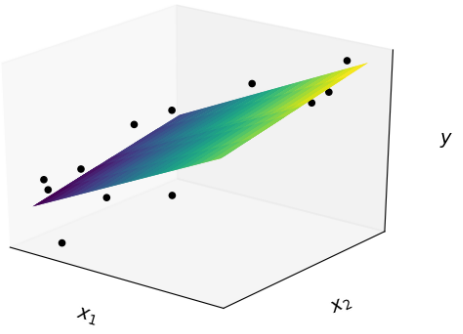


Figure 5: Here we have a dataset with two independent variables, x_1 and x_2. The hypothesis function forms a plane which is chosen to minimise the squared vertical distances between the samples and the plane.

The gradient descent algorithm is

$$\theta_0 \to \theta_0 - \frac{\alpha}{m}\sum_{i=1}^{m}[h_\theta(x^i) - y^i], \qquad \theta_j \to \theta_j - \frac{\alpha}{m}\sum_{i=1}^{m}[h_\theta(x^i) - y^i]{x_j}^i, \quad for\ \ j = 1, 2, ..., n \tag{14}$$

As in the single variable case, these steps must be performed simultaneously for all θ_i, until the minimum is reached.

The Normal Equation

The normal equation is an analytic approach to solving the cost function minimisation problem.

We start by writing a hypothesis column vector containing the hypothesis of each sample. If we have m samples with n features we can create the matrix X with dimensions $(m \times n)$, such that the hypothesis column vector is equal to this matrix multiplied by the column vector $\boldsymbol{\Theta}$:

$$\boldsymbol{h}_\Theta(x) = \begin{pmatrix} h_\theta(x^1) \\ h_\theta(x^2) \\ \vdots \\ h_\theta(x^m) \end{pmatrix} \tag{15}$$

$$= \begin{pmatrix} \theta_0 + \theta_1 {x_1}^1 + \theta_2 {x_2}^1 + \theta_3 {x_3}^1 + ... + \theta_n {x_n}^1 \\ \theta_0 + \theta_1 {x_1}^2 + \theta_2 {x_2}^2 + \theta_3 {x_3}^2 + ... + \theta_n {x_n}^2 \\ \vdots \\ \theta_0 + \theta_1 {x_1}^m + \theta_2 {x_2}^m + \theta_3 {x_3}^m + ... + \theta_n {x_n}^m \end{pmatrix} \tag{16}$$

$$= \begin{pmatrix} \longleftarrow & \mathbf{x}^1 & \longrightarrow \\ \longleftarrow & \mathbf{x}^2 & \longrightarrow \\ & \vdots & \\ \longleftarrow & \mathbf{x}^m & \longrightarrow \end{pmatrix} \begin{pmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{pmatrix} = X\boldsymbol{\Theta} \tag{17}$$

where $\mathbf{x}^i$ is the vector representing the i^{th} sample, and ${x_j}^i$ denotes the j^{th} feature of the i^{th} sample.

If we create a column vector of the y values of the samples

$$\boldsymbol{Y} = \begin{pmatrix} y^1 \\ y^2 \\ \vdots \\ y^m \end{pmatrix} \tag{18}$$

then

$$X\boldsymbol{\Theta} - \boldsymbol{Y} = \begin{pmatrix} h_\theta(x^1) - y^1 \\ h_\theta(x^2) - y^2 \\ \vdots \\ h_\theta(x^m) - y^m \end{pmatrix} \tag{19}$$

Multiplying this vector by its transpose yields

$$\begin{aligned}(X\boldsymbol{\Theta}-\boldsymbol{Y})^T(X\boldsymbol{\Theta}-\boldsymbol{Y}) &= [h_\theta(x^1)-y^1]^2+[h_\theta(x^2)-y^2]^2+...+[h_\theta(x^m)-y^m]^2 \\ &= \sum_{i=1}^{m}[h_\theta(x^i)-y^i]^2\end{aligned}$$

Therefore, the cost function can be expressed as

$$\begin{aligned}C(\boldsymbol{\Theta}) &= \frac{1}{2m}(X\boldsymbol{\Theta}-\boldsymbol{Y})^T(X\boldsymbol{\Theta}-\boldsymbol{Y}) \\ &= \frac{1}{2m}[(X\boldsymbol{\Theta})^T(X\boldsymbol{\Theta})-(X\boldsymbol{\Theta})^T\boldsymbol{Y}-\boldsymbol{Y}^T(X\boldsymbol{\Theta})+\boldsymbol{Y}^T\boldsymbol{Y}] \\ &= \frac{1}{2m}[(X\boldsymbol{\Theta})^TX\boldsymbol{\Theta}-2(X\boldsymbol{\Theta})^T\boldsymbol{Y}+\boldsymbol{Y}^T\boldsymbol{Y}] \qquad (20)\end{aligned}$$

where in the last line we have used the property that the dot product of vectors is symmetric with respect to its arguments, i.e., $(X\boldsymbol{\Theta})^T\boldsymbol{Y}=\boldsymbol{Y}^T(X\boldsymbol{\Theta})$.

The goal is to minimise C and determine $\boldsymbol{\Theta}$. So, first we differentiate the cost function with respect to $\boldsymbol{\Theta}$:

$$\frac{dC}{d\boldsymbol{\Theta}} = \frac{1}{2m}(2X^TX\boldsymbol{\Theta}-2X^T\boldsymbol{Y}) \qquad (21)$$

Next, we set the result equal to zero:

$$0 = \frac{1}{2m}(2X^TX\boldsymbol{\Theta}-2X^T\boldsymbol{Y})$$

$$X^TX\boldsymbol{\Theta} = X^T\boldsymbol{Y} \qquad (22)$$

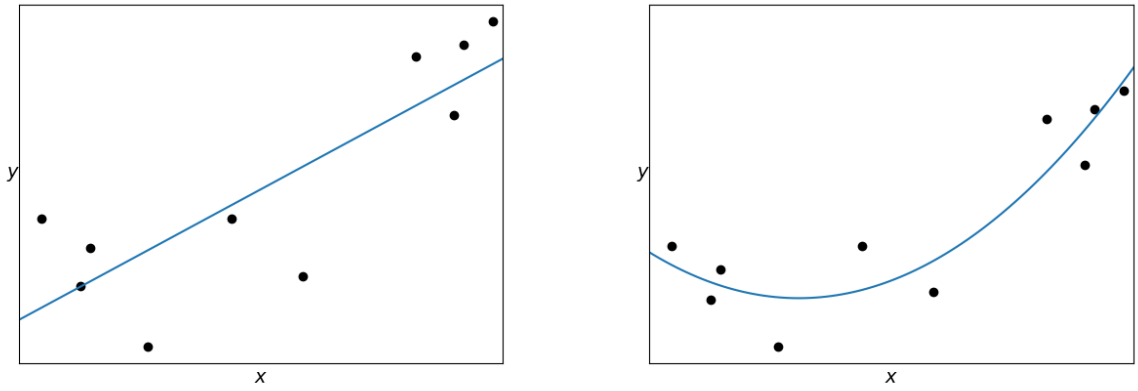
Assuming that there exists a matrix $(X^TX)^{-1}$ such that $(X^TX)^{-1}(X^TX)=I$, i.e., that X^TX is invertible, we obtain the result

$$\boldsymbol{\Theta} = (X^TX)^{-1}(X^T\boldsymbol{Y}) \qquad (23)$$

This is the normal equation, and it can be employed directly to find the θ_i. When the data has few features, using the normal equation is often preferable to gradient descent. However, for large numbers of features, gradient descent is usually the better option. This is because X^TX has the dimensions $(n\times n)$, meaning it becomes more demanding to compute as n increases.

Polynomial Regression

Linear regression can be employed in settings in which the relationship between the dependent variable and the independent variable is non-linear.



(a) Linear regression.

(b) Polynomial regression.

Figure 6: (a) The linear hypothesis function does not provide a good fit to this dataset, which is more suited to a quadratic hypothesis function (b).

The idea of polynomial regression is to use powers of the independent variable x, as additional features in the model. Therefore, the polynomial regression hypothesis function is given by

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + ... + \theta_n x^n \tag{24}$$

Clearly, polynomial regression is a special case of multivariable linear regression.

In Figure 6(a) the linear hypothesis function $h_\theta(x) = \theta_0 + \theta_1 x$ does not fit the data well. In Figure 6(b) we have used the quadratic hypothesis function $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$ which results in an improved fit.

Regularisation

Overfitting is a problem commonly encountered in Machine Learning. It occurs when a model generates an excellent fit to the training data but generalises poorly to the test data. The model learns noise that is not an inherent characteristic of the training data, to the extent that model performance on new data is adversely affected.

In Figure 7 we can see that the hypothesis function, a polynomial of degree 10, fits the training data perfectly. However, compared to the quadratic hypothesis function in Figure 6(b), the performance of the model on new data will be worse, especially at the extremes of the plot where the hypothesis tends to infinities. The problem is that the hypothesis function we are trying to fit is too complex for the data that we have, and as a result noise that is not a fundamental property of the data is learnt. So how do we go about rectifying this issue? In the present case where we have 10 features, we can reproduce the quadratic hypothesis function if we set the coefficients $\theta_3, \theta_4, ..., \theta_{10}$ equal to

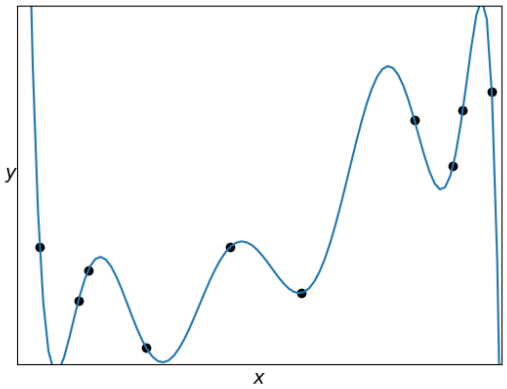


Figure 7: Here we have fitted a polynomial of degree 10 to the data from Figure 6. The hypothesis function passes through all samples, making it a perfect fit, but will the model generalise well to new data?

zero. This is the idea behind regularisation. We add a regularisation term to the cost function that aims to set all the θ_i equal to zero as the cost function is minimised. The only θ_i that remain large are those that are important in the minimisation of the original term in the cost function, i.e., those that ensure the greatest error reductions between the $h_\theta(x^i)$ and the y^i.

The (ridge) regularisation term added to the cost function is $\frac{\lambda}{2m}\sum_{j=1}^{n}{\theta_j}^2$, where λ is the regularisation parameter that determines the severity of the penalty applied to the θ_j. So, our regularised cost function for multivariable linear regression becomes

$$C(\theta_0, \theta_1, ..., \theta_n) = \frac{1}{2m}\left\{\sum_{i=1}^{m}[h_\theta(x^i) - y^i]^2 + \lambda\sum_{j=1}^{n}{\theta_j}^2\right\} \tag{25}$$

Note that the regularisation term is (strictly) convex (see Appendix), and as two or more convex functions added together result in a convex function, the regularised cost function remains convex.

If $\lambda = 0$, there is no regularisation. For increasingly larger values of λ, the parameters $\theta_1, \theta_2, ..., \theta_n$ will be penalised to a greater extent, i.e., they will tend to increasingly small values. If λ is very large then $h_\theta(x) \to \theta_0$, i.e., the hypothesis function will tend to a straight line and the data will be underfitted. This occurs when the hypothesis function is too simple to model the data.

The first term in the cost function aims to find the parameters that produce the best fit between the hypothesis function and the data, with no restriction on the values that the parameters can take or the complexity of the model. The sole goal of the regularisation term is to minimise the parameters, and produce a hypothesis function approximating a straight line. Therefore, the regularised cost function represents a balancing act between model complexity and simplicity. Large parameter values are only tolerated by the regularisation term if they make significant contributions to the reduction of the first term when the cost function is minimised.

$\partial C/\partial\theta_0$ remains unchanged with the addition of the regularisation term as the index j begins at 1. However, $\partial C/\partial\theta_j$ must be computed again:

$$\frac{\partial C}{\partial\theta_j} = \frac{1}{m}\left\{\sum_{i=1}^{m}[h_\theta(x^i) - y^i]{x_j}^i + \lambda\theta_j\right\}, \qquad for\ \ j = 1, 2, ..., n \tag{26}$$

As a consequence the gradient descent algorithm becomes

$$\theta_0 \to \theta_0 - \frac{\alpha}{m}\sum_{i=1}^{m}[h_\theta(x^i) - y^i], \qquad \theta_j \to \theta_j - \frac{\alpha}{m}\left\{\sum_{i=1}^{m}[h_\theta(x^i) - y^i]{x_j}^i + \lambda\theta_j\right\}, \quad for \;\; j = 1, 2, ..., n \tag{27}$$

where as usual, the steps are repeated simultaneously for all θ_i , until the minimum is reached.

References

Ng, A. *Machine Learning.* Offered by Stanford University on Coursera.

Appendix

0.1 The MSE is always convex for linear regression

The MSE for univariate linear regression is

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(\theta_0 + \theta_1 x^i - y^i)^2 \tag{28}$$

Let's discard the $1/m$ factor and define $J^i(\theta_0, \theta_1)$ as the i^{th} term of the sum so that

$$J^i(\theta_0, \theta_1) = (\theta_0 + \theta_1 x^i - y^i)^2 \tag{29}$$

Now we find the second partial derivatives of J^i:

$$\frac{\partial^2 J^i}{\partial \theta_0^2} = 2, \quad \frac{\partial^2 J^i}{\partial \theta_1^2} = 2{x^i}^2, \quad \frac{\partial^2 J^i}{\partial \theta_0 \partial \theta_1} = 2x^i, \quad \frac{\partial^2 J^i}{\partial \theta_1 \partial \theta_0} = 2x^i \tag{30}$$

The Hessian matrix of J^i is

$$H = \begin{pmatrix} \frac{\partial^2 J^i}{\partial \theta_0^2} & \frac{\partial^2 J^i}{\partial \theta_0 \partial \theta_1} \\ \frac{\partial^2 J^i}{\partial \theta_1 \partial \theta_0} & \frac{\partial^2 J^i}{\partial \theta_1^2} \end{pmatrix} = \begin{pmatrix} 2 & 2x^i \\ 2x^i & 2{x^i}^2 \end{pmatrix} \tag{31}$$

A convex function has the property that its Hessian matrix is positive semidefinite. There are several ways of showing that the Hessian matrix of J^i is positive semidefinite. A matrix is positive semidefinite if it is symmetric and all its eigenvalues are non-negative, with at least one equal to zero. We proceed to find the eigenvalues of H:

The equation to solve for finding the eigenvalues is

$$\begin{vmatrix} 2-\lambda & 2x^i \\ 2x^i & 2{x^i}^2 - \lambda \end{vmatrix} = 0 \tag{32}$$

This yields

$$\lambda^2 - 2({x^i}^2 + 1)\lambda = 0$$

Therefore, the eigenvalues of H are

$$\lambda = 0, \qquad \lambda = 2({x^i}^2 + 1) \tag{33}$$

Hence, the Hessian matrix of J^i is positive semidefinite, and J^i is a convex function. The sum of two or more convex functions is also a convex function. As the MSE is a sum of all the J^i (multiplied by a constant) it must be convex. This result holds for multiple linear regression.

0.2 The ridge regularisation term is strictly convex

The second derivative of ${\theta_j}^2$ with respect to θ_j is

$$\frac{d}{d\theta_j}({\theta_j}^2) = 2 \tag{34}$$

As its second derivative is positive everywhere, ${\theta_j}^2$ is strictly convex (it has a unique minimum). As mentioned before, the sum of convex functions is convex. Therefore, $\sum_{j=1}^{n} {\theta_j}^2$ is strictly convex.