McGill **Artificial Intelligence** Society

Lecture 2: Regression

Slides based off of Machine Learning at Berkeley
https://github.com/mlberkeley/Machine-Learning-Decal-Fall-2018

Today's Lesson Plan

Linear Regression

Optimization Via Gradient Descent

Logistic Regression

Multinomial Regression

Recall two main types of supervised algorithms

Regression:

- Input maps directly to a continuous output space
- Involves estimating or predicting a response
- Ex: predicting housing prices, computing trends in stock market

Classification:

- Input maps to a class label
- Classification is the act of identifying group membership
- Ex: image classification, semantic classification in text

Linear Regression

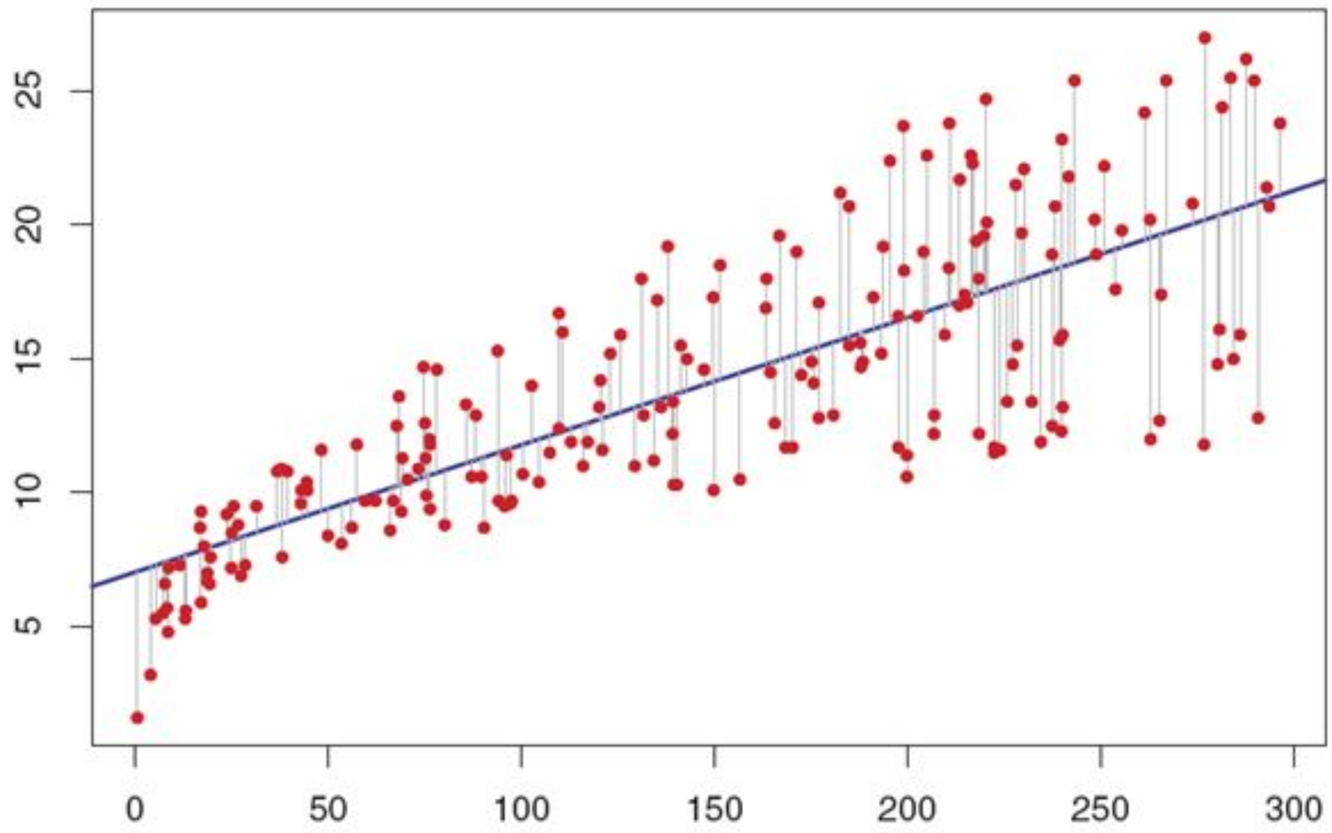


Image credits to Rachna Devasthali from towarddatascience.com

In statistics, linear regression is a linear approach to modelling the relationship between a dependent variable and one or more independent variables.

Linear Regression

We begin with the general format of a linear regression problem

$$y = \theta_1 x + \theta_0 + \epsilon$$ Error due to the variance

Where we model real-world practicalities with standard Gaussian noise

$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

In vector(compact) form, we write:

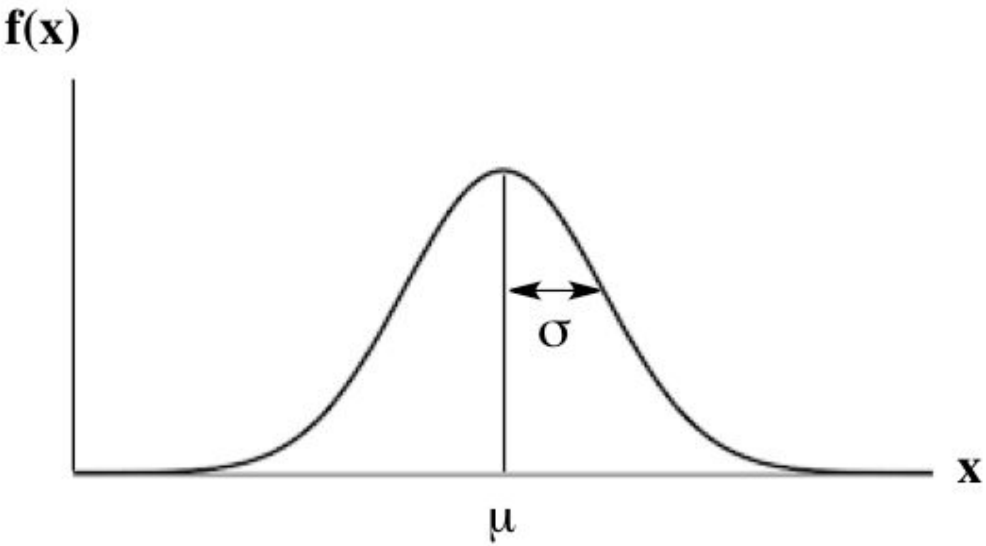
$$y = \theta^T X + \epsilon$$

Probabilistic interpretation:

$$p(y|x, \theta) = \mathcal{N}(y|w^T x, \sigma^2)$$

Quick Review Of Gaussian Distribution!

The Gaussian Distribution



$$f(x) = \frac{1}{\boxed{\sigma}\sqrt{2\pi}} e^{-(x-\boxed{\mu})^2/2\sigma^2}$$

$e = 2.71828$

Distribution defined by its mean, variance

What are we trying to solve?

We can't guaranty that solution is correct, but we can guaranty that our solution is the most likely to be correct based on our data.

In essence, we want to solve the optimization problem

most likely solution

$$\hat{\theta} = argmax_{\theta}\, log\, p(D|\theta)$$

Where D is a representation of the dataset. The log-likelihood is therefore written as follows:

$$l(\theta) = log\, p(D|theta) = \sum_{i=1}^{N} log\, p(y_i|x_i, \theta)$$

In practice, negative log likelihood is used

we use log function because
1. its differentiable
2. Probability is monotonically increasing

$$NLL(\theta) = -\sum_{i=1}^{N} log\, p(y_i|x_i, \theta)$$

It's a lot easier to minimize a function that to maximize a function

minimize negative likelihood to maximize probability

Optimization is : Optimization allows us to select the best parameters, associated with the machine learning algorithm or method we are using, for our problem case.

Framing the Optimization Problem

We expand the likelihood equation to its full form

distance btwn actual value and predicted value

$$\text{NLL}(\theta) = -l(\theta) = -\sum_{i=1}^{N} log[(\frac{1}{2\pi\sigma^2})^{1/2} exp(\frac{-1}{2\sigma^2}(y_i - w^T x_i)^2)]$$

$$f(x) = \frac{1}{\boxed{\sigma}\sqrt{2\pi}} e^{-(x-\boxed{\mu})^2/2\sigma^2}$$

$$\boxed{\text{NLL}(\theta) = \frac{\boxed{-1}}{2\sigma^2} RSS(w)} - \cancel{\frac{N}{2} log(2\pi\sigma^2)}$$

We do not consider this term in our optimization problem as it is constant with respect to the parameters of the model

Where the residual sum of squares is:

$$\boxed{RSS(w) = \sum_{i=1}^{N} (y_i - w^T x_i)^2} = (y - Xw)^T (y - Xw)$$

Residual sum of squares

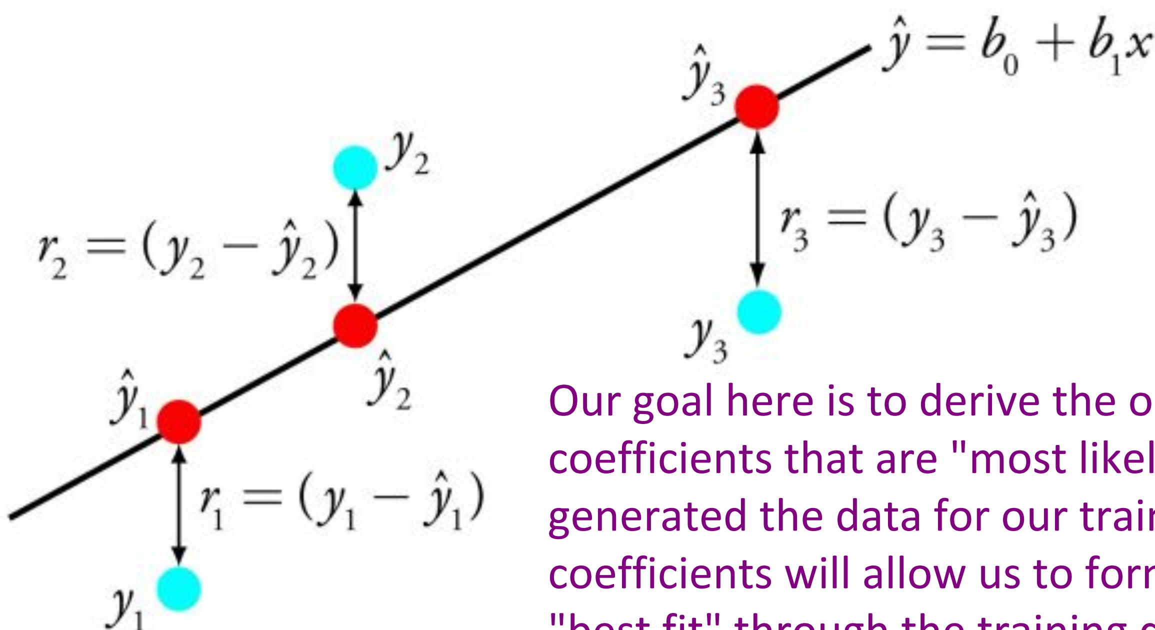
Summing distance between actual value and predicted value

When your function is strictly convexe, the gradient = 0 is definitely a minima

Linear Regression -Least Squares Method

Let $\hat{y}_i = h(x) = b_0 + b_1 x$

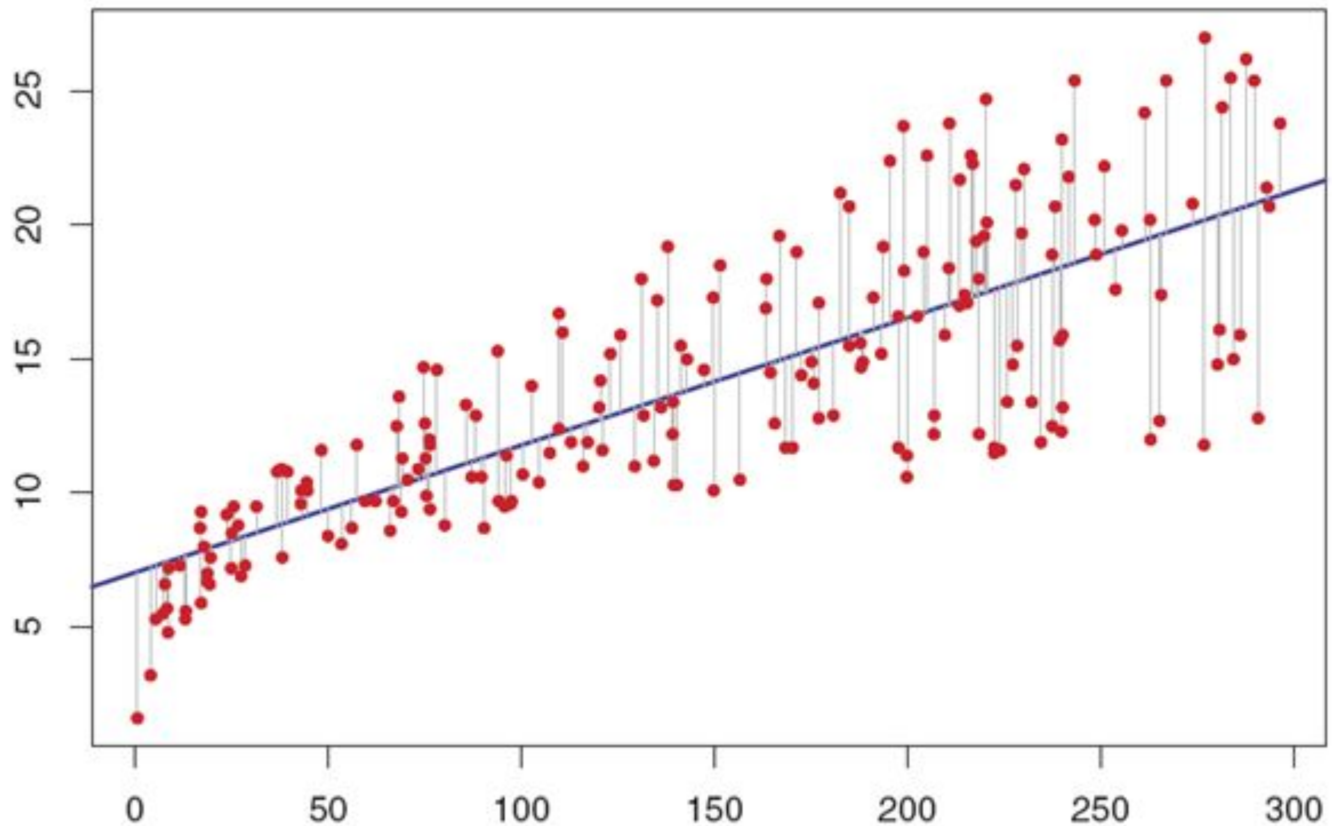
$$\min J(b_0, b_1)$$



Our goal here is to derive the optimal set of β coefficients that are "most likely" to have generated the data for our training problem. These coefficients will allow us to form a hyperplane of "best fit" through the training data.

Cost function ： Cost functions are used to estimate how badly models are performing. A high cost value means it's expensive—our approximation is far from describing the real relationship. On the other hand, a low cost value means it's cheap—our approximation is close to describing the relationship.
The mean squared error is often used as a type of cost function.

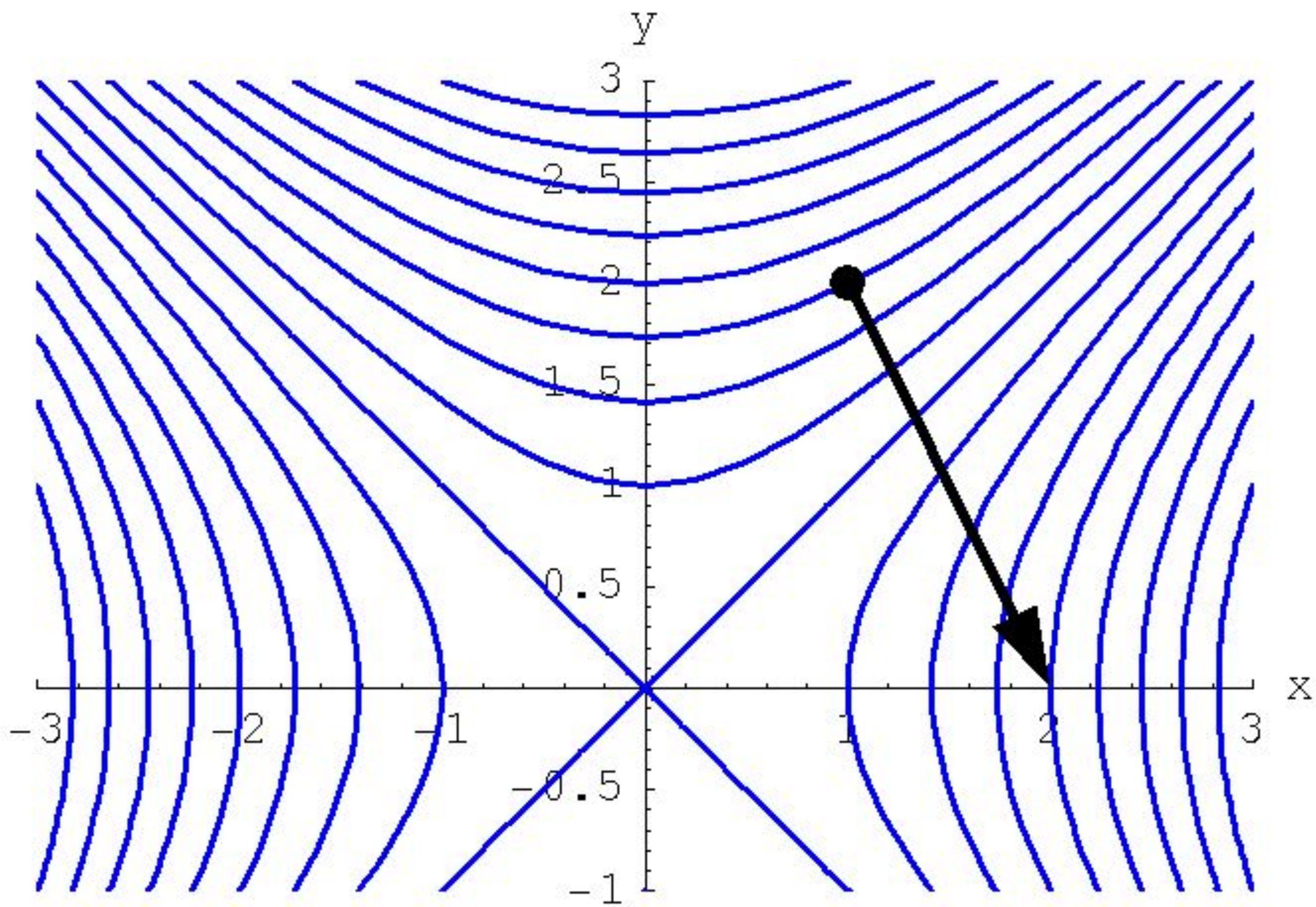
Linear Regression -Least Squares Method



We care more about the average mistakes

Image credits to Rachna Devasthali from towarddatascience.com

Optimization Via Gradient Descent



Derivation of the MLE

it is often easier to minimise the negative of the log-likelihood rather than maximise the log-likelihood itself

Rewriting the objective in a form that is amenable to differentiation

Neg log function

$$NLL(w) = \frac{1}{2}(y - Xw)^T(y - Xw) = \frac{1}{2}w^T(X^TX)w - w^T(X^Ty)$$

Where:

$$X^TX = \sum_{i=1}^{N} x_i x_i^T$$

This is the function we need to minimise. By doing so we will derive the ordinary least squares estimate for the β coefficients. (h(x) = b0 + b1x

And XTY follows, we can compute the gradient of the NLL, and we wish to set it to 0: We want to derive the NLL function and set its gradient to 0 to find where the function is at it minimum (least error)

$$g(w) = [X^TXw - X^Ty] = \sum_{i=1}^{N} x_i(w^Tx_i - y_i)$$

quadratic function

How do we know this reaches a minima? function is stically converxte we can guarantee that it has only one local minima.

Derivation of the MLE

Maximum likelihood estimation

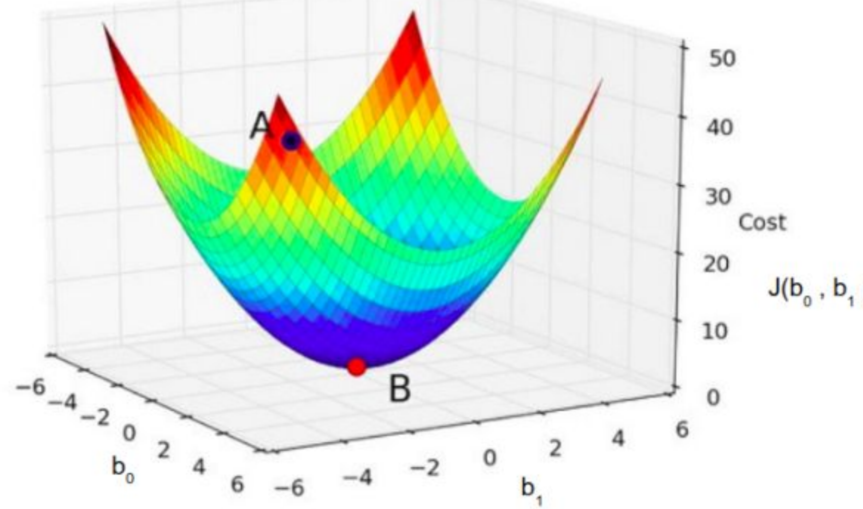
Given that this problem is convex (proof omitted), we know that it has a unique global minimizer, which we can find by setting the gradient to 0, where the solution to the problem is:

$$X^T X w = X^T y$$

$$g(w) = X^T X w - X^T y$$

$$0 = X^T X w - X^T y$$

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



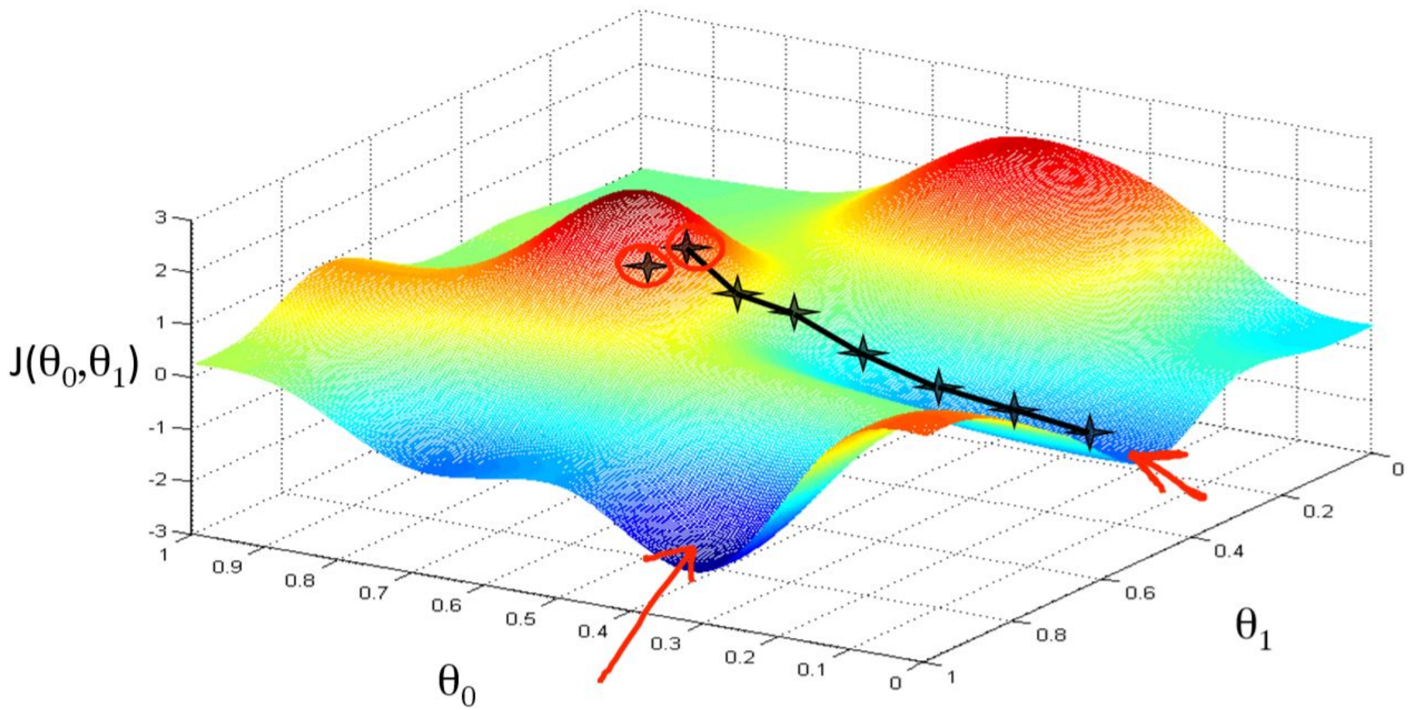
Rearranging the terms, we get the ordinary least squares solution in closed form:

$$\hat{w}_{OLS} = (X^T X)^{-1} X^T y$$

Observe complexity - 3 matrix multiplications, 1 matrix inverse: can compute in polynomial time, **bad for large datasets with many examples, many features**.

Gradient Descent

If we pick a point and find that the derivative is negative (for example, if x = 1) we know we need to pick a bigger x since we want to move downhill. If the derivative is positive, (say x = 6) we need to pick a smaller x.



Arrows are two minima

Gradient Descent

Gradient Descent is an optimization algorithm that helps machine learning models converge at a minimum value through repeated steps (find the minimum gradient of NLL function). Essentially, gradient descent is used to minimize a function by finding the value that gives the lowest output of the loss function. Loss functions measure how bad our model performs compared to actual occurrences. Hence, it only makes sense that we should reduce this loss. One way to do this is via Gradient Descent. Lost function is for 1 point, cost function is for the summation of every points

We essentially want to iteratively get closer to the minimum of our objective function (defined as the MSE with respect to our weights). For linear regressions we use a cost function known as the mean squared error or MSE.

- w_o , w_1 , w_2 , ... such that $MSE(w_o) > MSE(w_1) > MSE(w_2) > \ldots$

1. Pick initial w_0
2. For k = 1, 2, ...,

   $w_{k+1} = w_k - \alpha\, g(w_k)$ (gradient(derivative of NLL))

   where $\alpha>0$ is called the "learning rate" magnitude of everystep

   We take $-\alpha$ because, we wanna move towards local minima.

End when $|w_{k+1} - w_k| < \varepsilon$

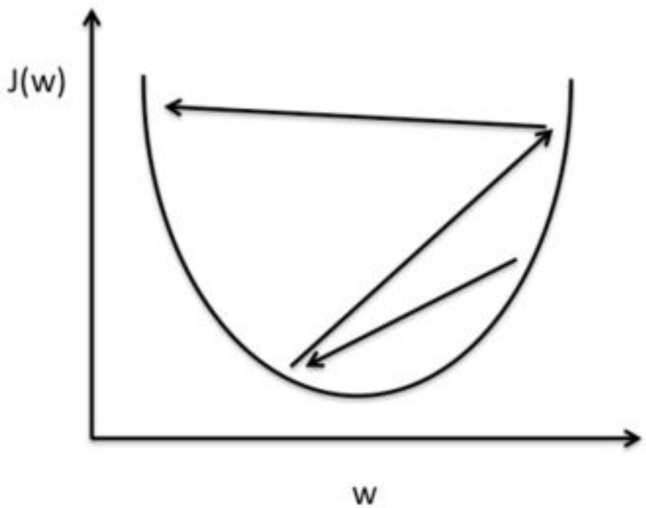
Picking α

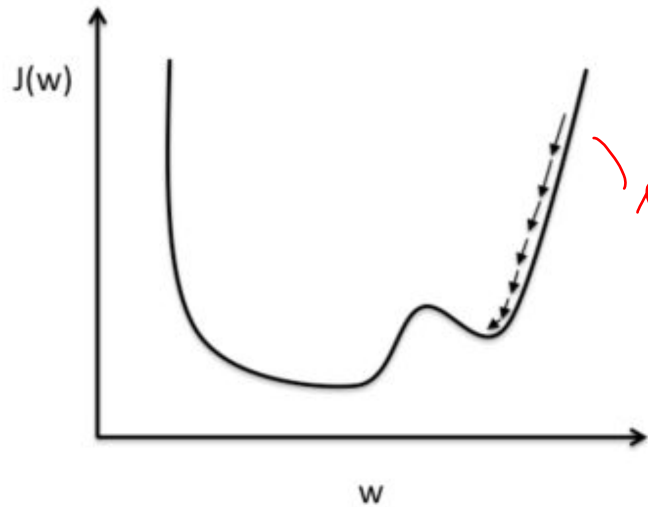
Wk+1 = wk -a g(wk) is because:

Xnew = Xold - d where d is the derivative

If we pick an x and find the derivative is positive, we know we overshot and need to move backwards on the x-axis. Mathematically, we want to subtract from our guess x, and since the derivative is positive, it gives us a number with the correct sign.

If on the other hand we undershot it, the derivative will be negative, and need to move forward to move down the hill. If our guess is 5 and the derivative is -1, our new guess will be 5-(-1) = 6. Since we undershot, we increase our x value.





Non-convexe function

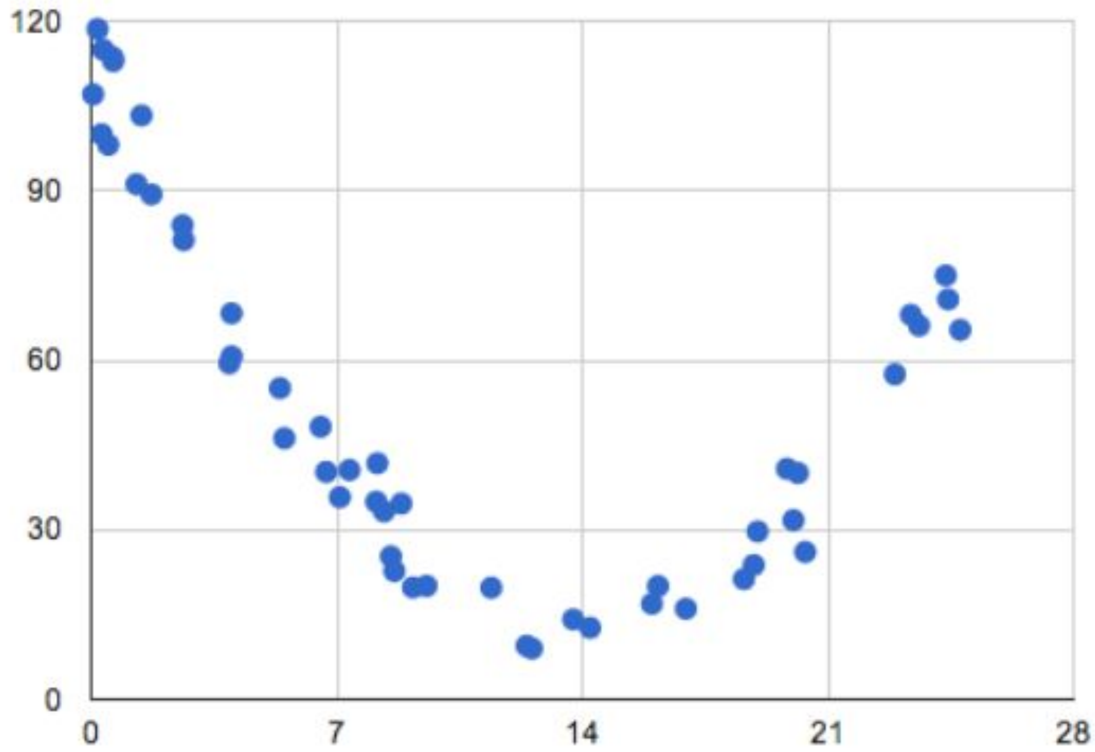
We want to approximate with a convexe function

Too large: we “overshoot” and don’t converge to the global minima

Too small: the weights might not move far enough to reach a local minima, slow convergence

What if Data is Non-Linear?

Can we still use linear regression?



$$h(x) = b_0 + b_1 x + b_2 x^2$$

Introducing Polynomial Regression

It doesn't have to be 2D

We linearize our hypothesis h(x):

$$h(x) = b_0 + b_1 x + b_2 x^2$$

$$h(x_1, x_2) = b_0 + b_1 x_1 + b_2 x_2$$

Such that $x_1 = x$, and $x_2 = x^2$

This way, the model is still **linear** with respect to its **parameters**.

Introducing Polynomial Regression

Instead of just using X, we apply a basis function expansion by replacing x with some non-linear function of the inputs s.t.

$$p(y|x,\theta) = \mathcal{N}(y|w^T\phi(X), \sigma^2)$$

Where

$$\phi(X) = [1, x, x^2, ..., x^d]$$

$x_0 \quad x_1 \quad x_2$

:

- model is still linear in parameters **w**
- allows to fit nonlinear data (**ϕ**(X) can be replaced with many other basis function expansions or kernels)

Overfitting vs. Underfitting

Intuitively, a linear (or a low dimensional polynomial) will not be powerful to fit more complex models → **underfitting**.

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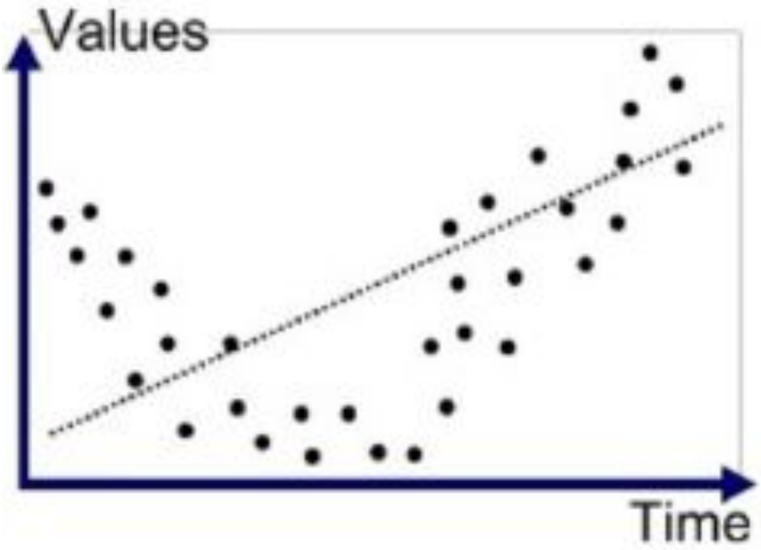
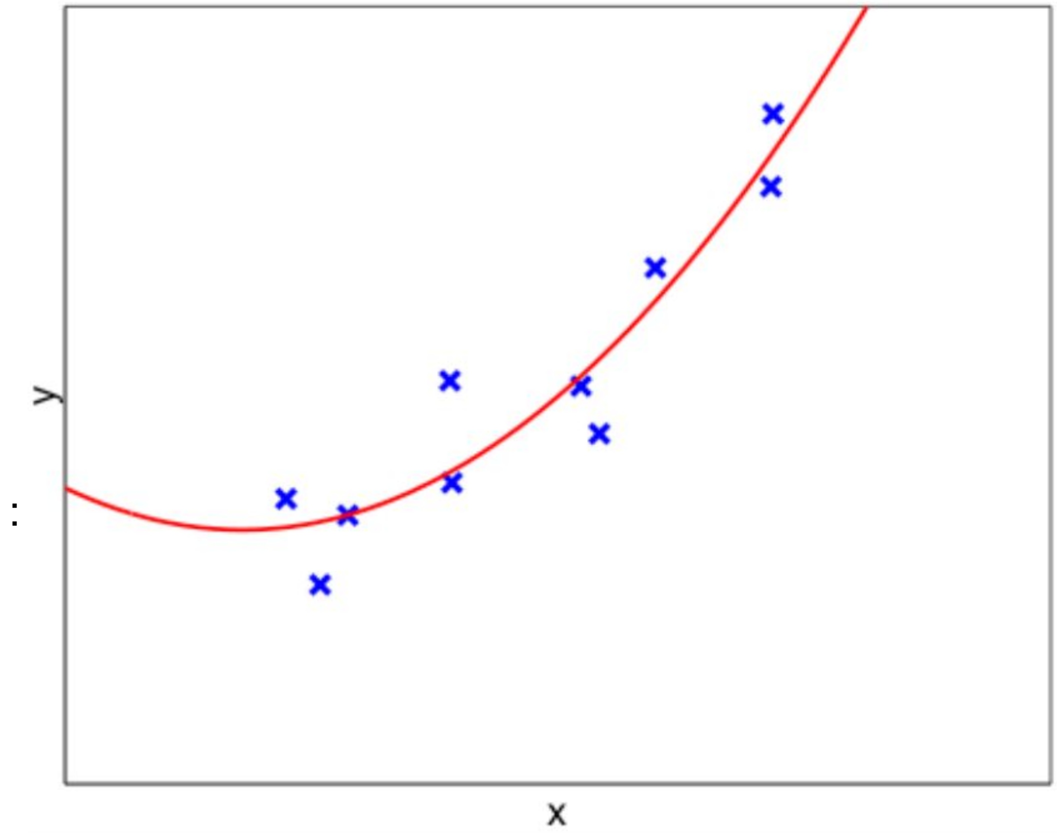


Overfitting -the phenomena by which the model is so adapted to the training set that it no longer generalizes well to the underlying model

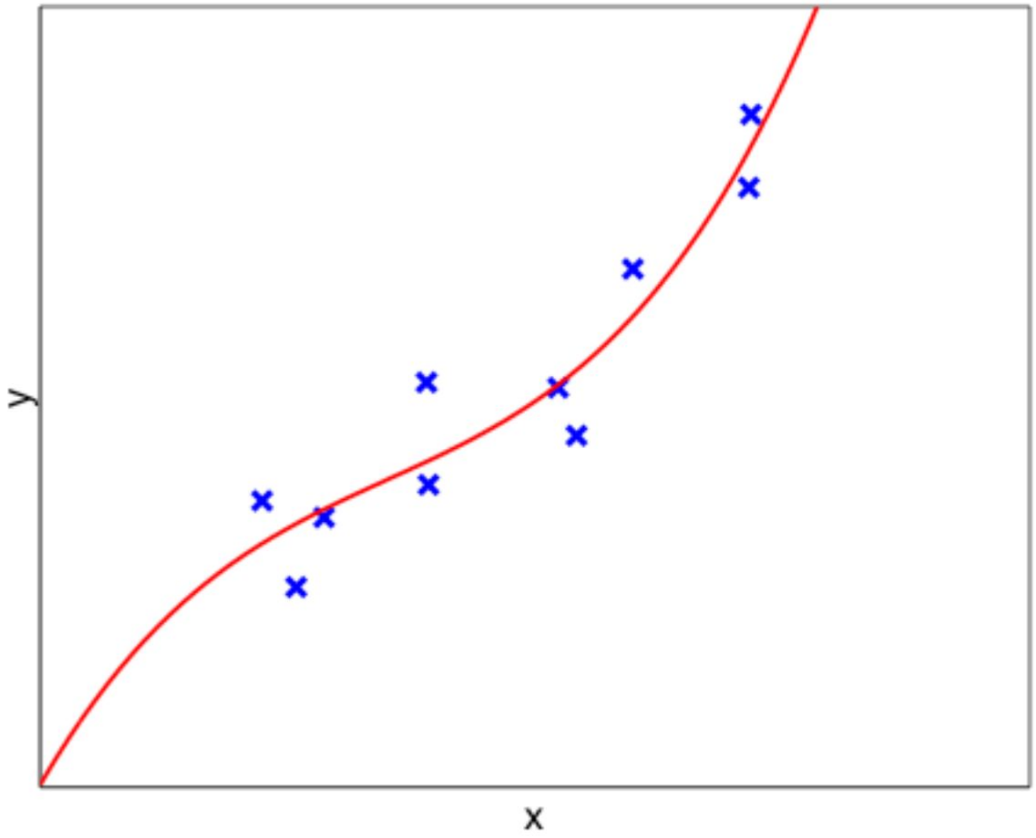
Learning the noise of the data
(variance)

Slides 21-25 adapted from Joelle Pineau - COMP 551 Lecture 3 on Linear Regression

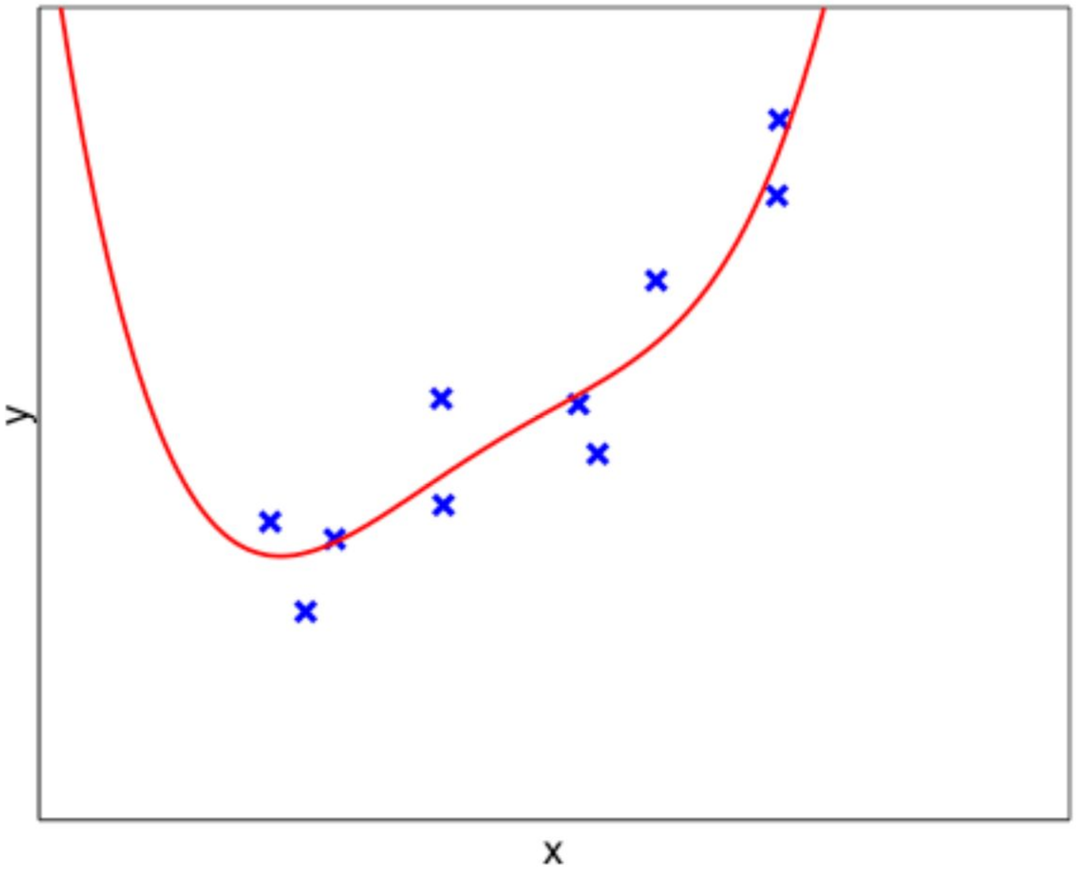
Order 2 fit



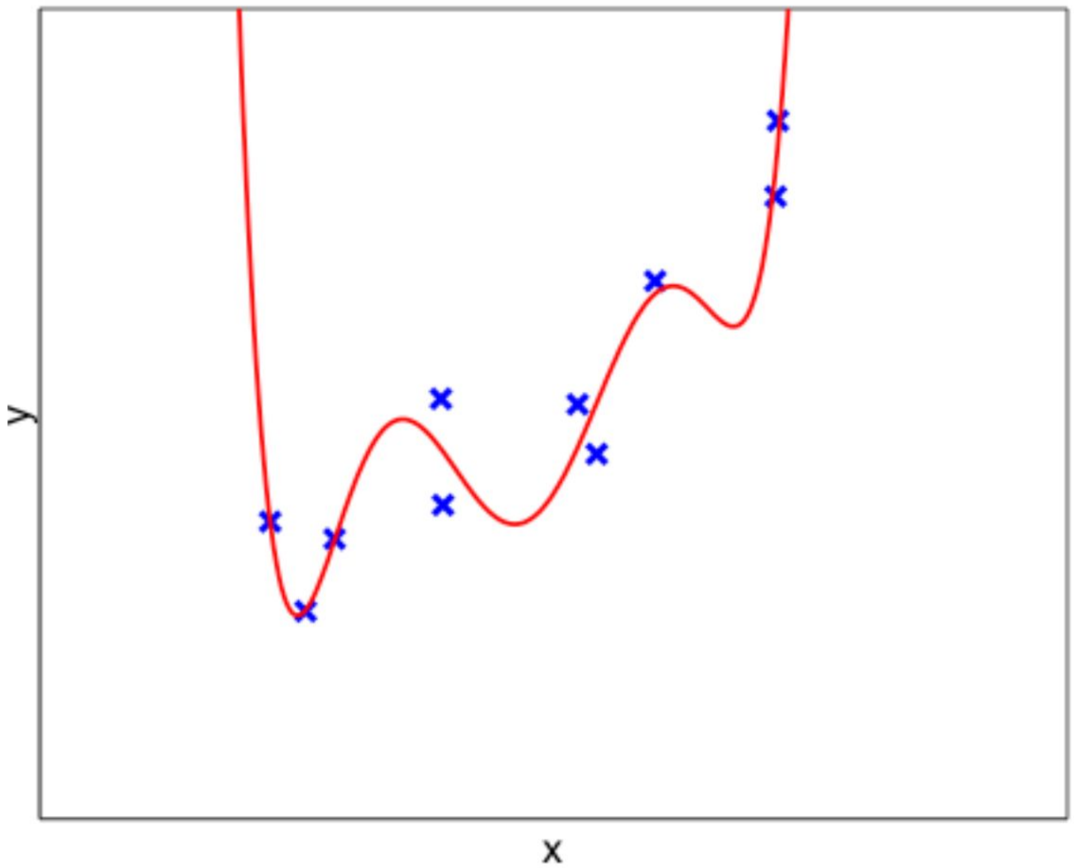
Order 3 fit



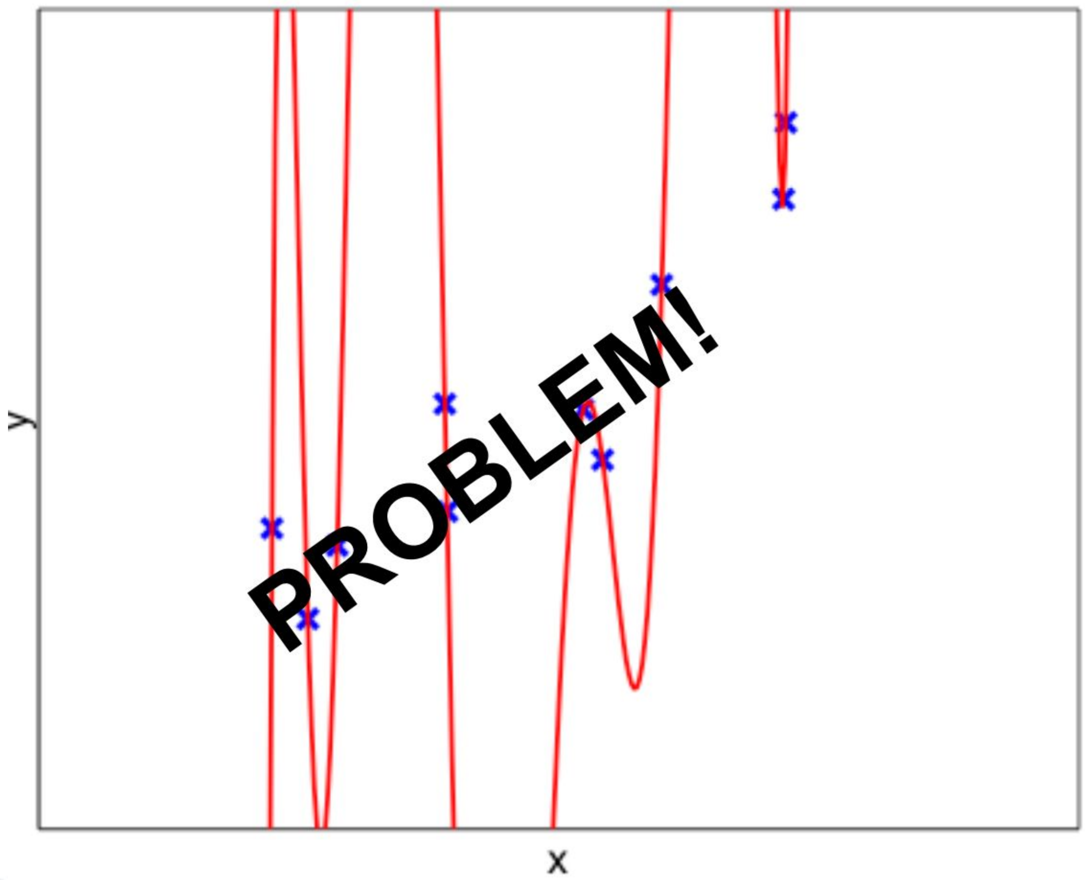
Order 4 fit



Order 6 fit



Order 9 fit



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Addressing Overfitting

Need training set
and validation set

How to address overfitting -

1) **Hyperparameter tuning -**
   Simply modify hyperparameters that control the complexity of the model (in this case, the value of d) until you get the validation set accuracy optimized

2) **Adding more data-**
   Adding more data, so simply having more training set data can allow for a more complex model without overfitting

More sophisticated methods: Ridge regression (L2 regularization), dropout in neural networks, lasso regression (L1 regularization), cross-validation, etc.

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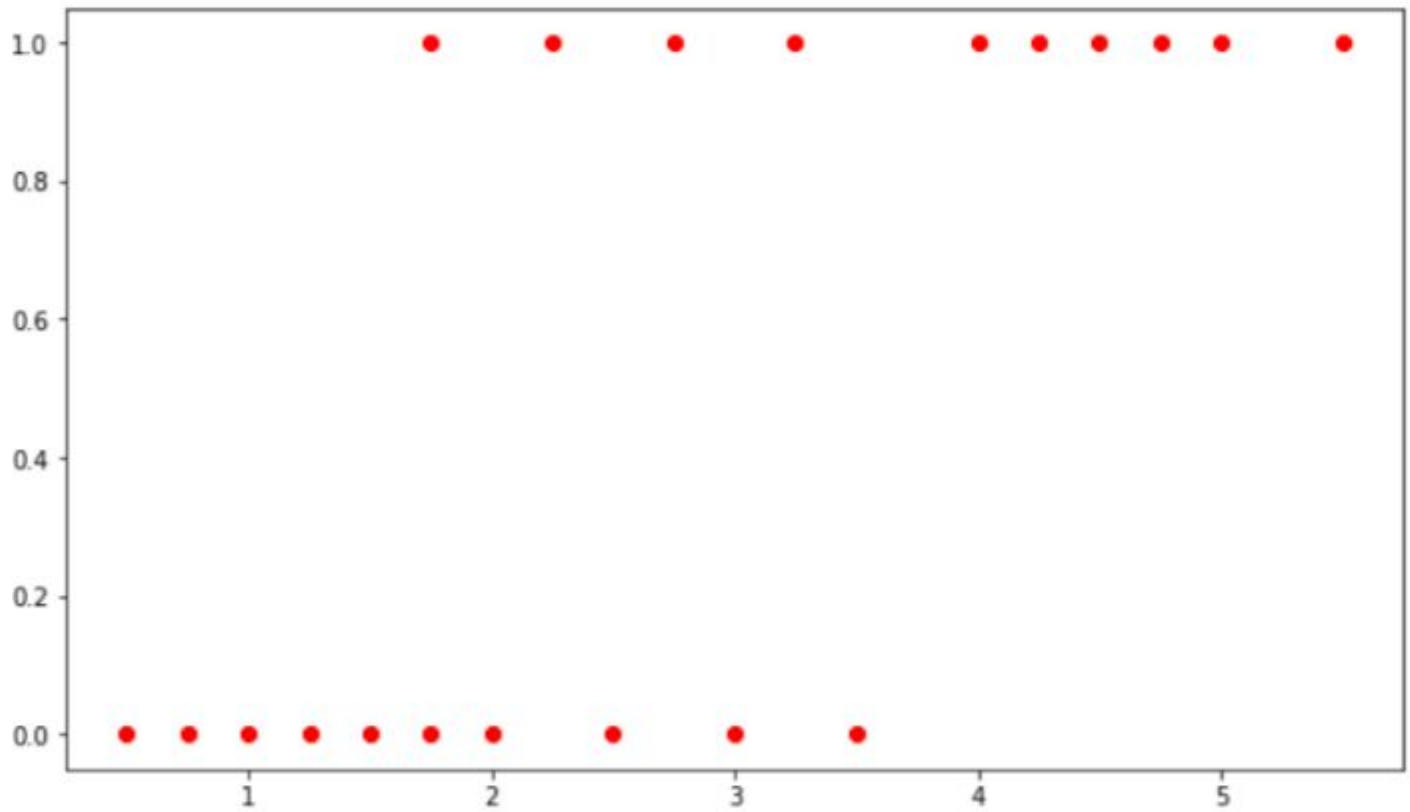
5-MINUTE BREAK

Now Consider the Following Problem…



Data classify either as 0 or 1 EX: classing e-mail as a spam or not

Image credits to Berkeley DeCal Course

Problem of linear regression: data is discrete, if we draw a line which is continuous, everything in the middle would mean anything
Prediction can exceed the range
No matter what the input is, we want the ouput is exactly 0 or 1

Why Linear Regression Doesn't Work Here

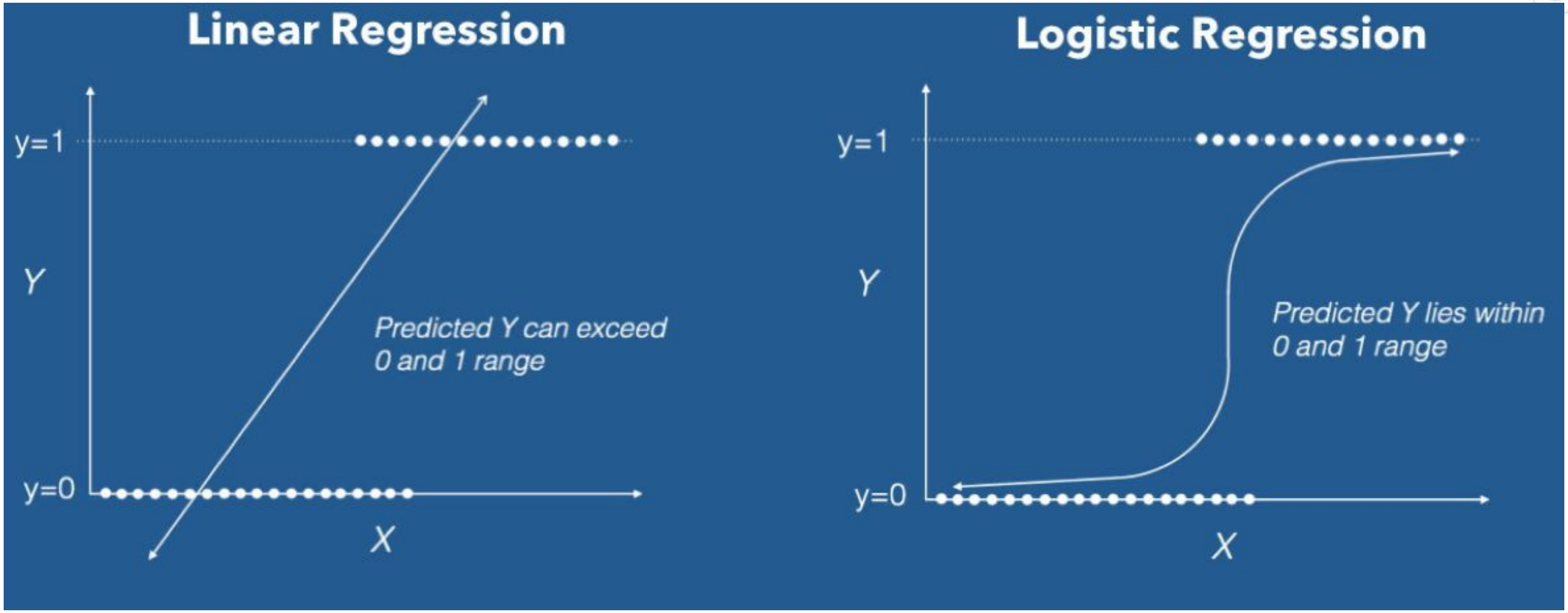


Image Credits

Logistic Regression

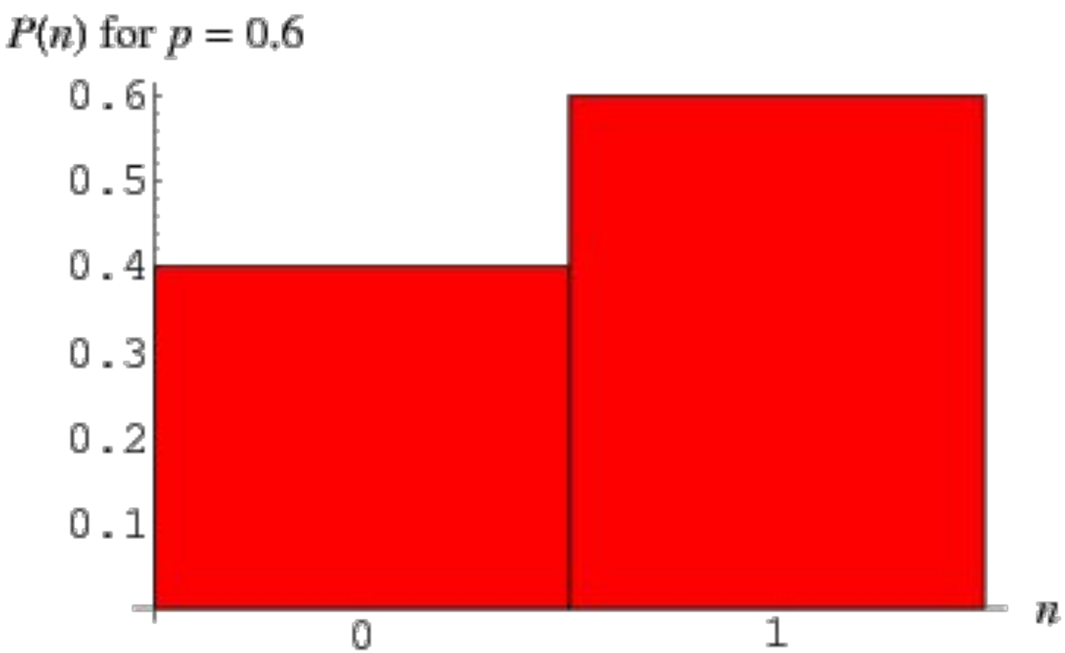
Instead of modeling our response directly, logistic regression models the probability that y belongs to a certain class:

$$p(y|x, w) = \boxed{Ber}(y|\boxed{sigm}(w^T x)$$

Bernoulli, sigmoid… what are those??

s shape curve that restrict function btwn 0 and 1

Bernoulli Random Variable



Sigmoid/ Logistic Function

We want a function f s.t. range$(f) \in [0, 1]$ $\forall$ X

such that

We can round the output to 0 or 1

Logistic Function (Ct'd)

$$P(X) = \frac{e^{\beta_0+\beta_1 X}}{1+e^{\beta_0+\beta_1 X}}$$

$$= \frac{1}{1+e^{-(\beta_0+\beta_1)X}}$$

$$\frac{P(X)}{1-P(X)} = e^{\beta_0+\beta_1 X}$$

$$\boxed{\ln\left(\frac{P(X)}{1-P(X)}\right)} = \beta_0+\beta_1 X$$

The "logit/ log-odds" function is linear in X

Computing Regression Coefficients

Although we can use the least-squares method and estimate using our training data, we prefer the maximum likelihood approach due to its better statistical properties (out of the scope of the course).

$$\ell(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i':y_{i'}=0} (1 - p(x_{i'})).$$

likelihood of B0 and B1

we want all the probability to happen at the same time based on these parameters

:

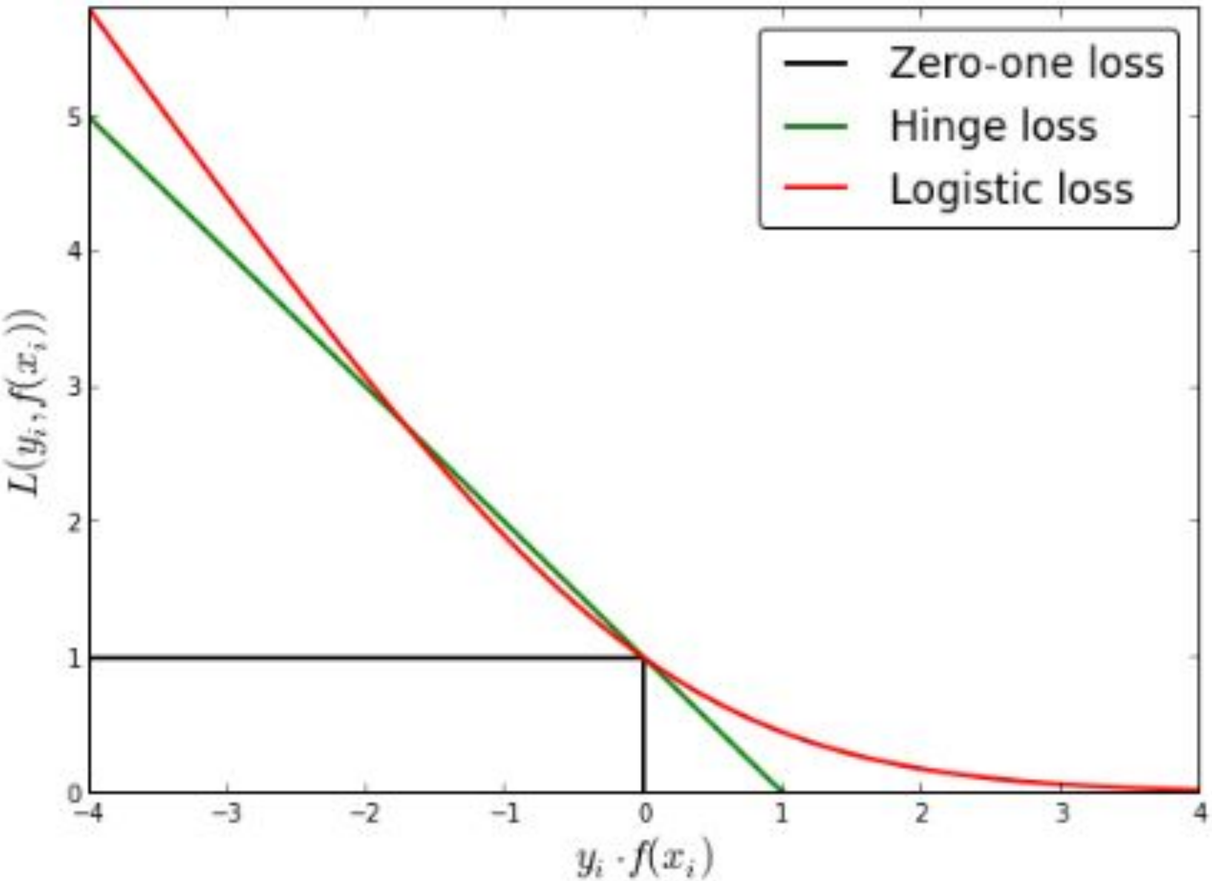
We seek to minimize logistic loss:

'Log' everything to get a sum

$$J(b) = -\sum_{i=1}^{m} \left(y^{(i)} \cdot \ln z^{(i)} + (1 - y^{(i)}) \cdot \ln (1 - z^{(i)}) \right)$$

$$z = h(x) = \frac{1}{1+e^{-\vec{b}^T \vec{x}}}$$

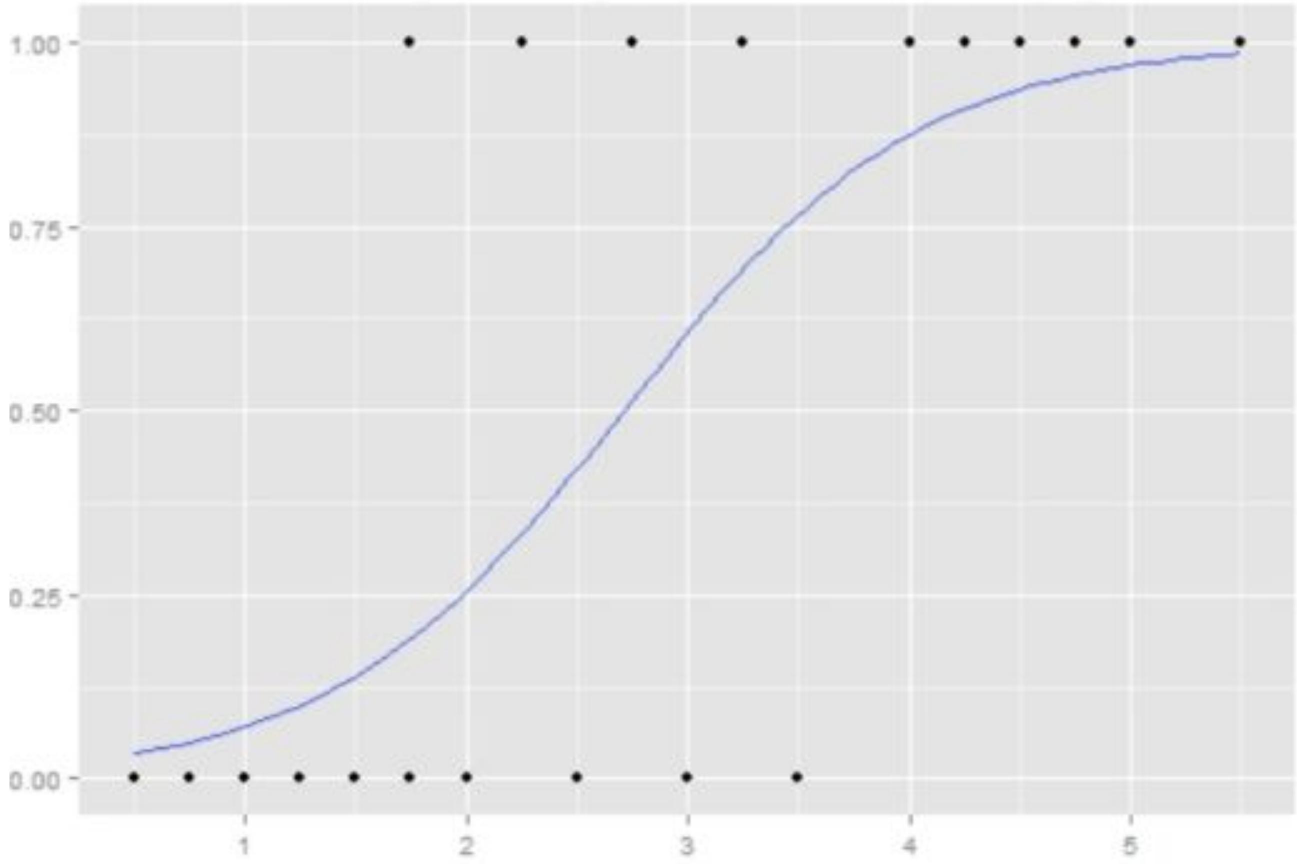
Logistic Loss



$$J(b) = -\sum_{i=1}^{m} \left(y^{(i)} \cdot \ln z^{(i)} + (1 - y^{(i)}) \cdot \ln (1 - z^{(i)}) \right)$$

Image from Stack Exchange

Coefficients should return something like this...



SUMMARY

	Linear	Logistic
Label Type	Continuous	Categorical
Problem Type	Actual Regression	Actually Classification
Hypothesis	$\theta^T x$	$s(\theta^T x)$
Loss	Mean Squared	Logistic
Analytical Solution	Yes	No

Thanks!

Any questions?

Reminders:

Homework 1 and deliverable 1 due before next lecture.