Error Functions & Linear Regression (1)

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Machine Learning @ DIT

Univariate Linear Regression

- There are a family of machine learning approaches that can be thought of as directly searching for a set of parameters that maximise the performance of a particular prediction model.
- In this lecture we will look at linear regression and how it can be used for both categorical and continuous prediction problems.

Linear Regression

- Remember that the equation of a line, $y = mx + b$, can be used to represent the relationship between two variables, x and y.
- For simplicity we will rewrite the equation of a line as:

$$h_{\mathbf{w}}(x) = w_0 + w_1 x$$

where $\mathbf{w}$ is the vector $[w_0, w_1]$ and w_0 and w_1 are referred to as weights.

- We now just need to find the weight values that maximise the performance of this model - i.e. the weight values that allow us best predict y given x.

Loss Function

- In order to find the best values for $[w_0, w_1]$ we can measure the fit of a model by measuring squared loss function, L_2 over all training examples
- The loss function can be defined as:

$$\begin{aligned} Loss(h_{\mathbf{w}}) &= \sum_{j=1}^{N} L_2(y_j, h_{\mathbf{w}}(x)) \\ &= \sum_{j=1}^{N} (y_j - h_{\mathbf{w}}(x))^2 \\ &= \sum_{j=1}^{N} (y_j - (w_0 + w_1 x_j))^2 \end{aligned}$$

House Size	House Price
500	320
550	380
620	400
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700	410
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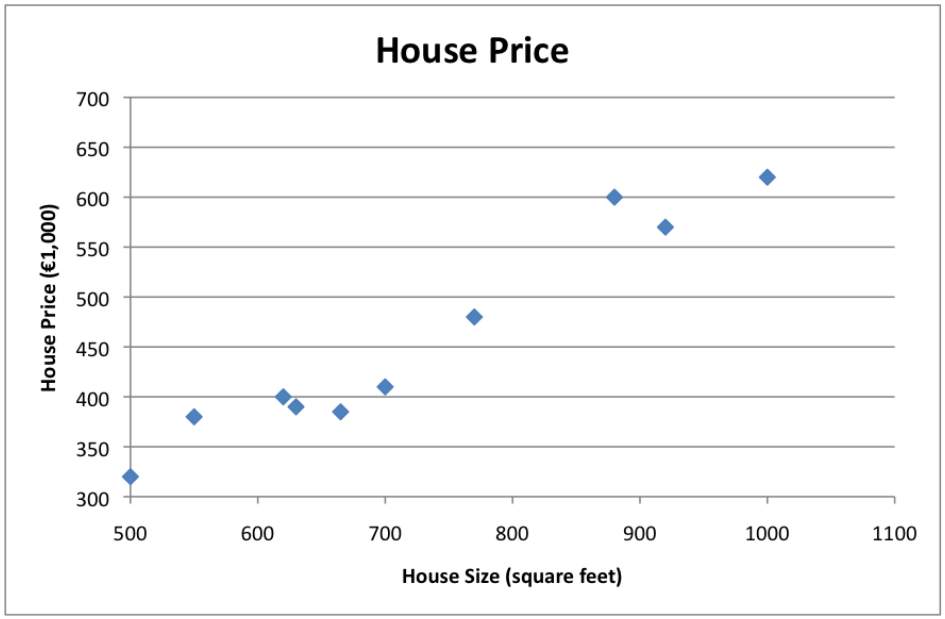
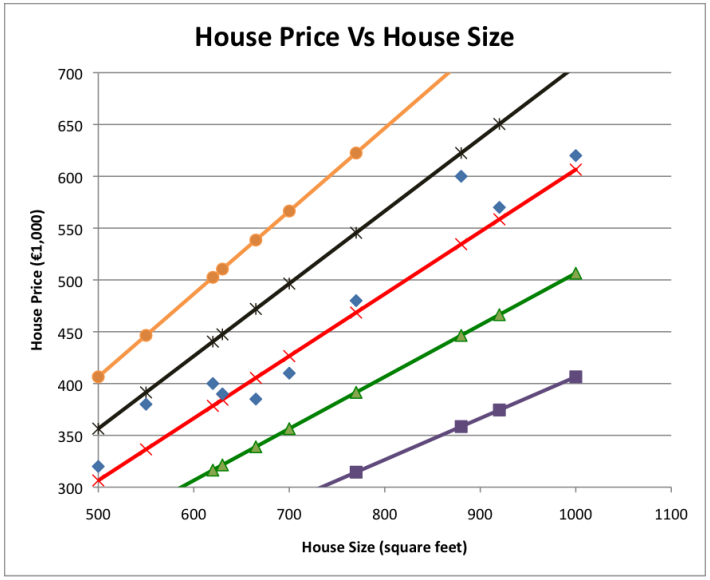
920	570
1000	620

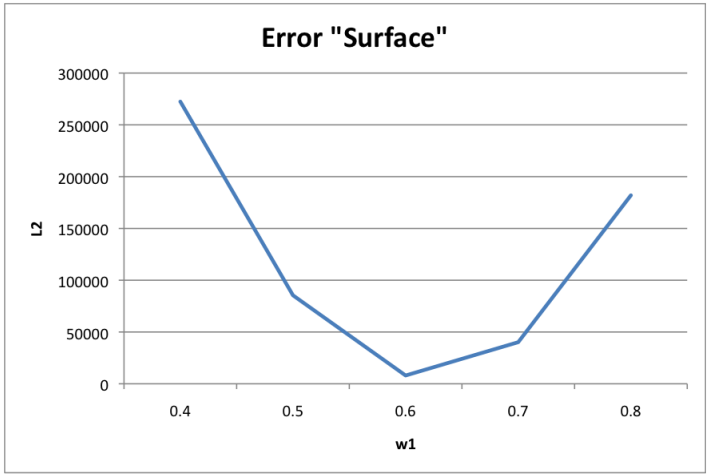


Practice

Assuming $w_0 = 6.47$ what would be the most accurate value of w_1 based on the given training set (select from 0.4, 0.5, 0.6, 0.7, 0.8).

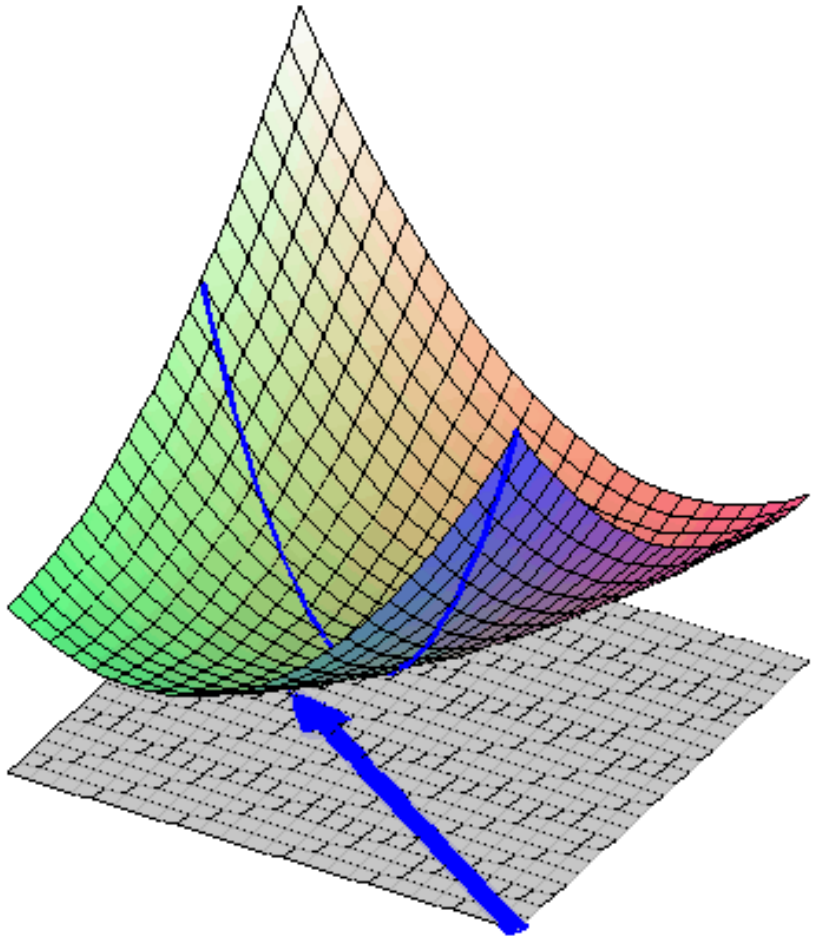
w_1	L_2
0.4	272,436
0.5	85,424
0.6	8,006
0.7	40,183
0.8	181,955





- The *Loss* depending on the weights $[w_0, w_1]$ can be viewed as a surface - in fact a surface that is convex and that has a global minimum.
- We need to find the lowest point on this surface and use it as our weight values.

Linear Regression



- So we want to find $\mathbf{w}^* = argmin_{\mathbf{w}} Loss(h_{\mathbf{w}})$.
- The sum $Loss(h_{\mathbf{w}})$ is minimised when its partial derivatives with respect to w_0 and w_1 are equal to 0.

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Partial What????

Who knows what a derivative is?

Who knows what a partial derivative is?

In order to compute slopes we need to know some calculus:

Fundamental Calculus:

- In mathematics, the derivative is a measurement of how a function changes when the values of its inputs change and a partial derivative (denoted by the symbol ∂) of a function of several variables is its derivative with respect to one of those variables with the others held constant.

- There are really only three things we need to know about calculus for working on linear regression. First:

$$\frac{\partial}{\partial x} x = 1$$

$$\frac{\partial}{\partial x} x^2 = 2x$$

Practice

- Calculate the following:

$$\frac{\partial}{\partial x} x + 1 =$$

$$\frac{\partial}{\partial x} 6x =$$

$$\frac{\partial}{\partial x} x^2 =$$

$$\frac{\partial}{\partial x} 3x^2 =$$

$$\frac{\partial}{\partial x} x^2 + 2x + 4 =$$

Practice

- Calculate the following:

$$\frac{\partial}{\partial x} x + 1 = 1$$

$$\frac{\partial}{\partial x} 6x = 6$$

$$\frac{\partial}{\partial x} x^2 = 2x$$

$$\frac{\partial}{\partial x} 3x^2 = 6x$$

$$\frac{\partial}{\partial x} x^2 + 2x + 4 = 2x + 2$$

Fundamental Calculus:

- The second thing is the Chain Rule
- The Chain Rule allows us calculate the derivative of a composition of two or more functions.
- Chain rule: $\frac{\partial}{\partial x} g(f(x)) = \frac{\partial}{\partial f(x)} g(f(x)) \frac{\partial}{\partial x} f(x)$
- Ex.1: $\frac{\partial}{\partial x}(x^2 + 1)^2 = 2(x^2 + 1)(2x)$
- Ex.2: $\frac{\partial}{\partial x} \frac{1}{2}(c - x)^2 =$

  $\frac{2}{2}(c - x)(\frac{\partial}{\partial x}(c - x)) = (c - x)(-1) = -(c - x)$

Practice

- $\frac{\partial}{\partial x}(x^2 + 2)^2 =$
- $\frac{\partial}{\partial x}(3x^2 + 3x + 3)^2 =$

Practice

- $\frac{\partial}{\partial x}(x^2+2)^2 = 2(x^2+2)(2x)$
- $\frac{\partial}{\partial x}(3x^2+3x+3)^2 = 2(3x^2+3x+3)(6x+3)$

- So we want to find $\mathbf{w}^* = argmin_{\mathbf{w}} Loss(h_{\mathbf{w}})$.
- The sum $Loss(h_{\mathbf{w}})$ is minimised when its partial derivatives with respect to w_0 and w_1 are equal to 0.
- So:

$$\frac{\partial}{\partial w_0} \sum_{j=1}^{N} (y_j - (w_0 + w_1 x_j))^2 = 0$$

and

$$\frac{\partial}{\partial w_1} \sum_{j=1}^{N} (y_j - (w_0 + w_1 x_j))^2 = 0$$

- Fortunately, these equations have a unique solution*:

$$w_1 = \frac{N(\sum x_j y_j) - (\sum x_j)(\sum y_j)}{N(\sum x_j^2) - (\sum x_j)^2}$$

and

$$w_0 = \frac{(\sum y_j - w_1(\sum x_j))}{N}$$

*based on assumptions that there is normally distributed noise and the stationarity assumption amongst other things

Practice

House Size	House Price
500	320
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- Let's work out the optimal values for $[w_0, w_1]$ for the house price dataset we looked at previously.
- See the associated Excel sheet for the solution!

- While it was great to have a unique solution to our system of equations in the previous example, this will not always be the case.
- We need an alternative way to find the best weights to use in our model.
- **Any ideas?**

- We need to perform a search through the weight space for the best values to use.
- An exhaustive search is just not reasonable.
- Instead we can use the common approach of gradient descent:
  - Start at any point in weight space
  - Move to a neighbouring point that is *downhill*
  - Repeat until we converge on the point of minimum loss.

Gradient descent

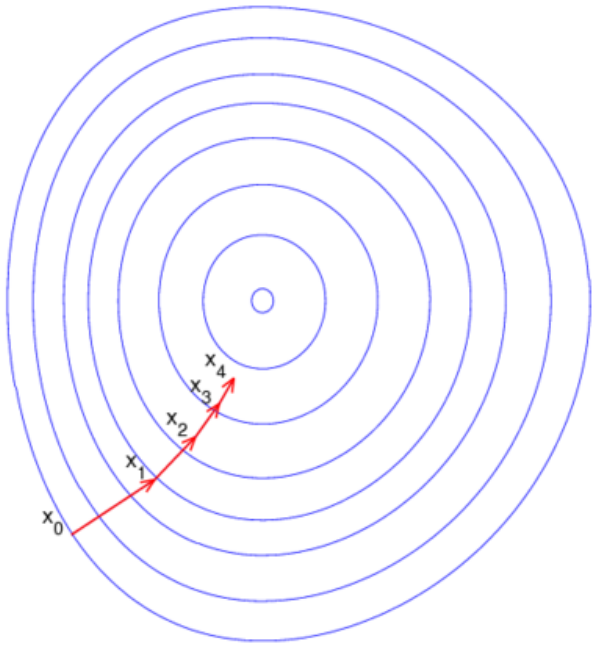
$\mathbf{w} \leftarrow$ any point in the parameter space

loop until convergence **do**

for each w_i **in w do**

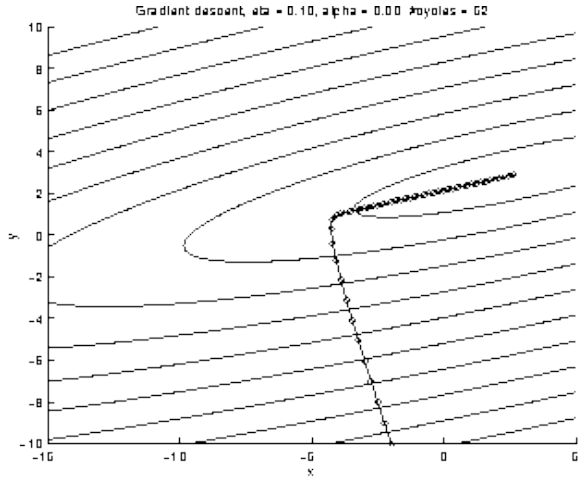
$$w_i \leftarrow w_i - \alpha \frac{\partial}{\partial w_i} Loss(\mathbf{w})$$

- α is referred to as the learning rate and determines the amount by which weights are changed at each step.
- This can be a fixed constant or can decay over time as learning proceeds.

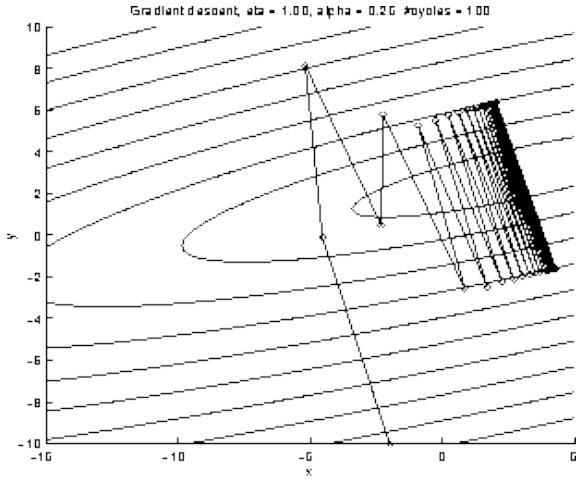


Nice gradient descent animations: http://animation.yihui.name/compstat:gradient_descent_algorithm

Gradient Descent



(a)



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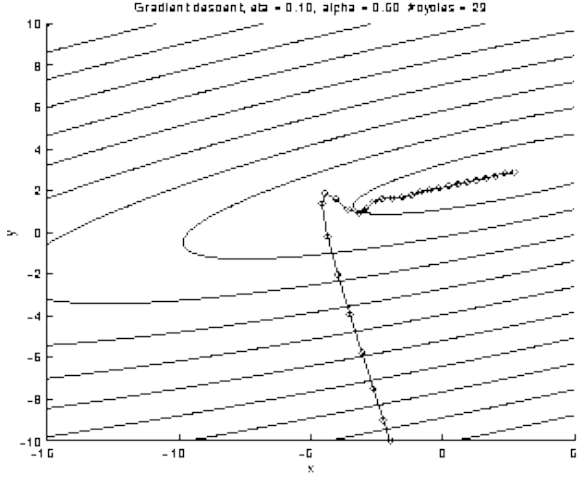

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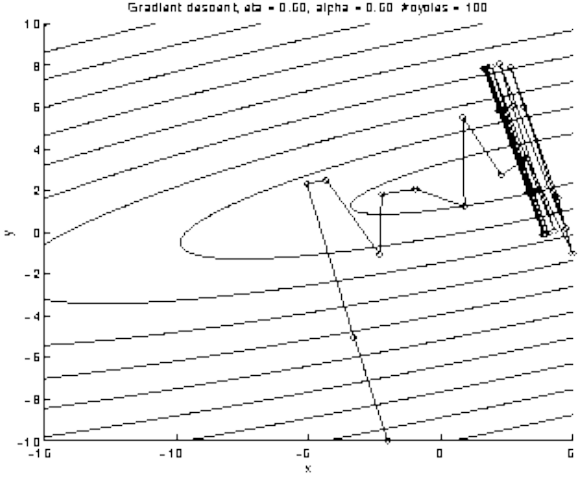

(d)

Imagine there was just one training example (x, y). Then the gradient would be given as (note use of chain rule):

$$\begin{aligned}\frac{\partial}{\partial w_i} Loss(\mathbf{w}) &= \frac{\partial}{\partial w_i}(y - h_{\mathbf{w}}(x))^2 \\ &= 2(y - h_{\mathbf{w}}(x)) \times \frac{\partial}{\partial w_i}(y - h_{\mathbf{w}}(x)) \\ &= 2(y - h_{\mathbf{w}}(x)) \times \frac{\partial}{\partial w_i}(y - (w_0 + w_1 x))\end{aligned}$$

Applying to both w_0 and w_1 we get:

$$\frac{\partial}{\partial w_0} Loss(\mathbf{w}) = -2(y - h_{\mathbf{w}}(x))$$
$$\frac{\partial}{\partial w_1} Loss(\mathbf{w}) = -2(y - h_{\mathbf{w}}(x)) \times x$$

Plugging these into our weight update rule we get:

$$w_0 \leftarrow w_0 + \alpha(y - h_{\mathbf{w}}(x))$$
$$w_1 \leftarrow w_1 + \alpha(y - h_{\mathbf{w}}(x)) \times x$$

Intuitively this makes sense:

- if $h_{\mathbf{w}}(x)$ is too high reduce w_0 a little bit and reduce w_1 if x was positive but increase it if x was negative.
- if $h_{\mathbf{w}}(x)$ is too low do the opposite.

The previous example only considered a single training example.
However, adjusting this to deal with a full training set of N examples simply involves introducing a sum:

$$w_0 \leftarrow w_0 + \alpha \sum_j (y_j - h_{\mathbf{w}}(x_j))$$

$$w_1 \leftarrow w_1 + \alpha \sum_j (y_j - h_{\mathbf{w}}(x_j)) \times x_j$$

This is known as batch gradient descent.

An alternative to batch gradient descent is stochastic gradient descent in which the update rule is applied one example at a time and the examples are chosen, usually randomly, from the training set.

Multivariate Linear Regression

- We have seen how linear regression can be used to make continuous predictions from a single variable.
- However, we like big data so one variable is no good to us!
- A multivariate linear regression does the same job using multiple variables.

Multi-variate Linear Regression

- Our hypothesis space is of the form:

$$\begin{aligned} h_{\mathbf{w}}(x) &= w_0 + w_1 x_1 + \cdots + w_n x_n \\ &= w_0 + \sum_i w_i x_i \end{aligned}$$

- We can make this look a little neater by inventing a dummy input attribute, x_0, that is always equal to 1. Then:

$$\begin{aligned} h_{\mathbf{w}}(x) &= \sum_i w_i x_i \\ &= \mathbf{w} \cdot \mathbf{x} \end{aligned}$$

Gradient Descent for Multi-variate Linear Regression

- The best set of weights, $\mathbf{w}^*$ minimizes the squared error loss, L_2, over a set of training examples:

$$\mathbf{w}^* = argmin_{\mathbf{w}} \sum_j L_2(y_j, \mathbf{w} \cdot \mathbf{x}_j)$$

- Gradient descent works for the multi-variate case just like it does for the univariate case and will minimise the loss function.
- The update rule for each weight is:

$$w_i \leftarrow w_i + \alpha \sum_j x_{j,i}(y_i - h_{\mathbf{w}}(\mathbf{x}_j))$$

Summary