CS 460200

Introduction to Machine Learning

Regression

Instructor: Po-Chih Kuo

Roadmap

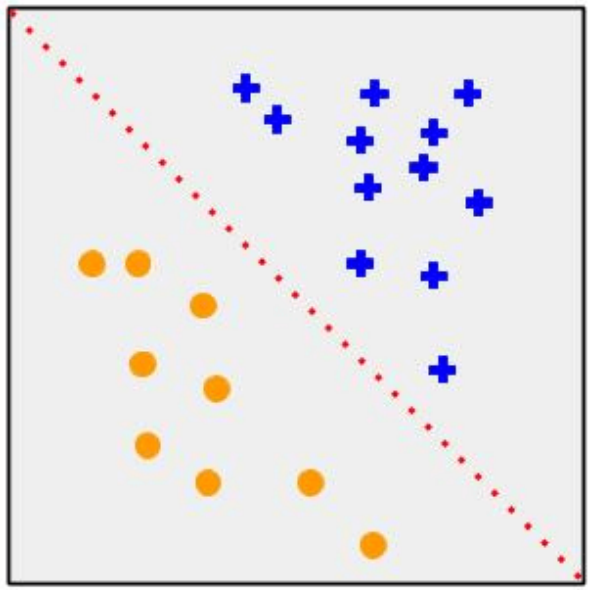
- Introduction and Basic Concepts
- Regression
- Bayesian Classifiers
- Decision Trees
- KNN
- Linear Classifier
- Neural Networks
- Deep learning
- Convolutional Neural Networks
  - Autoencoder
  - Adversarial
  - Transfer learning
  - …
- RNN/Transformer
- Reinforcement Learning
- Model Selection and Evaluation
- Clustering
- Data Exploration & Dimensionality reduction

Supervised learning

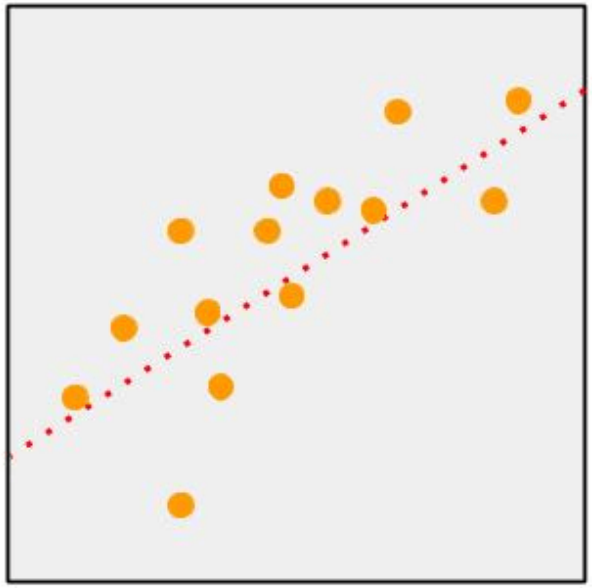
This week

- Regression *vs* Classification
- Linear regression – another discriminative learning method
  - As matrix inversion (Ordinary Least Squares)
  - As optimization: Gradient descent
    - Batch gradient decent
    - Stochastic gradient descent
- Overfitting and regularization
- Autoregression
- Logistic regression (more like classification)

Regression vs Classification

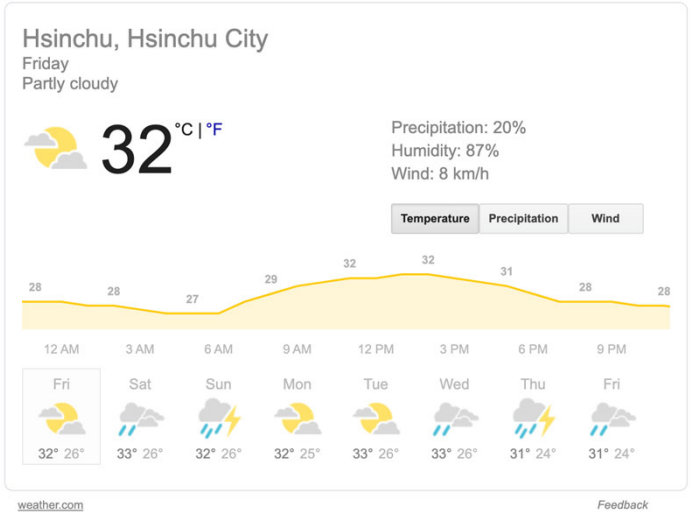


Classification



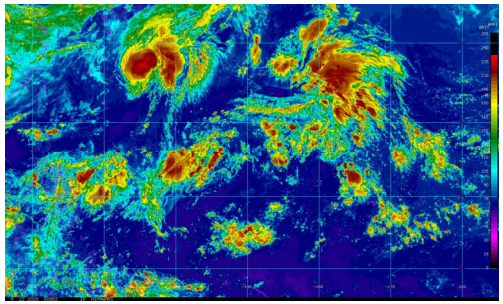
Regression

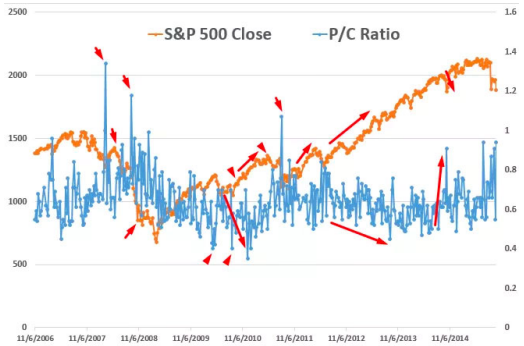
Regression examples



Weather prediction

Stock market





Example: House price in the U.S

	X_i	Y_i
i	sqft	price
1	5650	221900
2	7242	538000
3	10000	180000
4	5000	604000
5	8080	510000
6	101930	1230000

Training data

$\{(X_i, Y_i)\}_{i=1}^{n}$

Machine learning algorithm

Prediction function

$f(X_i)$

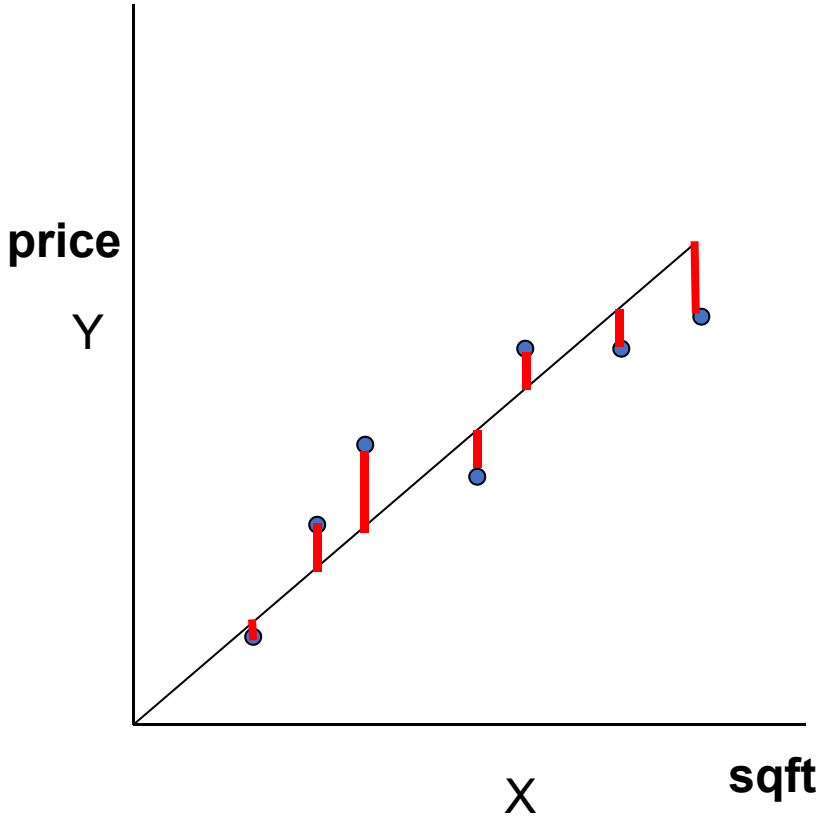
Linear regression

- Given an input x we would like to compute an output y
- In linear regression we assume that y and x are related with the following equation:

What we are trying to predict

$$y = f(x)=wx+\varepsilon$$

where w is a parameter and ε represents measurement noise



Linear regression

- Our goal is to estimate *w* from a training data of <x_i,y_i> pairs
- Optimization goal: minimize squared error (least squares):

$$\text{argmin}_w \sum_i (y_i - wx_i)^2$$

L(w)

- Why least squares?
  - Straightforward! minimizes squared distance between measurements and predicted line
  - Has probabilistic interpretation: equivalent to maximum likelihood estimation. (http://people.math.gatech.edu/~ecroot/3225/maximum_likelihood.pdf)
  - the math is pretty

Solving linear regression

- To optimize – closed form:
- Let's take the derivative w.r.t. to w and set to 0:

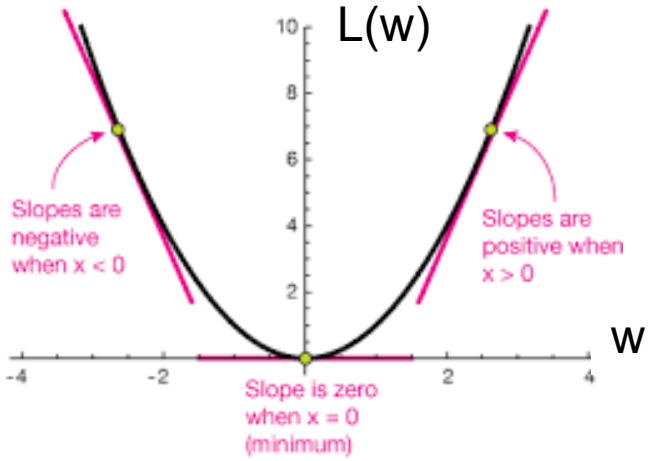
$$\frac{\partial}{\partial w}\sum_i (y_i - wx_i)^2 = 0$$

$$2\sum_i -x_i(y_i - wx_i) = 0$$

$$2\sum_i x_i(y_i - wx_i) = 0$$

$$2\sum_i x_i y_i - 2\sum_i wx_i x_i = 0$$

$$\sum_i x_i y_i = \sum_i w{x_i}^2$$



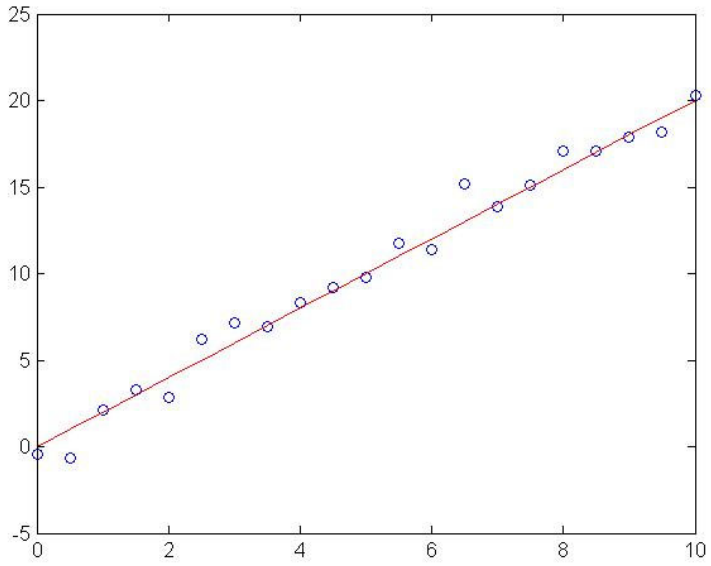
$$w = \frac{\sum_i x_i y_i}{\sum_i {x_i}^2} = \frac{COVAR(X,Y)}{VAR(X)}$$

if mean(X)=mean(Y)=0

Example-1

- Generated: w=2
- Noise: std=1

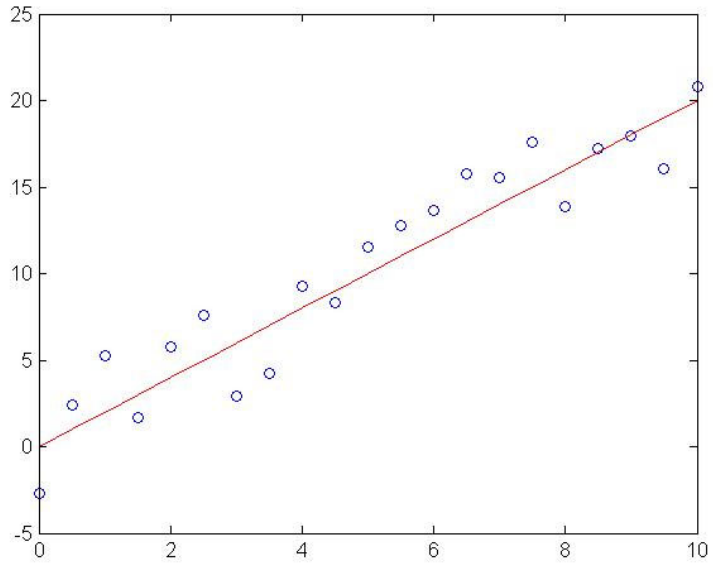
- Solved: w=2.03



Example-2

- Generated: w=2
- Noise: std=2

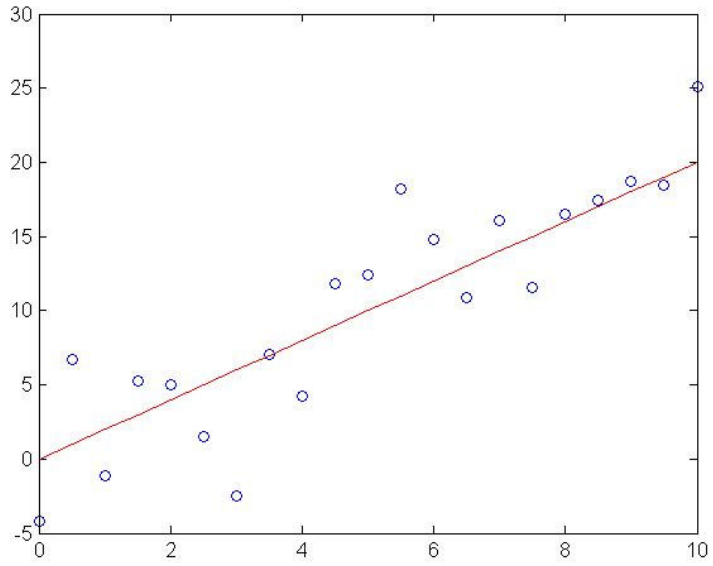
- Solved: w=2.05



Example-3

- Generated: w=2
- Noise: std=4

- Solved: w=2.08

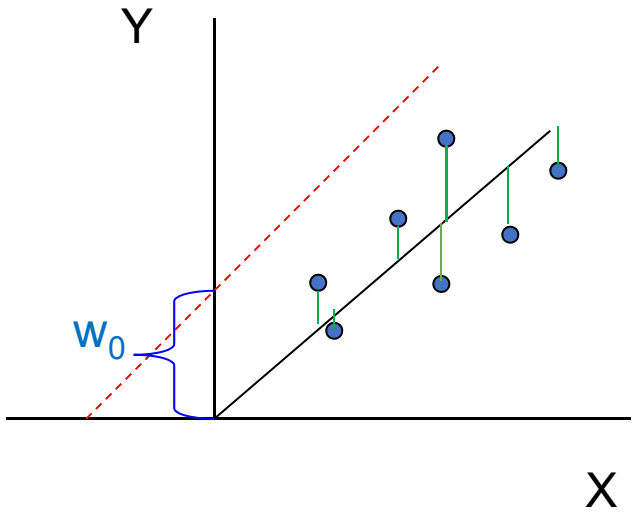


Intercept/Bias term

- So far we assumed that the line passes through the origin. What if the line does not?
- Simply change the model to:

$$y = w_0 + w_1 x + \varepsilon$$

- Can use least squares to determine w_0 , w_1



$$w_0 = \frac{\sum_i y_i - w_1 x_i}{n} \qquad w_1 = \frac{\sum_i x_i (y_i - w_0)}{\sum_i x_i^2}$$

Error vs Residual

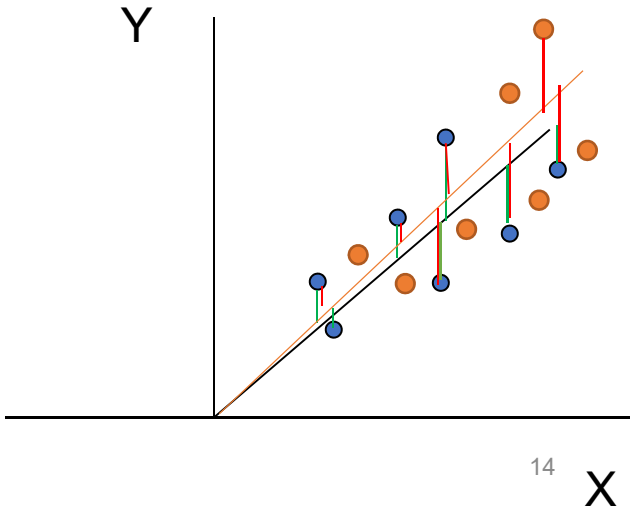
- The **error** of an observed value is the deviation of the observed value from the (unobservable) *true(theoretical)* value of a quantity of interest (for example, a population mean)
- The **residual** of an observed value is the difference between the observed value and the *estimated* value of the quantity of interest (for example, a sample mean).
- The error term accounts for the variation in the dependent variable(Y) that the independent variables(X) do not explain.
- Least square error?
  - "Model" error

$$y = wx + \varepsilon$$

$$\hat{y} = wx$$

$$\text{argmin}_w \sum_i (y_i - \hat{y}_i)^2$$

$$|y - \hat{y}|$$



- What if we have several inputs?

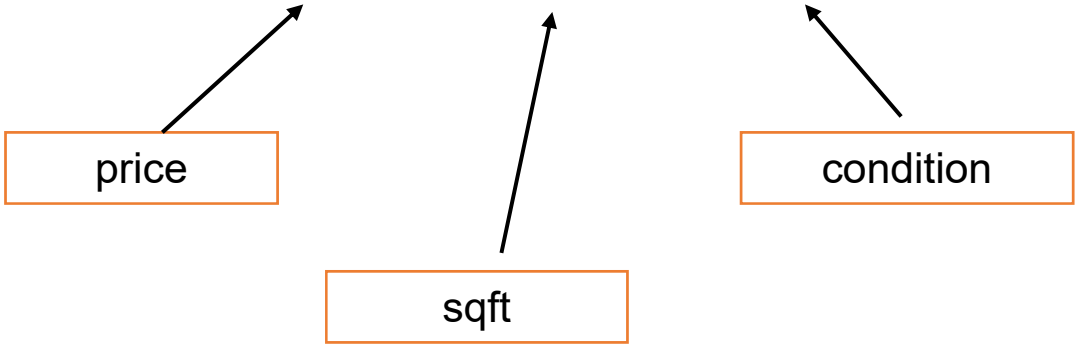
	X_1	X_2	X_3	X_4	Y
I	bedrooms	bathrooms	condition	sqft	price
1	3	1	3	5650	221900
2	3	2.25	3	7242	538000
3	2	1	3	10000	180000
4	4	3	5	5000	604000
5	3	2	3	8080	510000
6	4	4.5	3	101930	1230000

Multiple regression

"Multivariate" Regression : more than one independent variable (predictors) and more than one dependent variable (responses)

- This becomes a multiple regression problem
- Again, its easy to model:

$$y = w_0 + w_1 x_1 + \cdots + w_k x_k + \varepsilon$$



Non-linear basis functions

- So far we only used the observed values x_1,x_2,…
- However, linear regression can be applied in the same way to **functions** of these values
  - Eg: to add a term w x_1x_2 add a new variable $z=x_1x_2$ so each example becomes: x_1, x_2, …. z
- As long as these functions can be directly computed from the observed values the parameters are still **linear** in the data and the problem remains a multiple linear regression problem:

$$y = w_0 + w_1 x_1^{(2)} + \ldots + w_k x_k^{(2)} + \varepsilon$$

Linear in W, not necessarily in x

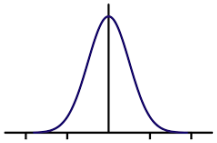
Non-Linear basis functions

- What type of functions can we use?
- A few common examples:
  - Polynomial:

$$\phi_j(x) = x^j$$

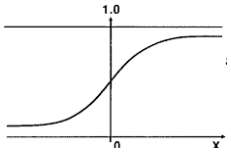
  - Gaussian:

$$\phi_j(x) = \exp(-\frac{(x-\mu_j)^2}{2s^2})$$



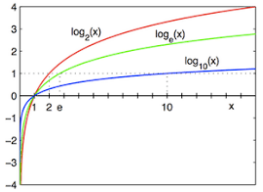
  - Sigmoid:

$$\phi_j(x) = \sigma(\frac{x-\mu_j}{s}) \qquad \sigma(a) = \frac{1}{1+\exp(-a)}$$



  - Logs:

$$\phi(x) = log(x+1)$$



Any function of the input values can be used. The solution for the parameters of the regression remains the same.

General linear regression problem

- Using our new notations for the basis function linear regression can be written as

$$y = \sum_{j=0}^{n} w_j \phi_j(x)$$

- Where $\phi_j(\mathbf{x})$ can be either x_j for multiple regression or one of the non-linear basis functions we defined
- $\phi_0(\mathbf{x})=1$ for the intercept term

Learning/Optimizing Multivariate Least Squares

Approach 1: Matrix Inversion

Approach 2: Gradient Descent

OLS (Ordinary Least Squares Solution)

OLS Assumption: The error term has a population mean of zero

$$\text{predict with}: \hat{y}^i = \sum_j^n w_j \phi_j(\mathbf{x}^i)$$

Goal: minimize the following loss function:

$$J_{\mathbf{X},\mathbf{y}}(\mathbf{w}) = \sum_i \left(y^i - \hat{y}^i\right)^2 = \sum_i \left(y^i - \sum_j w_j \phi_j(\mathbf{x}^i)\right)^2$$

sum over *n* examples

sum over *k+1* basis vectors

OLS (Ordinary Least Squares Solution)

Goal: minimize the following loss function:

$$J_{\mathbf{X},\mathbf{y}}(\mathbf{w}) = \sum_i \left(y^i - \hat{y}^i\right)^2 = \sum_i \left(y^i - \sum_j w_j \phi_j(\mathbf{x}^i)\right)^2$$

$$\frac{\partial}{\partial w_j} J(\mathbf{w}) = \frac{\partial}{\partial w_j} \sum_i \left(y^i - \hat{y}^i\right)^2$$

$$= -2 \sum_i \left(y^i - \hat{y}^i\right) \frac{\partial}{\partial w_j} \hat{y}^i$$

$$= -2 \sum_i \left(y^i - \hat{y}^i\right) \frac{\partial}{\partial w_j} \sum_j w_j \phi_j(\mathbf{x}^i)$$

$$= -2 \sum_i \left(y^i - \hat{y}^i\right) \phi_j(\mathbf{x}^i)$$

$$J_{\mathbf{X},\mathbf{y}}(\mathbf{w}) = \sum_i \left(y^i - \hat{y}^i\right)^2 = \sum_i \left(y^i - \sum_j w_j \phi_j(\mathbf{x}^i)\right)^2$$

$$\frac{\partial}{\partial w_j} J(\mathbf{w}) = -2 \sum_i \left(y^i - \hat{y}^i\right) \phi_j(\mathbf{x}^i)$$

Notation:

k+1 basis vectors

$$\mathbf{y} = \begin{pmatrix} y^1 \\ \cdots \\ \cdots \\ y^n \end{pmatrix} \quad \Phi = \begin{pmatrix} \phi_0(\mathbf{x}^1) & \phi_1(\mathbf{x}^1) & \cdots & \phi_k(\mathbf{x}^1) \\ \phi_0(\mathbf{x}^2) & \phi_1(\mathbf{x}^2) & \cdots & \phi_k(\mathbf{x}^2) \\ \vdots & \vdots & \cdots & \vdots \\ \phi_0(\mathbf{x}^n) & \phi_1(\mathbf{x}^n) & \cdots & \phi_k(\mathbf{x}^n) \end{pmatrix} \quad \mathbf{w} = \begin{pmatrix} w_0 \\ .. \\ w_k \end{pmatrix}$$

n examples

k+1 basis vectors

$$\mathbf{y} = \begin{pmatrix} y^1 \\ \cdots \\ \cdots \\ y^n \end{pmatrix} \quad \Phi = \begin{pmatrix} \phi_0(\mathbf{x}^1) & \phi_1(\mathbf{x}^1) & \cdots & \phi_k(\mathbf{x}^1) \\ \phi_0(\mathbf{x}^2) & \phi_1(\mathbf{x}^2) & \cdots & \phi_k(\mathbf{x}^2) \\ \vdots & \vdots & \cdots & \vdots \\ \phi_0(\mathbf{x}^n) & \phi_1(\mathbf{x}^n) & \cdots & \phi_k(\mathbf{x}^n) \end{pmatrix} = \begin{pmatrix} \vec{\phi}^1 \\ \cdots \\ \cdots \\ \vec{\phi}^n \end{pmatrix} \quad \mathbf{w} = \begin{pmatrix} w_0 \\ .. \\ w_k \end{pmatrix}$$

n examples

$$\frac{\partial}{\partial w_j} J(\boldsymbol{w}) = \begin{pmatrix} \frac{\partial}{\partial w_0} J(\boldsymbol{w}) = 2 \sum_i (y^i - \widehat{y^i}) \emptyset_0(\boldsymbol{x}^i) \\ \cdots \\ \frac{\partial}{\partial w_k} J(\boldsymbol{w}) = 2 \sum_i (y^i - \widehat{y^i}) \emptyset_k(\boldsymbol{x}^i) \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial w_0} J(\boldsymbol{w}) = 2 \sum_i (y^i \emptyset_0^i - \hat{y}^i \emptyset_0^i) \\ \cdots \\ \frac{\partial}{\partial w_k} J(\boldsymbol{w}) = 2 \sum_i (y^i \emptyset_k^i - \hat{y}^i \emptyset_k^i) \end{pmatrix}$$

notation: $\phi_j^i \equiv \phi_j(\mathbf{x}^i)$

$$\text{recall } \hat{y}^i = \sum_j^n w_j \phi_j^i$$

$$= \vec{\phi}^i \mathbf{w}$$

$$\begin{pmatrix} \frac{\partial}{\partial w_0} J(\boldsymbol{w}) = 2 \sum_i (y^i \phi_0^i - \hat{y}^i \phi_0^i) \\ \cdots \\ \frac{\partial}{\partial w_k} J(\boldsymbol{w}) = 2 \sum_i (y^i \phi_k^i - \hat{y}^i \phi_k^i) \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial w_0} J(\boldsymbol{w}) = 2 \sum_i (y^i \phi_0^i - \phi^i \mathbf{w} \phi_0^i) \\ \cdots \\ \frac{\partial}{\partial w_k} J(\boldsymbol{w}) = 2 \sum_i (y^i \phi_k^i - \phi^i \mathbf{w} \phi_k^i) \end{pmatrix}$$

$$= \begin{pmatrix} \frac{\partial}{\partial w_0} J(\boldsymbol{w}) = 2 \sum_i (\phi_0^i y^i - \phi_0^i \phi^i \mathbf{w}) \\ \cdots \\ \frac{\partial}{\partial w_k} J(\boldsymbol{w}) = 2 \sum_i (\phi_k^i y^i - \phi_k^i \phi^i \mathbf{w}) \end{pmatrix}$$

n examples

$$\Phi^T = \begin{pmatrix} \phi_0(\mathbf{x}^1) & \phi_0(\mathbf{x}^2) & \cdots & \phi_0(\mathbf{x}^n) \\ \vdots & \vdots & \cdots & \vdots \\ \phi_k(\mathbf{x}^1) & \phi_k(\mathbf{x}^2) & \cdots & \phi_k(\mathbf{x}^n) \end{pmatrix} \quad k+1 \qquad \mathbf{y} = \begin{pmatrix} y^1 \\ \cdots \\ \cdots \\ \cdots \\ y^n \end{pmatrix}$$

$$\begin{pmatrix} \frac{\partial}{\partial w_0} J(\boldsymbol{w}) = 2\sum_i (\phi_0^i y^i - \phi_0^i \phi^i \mathbf{w}) \\ \cdots \\ \frac{\partial}{\partial w_k} J(\boldsymbol{w}) = 2\sum_i (\phi_k^i y^i - \phi_k^i \phi^i \mathbf{w}) \end{pmatrix} = 2\Phi^T \mathbf{y} - \ldots$$

n examples

k+1 basis vectors

$$\begin{pmatrix} \phi_0(\mathbf{x}^1) & \dots & \cdots & \phi_0(\mathbf{x}^n) \\ \phi_1(\mathbf{x}^1) & & & \phi_1(\mathbf{x}^n) \\ \vdots & \vdots & \cdots & \vdots \\ \phi_k(\mathbf{x}^1) & & \cdots & \phi_k(\mathbf{x}^n) \end{pmatrix} \quad \begin{pmatrix} \phi_0(\mathbf{x}^1) & \cdots & \phi_k(\mathbf{x}^1) \\ \phi_0(\mathbf{x}^2) & \cdots & \phi_k(\mathbf{x}^2) \\ \vdots & \vdots & \vdots \\ \phi_0(\mathbf{x}^n) & \cdots & \phi_k(\mathbf{x}^n) \end{pmatrix} \quad \begin{pmatrix} w_0 \\ .. \\ w_k \end{pmatrix}$$

$$\begin{pmatrix} \frac{\partial}{\partial w_0} J(\boldsymbol{w}) = 2\sum_i (\phi_0^i y^i - \phi_0^i \phi^i \mathbf{w}) \\ \cdots \\ \frac{\partial}{\partial w_k} J(\boldsymbol{w}) = 2\sum_i (\phi_k^i y^i - \phi_k^i \phi^i \mathbf{w}) \end{pmatrix} = \ldots - 2\Phi^T \Phi \mathbf{w}$$

k+1 basis vectors

$$\mathbf{w} = \begin{pmatrix} w_0 \\ .. \\ w_k \end{pmatrix} \qquad \Phi = \begin{pmatrix} \phi_0(\mathbf{x}^1) & \phi_1(\mathbf{x}^1) & \cdots & \phi_k(\mathbf{x}^1) \\ \phi_0(\mathbf{x}^2) & \phi_1(\mathbf{x}^2) & \cdots & \phi_k(\mathbf{x}^2) \\ \vdots & \vdots & \cdots & \vdots \\ \phi_0(\mathbf{x}^n) & \phi_1(\mathbf{x}^n) & \cdots & \phi_k(\mathbf{x}^n) \end{pmatrix} \quad \text{n examples} \qquad \mathbf{y} = \begin{pmatrix} y^1 \\ \cdots \\ \cdots \\ y^n \end{pmatrix}$$

$$\begin{pmatrix} \frac{\partial}{\partial w_0} J(\boldsymbol{w}) = 2\sum_i (\phi_0^i y^i - \phi_0^i \phi^i \mathbf{w}) \\ \cdots \\ \frac{\partial}{\partial w_k} J(\boldsymbol{w}) = 2\sum_i (\phi_k^i y^i - \phi_k^i \phi^i \mathbf{w}) \end{pmatrix} = 2\Phi^T \mathbf{y} - 2\Phi^T \Phi \mathbf{w} \quad = 0$$

$$\mathbf{w} = \left(\Phi^T \Phi\right)^{-1} \Phi^T \mathbf{y}$$

OLS for general linear regression

$$w = \frac{\sum_i x_i y_i}{\sum_i x_i^2} = \frac{COVAR(X,Y)}{VAR(X)}$$

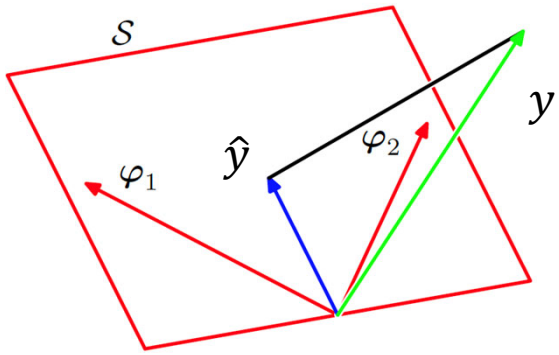
$$J(w) = \sum_i (y^i - w^T \phi(x^i))^2$$

Deriving w we get: $w = (\Phi^T \Phi)^{-1} \Phi^T y$

k+1 entries vector

n by k+1 matrix

n entries vector



This solution is also known as '**pseudo inverse**'

Learning/Optimizing Multivariate Least Squares

Approach 1: Matrix Inversion

Approach 2: Gradient Descent

Gradient descent for linear regression

$$\text{predict with}: \hat{y}^i = \sum_j^n w_j \phi_j(\mathbf{x}^i)$$

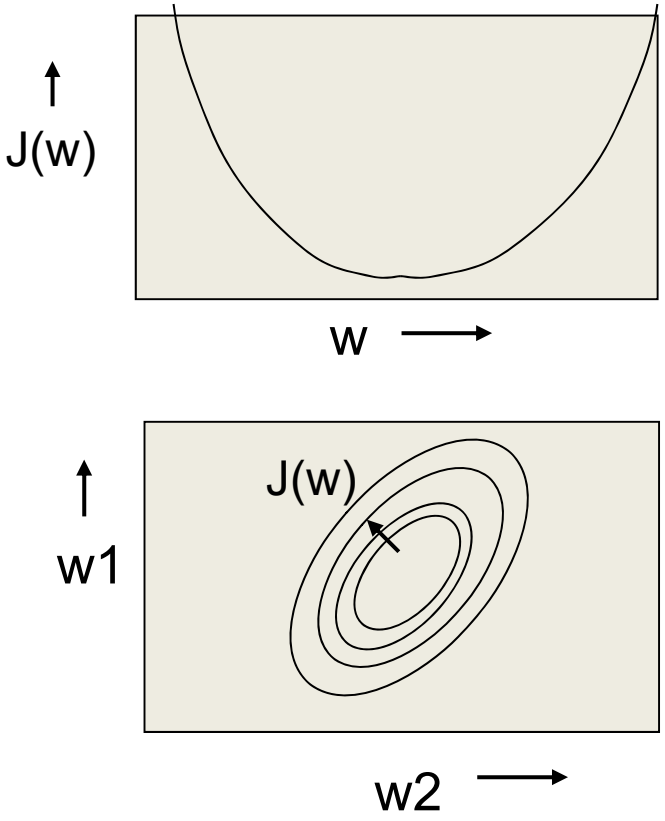
Goal: minimize the following loss function:

$$J_{\mathbf{X},\mathbf{y}}(\mathbf{w}) = \sum_i \left(y^i - \hat{y}^i\right)^2 = \sum_i \left(y^i - \sum_j w_j \phi_j(\mathbf{x}^i)\right)^2$$

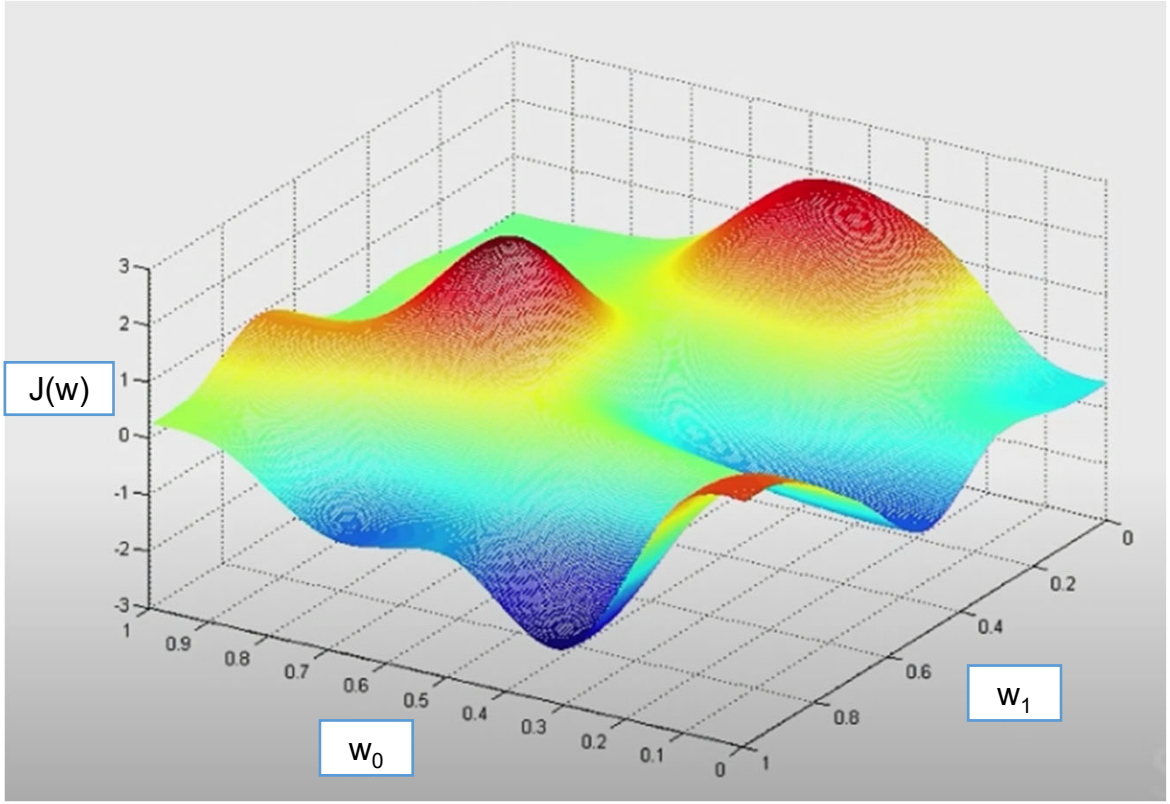
sum over *n* examples

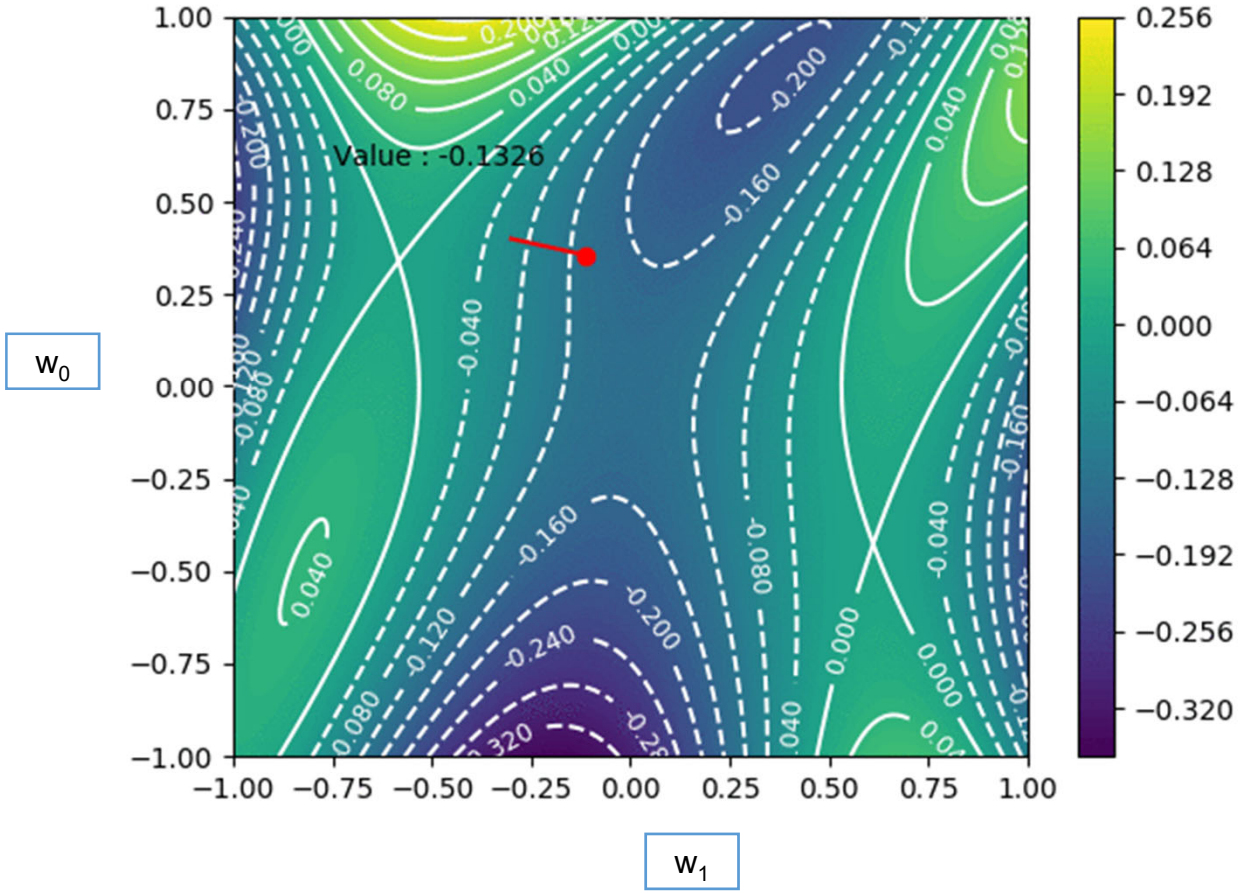
sum over *k+1* basis vectors

Gradient descent



Gradient descent





(https://github.com/Shathra/gradient-descent-demonstration)

Gradient descent for linear regression

Goal: minimize the following loss function:

$$J_{\mathbf{X},\mathbf{y}}(\mathbf{w}) = \sum_i \left(y^i - \hat{y}^i\right)^2 = \sum_i \left(y^i - \sum_j w_j \phi_j(\mathbf{x}^i)\right)^2$$

$$\frac{\partial}{\partial w_j} J(\mathbf{w}) = \frac{\partial}{\partial w_j} \sum_i \left(y^i - \hat{y}^i\right)^2$$

$$= -2 \sum_i \left(y^i - \hat{y}^i\right) \frac{\partial}{\partial w_j} \hat{y}^i$$

$$= -2 \sum_i \left(y^i - \hat{y}^i\right) \frac{\partial}{\partial w_j} \sum_j w_j \phi_j(\mathbf{x}^i)$$

$$= -2 \sum_i \left(y^i - \hat{y}^i\right) \phi_j(\mathbf{x}^i)$$

Gradient descent for linear regression

Learning algorithm:

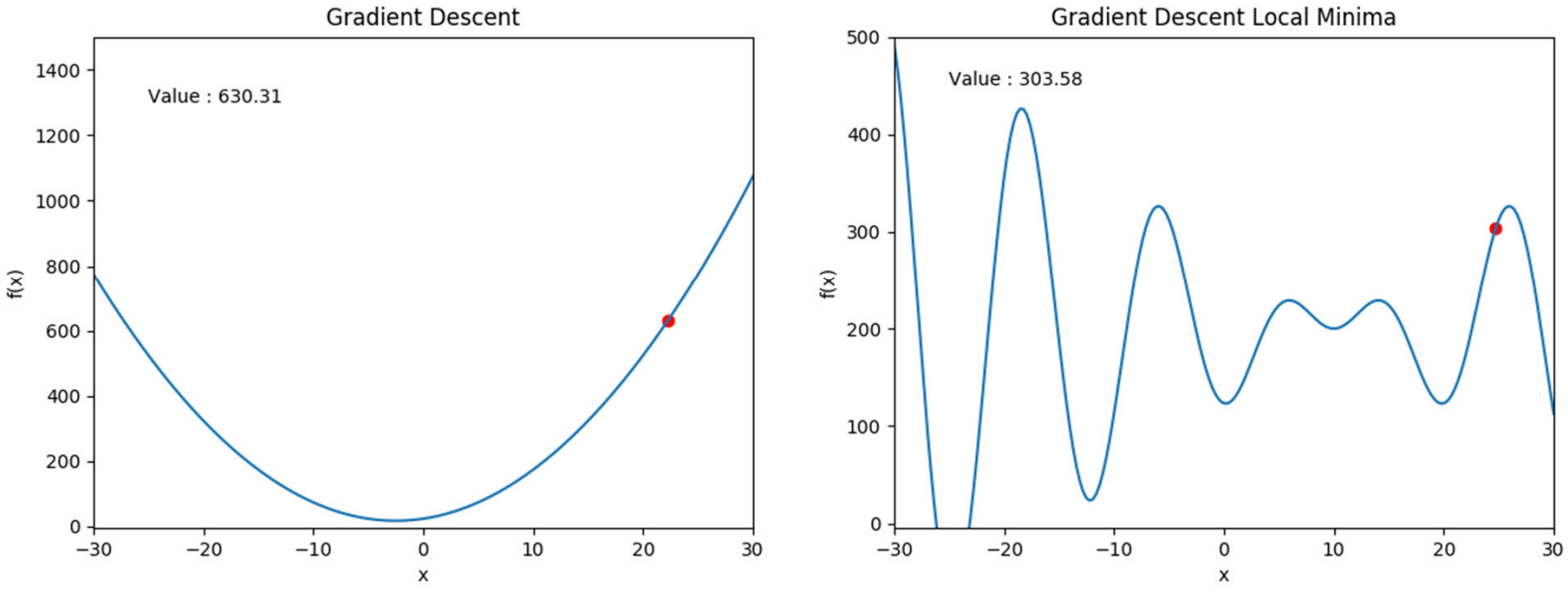
- Initialize weights **w=0**
- For t=1,… until convergence:
  - Predict for each example $\boldsymbol{x}^i$ using **w:** $\hat{y}^i = \sum_{j=0}^{k} w_j \phi_j(\mathbf{x}^i)$
  - Compute gradient of loss: $\frac{\partial}{\partial w_j} J(\mathbf{w}) = 2\sum_i \left(y^i - \hat{y}^i\right) \phi_j(\mathbf{x}^i)$
  - This is a vector **g**
  - Update: **w = w** – α**g,** α is the learning rate

$$\mathrm{w}=\mathrm{w}-\alpha\nabla J(w)$$

(bowl shaped)

Linear regression is a convex optimization problem

gradient descent can reach a *global* optimum

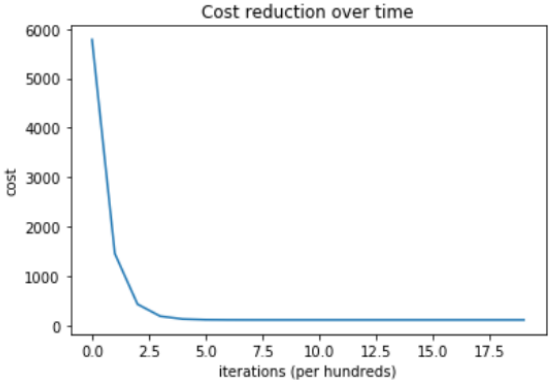


(https://github.com/Shathra/gradient-descent-demonstration)

Non-convex optimization

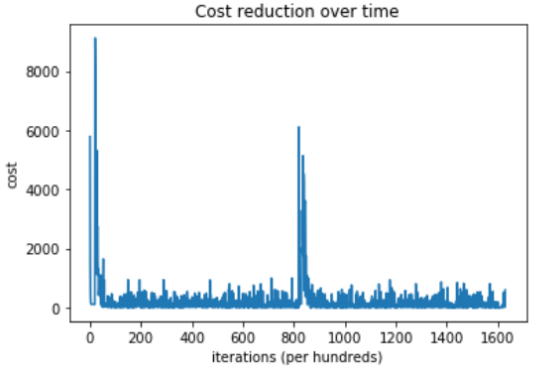
- NP-hard in general
- Deep learning

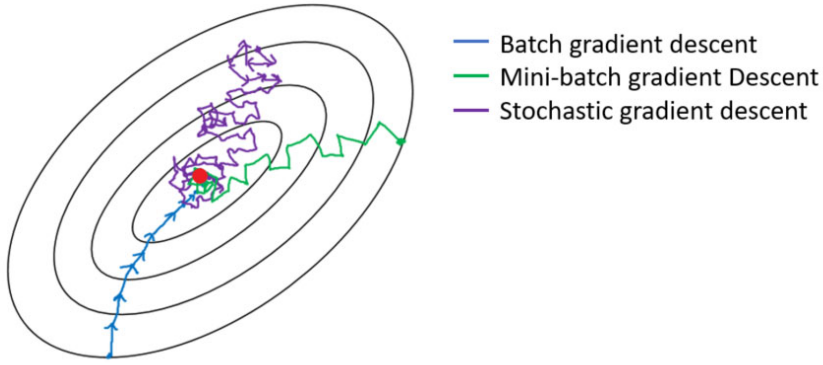
Stochastic gradient descent



- What we just see is “Batch” gradient decent
  - The gradient will be computed using the whole training data set
  - Since it uses the whole dataset at every iteration, hence, it makes the computation very, very slow especially when the data set is very large.

- Idea: rather than using the full gradient, just use one training example
  - Fast to compute $\mathrm{w}=\mathrm{w}-\alpha\nabla J(w; y_i)$





(Ref: https://suniljangirblog.wordpress.com/2018/12/13/variants-of-gradient-descent/)

OLS versus gradient descent

$$J(\mathrm{w}) = \sum_i (y^i - \mathrm{w}^{\mathrm{T}} \phi(x^i))^2 \qquad \mathrm{w} = (\Phi^T \Phi)^{-1} \Phi^T \mathrm{y}$$

Ordinary Least Squares (OLS) solution:

+ Very simple in programming

-Requires matrix inverse, which is expensive for a large matrix.

Gradient descent:

+ Fast for large matrices

+ Stochastic GD is very memory efficient

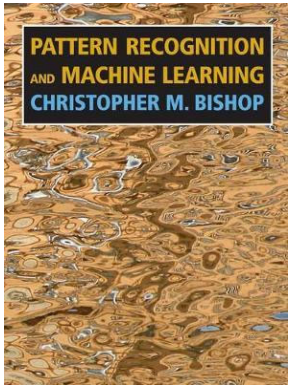
+ Easily extended to other cases

- Parameters to tune (how to decide convergence? what is the learning rate? ….)

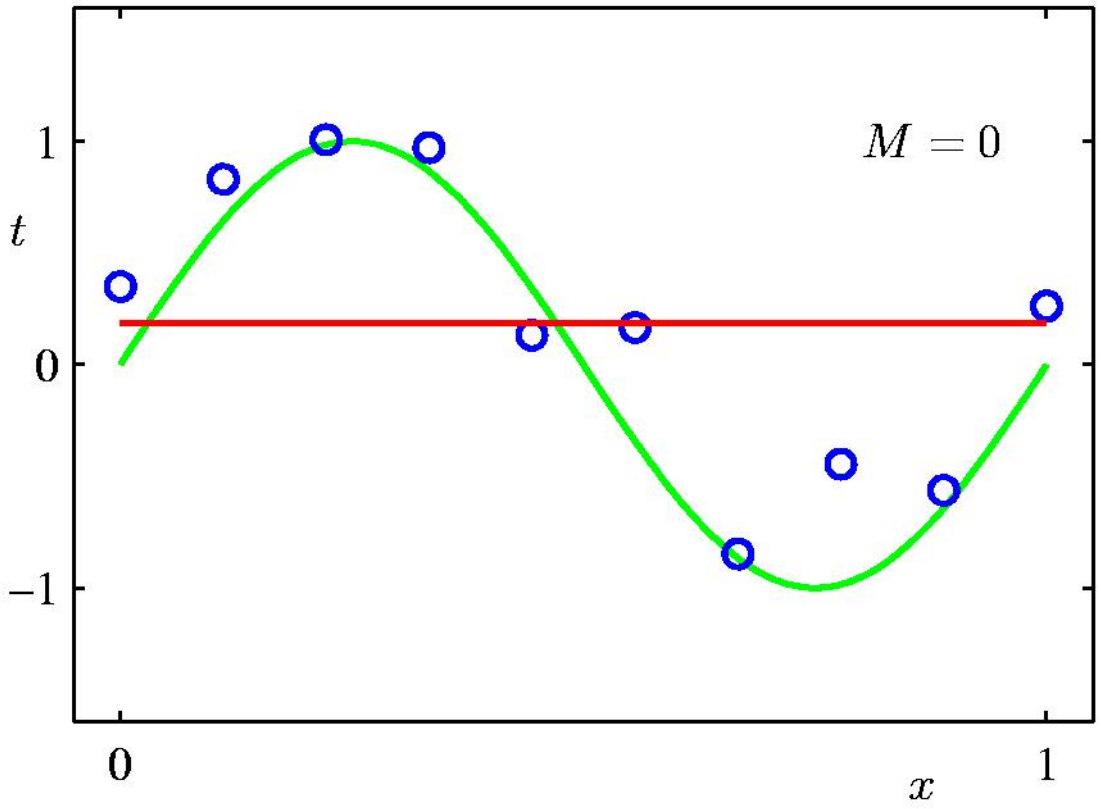
Overfitting and Regularization

An example: polynomial basis vectors on a small dataset

(From Bishop Ch 1)

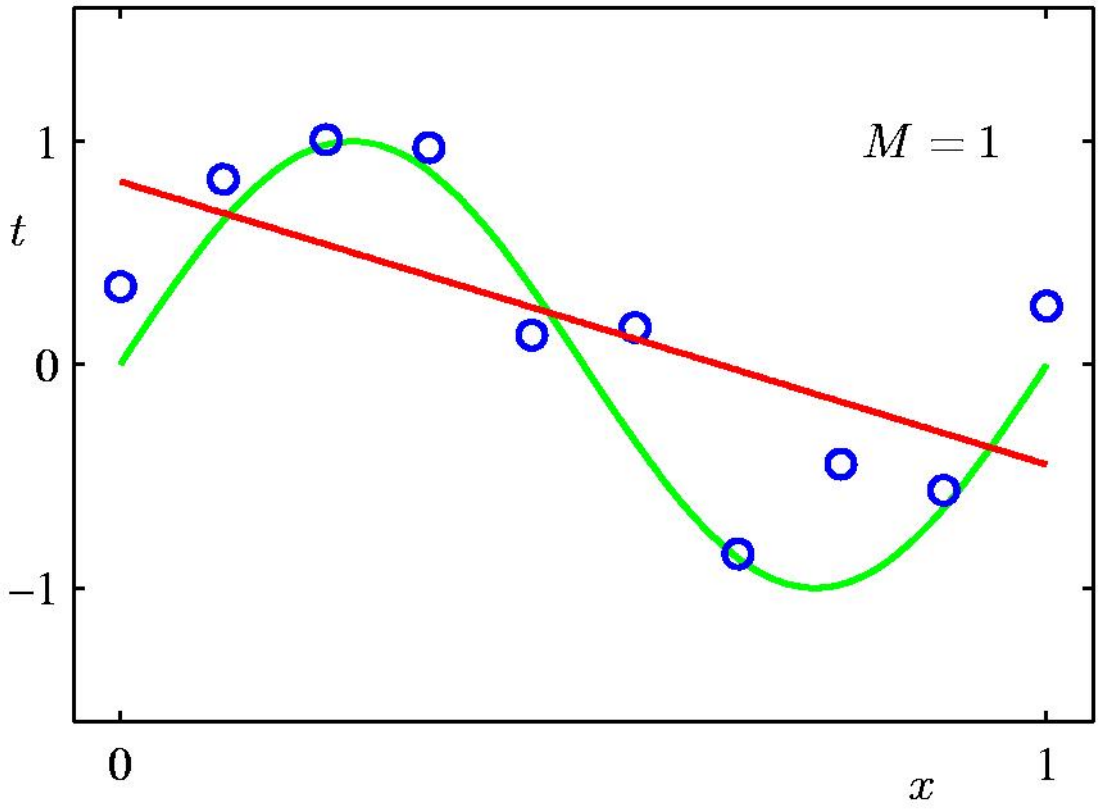


0^{th} Order Polynomial

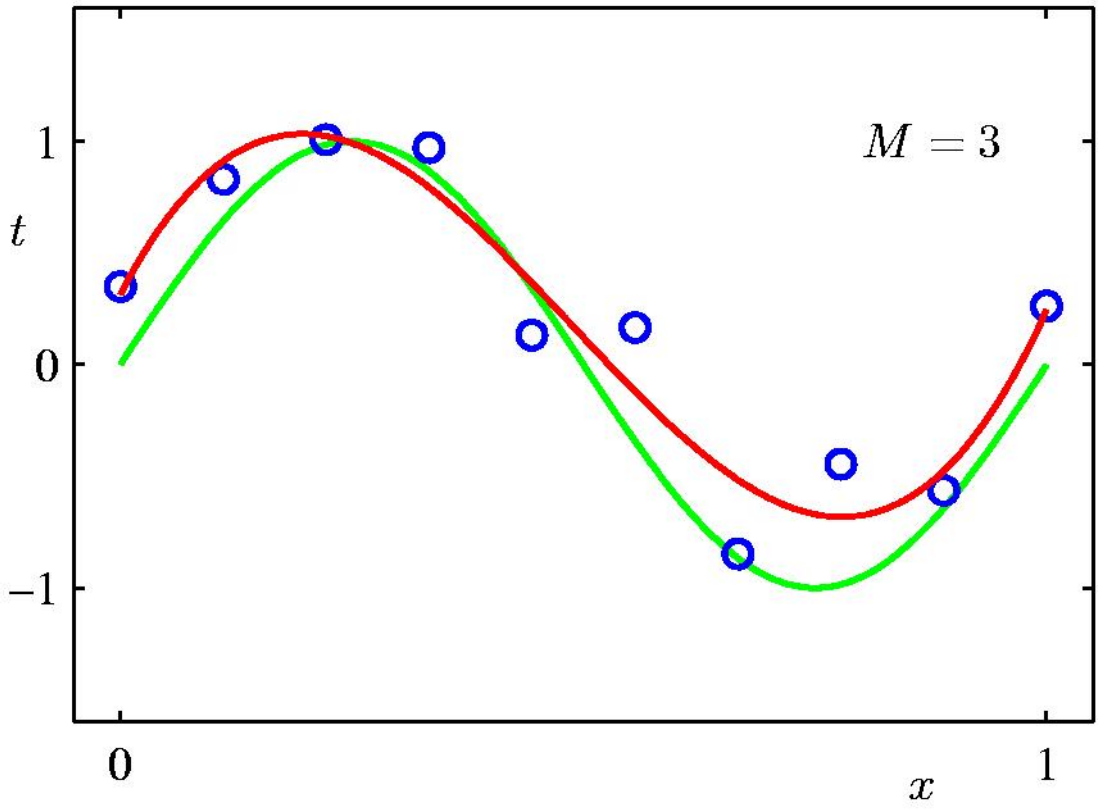


n=10

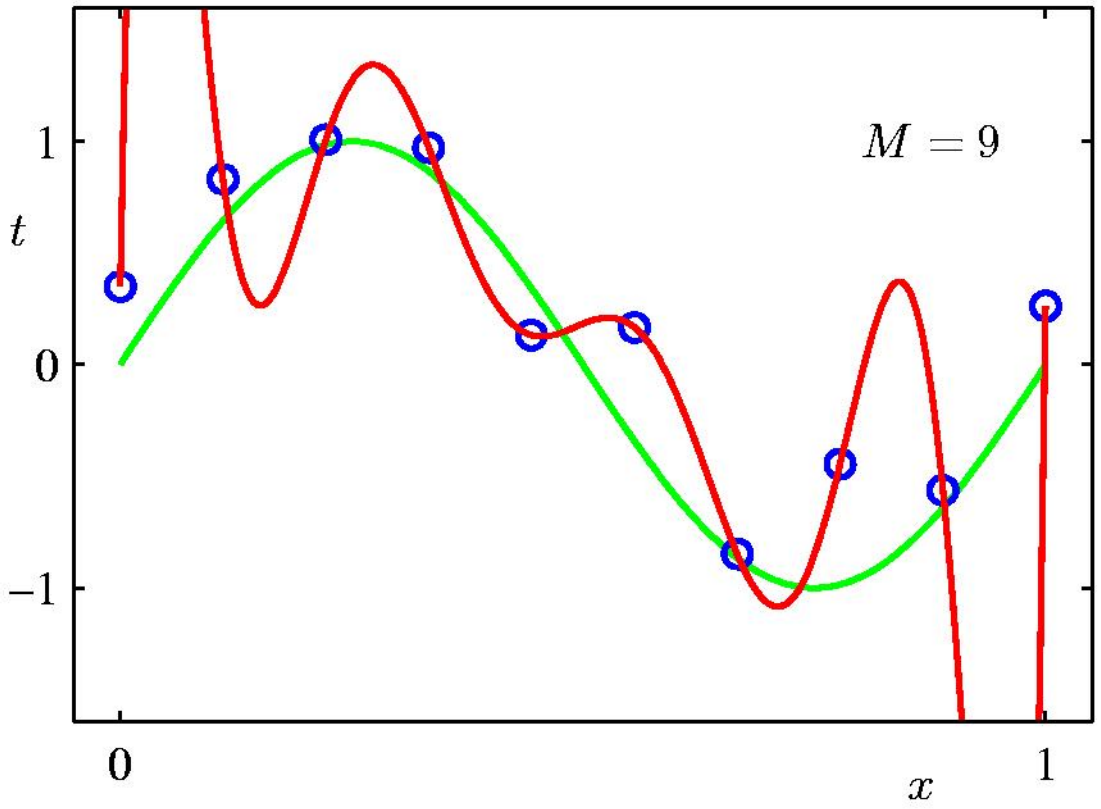
1st Order Polynomial



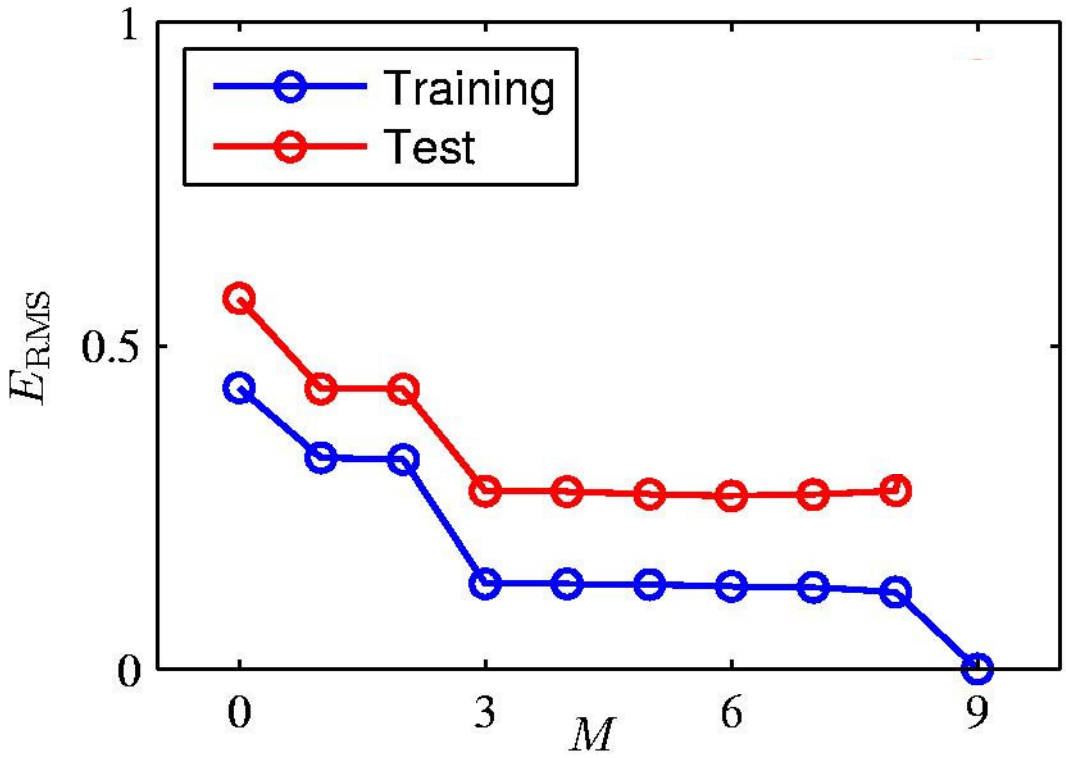
3rd Order Polynomial



9th Order Polynomial



Over-fitting



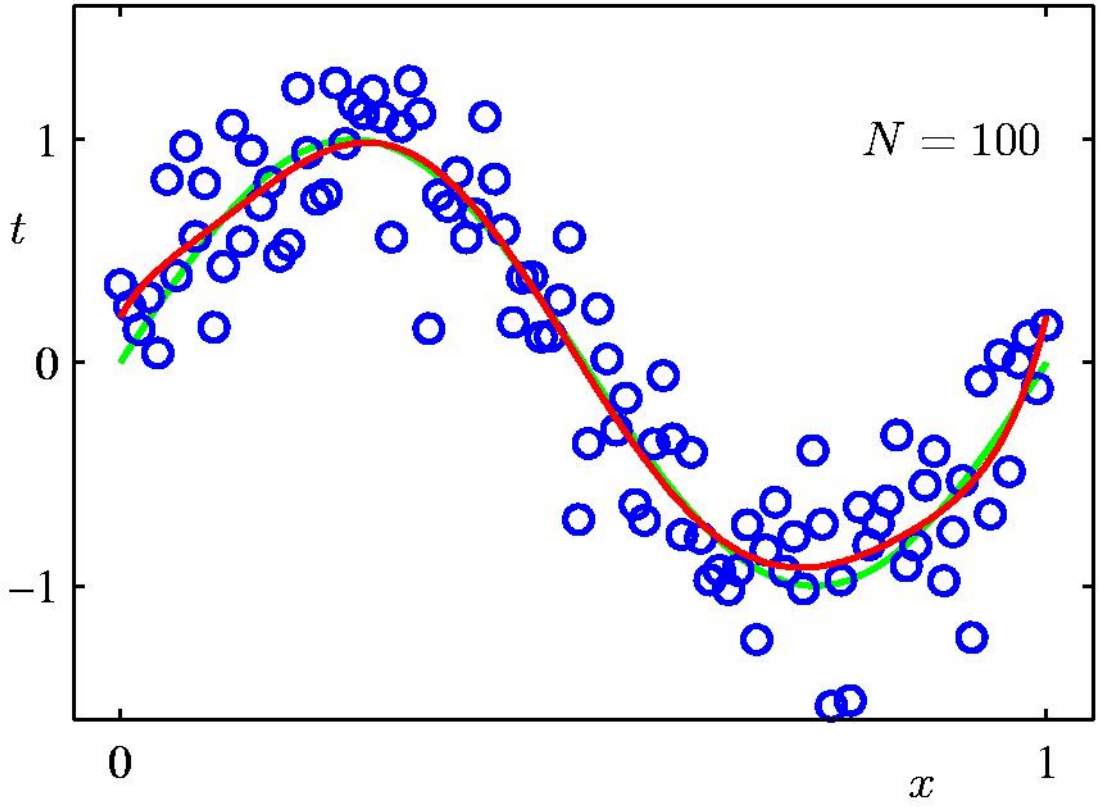
Root-Mean-Square (RMS) Error: $E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$

Polynomial Coefficients

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

Data Set Size:

9th Order Polynomial $N = 100$

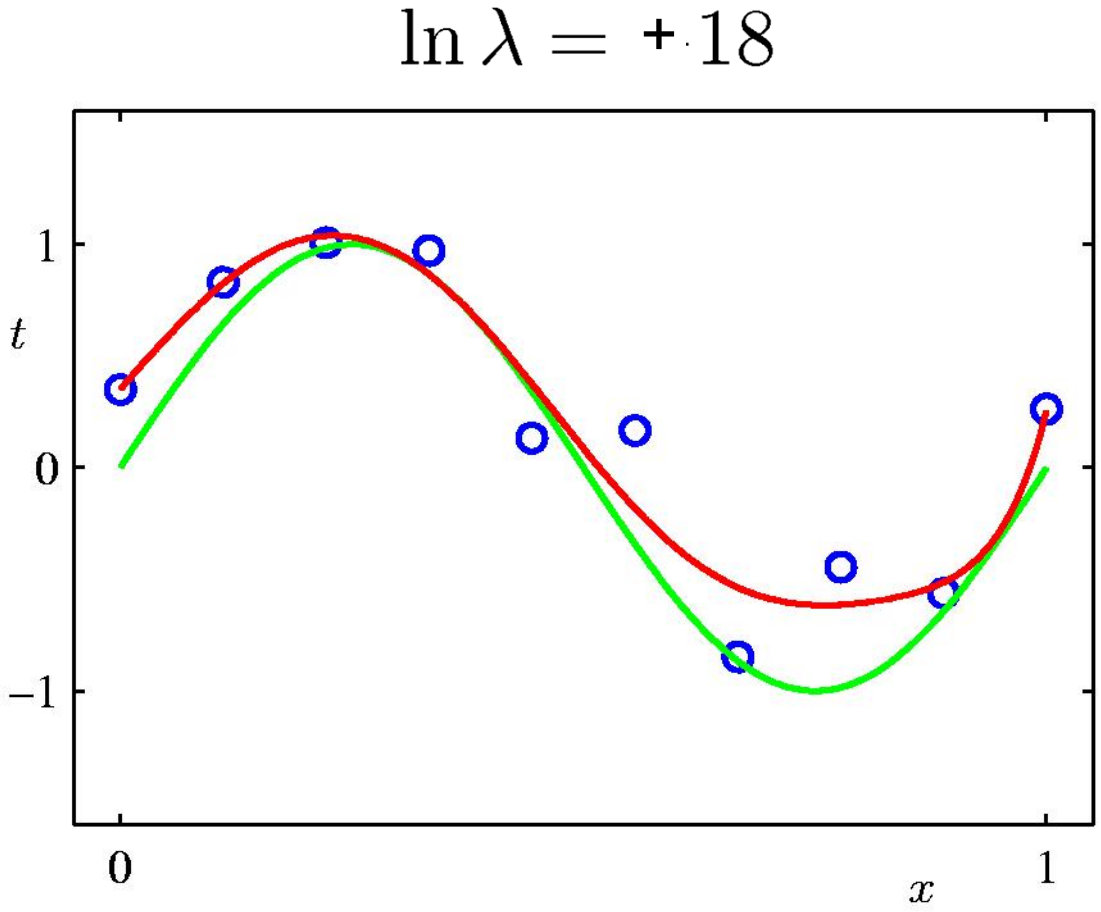


Regularization

Penalize large coefficient values

$$J_{\mathbf{X},\mathbf{y}}(\mathbf{w}) = \frac{1}{2}\sum_i \left(y^i - \sum_j w_j \phi_j(\mathbf{x}^i) \right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

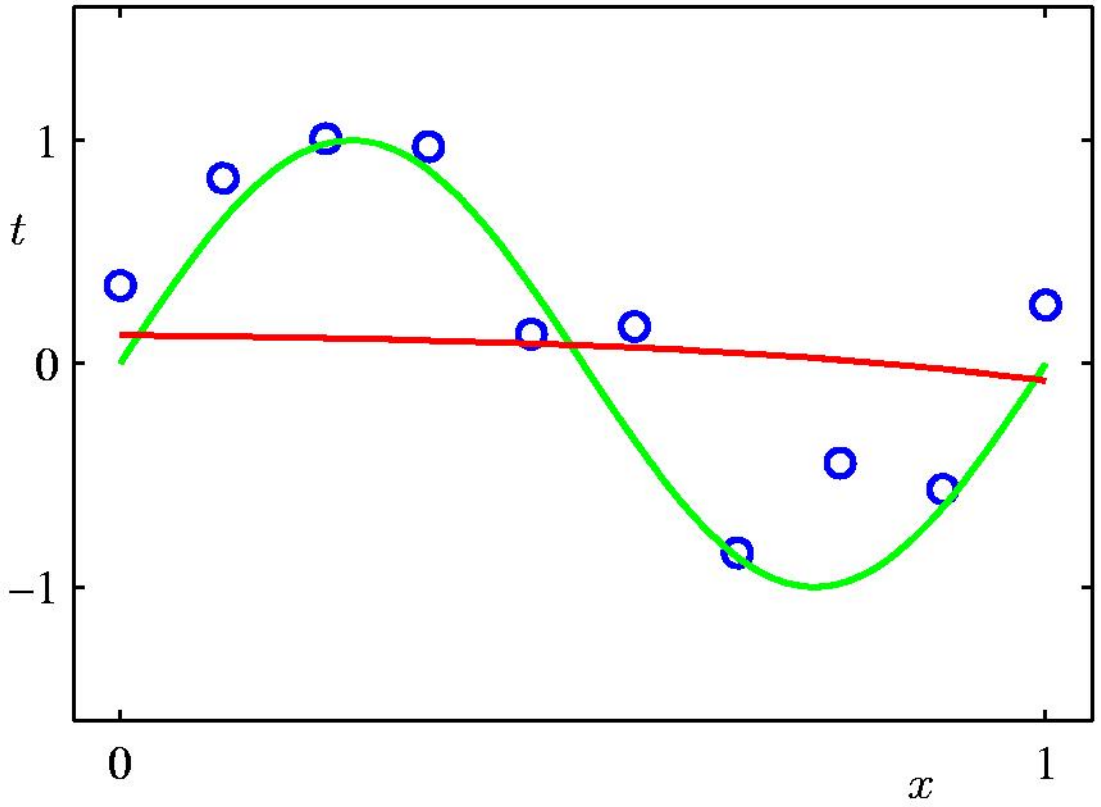
Regularization:



Polynomial Coefficients

	none	exp(18)	huge
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

Over Regularization:



Example in Google colab notebook:

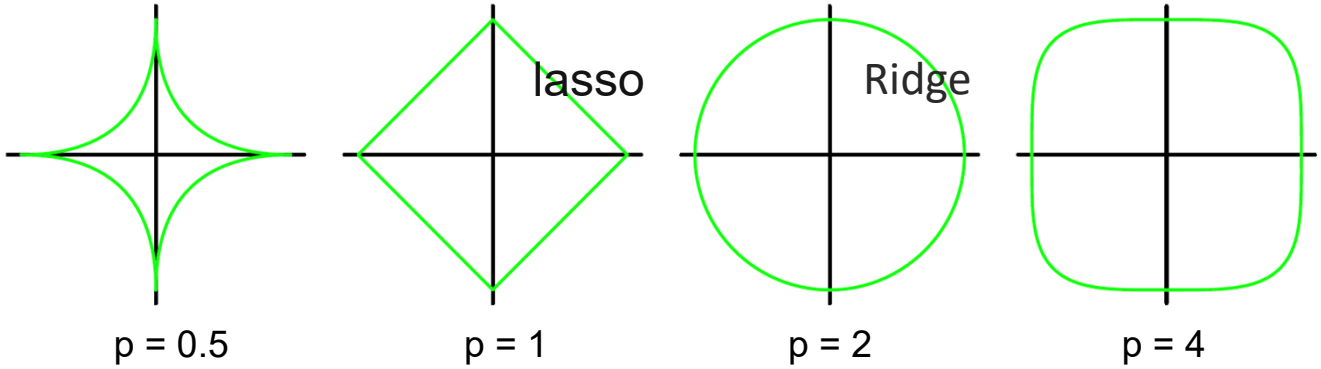
https://colab.research.google.com/github/jakevdp/PythonDataScienceHandbook/blob/master/notebooks/05.06-Linear-Regression.ipynb#scrollTo=xW7yPbeMBvwy

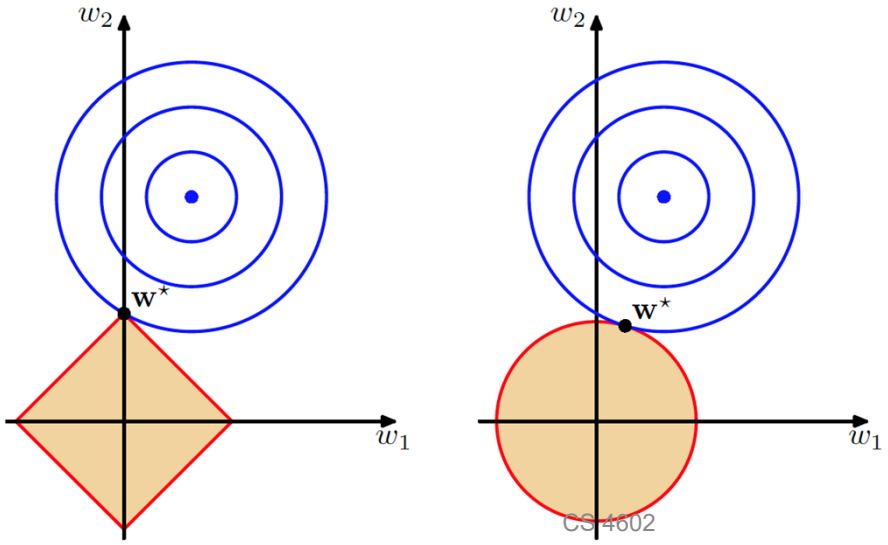
$$J(\boldsymbol{w}) = (\sum_i y^i - \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}^i)^2 + \lambda \|\boldsymbol{w}\|_p$$

$$||x||_p = \left(\sum_i |x_i|^p \right)^{1/p}$$

$$||x||_2 = \sqrt{\left(\sum_i x_i^2 \right)} = \sqrt{x_1^2 + x_2^2 + \ldots + x_i^2}$$

$$||x||_1 = \sum_i |x_i| = |x_1| + |x_2| + \ldots + |x_i|$$





- What if we are going to forecast the future?

Autoregressive (AR) Modeling

- Used for forecasting
- Takes Advantage of Autocorrelation
  - 1st order - correlation between consecutive values
  - 2nd order - correlation between values 2 periods apart
- Autoregressive Model for *p-th* order:

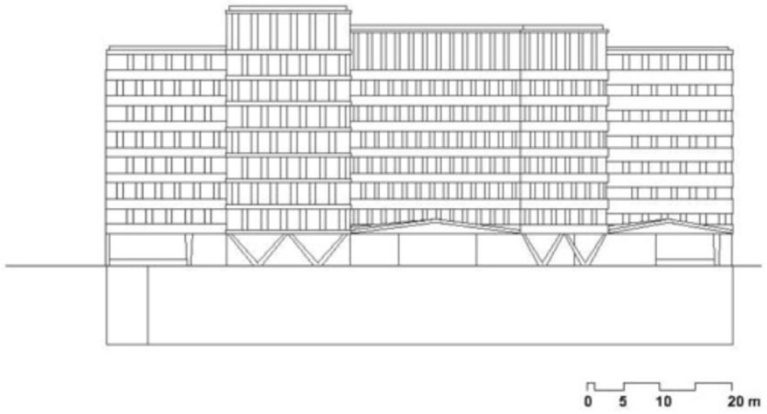
Random Error

$$Y_i = A_0 + A_1 Y_{i-1} + A_2 Y_{i-2} + \cdots + A_p Y_{i-p} + \delta_i$$

Autoregressive Model: Example

The Office Concept Corp. has acquired a number of office units (in thousands of square feet) over the last 8 years. Develop the 2nd order Autoregressive models.

Year	Units
92	4
93	3
94	2
95	3
96	2
97	2
98	4
99	6



Autoregressive Model: Example Solution

- Develop the 2nd order table
- Run a regression model

	Coefficients
Intercept	3.5
X Variable 1	0.8125
X Variable 2	-0.9375

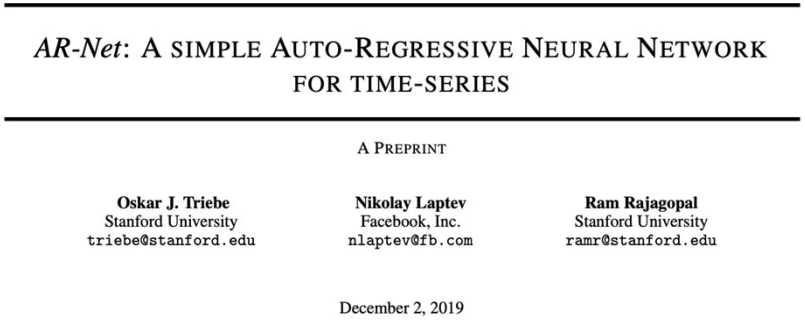
Year	Y_i	Y_{i-1}	Y_{i-2}
92	4	---	---
93	3	4	---
94	2	3	4
95	3	2	3
96	2	3	2
97	2	2	3
98	4	2	2
99	6	4	2
100	?	6	4

$$Y_i = 3.5 + 0.8125\ Y_{i-1} - 0.9375\ Y_{i-2}$$

$$Y_{100} = 3.5 + 0.8125 \times 6 - 0.9375 \times 4 = 4.625$$

AR family

- The Autoregressive Moving Average (ARMA) Model
  - The ARMA (p,q) model is a combination of AR (autoregressive) and MA (moving average) terms.
- The Autoregressive Integrated Moving Average (ARIMA) Model
  - The BJ methodology is based on the assumption that the underlying time series is stationary or can be made stationary by differencing it one or more times.
- AR + NN



AR-Net: A SIMPLE AUTO-REGRESSIVE NEURAL NETWORK FOR TIME-SERIES

A PREPRINT

Oskar J. Triebe
Stanford University
triebe@stanford.edu

Nikolay Laptev
Facebook, Inc.
nlaptev@fb.com

Ram Rajagopal
Stanford University
ramr@stanford.edu

December 2, 2019

Classification by regression?

- Linear regression is not suitable for classification problem.

Example

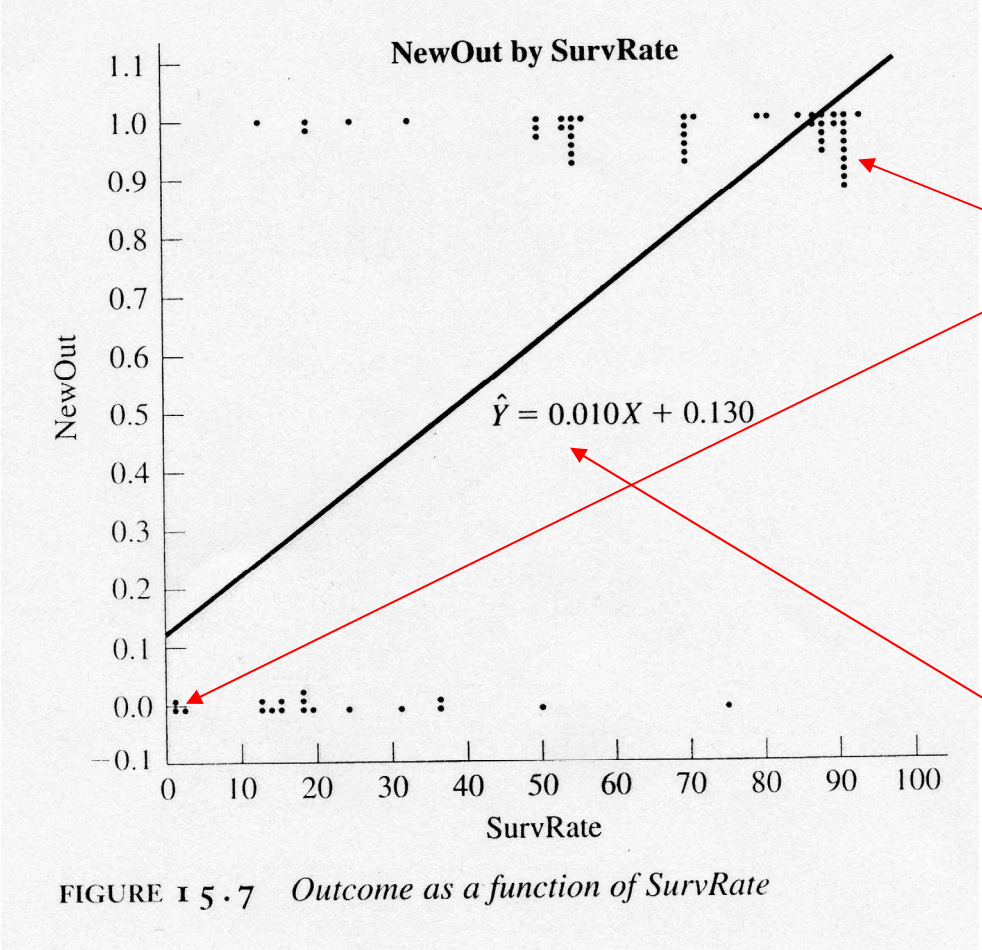


FIGURE 15.7 *Outcome as a function of SurvRate*

Observations:
For each value of SurvRate, the number of dots is the number of patients with that value of NewOut

Regression:
Standard linear regression

Problem: extending the regression line a few units left or right along the X axis produces predicted probabilities that fall outside of [0,1]

Logistic Regression: A better solution!

- To fit a curve to data in which the dependent variable is binary
- Typical application: Medicine
  - We might want to predict response to treatment, where we might code survivors as 1 and those who don't survive as 0

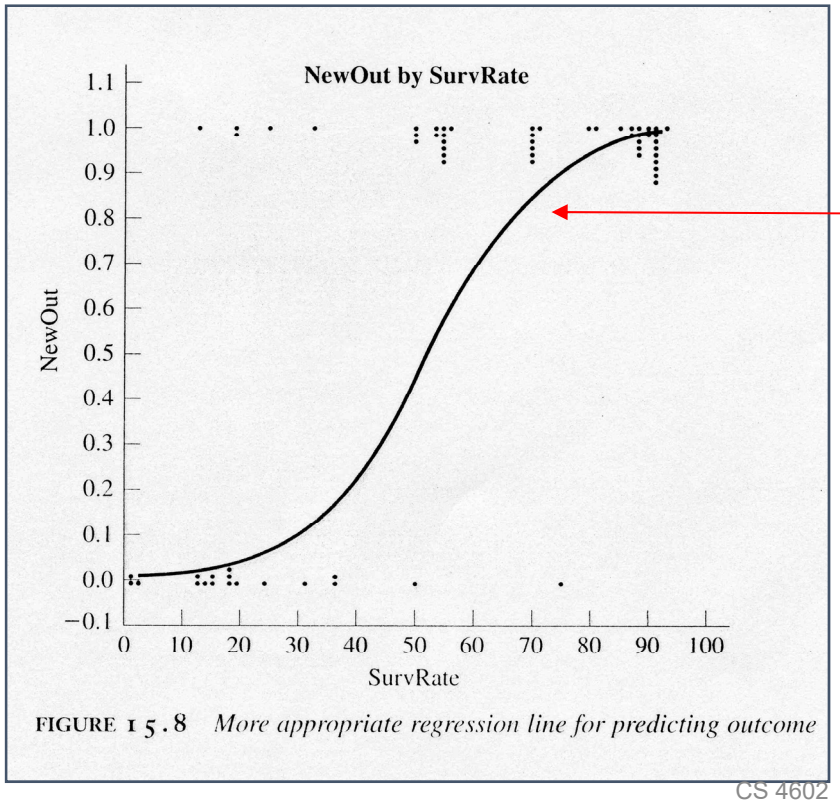


FIGURE 15.8 *More appropriate regression line for predicting outcome*

Regression Curve:
Sigmoid function!
(Logistic function)
(bounded by asymptotes y=0 and y=1)

$$S(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$$

Logistic Regression

- In logistic regression, we seek a model:

$$\underbrace{\text{logit}(p)}_{Y} = \beta_0 + \beta_1 X$$

- That is, **the log odds (logit)** is assumed to be linearly related to the independent variable X
- So, now we can focus on solving an ordinary (linear) regression!

Odds

- Given some event with probability *p* of being 1, the odds of that event are given by: $\text{odds} = p / (1-p)$
- Consider the following data

		Delinquent		
		Yes	No	Total
Testosterone	Normal	402	3614	4016
	High	101	345	446
		503	3959	4462

- The odds of being delinquent if you are in the Normal group are:

$p_{delinquent}/(1-p_{delinquent}) = (402/4016) / (1 - (402/4016)) = 0.1001 / 0.8889 = 0.111$

Odds Ratio

- The odds of being not delinquent in the Normal group is the reciprocal of this:
  - 0.8999/0.1001 = 8.99
- Now, for the High testosterone group
  - odds(delinquent) = 101/345 = 0.293
  - odds(not delinquent) = 345/101 = 3.416
- When we go from Normal to High, the odds of being delinquent nearly triple:
  - Odds ratio: 0.293/0.111 = 2.64
  - 2.64 times more likely to be delinquent with high testosterone levels

logit(p) = ln(odds)

$$\text{logit}(p) = \beta_0 + \beta_1 x$$

$$\ln\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x$$

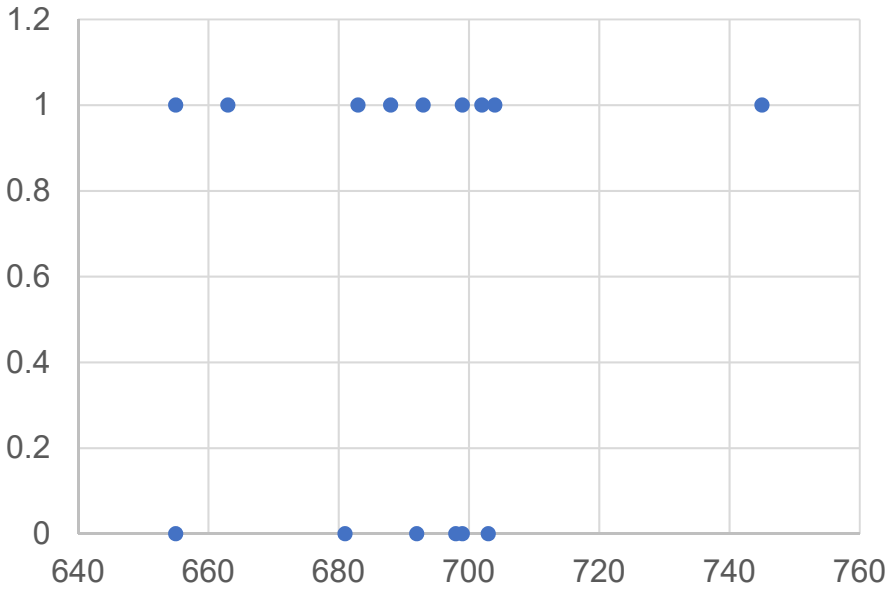
$$\frac{p}{1-p} = e^{\beta_0+\beta_1 x}$$

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

An example- Home Mortgage Loan

Credit Score (FICOscore)	Approved
655	0
692	0
681	0
663	1
688	1
693	1
699	0
699	1
683	1
698	0
655	1
703	0
704	1
745	1
702	1

Approved = 1
Not approved = 0



Ref: https://www.youtube.com/watch?v=Rj3pVkjAwY0

Binary Logistic Regression: Approve versus FICOscore

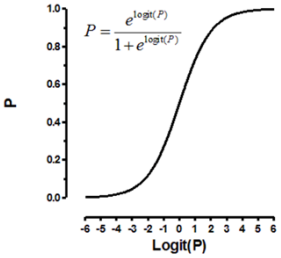
Coefficients

Term	Coef	SE Coef	95% CI	Z-Value	P-Value	VIF
Constant	**-9.346**	0.637	(-10.594, -8.097)	-14.67	0.000	
FICOscore	**0.014634**	0.000940	(0.012791, 0.016476)	15.56	0.000	1.00

Sigmoid function: $S(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$

Regression equation:

Estimated probability of being approved $\hat{p} = \frac{e^{\beta_0 + \beta_1 x_1}}{1+e^{\beta_0 + \beta_1 x_1}}$



FICOscore

$$\hat{p} = \frac{e^{-9.346+0.014634x_1}}{1+e^{-9.346+0.014634x_1}}$$

Credit Score (FICOscore)	Approved
655	0
692	0
681	0
663	1
688	1
693	1
699	0
699	1
683	1
698	0
655	1
703	0
704	1
745	1
702	1

$$\hat{p} = \frac{e^{-9.346+0.014634(655)}}{1+e^{-9.346+0.014634(655)}} = \frac{1.270321477}{2.270321477} = 0.559533744$$

$$odds = \frac{0.559533744}{1-0.559533744}$$

$$\text{Odds ratio for 655 to 745} = \frac{\frac{0.825826101}{1-0.825826101}}{\frac{0.559533744}{1-0.559533744}} = \frac{4.74138838}{1.270321477}$$

$$= 3.732431881$$

$$\hat{p} = \frac{e^{-9.346+0.014634(745)}}{1+e^{-9.346+0.014634(745)}} = \frac{4.74138838}{5.74138838} = 0.825826101$$

$$odds = \frac{0.825826101}{1-0.825826101}$$

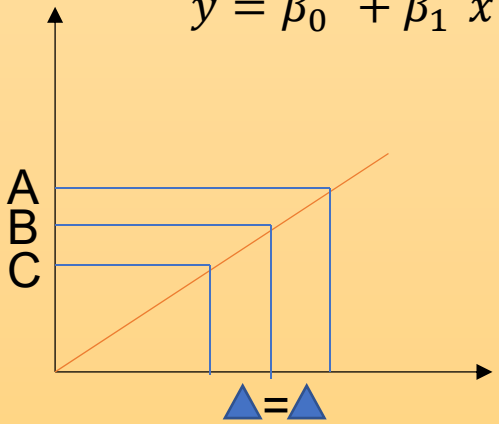
$$\text{Odds ratio for } 655 \overset{90}{\text{ to }} 745 = \frac{\frac{0.825826101}{1-0.825826101}}{\frac{0.559533744}{1-0.559533744}} = \frac{4.74138838}{1.270321477}$$

$$= 3.732431881$$

$$\text{Odds ratio for } 600 \overset{90}{\text{ to }} 690 = \frac{\frac{0.679496743}{1-0.679496743}}{\frac{0.362252721}{1-0.362252721}} = \frac{2.120093094}{0.568019233}$$

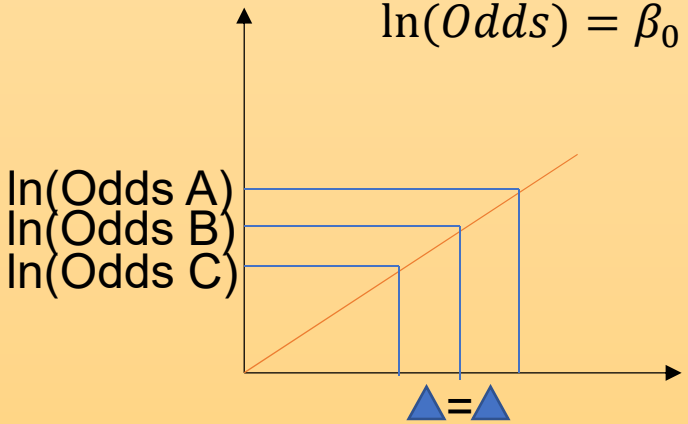
$$= 3.732431881$$

$y = \beta_0 + \beta_1 x$



A - B = B - C

$\ln(Odds) = \beta_0 + \beta_1 x$



Odds A/Odds B = Odds B/Odds C

ln(Odds A/Odds B) = ln(Odds B/Odds C)

ln(Odds A) – ln(Odds B) = ln(Odds B) – ln(Odds C)

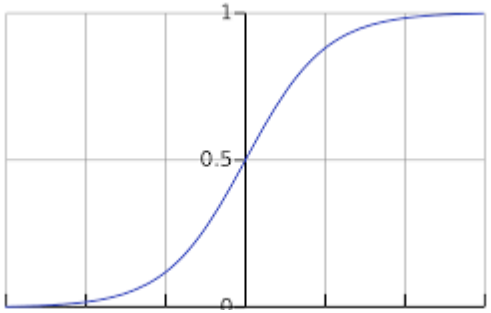
FICO	$\hat{p}$	$1-\hat{p}$	ODDS
600	0.362253	0.637747	0.568019
610	0.396694	0.603306	0.657533
620	0.43219	0.56781	0.761154
630	0.468397	0.531603	0.881104
640	0.50494	0.49506	1.019957
650	0.54143	0.45857	1.180691
660	0.577481	0.422519	1.366756
670	0.612725	0.387275	1.582143
680	0.646827	0.353173	1.831472
690	0.679497	0.320503	2.120093
700	0.710497	0.289503	2.454198

$$+0 = \frac{0.568019}{0.568019} = 1$$

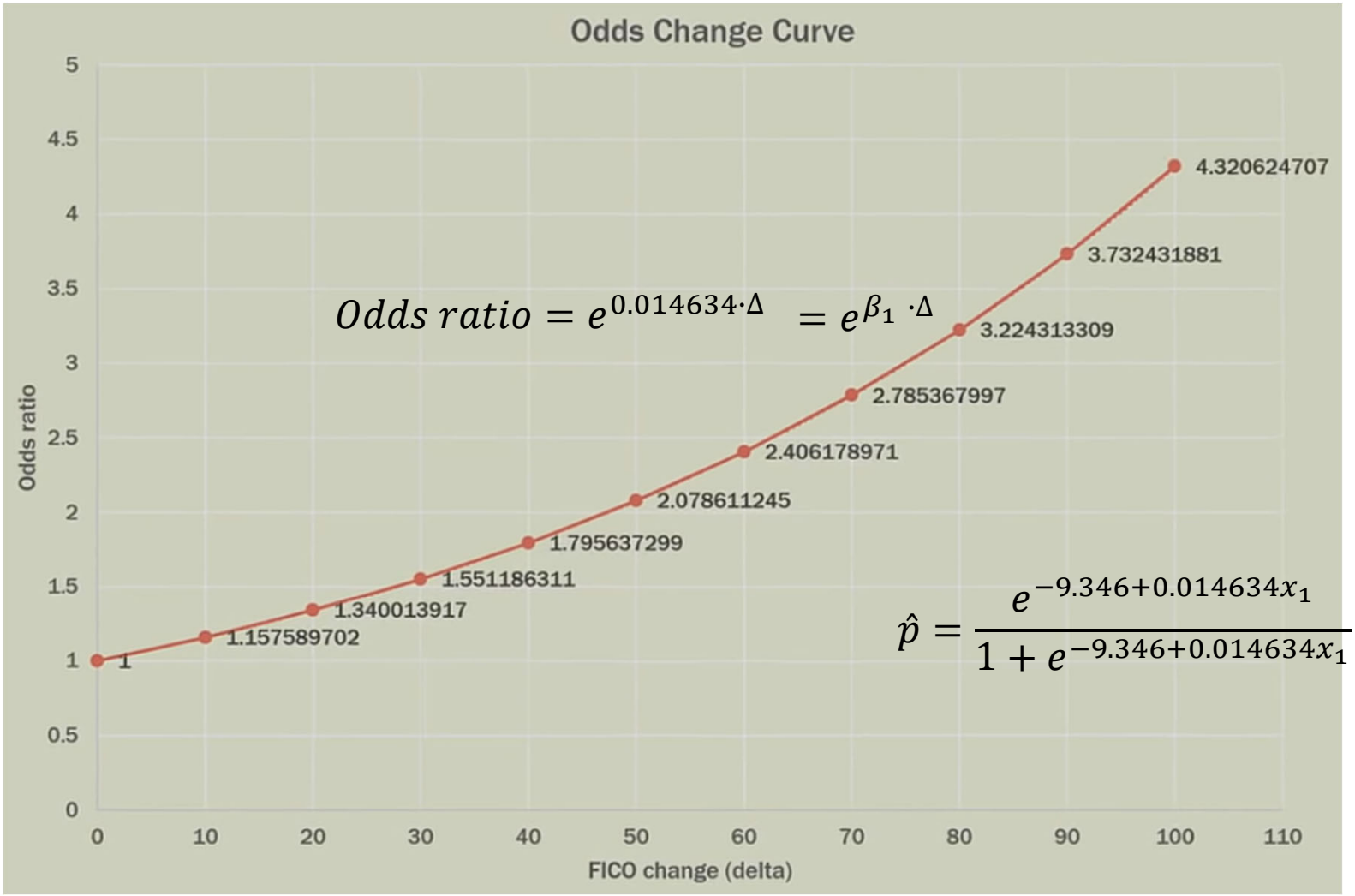
$$+10 = \frac{0.657533}{0.568019} = 1.157589702$$

$$+20 = \frac{0.761154}{0.568019} = 1.340013917$$

$$+30 = \frac{0.881104}{0.568019} = 1.551187548$$



630~640



$$Odds\ ratio = e^{0.014634 \cdot \Delta} = e^{\beta_1 \cdot \Delta}$$

$$\hat{p} = \frac{e^{-9.346+0.014634x_1}}{1 + e^{-9.346+0.014634x_1}}$$

Binary Logistic Regression: Approve versus FICOscore

Coefficients

Term	Coef	SE Coef	95% CI	Z-Value	P-Value	VIF
Constant	**-9.346**	0.637	(-10.594, -8.097)	-14.67	0.000	
FICOscore	**0.014634**	0.000940	(0.012791, 0.016476)	15.56	0.000	1.00

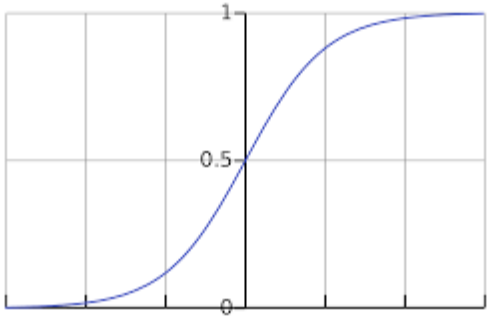
FICO for even odds (50/50)

$$ln\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1$$

$$ln\left(\frac{.5}{.5}\right) = -9.346 + 0.014634x_1$$

$$0 = -9.346 + 0.014634x_1$$

$$x_1 = 638.65$$



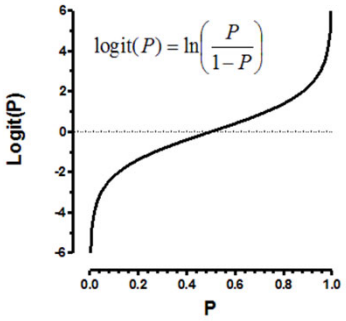
639

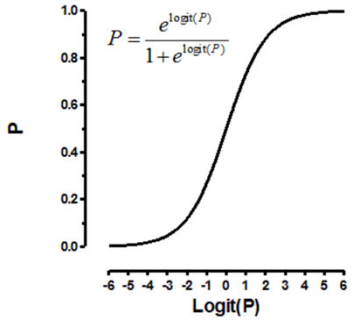
To have even odds for approve/disapprove, you will need to have FICO score = 639

Logit Transform

- p is the probability that the event Y occurs, p(Y=1)
  - [range=0 to 1]
- p/(1-p) is the "odds"
  - [range=0 to ∞]
- ln[p/(1-p)]: log odds, or "logit“
  - [range=-∞ to +∞]

- logit(p) = ln(odds) = ln (p/(1-p))





Logistic Regression: $\text{logit}(p) = \beta_0 + \beta_1 X$

We've learned

- Regression *vs* Classification
- Linear regression – another discriminative learning method
  - As matrix inversion (Ordinary Least Squares)
  - As optimization: Gradient descent
    - Batch gradient decent
    - Stochastic gradient descent
- Overfitting and regularization
- Autoregression
- Logistic regression (more like classification)

Questions?