

Introduction to Machine Learning

Ramon Fuentes^{1,2}

August 5, 2019

¹Visiting Researcher, Dynamics Research Group
The University of Sheffield

²Research Scientist, Callsign Ltd

A little bit about me...



The
University
Of
Sheffield.



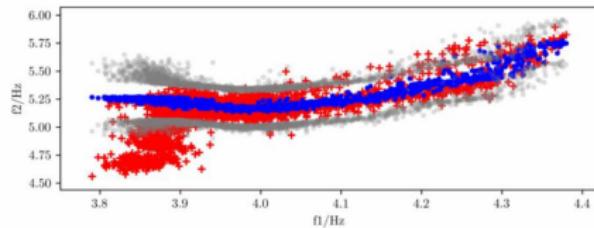
KONGSBERG

Callsign

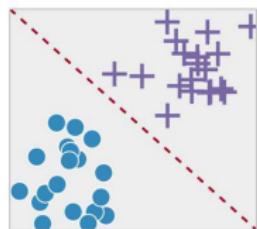


The tools of machine learning

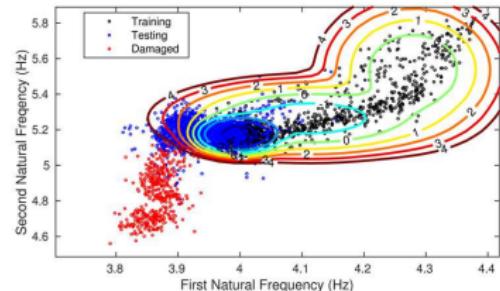
Regression



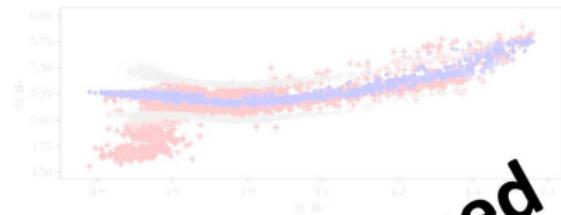
Classification



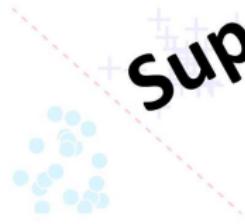
Density Estimation



The tools of machine learning

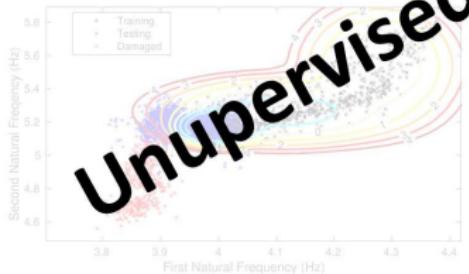


• Classification



Supervised

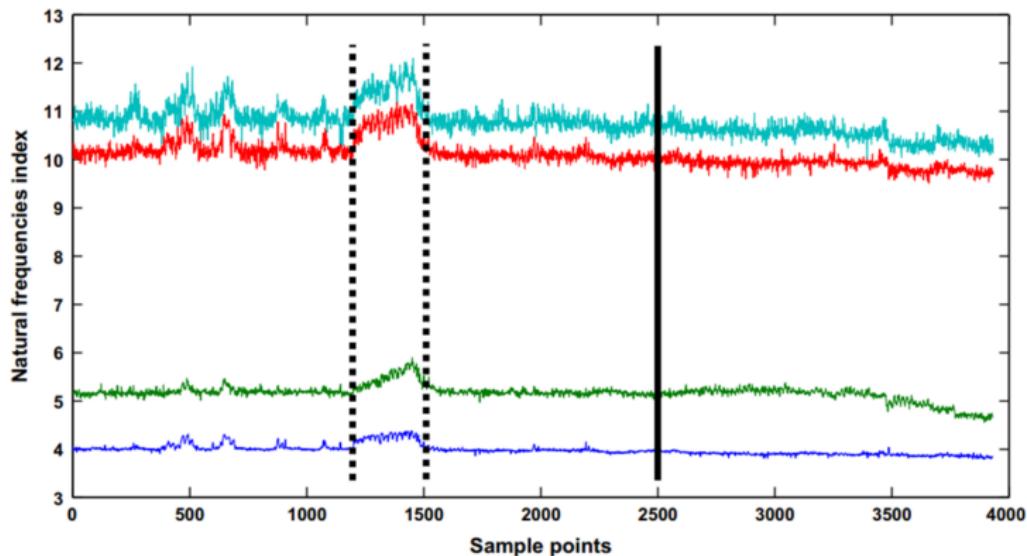
• Density Estimation



Unsupervised

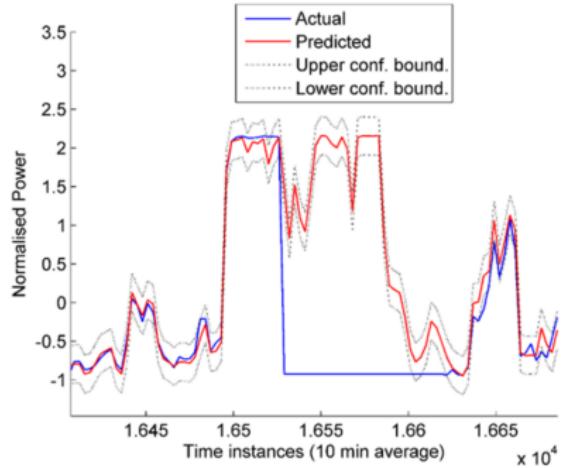
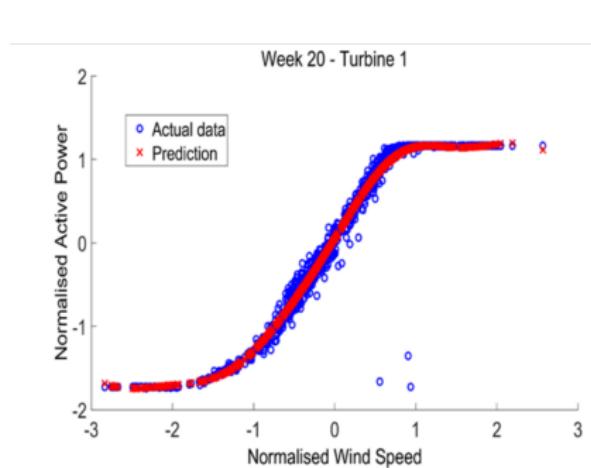
Motivating problem

Given a set of measured natural frequencies from a bridge, can we detect damage?



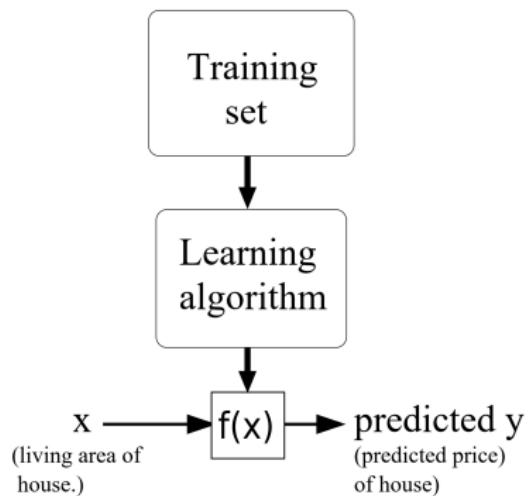
Motivating problem

Can we diagnose problems on a wind turbine,
given measured wind and power?



Supervised learning

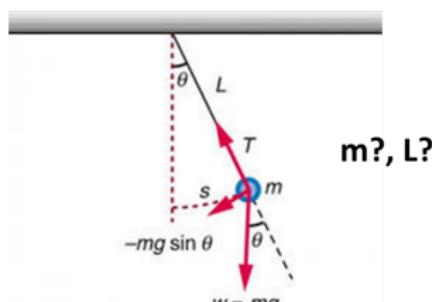
Supervised learning deals with the problem of modelling the relationship between a set of inputs, x and outputs y



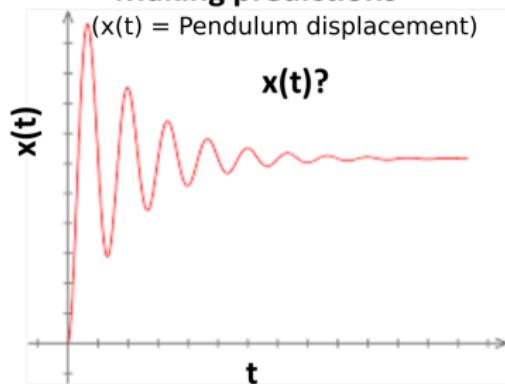
A first look at supervised learning: linear regression

Given some measured data,
there are generally two problems of interest:

Identifying a system



Making predictions



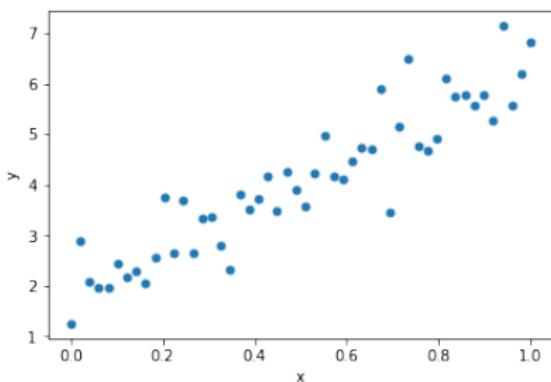
Linear Regression

Lets start with a simple toy example: a noisy $y = 5x + 1$

Can we learn the relationship
between x and y from the data
?

We need to things:

1. A model
2. A loss function, that
quantifies our error or
predictive performance



Linear Regression

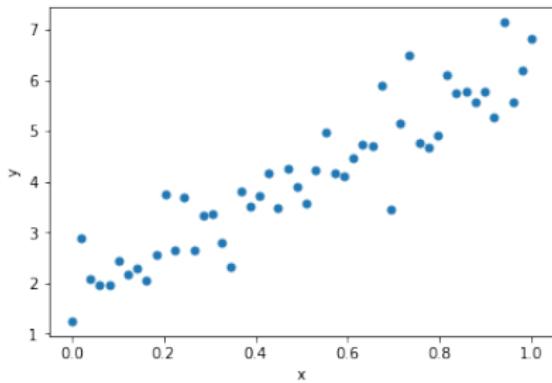
We need a model for the underlying function:

$$y = f(x)$$

Linear regression models $f(\mathbf{x})$ as:

$$y = x_0 w_0 + x_1 w_1 + x_2 w_2 + \dots$$

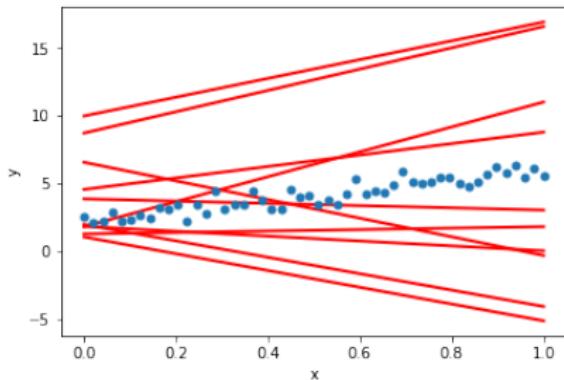
$$y = \sum_j x_j w_j$$



Linear Regression

So, we have a model, parametrised by \mathbf{w} , we now need to define a loss function so we can pick our weights appropriately

A bunch of models drawn at random, which fits the data best?

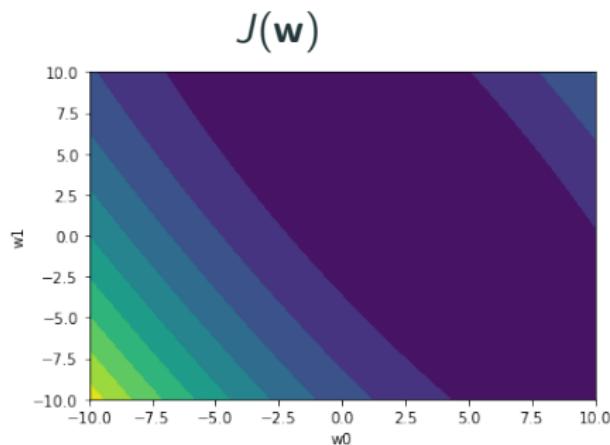


Squared error loss

One appropriate loss function is the mean of the squared prediction error:

$$J(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^n (y^{(i)} - f(x^{(i)}))^2$$

But how should we find the value of \mathbf{w} that minimises $J(\mathbf{w})$?



Gradient Descent

- There are many ways to *optimise w*, but one efficient way of doing so is via **gradient descent**.

Gradient Descent

- There are many ways to *optimise w*, but one efficient way of doing so is via **gradient descent**.
- The idea is that we'll start with an initial choice for w and improve it iteratively in a direction that decreases $J(w)$ - our cost function

Gradient Descent

- There are many ways to *optimise* \mathbf{w} , but one efficient way of doing so is via **gradient descent**.
- The idea is that we'll start with an initial choice for \mathbf{w} and improve it iteratively in a direction that decreases $J(\mathbf{w})$ - our cost function
- We take a step in the direction of the gradient $\frac{\partial J}{\partial \mathbf{w}}$

Gradient Descent

This leads us to the gradient descent algorithm:

$$w_j \leftarrow w_j - \alpha \frac{\partial}{\partial w_j} J(\mathbf{w})$$

Gradient Descent

This leads us to the gradient descent algorithm:

$$w_j \leftarrow w_j - \alpha \frac{\partial}{\partial w_j} J(\mathbf{w})$$

And recall our loss function was:

$$J(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^n (y^{(i)} - f(\mathbf{x}^{(i)}))^2$$

Gradient Descent

This leads us to the gradient descent algorithm:

$$w_j \leftarrow w_j - \alpha \frac{\partial}{\partial w_j} J(\mathbf{w})$$

And recall our loss function was:

$$J(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^n (y^{(i)} - f(\mathbf{x}^{(i)}))^2$$

and remember,

$$f(\mathbf{x}^{(i)}) = \sum_j^d w_j x_j^{(i)}$$

Gradient Descent

Lets derive $\frac{\partial}{\partial w_j} J(\mathbf{w})$ for the case where we have a single training example $x_j^{(i)} \ y^{(i)}$,

$$\begin{aligned}\frac{\partial}{\partial w_j} J(\mathbf{w}) &= \frac{\partial}{\partial w_j} \frac{1}{2} (y^{(i)} - f(\mathbf{x}^{(i)}))^2 \\&= 2 \frac{1}{2} (y^{(i)} - f(\mathbf{x}^{(i)})) \frac{\partial}{\partial w_j} (y^{(i)} - f(\mathbf{x}^{(i)})) \\&= (y^{(i)} - f(\mathbf{x}^{(i)})) \frac{\partial}{\partial w_j} \left(\sum_{k=0}^d x_k^{(i)} w_k - y^{(i)} \right) \\&= (y^{(i)} - f(\mathbf{x}^{(i)})) x_j^{(i)}\end{aligned}$$

Gradient Descent, learning rule

We now have an update rule, that we can apply whenever we encounter a new observation,

$$w_j = w_j + \alpha(y^{(i)} - f(\mathbf{x}^{(i)}))x_j^{(i)}$$

here, α is a *learning rate*

Batch Gradient Descent

When we have all training observations $x^{(1)}, \dots, x^{(n)}$ and $y^{(1)}, \dots, y^{(n)}$, we can assemble this into an algorithm

while not converged **do**

for every j , **do**

$$w_j \leftarrow w_j + \alpha \sum_{i=1}^n (y^{(i)} - \sum_j^d x_j^{(i)} w_j) x_j$$

end for

end while

this is called *batch gradient descent*

Back to our problem...

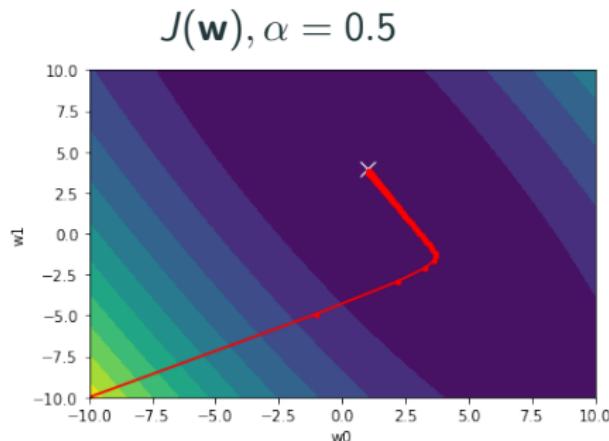
Applying 200 iterations of batch gradient descent to our toy problem, this is how our quadratic loss looks like

True function: $y = 5x + 1$

Estimated parameters:

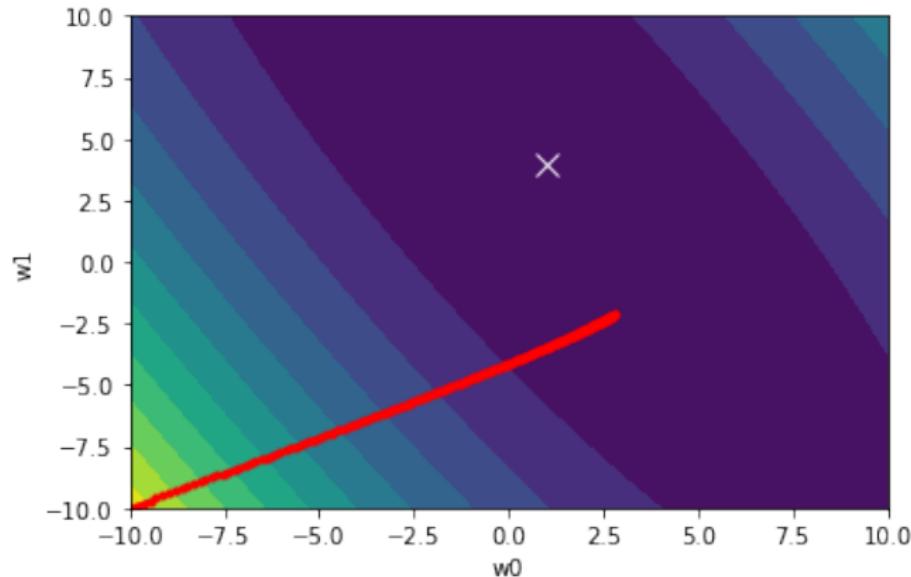
$w_0 = 1.05, w_1 = 3.75$

close enough...



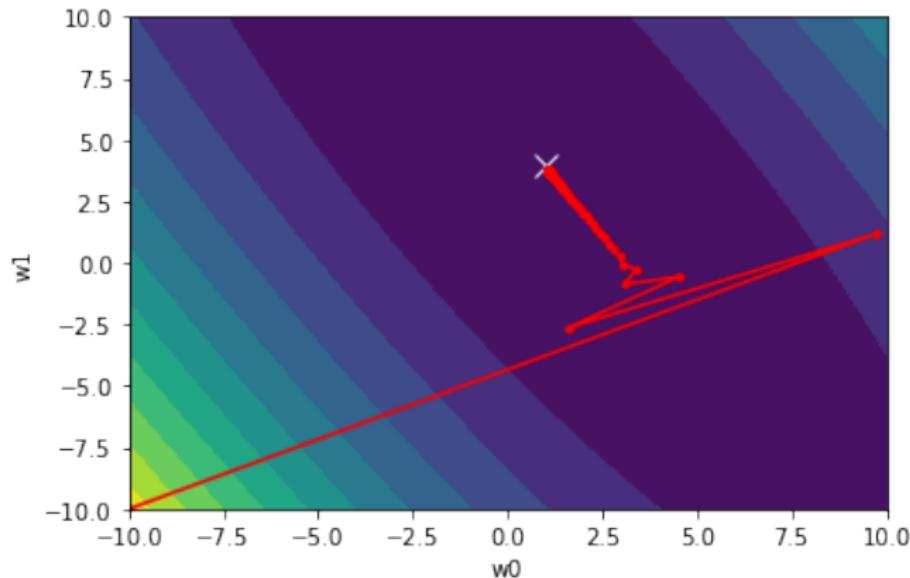
Back to our problem...

What happens if we choose a lower learning rate ($\alpha = 0.05$)?



Back to our problem...

What happens if we choose a higher learning rate($\alpha = 1.5$)?



Gradient Descent

Some notes on gradient descent:

- The learning rate has to be chosen wisely.

Gradient Descent

Some notes on gradient descent:

- The learning rate has to be chosen wisely.
- It is common to have a cooling rate - take large steps initially, and slow down as learning progresses. A bit of a heuristic

Gradient Descent

Some notes on gradient descent:

- The learning rate has to be chosen wisely.
- It is common to have a cooling rate - take large steps initially, and slow down as learning progresses. A bit of a heuristic
- It can get stuck in local optima. Not in this case though, as we have a well defined convex quadratic loss function.

Gradient Descent

Some notes on gradient descent:

- The learning rate has to be chosen wisely.
- It is common to have a cooling rate - take large steps initially, and slow down as learning progresses. A bit of a heuristic
- It can get stuck in local optima. Not in this case though, as we have a well defined convex quadratic loss function.
- For the basic linear regression problem, can we do better?

Gradient Descent

Some notes on gradient descent:

- The learning rate has to be chosen wisely.
- It is common to have a cooling rate - take large steps initially, and slow down as learning progresses. A bit of a heuristic
- It can get stuck in local optima. Not in this case though, as we have a well defined convex quadratic loss function.
- For the basic linear regression problem, can we do better?
- yes!

Analytical solution

- There is in fact a closed form analytical solution that optimises $J(\mathbf{w})$.

Analytical solution

- There is in fact a closed form analytical solution that optimises $J(\mathbf{w})$.
- But first, lets re-write our problem in matrix notation

Analytical solution

- There is in fact a closed form analytical solution that optimises $J(\mathbf{w})$.
- But first, let's re-write our problem in matrix notation
- Our output is represented by a (column) vector: $\mathbf{y} = [y_1, \dots, y_n]$

Analytical solution

- There is in fact a closed form analytical solution that optimises $J(\mathbf{w})$.
- But first, let's re-write our problem in matrix notation
- Our output is represented by a (column) vector: $\mathbf{y} = [y_1, \dots, y_n]$
- And our inputs are assembled into a matrix, with each variable represented by a column $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_m]$,

Analytical solution

- There is in fact a closed form analytical solution that optimises $J(\mathbf{w})$.
- But first, let's re-write our problem in matrix notation
- Our output is represented by a (column) vector: $\mathbf{y} = [y_1, \dots, y_n]$
- And our inputs are assembled into a matrix, with each variable represented by a column $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_m]$,
- where each column, $\mathbf{x}_j = [x_j^{(1)}, \dots, x_j^{(n)}]$

Analytical solution

Our linear regression problem is now:

$$\mathbf{y} = \mathbf{X}\mathbf{w}$$

Analytical solution

Our linear regression problem is now:

$$\mathbf{y} = \mathbf{X}\mathbf{w}$$

Our loss is:

$$\begin{aligned} J(\mathbf{w}) &= \frac{1}{2} \sum_{i=1}^n (y^{(i)} - \sum_j x_j^{(i)} w_j)^2 \\ &= \frac{1}{2} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) \end{aligned}$$

Analytical solution

The gradient of the loss is

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \nabla_{\mathbf{w}} \frac{1}{2} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

Analytical solution

The gradient of the loss is

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \nabla_{\mathbf{w}} \frac{1}{2} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

which (applying a few matrix identities...) leads to,

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbf{X}^T \mathbf{X}\mathbf{w} - \mathbf{X}^T \mathbf{y}$$

Analytical solution

The gradient of the loss is

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \nabla_{\mathbf{w}} \frac{1}{2} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

which (applying a few matrix identities...) leads to,

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbf{X}^T \mathbf{X}\mathbf{w} - \mathbf{X}^T \mathbf{y}$$

Setting $\nabla_{\mathbf{w}} J(\mathbf{w})$ to zero, leads to the normal equations,

$$\mathbf{X}^T \mathbf{X}\mathbf{w} = \mathbf{X}^T \mathbf{y}$$

Analytical solution

The gradient of the loss is

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \nabla_{\mathbf{w}} \frac{1}{2} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

which (applying a few matrix identities...) leads to,

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbf{X}^T \mathbf{X}\mathbf{w} - \mathbf{X}^T \mathbf{y}$$

Setting $\nabla_{\mathbf{w}} J(\mathbf{w})$ to zero, leads to the normal equations,

$$\mathbf{X}^T \mathbf{X}\mathbf{w} = \mathbf{X}^T \mathbf{y}$$

and solving for \mathbf{w} , gives us

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Back to our problem again

Using the normal equation,

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Back to our problem again

Using the normal equation,

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

$$w_0 = 1.05, w_1 = 3.75$$

Back to our problem again

Using the normal equation,

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

$$w_0 = 1.05, w_1 = 3.75$$

Similar solution as gradient descent!

Back to our problem again

Using the normal equation,

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

$$w_0 = 1.05, w_1 = 3.75$$

Similar solution as gradient descent!

but rather easier ?

Recap

We've looked at two ways of optimising the parameters/weights in a linear regression setting:

- through gradient descent, leading to the batch gradient descent algorithm

Recap

We've looked at two ways of optimising the parameters/weights in a linear regression setting:

- through gradient descent, leading to the batch gradient descent algorithm
- analytically, through the matrix normal equations

Recap

We've looked at two ways of optimising the parameters/weights in a linear regression setting:

- through gradient descent, leading to the batch gradient descent algorithm
- analytically, through the matrix normal equations
- both of these useful on their own, and key ingredients when solving more complex problems, as we'll see...

Conclusions

What have we learned today?

- Basics of supervised vs. unsupervised learning
- Linear models for regression
- The least means squares algorithm
- Analytical solution to the unconstrained linear regression problem

So... what next?

Tomorrow, we'll learn how to deal with more complex nonlinear problems, using the tools we've worked through today ;)