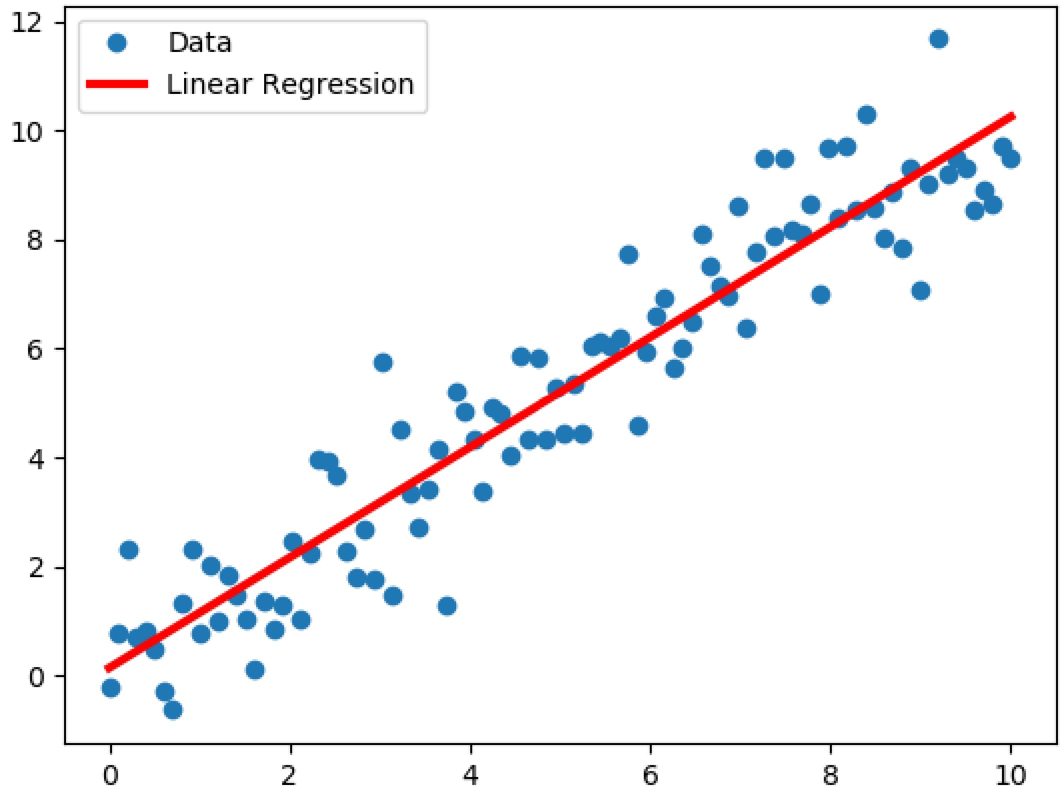
Optimisation

Motivation



We want to find a and b which minimize the sum square errors J which is given by

$$J(a,b) = \frac{1}{2}\sum_{i=1}^{n}(y_i - (ax_i + b))^2$$

The build-up

- Interactively create a dummy data in excel (data **A**)
- Visualise how different choices of slopes and intercept will affect the error
- Gradient descent applied to one variable function
- Gradient descent applied to two variables function (using **A**)
- How can we check our results numerically?
- **Exercise**: Using the built-up knowledge so far to estimate the coeffients of:
  - linear regression on real dataset.
  - logistic regression on real dataset.

Note: This will combine Excel. Pandas, Numpy, and Basic Math knowledge

Matrix Representation

Recall that we would like to minimize

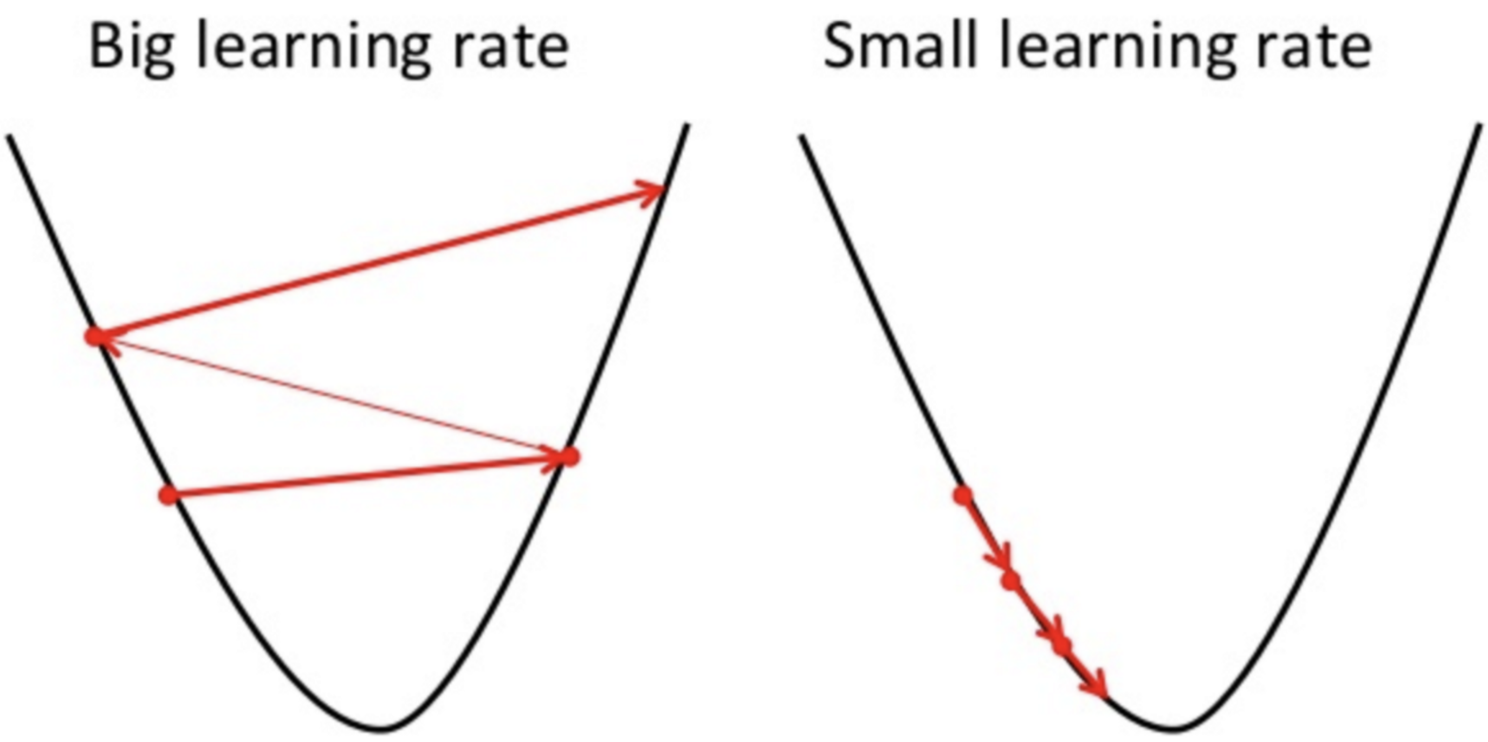
$$J(a,b) = \frac{1}{2}\sum_{i=1}^{n}(y_i - (ax_i + b))^2$$

Suppose that we have n observations and m features. We can stack these observations in a matrix X with size $n \times m$.

If $J(\beta) = \frac{1}{2}(y - X\beta)^T(y - X\beta)$, then $\hat{\beta}$ which minimize J is given by

$$\beta = (X^TX)^{-1}X^Ty$$

Gradient Descent - Intuition



Gradient Descent - algorithm

For one variable, the iteration logic is given by:

$$x_{n+1} = x_n - \eta Df(x_n)$$

where $Df(x_0)$ means $\frac{df(x)}{dx}$ evaluated at $x = x_0$

If it is extended to multi-variable scheme, then the iteration logic becomes:

$$\beta_{n+1} = \beta_n - \eta \nabla J(\beta_n)$$

Remarks: η is called *learning rate*.

Gradient Descent - algorithm

Recall the cost function of the original problem

$$J(a,b) = \frac{1}{2}\sum_{i=1}^{n}(y_i - (ax_i + b))^2$$

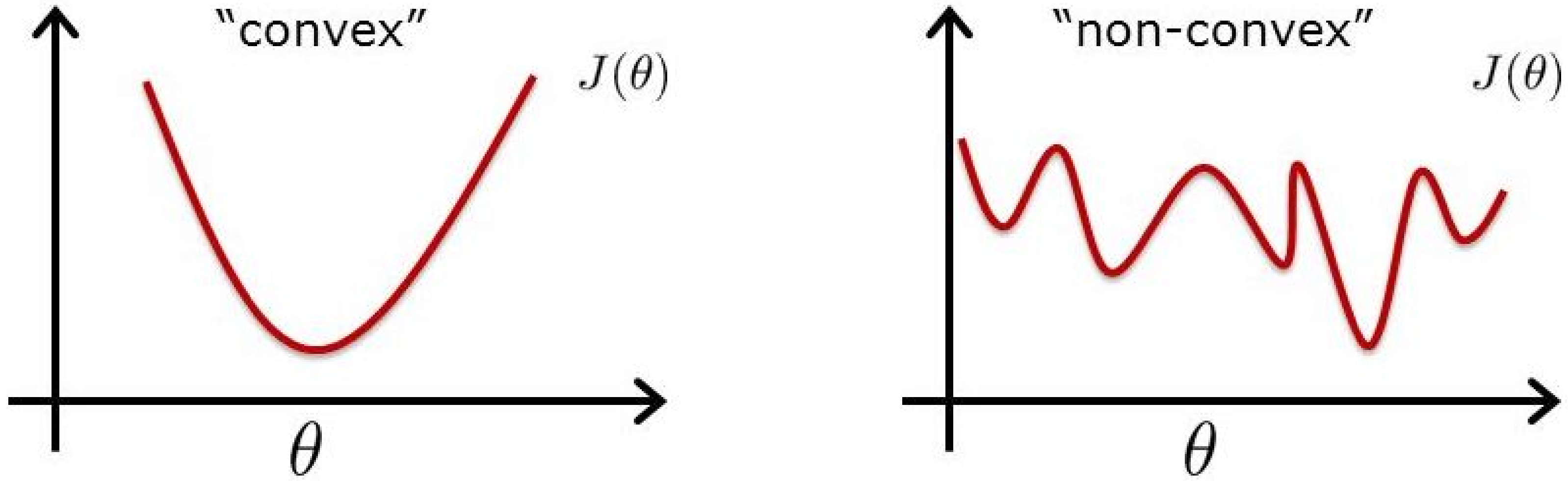
Partial derivaties with respect to a and b are given by

$$\frac{\partial J}{\partial a} = \sum_{i=1}^{n}(y_i - (ax_i + b))(-x_i)$$

and

$$\frac{\partial J}{\partial b} = \sum_{i=1}^{n}(y_i - (ax_i + b))(-1)$$

Differences between Convex vs Non-Convex



Appendix

Derivation of linear regression MLE

Using the previous notation, we would like to minimize

$$J(\beta) = (y - X\beta)^T (y - X\beta)$$

Calculating the gradient of J gives us

$$\nabla J = 2 \times \nabla (y - X\beta)^T \times (y - X\beta)$$

$$\nabla J = 2 \times (\nabla y^T - \nabla (X\beta)^T) \times (y - X\beta)$$

Knowing $\nabla (X\beta)^T = X^T$ and setting gradient to be zero, we get

$$0 = 2 \times -X^T \times (y - X\beta) = -X^T y + X^T X\beta$$

Moving $-X^T\beta$ to the left hand side and multiplying both sides by $(X^T X)^{-1}$ gives us the solution

$$\hat{\beta} = (X^T X)^{-1} X^T y$$