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Least Squares Optimization: Linear Regression

- Regression Analysis
  - set of statistical processes for estimating the relationships between a dependent variable (often called the 'outcome' or 'response' or ' target ') and one or more independent variables (often called 'predictors', 'covariates', 'explanatory variables' or 'features')
- Linear regression
  - Simplest method to build a relationship between input and output while many relationships are nonlinear in science and engineering
  - Fundamental to understanding more advanced regression methods
  - Adrien-Marie Legendre(1805), Johann Carl Friedrich Gauss(1809)
    - Orbits of celestial bodies
  - Term "regression": Francis Galton (1800's)
    - Genetics of sweet peas: weights of planted and harvested peas

https://en.wikipedia.org/wiki/Regression_analysis

Linear Regression Model

consider a set of N data points $(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$

a generic equation through these points: regression model made of two weights

$$y_n^* = w_0 + w_1 x_n \approx y_n \quad \text{for} \quad n = 1, \ldots, N$$

$$\begin{cases} w_0 : \text{ bias (constant weight)}, w_1 : \text{ weight} \\ y_n^* : \text{ computed approximate value}, y_n : \text{ "}true\text{" value} \end{cases}$$

assess how accurate the model is: $\text{total error} = \sum_{n=1}^{N} \left(y_n^* - y_n\right)^2 = \sum_{n=1}^{N} \left(w_0 + w_1 x_n - y_n\right)^2$

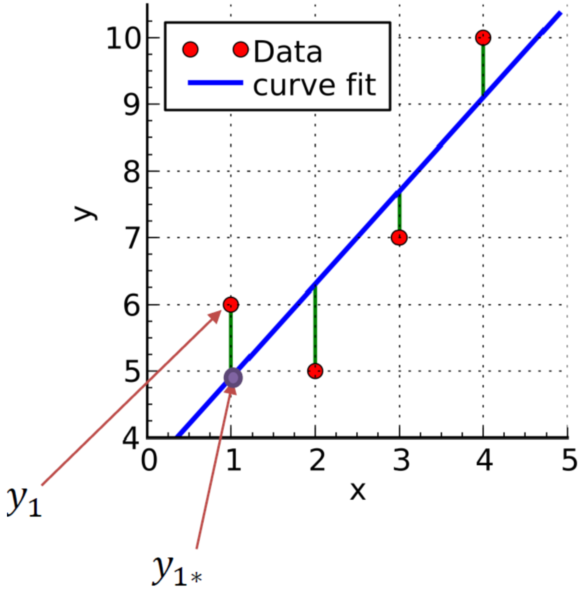
$$\text{cost function} = c(w_0, w_1) = \frac{1}{N} \sum_{n=1}^{N} \left(w_0 + w_1 x_n - y_n\right)^2 = \text{MSE (Mean Squared Error)}$$

$\rightarrow$ minimize the cost function to find optimal weights: $\arg\min_{\mathbf{w}} \text{ MSE}$

quantify how well the regression fit is: goodness of fit

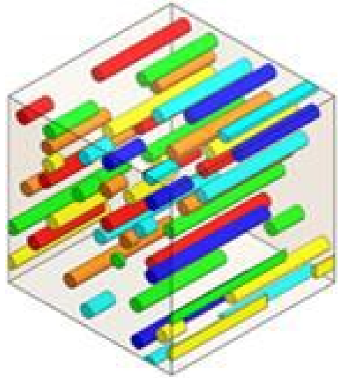
$$\text{coefficient of determination} = R^2 = \frac{\text{regression sum of squares}}{\text{total sum of squares}} = \frac{\sum_n \left(y_n^* - \bar{y}\right)^2}{\sum_n \left(y_n - \bar{y}\right)^2}$$

$\bar{y}$: average of the data points y_n



Background: Optimization (1)

- Process of finding the minimum (or maximum) value of a set of data or a function, generally performed mathematically
- Example
  - Let's say I'm an engineer at an automobile company tasked to design a new part. The part must satisfy a pre-determined list of requirements: strength, fatigue life weight manufacturability, etc. The part must also be economical to produce to keep profit margins up As such we want minimize the cost.
  - We've decided to go with Carbon Fiber Reinforced Polymer (CFRP) as our material. Yet, we need to determine several factors: volume fraction, fiber orientation, fiber radius, etc. while satisfying the pre-determined list of requirements. As such our cost function will be of high-dimensionality.



Background: Optimization (2)

- What is a cost function?
- Maximum and minimum of a cost function: local vs. global
- First, second, and higher order derivatives in multiple dimensions: gradients
- Gradient descents: a key concept behind optimization

Optimization: c vs. w

Optimization involves finding the maximum or minimum of a function.

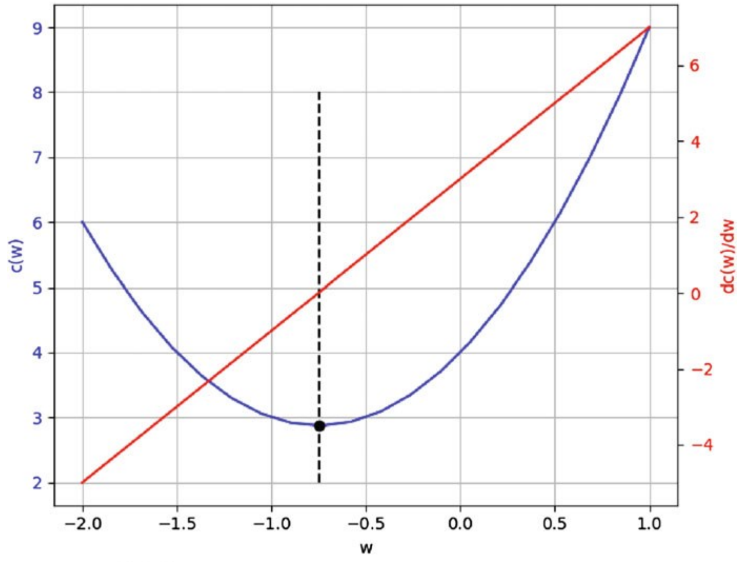
$$c(w) = 2w^2 + 3w + 4$$

First derivate test : $\frac{dc}{dw} = 0$ at maximum or minimum, find w^*

$$\frac{dc}{dw} = 4w + 3 = 0 \rightarrow w^* = -\frac{3}{4}$$

Second derivate test : $\frac{d^2c(w^*)}{dw^2} \begin{cases} > 0 \rightarrow \text{convex}(\text{minimum}) \\ < 0 \rightarrow \text{concave}(\text{maximum}) \\ = 0 \rightarrow (\text{inflection}) \end{cases}$

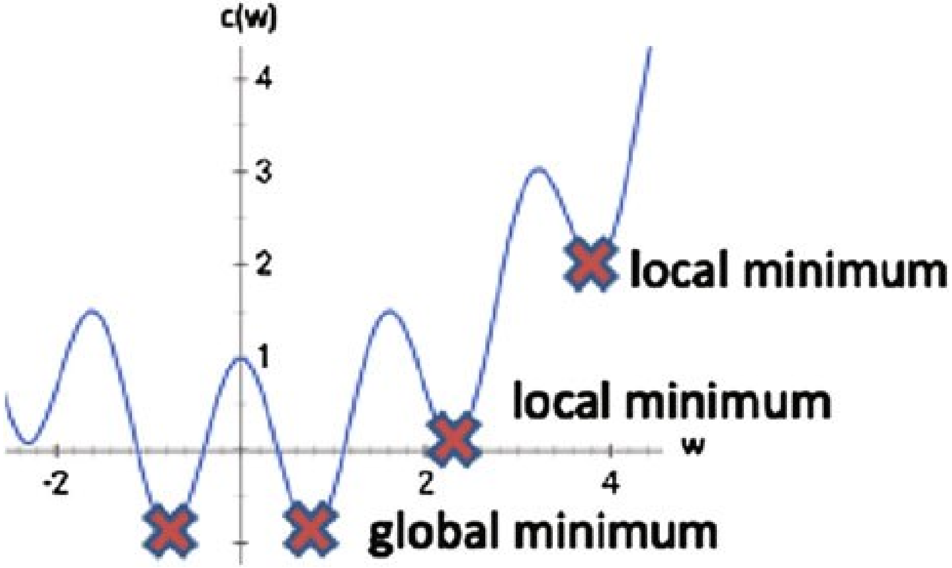
$$\frac{d^2c(w^*)}{dw^2} = 4 > 0 \rightarrow \text{minimum}$$



non-convex function with multiple local minimum

$$c(w) = \cos(4w) + 0.2w^2$$

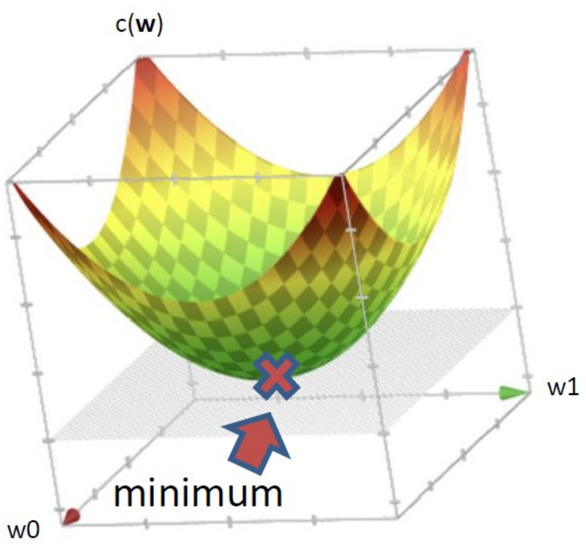
$$\frac{dc}{dw} = -4\sin(4w) + 0.4w = 0 \rightarrow w^* = ?$$

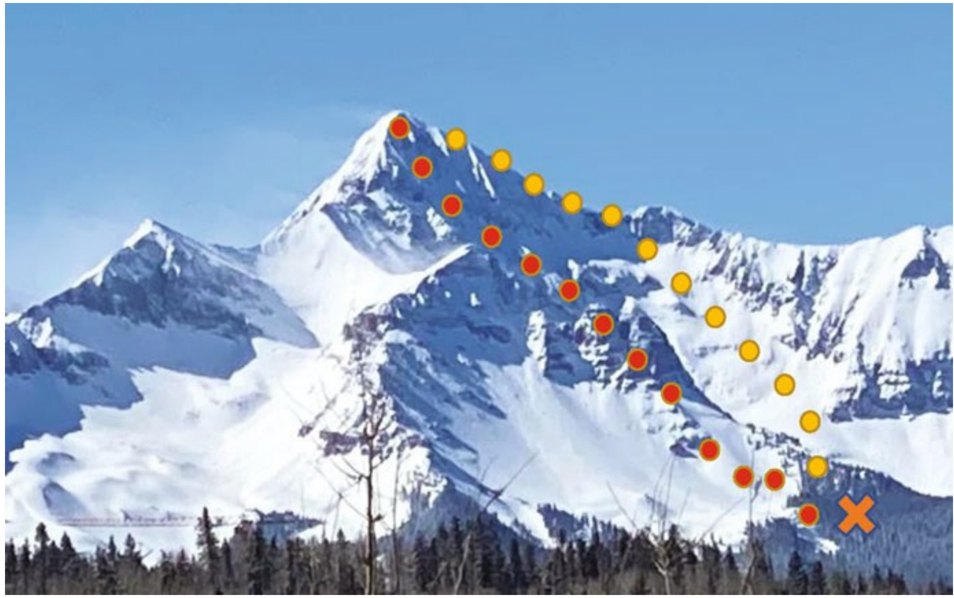


Optimization: c vs. $(w_0, w_1, \ldots, w_S)$

- Multidimensional Derivatives
- Gradient: slope or rate of change in a particular direction
  - find the minimum of high dimensionality functions

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_S \end{bmatrix} \to c(\mathbf{w}) \to \nabla c(\mathbf{w}) = \begin{bmatrix} \frac{\partial c(\mathbf{w})}{\partial w_0} \\ \frac{\partial c(\mathbf{w})}{\partial w_1} \\ \vdots \\ \frac{\partial c(\mathbf{w})}{\partial w_S} \end{bmatrix}$$





$$c(\mathbf{w}) = (w_0)^2 + 2(w_1)^2 + 1$$

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \to \nabla c(\mathbf{w}) = \begin{bmatrix} \frac{\partial c(\mathbf{w})}{\partial w_0} \\ \frac{\partial c(\mathbf{w})}{\partial w_1} \end{bmatrix} = \begin{bmatrix} 2w_0 \\ 4w_1 \end{bmatrix} = 0 \to \mathbf{w}^* = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

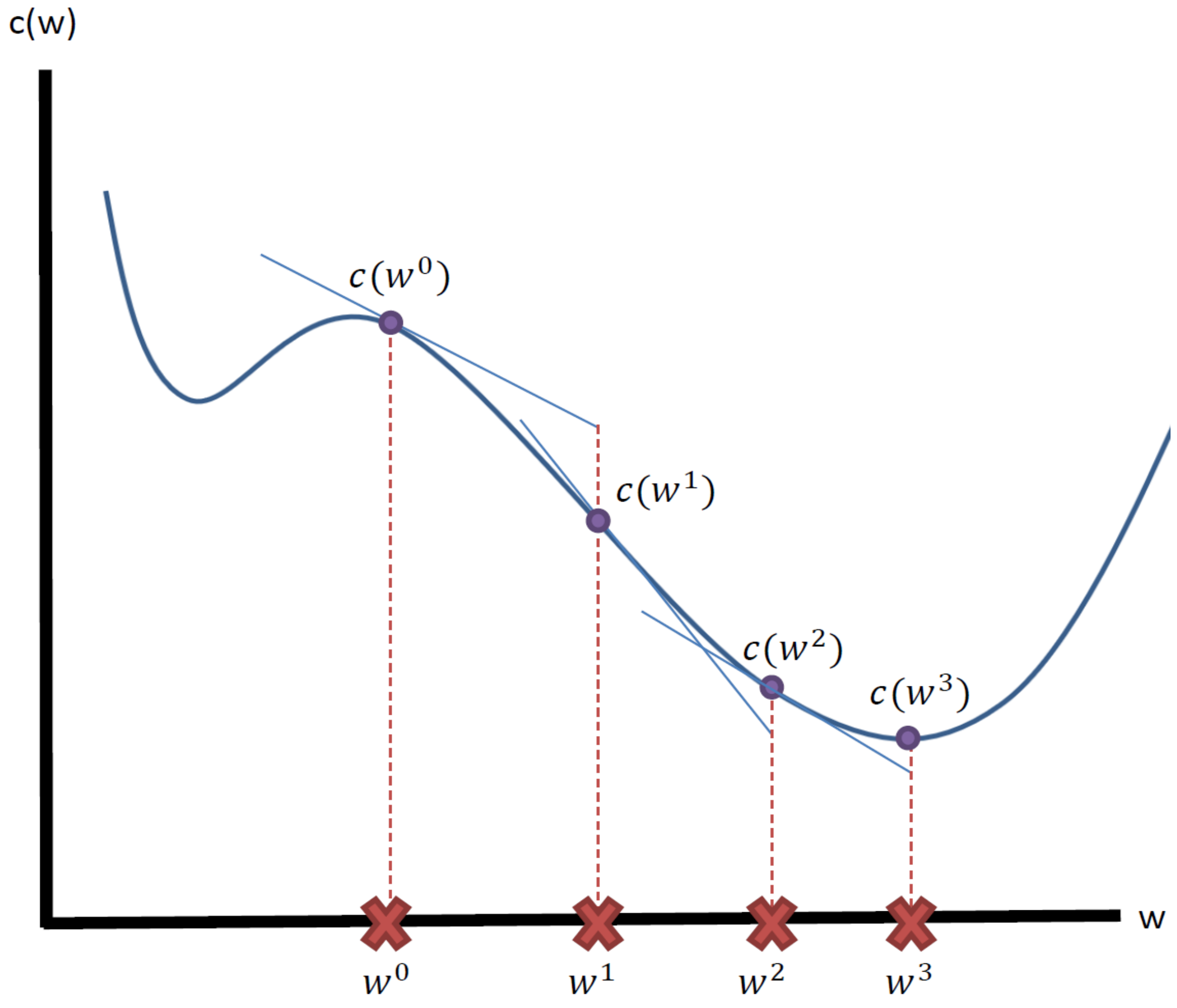
Gradient Descent

$$\begin{cases} w^{k+1} = w^k - \underbrace{\alpha}_{\text{step size}} \underbrace{\frac{dc\left(w^k\right)}{dw}}_{\text{search direction}} \\ \mathbf{w}^{k+1} = \mathbf{w}^k - \alpha \nabla c\left(\mathbf{w}^k\right) \end{cases}$$

1. Start at an arbitrary point w^0
2. Find the derivative of c at w^0
3. Descend to the next point through

the gradient descent equation: $w^1 = w^0 - \alpha \frac{dc\left(w^0\right)}{dw}$

4. Repeat the process: $w^2 = w^1 - \alpha \frac{dc\left(w^1\right)}{dw}$



Gradient Descent: Example

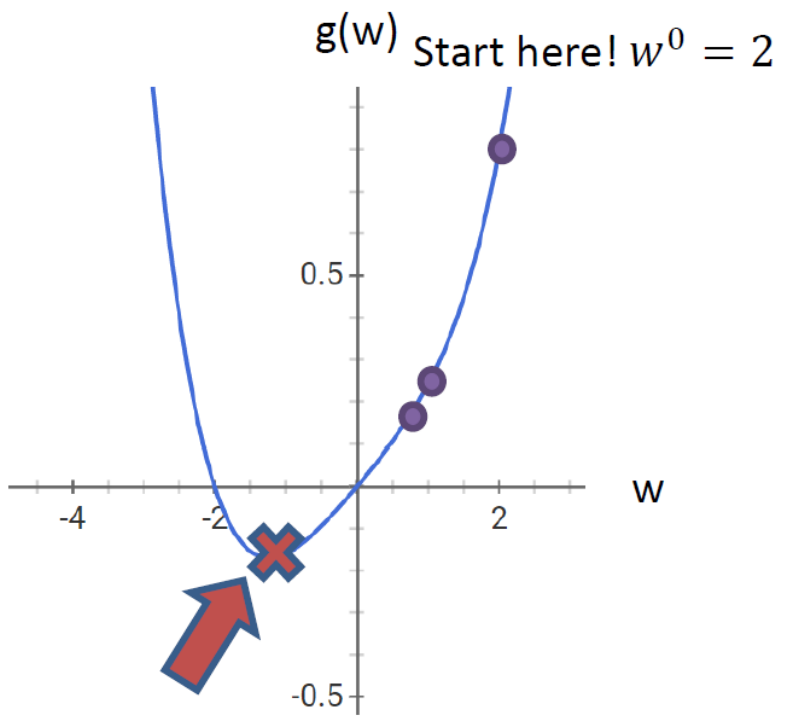
$$g(w) = \frac{1}{50}\left(w^4 + w^2 + 10w\right)$$

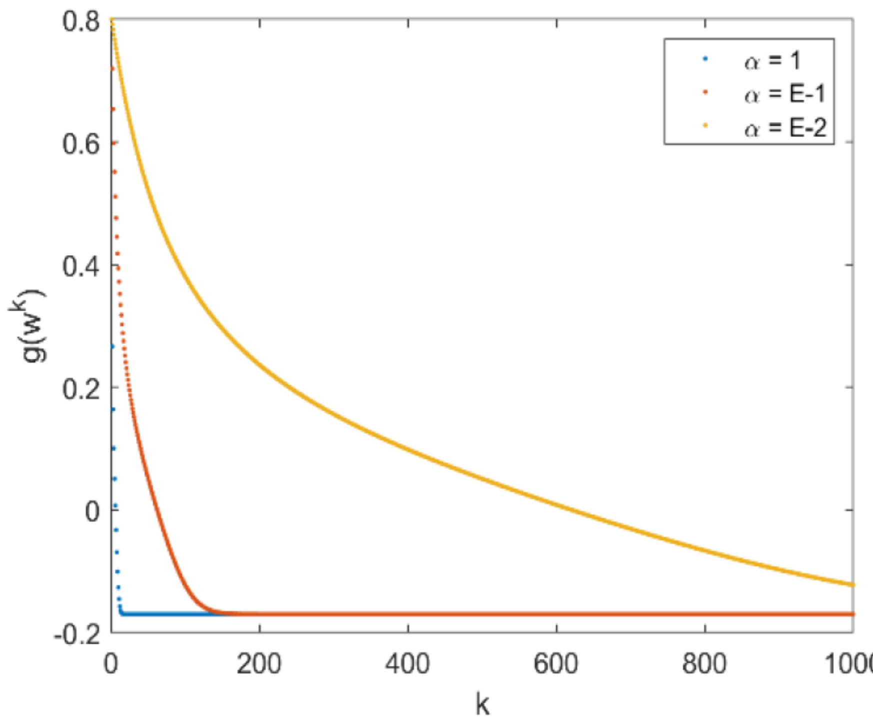
$$\frac{dg}{dw} = \frac{1}{50}\left(4w^3 + 2w + 10\right)$$

$$w^0 = 2,\ \alpha = 1$$

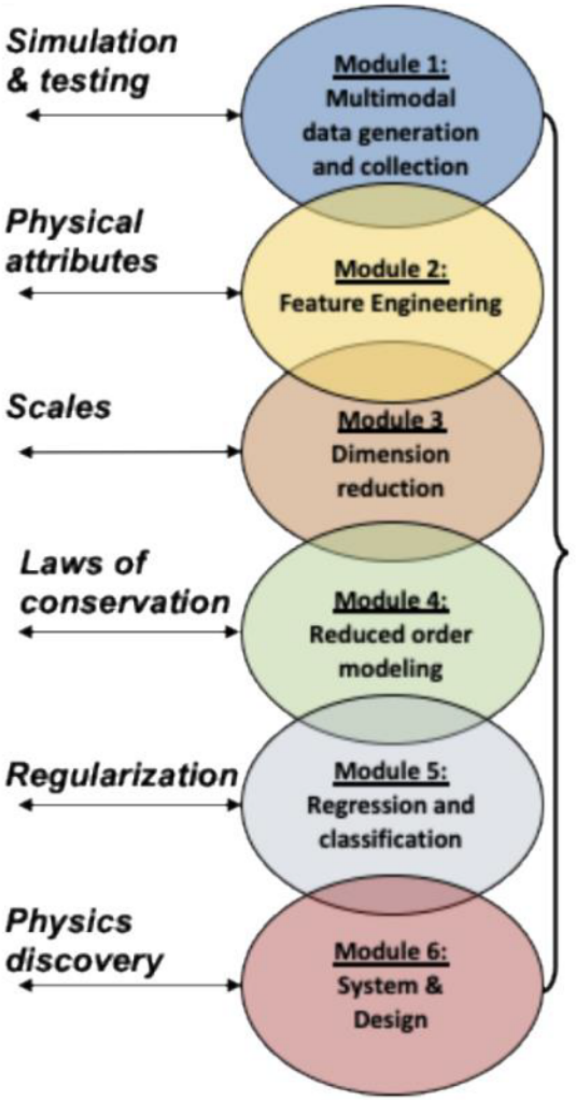
$$w^1 = w^0 - \alpha \frac{dg\left(w^0\right)}{dw} = 1.08$$

$$w^2 = w^1 - \alpha \frac{dg\left(w^1\right)}{dw} = 0.736$$





Example: Moneyball (1)



Baseball statistics are readily available. One such database is in Kaggle.

Various features are present in baseball sports analytics (OBP, SLG, RS, etc.).

Reduce dimension by only considering certain features (OBP, SLG, RS).

We reduce the order of the model by assuming it is linear.

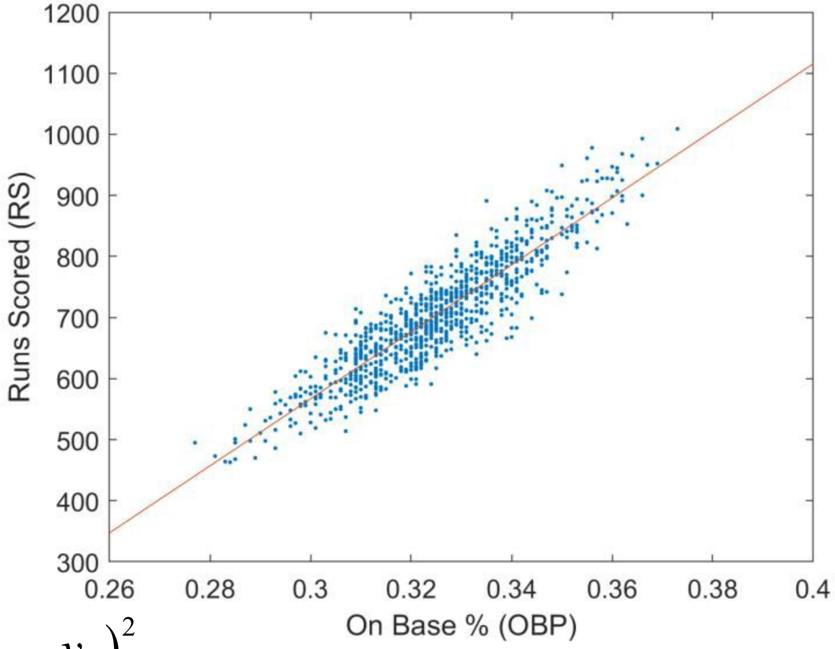
Use regression to determine model parameters

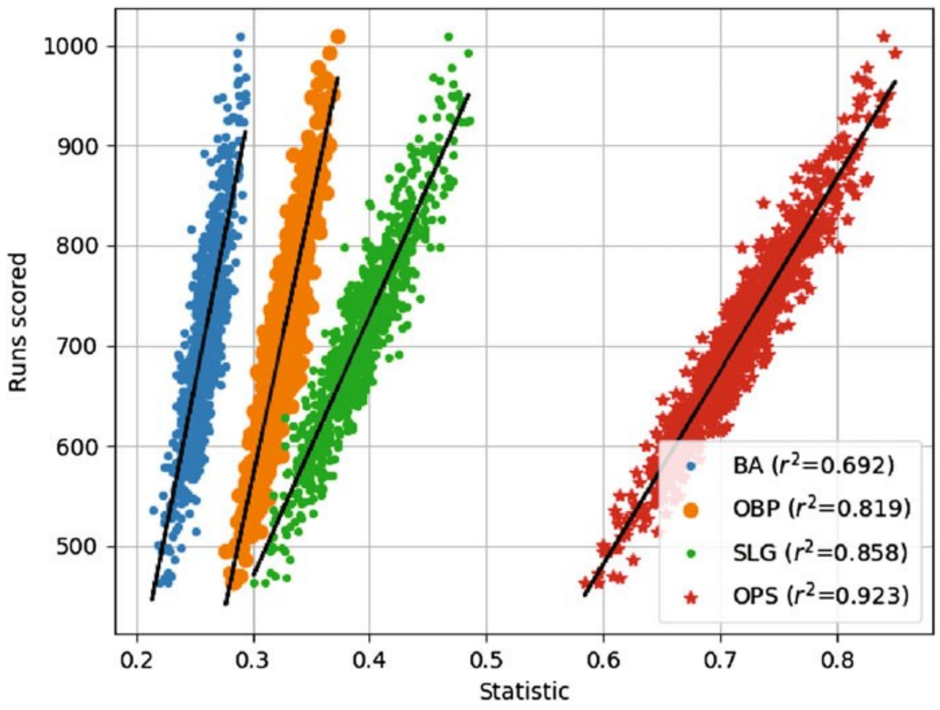
Use OBP and SLG to predict performance and therefore potential recruitment.

Example: Moneyball (2)

y_n	x_n
RS	OBP
691	0.327
818	0.341
729	0.324
687	0.319
772	0.334
777	0.336
798	0.334
735	0.324
897	0.35

n





$$c(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(w_0 + w_1 x_n - y_n\right)^2$$

$$x_n = \text{OBP} = \text{On Base Percentage}$$

$$y_n = \text{RS} = \text{Run Scored}$$

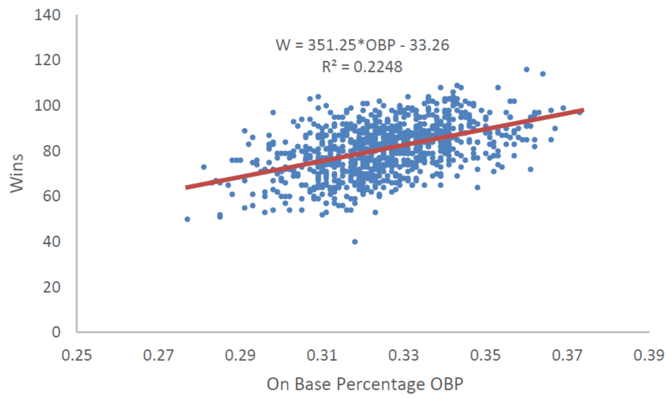
$$c(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left[\left(w_0 + w_1(0.327) - 691\right)^2 + \left(w_0 + w_1(0.341) - 818\right)^2 + \cdots\right]$$

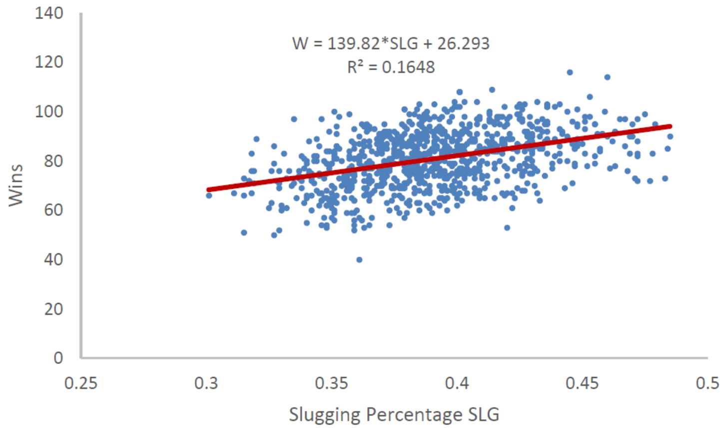
$$\mathbf{w}^{k+1} = \mathbf{w}^k - \alpha \nabla c\left(\mathbf{w}^k\right)$$

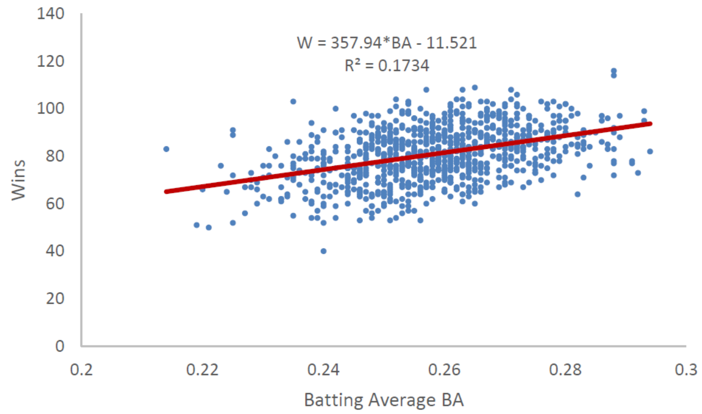
Can we get a better R-squared value if we include both OBP and SLG in a single regression?

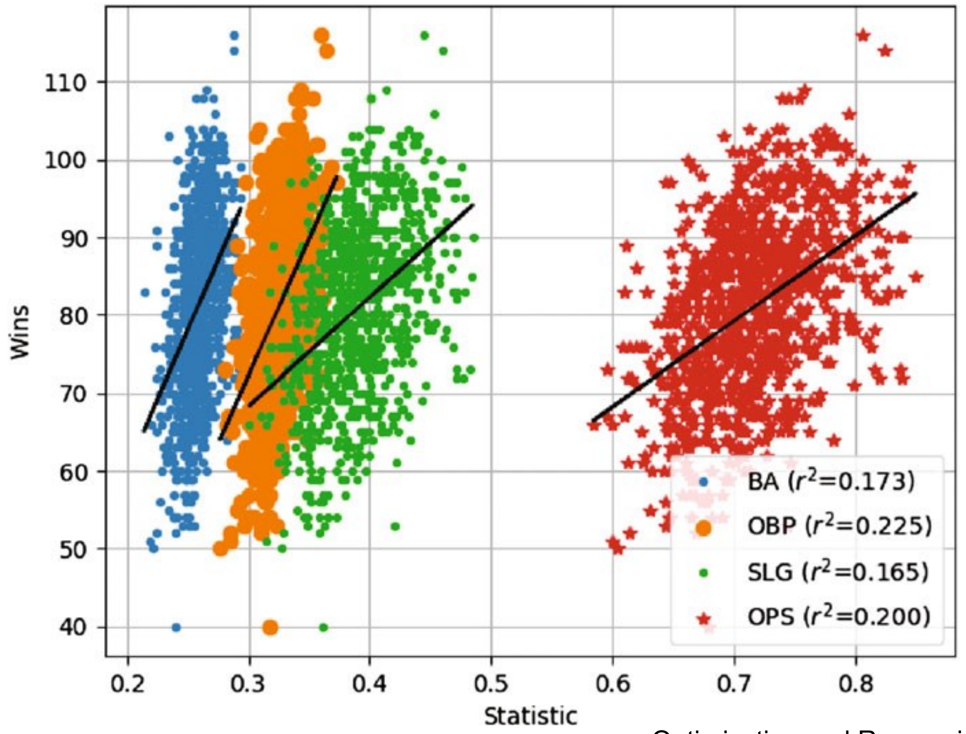
Example: Moneyball (3)

- correlation between W and any of these statistics? not good
  - do not account for pitching and defense, which are other important parts of winning baseball games









Multivariate Linear Regression Model

For high dimensions, consider a set of N data points $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)$

a generic equation through these points: regression model made of two weights

$$y_n^* = w_0 + w_1 x_{1,n} + w_2 x_{2,n} + \cdots + w_S x_{S,n} \approx y_n \quad \text{for } n = 1, \ldots, N$$

$$\hat{\mathbf{x}}_n = \begin{bmatrix} 1 \\ x_{1,n} \\ x_{2,n} \\ \vdots \\ x_{S,n} \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_S \end{bmatrix} \rightarrow y_n^* = \hat{\mathbf{x}}_n^T \mathbf{w} \rightarrow c_n = \left(\hat{\mathbf{x}}_n^T \mathbf{w} - y_n\right)^2$$

$$c = \frac{1}{N} \sum_{n=1}^{N} \left(\hat{\mathbf{x}}_n^T \mathbf{w} - y_n\right)^2 \rightarrow \nabla c = \frac{2}{N} \sum_{n=1}^{N} \left(\hat{\mathbf{x}}_n^T \mathbf{w} - y_n\right) \hat{\mathbf{x}}_n$$

$$\mathbf{w}^{k+1} = \mathbf{w}^k - \alpha \nabla c\left(\mathbf{w}^k\right) = \mathbf{w}^k - \alpha \frac{2}{N} \sum_{n=1}^{N} \left(\hat{\mathbf{x}}_n^T \mathbf{w} - y_n\right) \hat{\mathbf{x}}_n$$

Pitfall: For various features of dissimilar magnitudes, you might face convergence issues

$\rightarrow$ normalize your features: $z = \dfrac{x - \bar{x}}{\sigma}$ (standard normalization)

Example: Moneyball

y_n $x_{1,n}$ $x_{2,n}$ $\boldsymbol{x}_1$

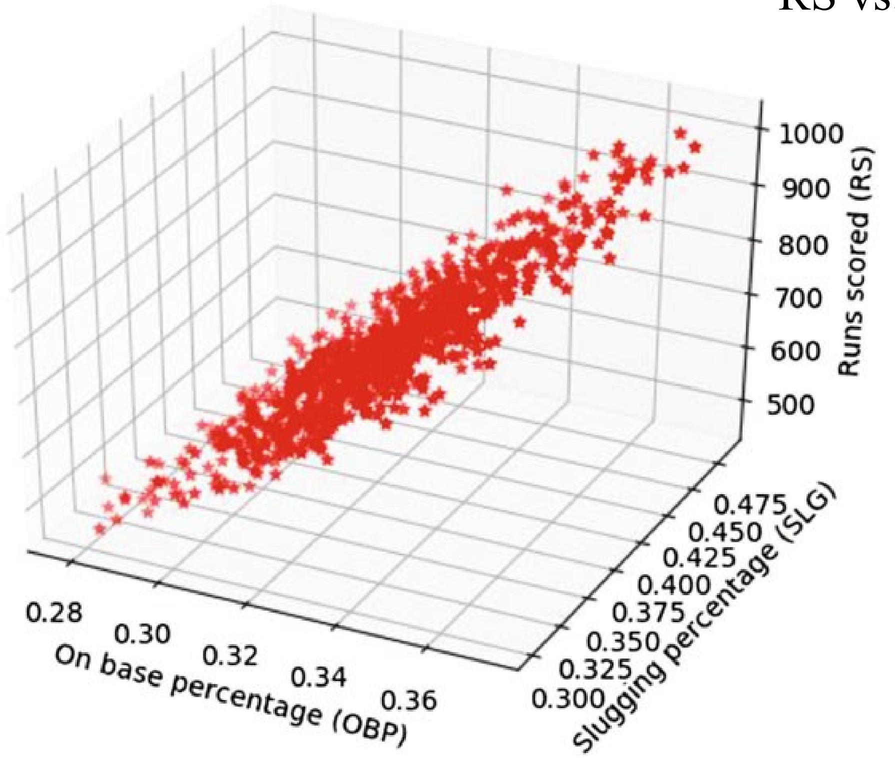
RS	OBP	SLG
691	0.327	0.405
818	0.341	0.442
729	0.324	0.412
687	0.319	0.38
772	0.334	0.439
777	0.336	0.43
798	0.334	0.451
735	0.324	0.419
897	0.35	0.458
923	0.354	0.483

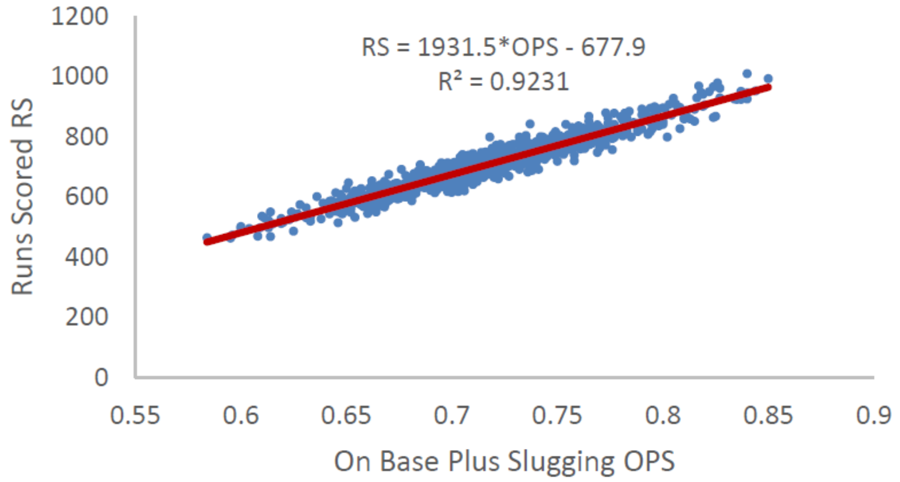
y_1 n

$$w_0 + w_1(\text{OBP})_n + w_2(\text{SLG})_n \approx (\text{RS})_n \quad \text{for } n = 1, \ldots, N$$

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} -803 \\ 2729 \\ 1587 \end{bmatrix} \rightarrow R^2 = 0.93$$

$$\text{RS vs. OPB}(=\text{OBP} + \text{SLG}) \rightarrow R^2 = 0.92$$





Python Code: Fig.3.24 (1)

```
import pandas as pd
import numpy as np
from scipy import stats
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
# Load team data
df = pd.read_csv('baseball.csv',sep=',').fillna(0)
df['OPS'] = df.OBP + df.SLG
df2002 = df.loc[df.Year < 2002]

# Linear regression for Runs scored

slBA, intBA, r_valBA, p_valBA, ste_errBA = stats.linregress(df2002.BA,df2002.RS)
rsqBA = r_valBA**2
slOBP, intOBP, r_valOBP, p_valOBP, ste_errOBP = stats.linregress(df2002.OBP,df2002.RS)
rsqOBP = r_valOBP**2
slSLG, intSLG, r_valSLG, p_valSLG, ste_errSLG = stats.linregress(df2002.SLG,df2002.RS)
rsqSLG = r_valSLG**2
slOPS, intOPS, r_valOPS, p_valOPS, ste_errOPS = stats.linregress(df2002.OPS,df2002.RS)
rsqOPS = r_valOPS**2

plt.plot(df2002.BA,df2002.RS,'.',label='BA ($r^2$=%.3f)' %rsqBA)
plt.plot(df2002.OBP,df2002.RS,'o',label='OBP ($r^2$=%.3f)' %rsqOBP)
plt.plot(df2002.SLG,df2002.RS,'.',label='SLG ($r^2$=%.3f)' %rsqSLG)
plt.plot(df2002.OPS,df2002.RS,'*',label='OPS ($r^2$=%.3f)' %rsqOPS)
plt.xlabel('Statistic')
plt.ylabel('Runs scored')
plt.legend(loc='lower right')
plt.grid()
```

https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.linregress.html

Python Code: Fig.3.24 (2)

```
yBA = slBA*df2002.BA + intBA
plt.plot(df2002.BA,yBA,'k-')
yOBP = slOBP*df2002.OBP + intOBP
plt.plot(df2002.OBP,yOBP, 'k-')
ySLG = slSLG*df2002.SLG + intSLG
plt.plot(df2002.SLG,ySLG, 'k-')
yOPS = slOPS*df2002.OPS + intOPS
plt.plot(df2002.OPS,yOPS, 'k-')
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.scatter(df2002.OBP,df2002.SLG,df2002.RS,marker='*',color='r')
ax.set_xlabel('On base percentage (OBP)')
ax.set_ylabel('Slugging percentage (SLG)')
ax.set_zlabel('Runs scored (RS)’)

x = df2002.OBP
y = df2002.SLG
x,y = np.meshgrid(x,y)
z = -803 + 2729*x + 1587*y
# Linear regression for Wins
slWBA, intWBA, r_valWBA, p_valWBA, ste_errWBA = stats.linregress(df2002.BA,df2002.W)
```

Matlab Code

```
%Gradient Descent
clear all
close all
%num of iterations, learning rate, initial guess
ite = 50000;
alpha = .0005;
wa = [-1000; 1000; 1000];
%imported data, 3 columns: RS, OBP, SLG
A = readtable ('baseball.csv');
%size(A)
%a1 is OBP, a2 is SLG, a3 is RS
a1 = A.OBP;
a2 = A.SLG;
a3 = A.RS;
%length of data
spac = length(a1);
%group OBP and SLG in a matrix
Af = [a1, a2];
```

```
%define symbolic variables
syms w0 w1 w2
whold = [w1; w2];
%cost function for first point
g(w0,w1,w2) = (w0+Af(1,:)*whold - a3(1))^2;
%cost function for the rest of points (wo+x.T *w y)^2
for i=2:spac
g = g + (w0+Af(1,:)*whold - a3(i))^2;
end
%take the grad of g
gradd(w0,w1,w2) = gradient(g,[w0,w1,w2]);
%loop through iterations
for i=1:ite
%value of gradient at wa
bloop1 = double(gradd(wa(1),wa(2),wa(3)));
%gradient descent, new value of w
wnew = wa - alpha*bloop1;
%update wa
wa = wnew;
end
wnew
```

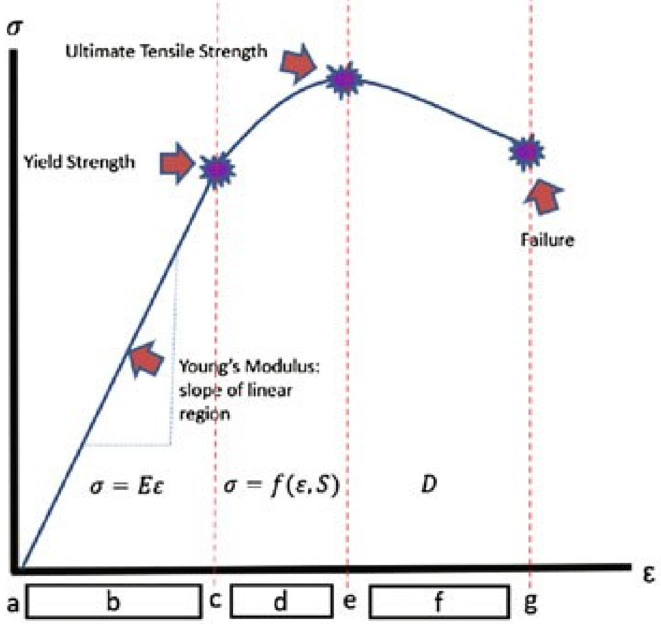
Matlab

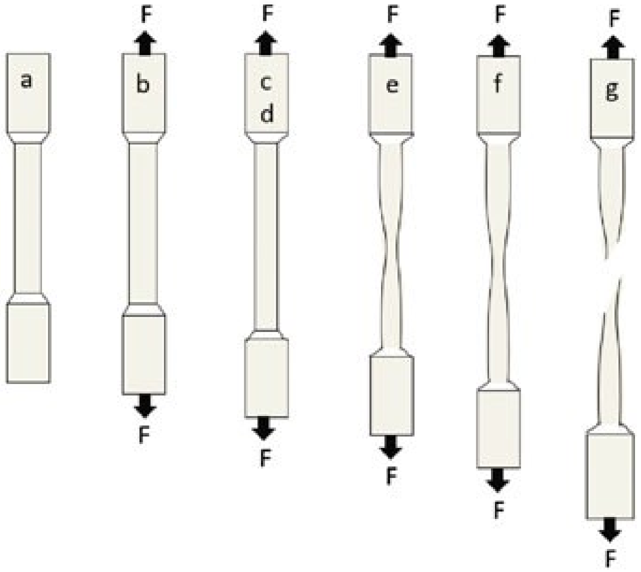
- statistics and machine learning toolbox
  - regress
  - lasso

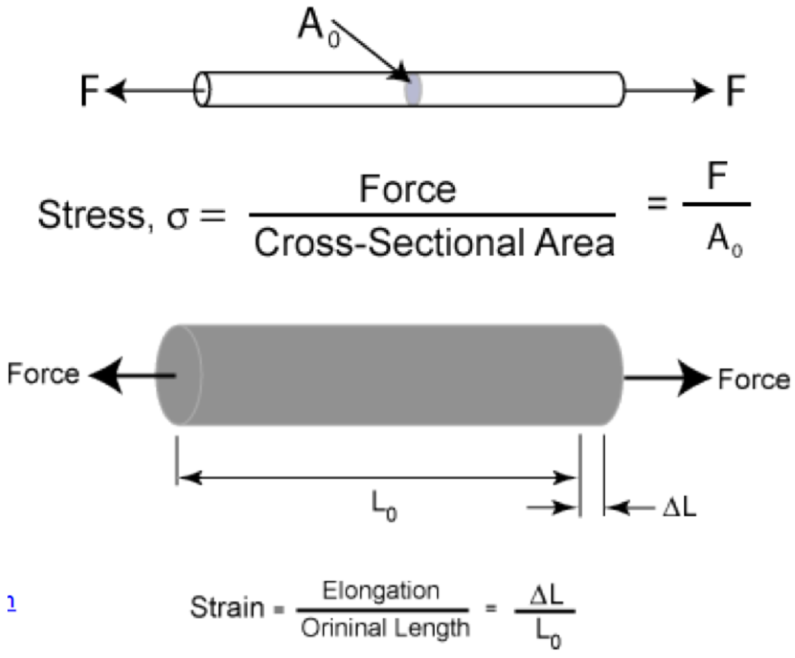
Example: Indentation for Material Hardness and Strength

- Stress-strain curve

Why stress instead of force?

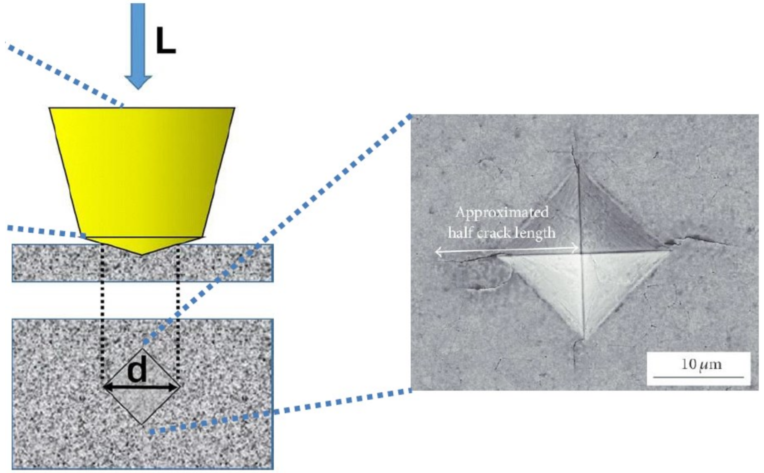






- Vickers Hardness (HV)

$$HV = \frac{F}{A} = \frac{F}{\dfrac{d^2}{2\sin(68°)}} = 1.8544\frac{F}{d^2}$$

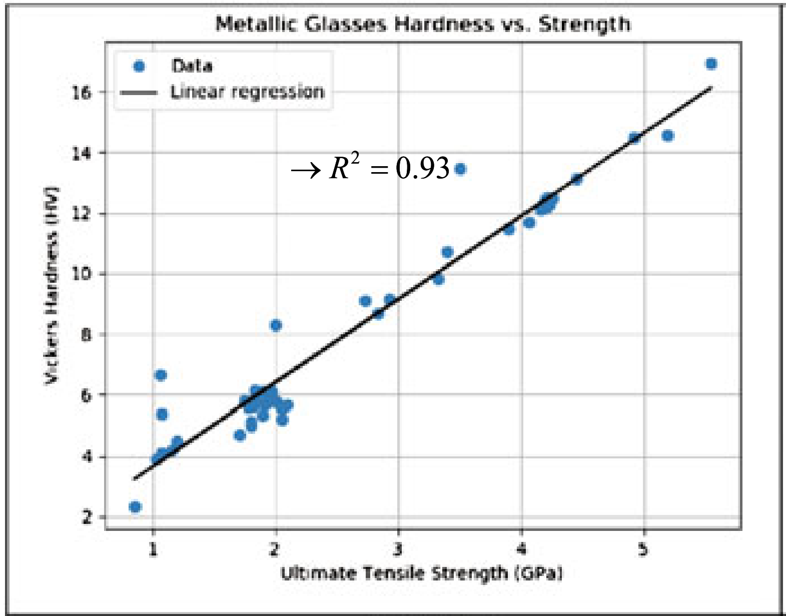


Example: Indentation for Material Hardness and Strength

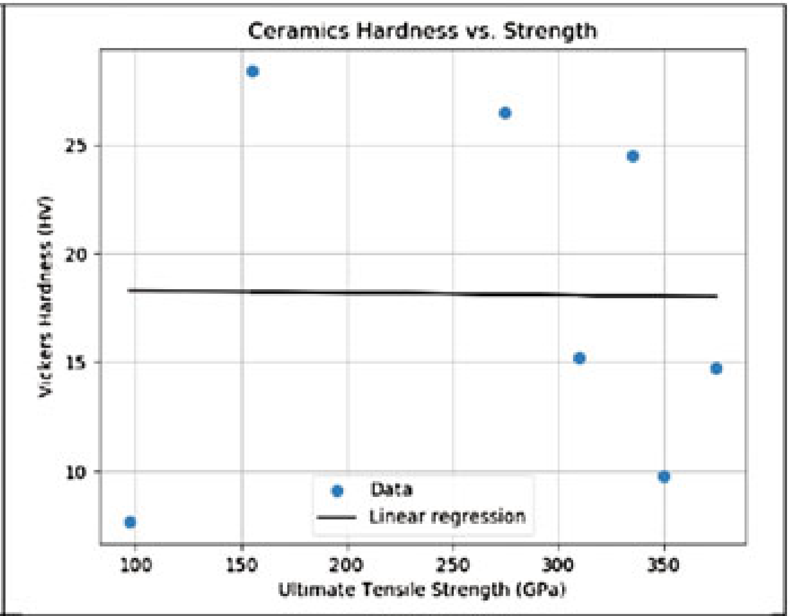
– Previous linear empirical equations in literature have been found to accurately relate Vickers Hardness (HV) and yield strength σ)for some materials

– why there should be a relationship between HV and σ?

Material	Ultimate Tensile Strength (Gpa)	Vickers Hardness (HV)
Zr52.5Ni14.6Al10Cu17.9Ti5	1.8	5.15
(Co0.942Fe0.058)69Nb3B22.4Si5.6	3.32	9.82
Zr55Cu30Al10Ni5	1.8	5
Pd40Ni40P20	1.78	5.6
Fe41Co7Cr15Mo14C15B6Y2	3.5	13.45
Fe74Ni9Cr4Si3B10	2.93	9.16
Fe66Ni7Zr6Cr8Si3B10	2	8.31
Fe63Ni7Zr6Cr8W3Si3B10	2.73	9.1
Zr53Cu30Ni9Al8	2.05	5.22
(Zr53Cu30Ni9Al8)99.75Si0.25	2.05	5.54
(Zr53Cu30Ni9Al8)99.5Si0.5	1.82	5.64
(Zr53Cu30Ni9Al8)99.25Si0.75	2.1	5.67
(Zr53Cu30Ni9Al8)99Si	1.75	5.82
Zr41.2Ti13.8Cu12.5Ni10Be22.5	1.95	5.95
Zr-400°C×5min	1.97	6.1



$$w = \begin{bmatrix} 0.9107 \\ 2.7436 \end{bmatrix}$$
$$HV = 2.7346\sigma + 0.9107$$
$$r^2 = 0.949$$



$$w = \begin{bmatrix} 18.377 \\ -0.001 \end{bmatrix}$$
$$HV = -0.001\sigma + 18.377$$
$$r^2 = 0.0002$$

Zhang, P. et al. (2011). General relationship between strength and hardness. Materials Science and Engineering: A, 529, 62-73.

Nonlinear Regression: Piecewise Linear Regression

- subdividing a set of nonlinear data into a series of segments that are approximately linear

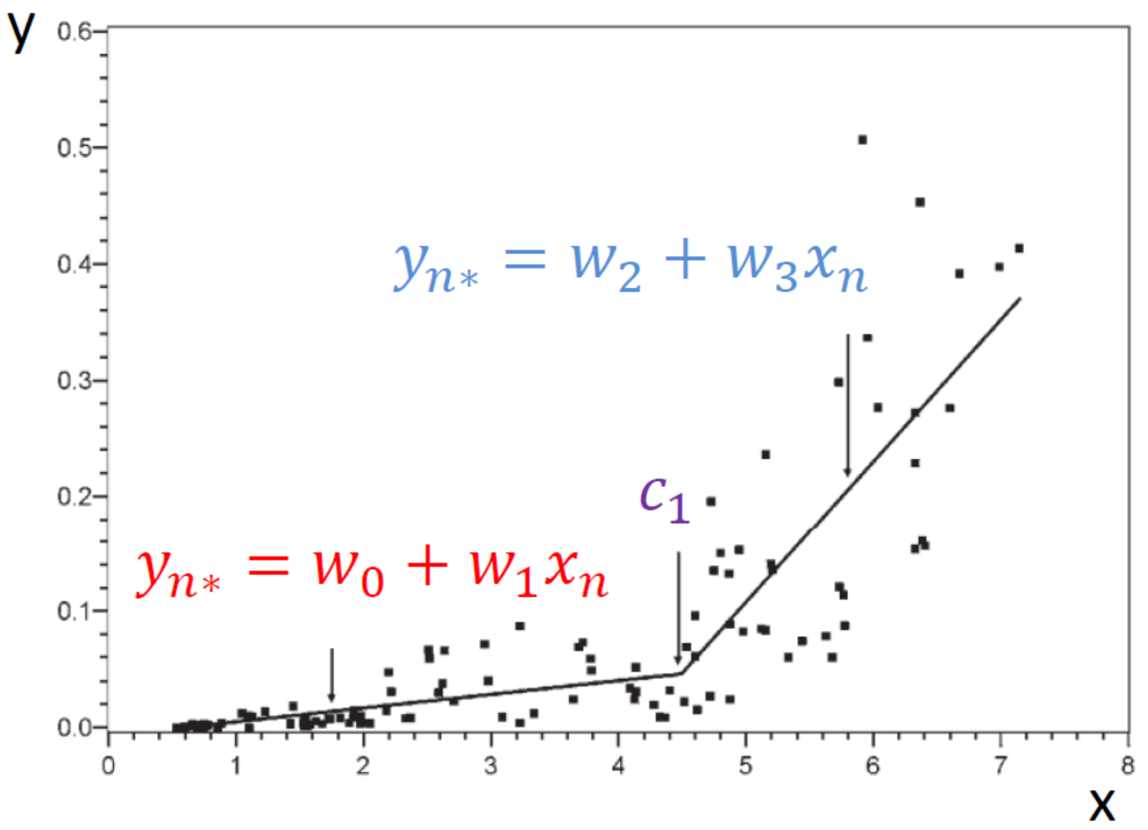
Split the data into two sets: N_1 and N_2

$$\left.\begin{array}{ll} y_n^* = w_0 + w_1 x_n & (x < c_1) \\ y_n^* = w_2 + w_3 x_n & (x > c_1) \end{array}\right\}$$

$$\xrightarrow[c_1 = -\frac{w_0 - w_2}{w_1 - w_3}]{w_0 + w_1 c_1 = w_2 + w_3 c_1} \begin{cases} y_n^* = w_0 + w_1 x_n & (x < c_1) \\ y_n^* = w_0 + (w_1 - w_3) c_1 + w_3 x_n & (x > c_1) \end{cases}$$

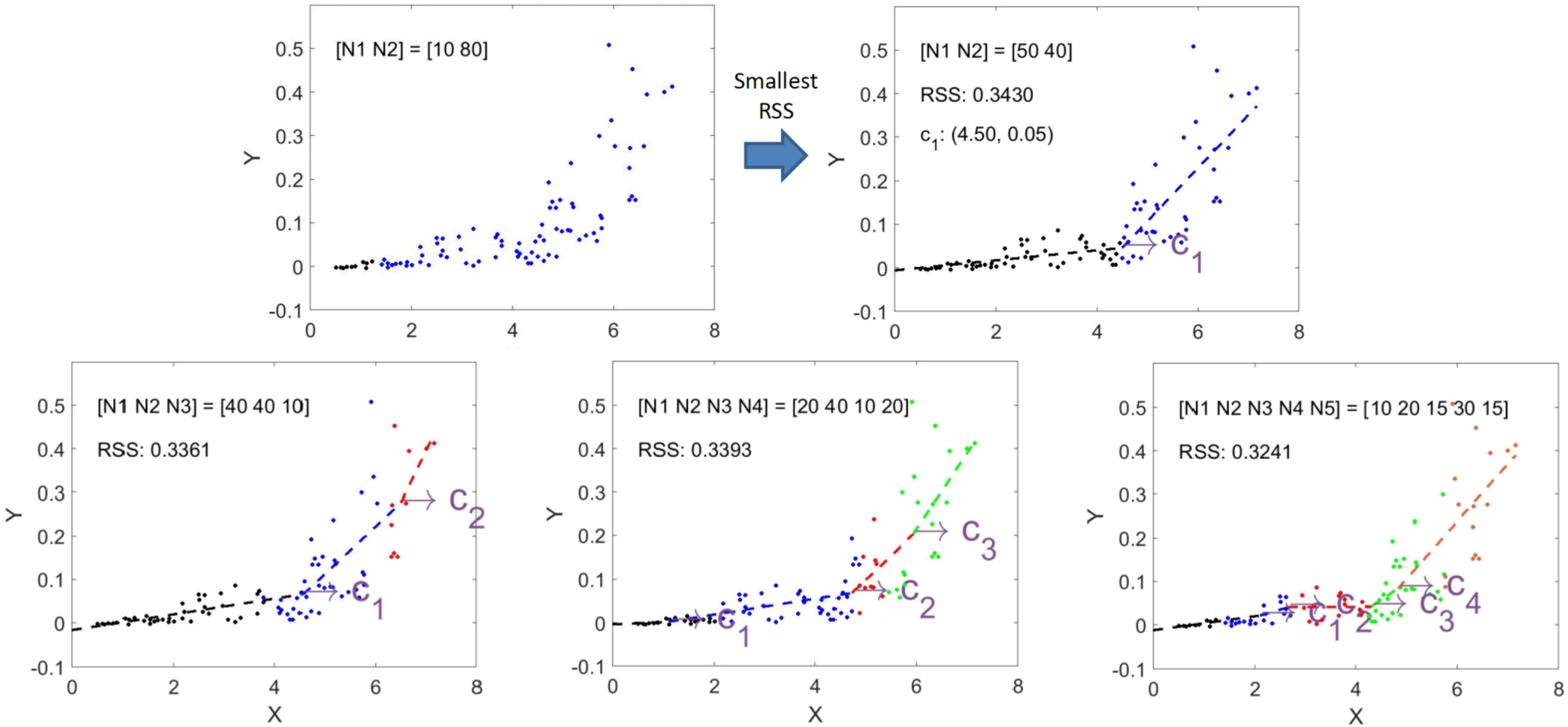
residual sum of squares (RSS)

$$c(\mathbf{w}) = \frac{1}{N_1} \sum_{n=1}^{N_1} \left(y_n^* - y_n \right)^2 + \frac{1}{N_2 - N_1} \sum_{n=N_1+1}^{N_2} \left(y_n^* - y_n \right)^2$$



Nonlinear Regression: Piecewise Linear Regression

- How can we choose the split point?
  - Use residual sum of squares (RSS) as a cost function

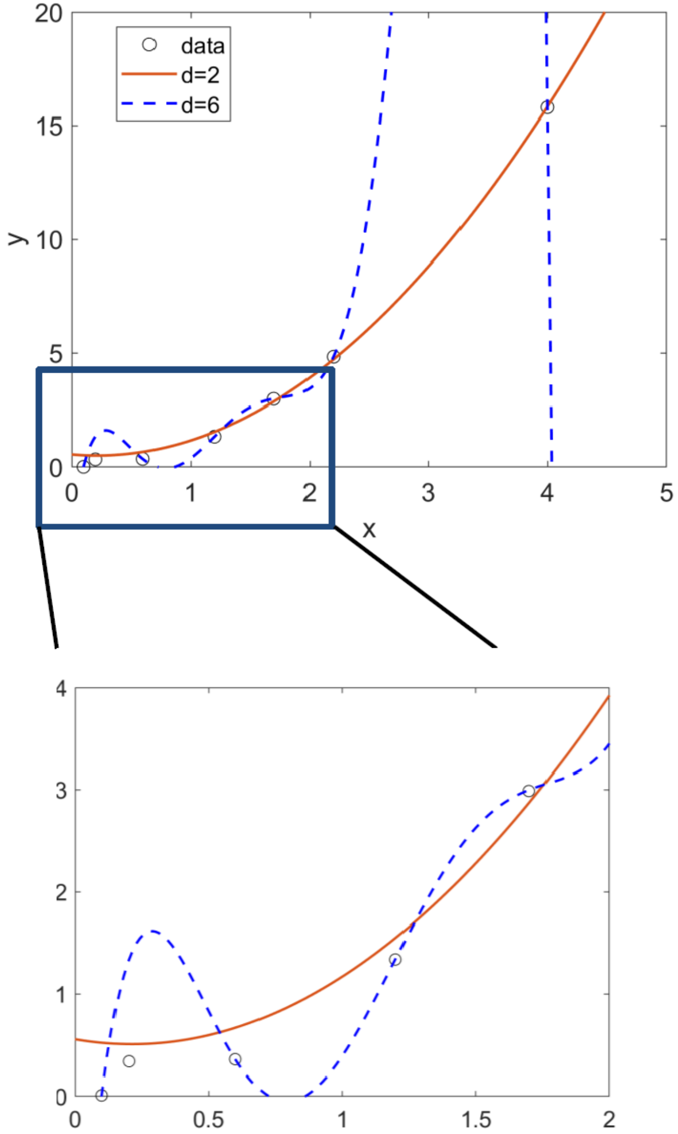


Polynomial Nonlinear Features

- We can increase our feature space by taking increasingly higher degrees of polynomials.
- Feature space: The n dimensions where the variables exist

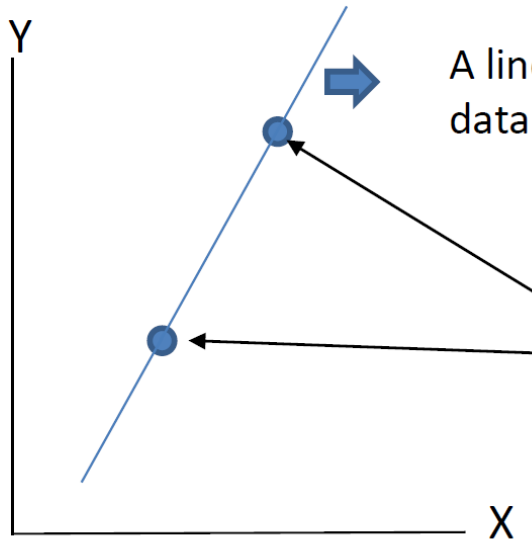
$$
\begin{cases}
\text{1-feature } x_n,\ d\text{-degree polynomial features: } 1, x_n, x_n^{\,2}, \dots, x_n^{\,d-1}, x_n^{\,d} \\
\text{polynomial basis: } \mathbf{p}(x_n)^T = \left[1, x_n, x_n^{\,2}, \dots, x_n^{\,d-1}, x_n^{\,d}\right] \\
\text{polynomial model: } y_n^* = \mathbf{p}(x_n)^T \mathbf{w} = \left[1, x_n, x_n^{\,2}, \dots, x_n^{\,d-1}, x_n^{\,d}\right] \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix} \\
d = 2 \rightarrow \text{linear}
\end{cases}
$$

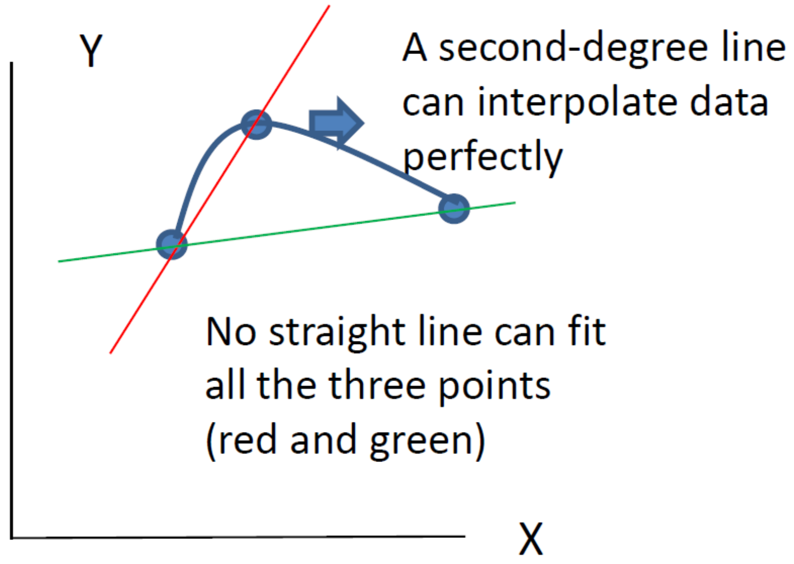
- Pitfall: For an increasingly higher d degree, you can start overfitting
- Overfitting: A model that fits the training data too well and therefore lacks generality.



Higher Order Interpolation May Lead to Overfitting

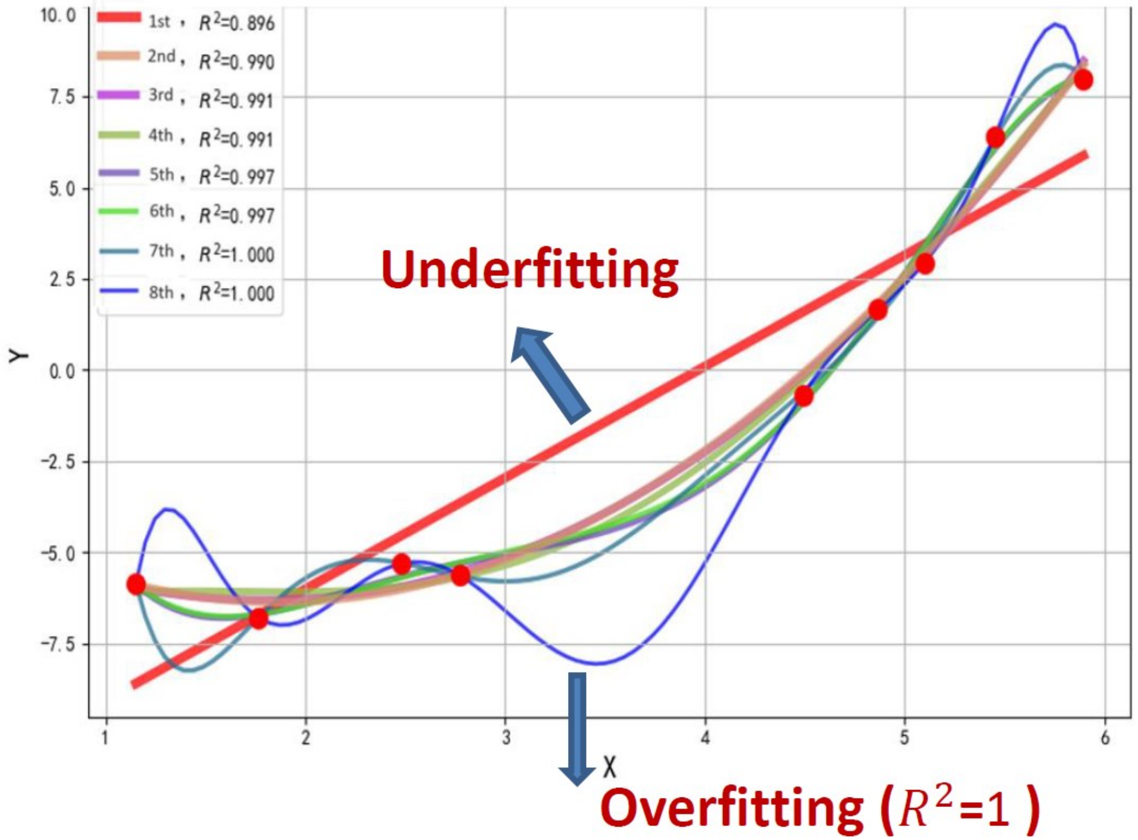
- Suppose you have a set N data points (x(i),y(i)) in the plane where no two x(i) are the same. Then there exists a polynomial P of degree N−1 or less which perfectly interpolates the data points. That is, P(x(i))=y(i) for all I
- According to the theorem, for two points there exists a line and for three points there exists a quadratic polynomial that perfectly fits the data points.
- But if we have a large number of data say 30,000, should we use a very high degree polynomial to fit it? The answer is NO.





Avoid High Order Polynomials

– By increasing the order of regression model, we can have more accurate regression result (regression curve corresponds too closely to data).
– This causes "Overfitting" and "Runge's Phenomenon oscillation".

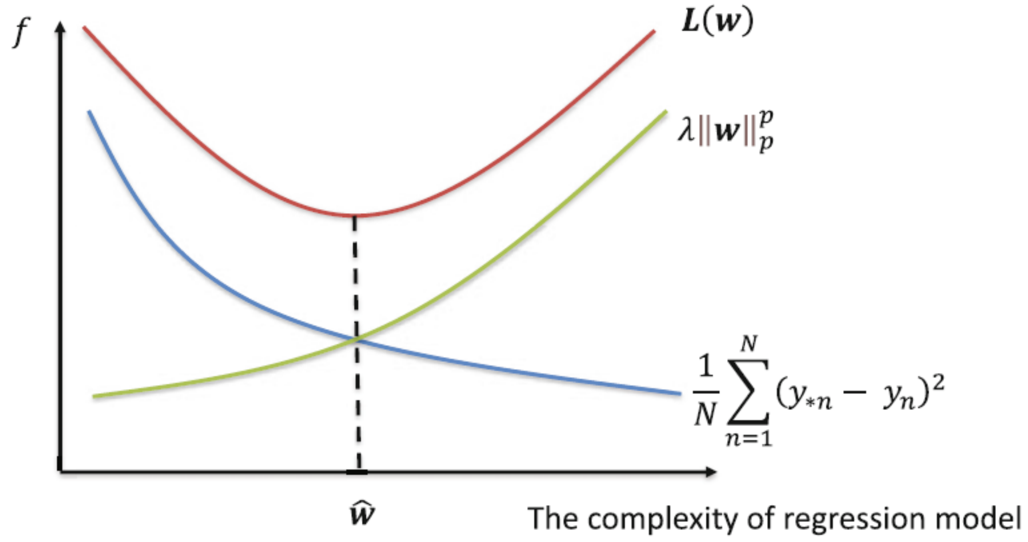


Use Regularization To Avoid Overfitting

- Find a good balance between model complexity and accuracy
  - complicated, higher order regression models to achieve accuracy → may lose generality for the regression models
- Regularized loss function
  - By tuning λ a model can be pushed to converge to the actual function
  - Larger λ: more simplicity, smaller λ: more accuracy
  - How to choose λ?

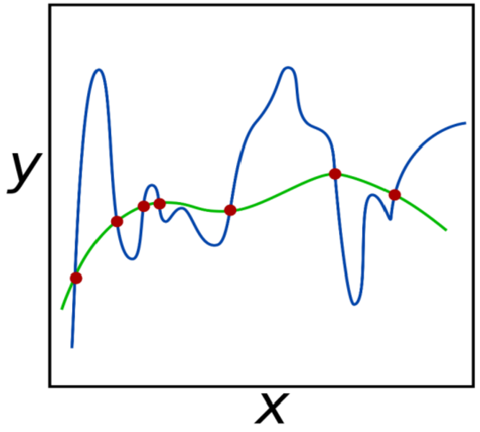
$$L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda\|\mathbf{w}\|_p \quad \text{where} \quad \|\mathbf{w}\|_p = \left(\sum_{j=1}^{N}|w_j|^p\right)^{1/p}$$

$$\begin{cases} \lambda: \text{ predefined regularization parameter with nonnegative value} \\ y_n: \text{ original data} \\ y_n^*: \text{ regression model} \\ N: \text{ number of data points} \end{cases}$$



Regularization Can Avoid Overfitting

- We consider the green curve to be smoother an “easier" path to traverse in comparison to the blue curve. Smaller weights will get us better or smoother results. By tuning $\boldsymbol{\lambda}$ a model can be pushed to converge at the green curve.
- Think of regularization in two ways
  - You are penalizing high weights by adding a positive term to the cost function. The higher the magnitude of $\boldsymbol{w}$the higher the cost will be.
  - By adjusting λ, you can modify the cost function to achieve convergence to a minimum.



$$L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda\|\mathbf{w}\|_{p=2}^2 \xrightarrow{\lambda\to\infty} L(\mathbf{w}) \approx \lambda\|\mathbf{w}\|_{p=2}^2 \ (\text{convex})$$

$$\begin{cases} L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda\|\mathbf{w}\|_1 = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda\sum_{n=1}^{S}|w_n| : \text{ LASSO}(\text{least absolute shrinkage and selection operator}) \\ L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda\|\mathbf{w}\|_2 = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda\sum_{n=1}^{S}|w_n|^2 : \text{ Ridge} \\ L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda\left(\alpha\|\mathbf{w}\|_1 + (1-\alpha)\|\mathbf{w}\|_2\right) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \beta_1\|\mathbf{w}\|_1 + \beta_2\|\mathbf{w}\|_2 : \text{ Elastic Net} \end{cases}$$

L_p-Norm

- L1-norm can be used to relieve overfitting: eliminate some high order terms in the regression model (may omit the intricate details)
- L2-norm uses the concept of "sum of squares", and thus has useful properties such as convexity, smoothness and differentiability (capture those details)

$$\|\mathbf{w}\|_p = \left(\sum_{j=1}^{N} |w_j|^p \right)^{1/p}$$

$$p = 1: \ \|\mathbf{w}\|_1 = \sum_{j=1}^{N} |w_j| = |w_1| + |w_2| + \cdots + |w_N|$$

$$p = 2: \ \|\mathbf{w}\|_2 = \left(\sum_{j=1}^{N} |w_j|^2 \right)^{1/2} = \sqrt{|w_1|^2 + |w_2|^2 + \cdots + |w_N|^2}$$

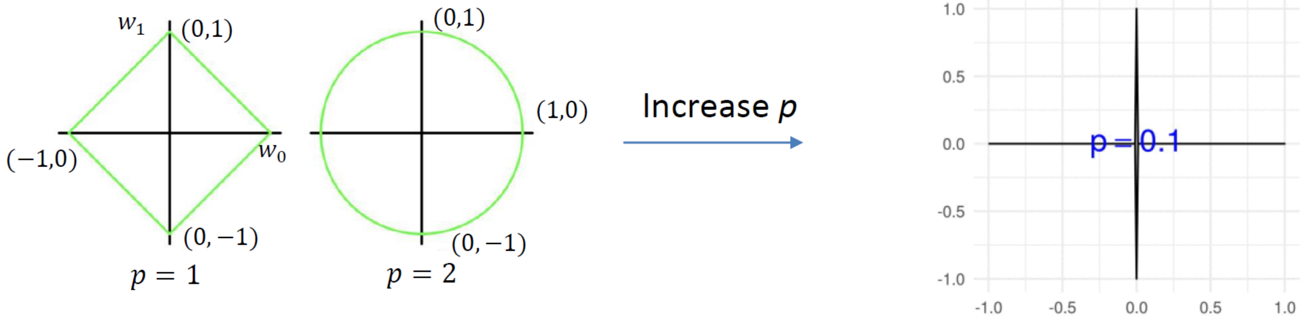
$$p = \infty: \ \|\mathbf{w}\|_\infty = \max\left(|w_j|\right) = \max\left(|w_1|, |w_2|, \ldots, |w_N|\right)$$

$N = 2, \ \|\mathbf{w}\|_p = 1$

$\|\boldsymbol{w}\|_{p=1}$ — Rhombus — $|w_0| + |w_1| = 1$

$\|\boldsymbol{w}\|_{p=2}$ — Circle — $|w_0|^2 + |w_1|^2 = 1$

$\|\omega\|_\infty = \max(|\omega_j|)$ — Square



L1 norm **L2 norm** **Convergence to L∞ norm**

Example: Regularized Regression

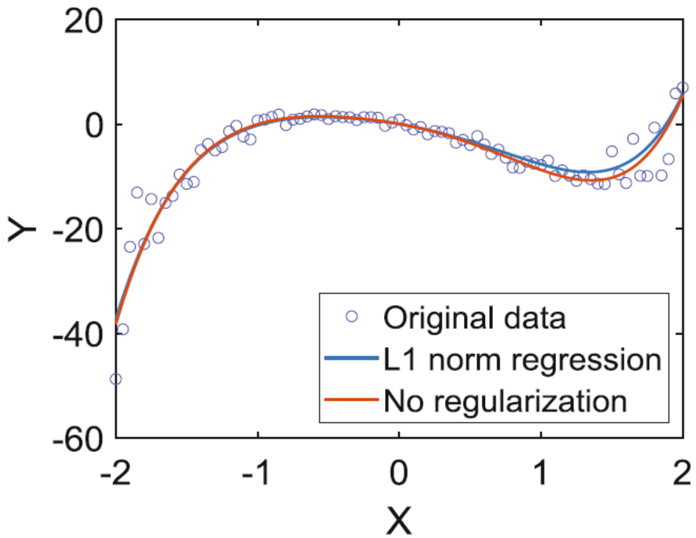
$$y = 1(x+\varepsilon_1)^5 - 4(x+\varepsilon_2)^2 - 5(x+\varepsilon_3) \quad \text{where } \ \varepsilon_i \sim Normal(0, 0.05), \text{ Gaussian noise}$$

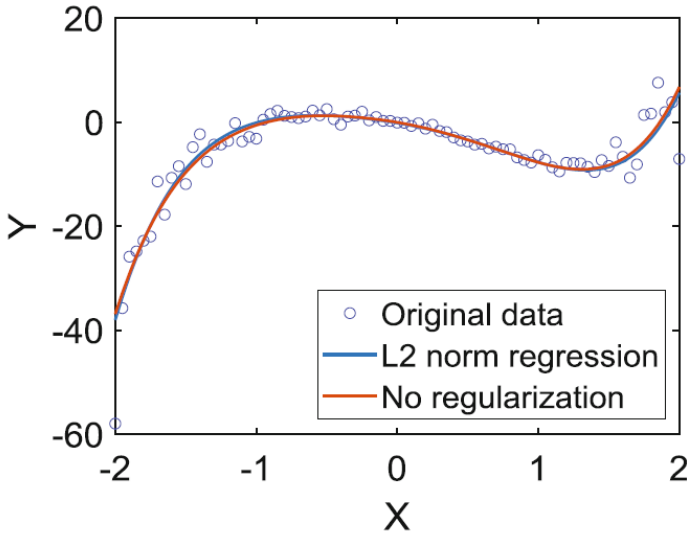
$$y_n^* = w_0 + w_1 x_n + w_2 x_n^{\ 2} + \cdots + w_5 x_n^{\ 5}$$

$$L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 \rightarrow \mathbf{w} = \begin{bmatrix} -0.0018 & -4.8456 & -4.5166 & -0.1003 & 0.2190 & 1.0498 \end{bmatrix}^T \ (\text{MATLAB: polyfit})$$

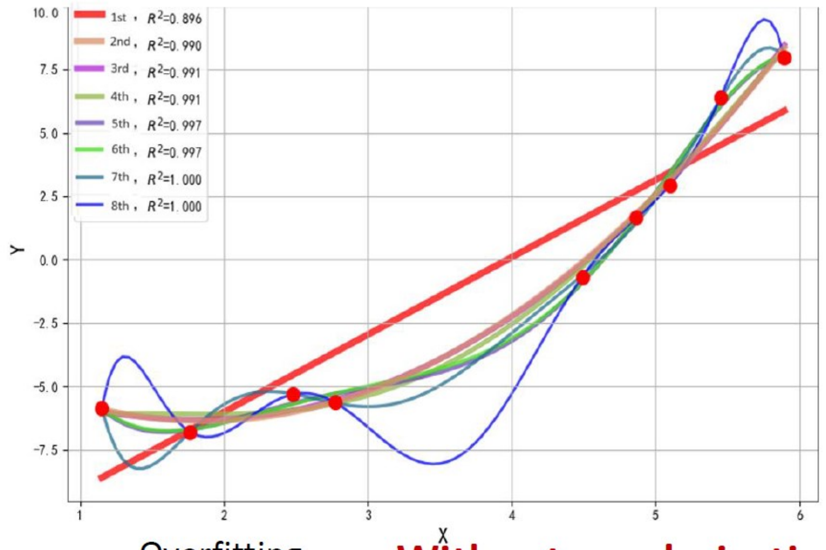
$$L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda \left\|\mathbf{w}\right\|_{p=1} \xrightarrow{\lambda=0.074} \mathbf{w} = \begin{bmatrix} 0 & -4.6723 & -3.9175 & 0 & 0 & 0.9671 \end{bmatrix}^T$$

$$L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2 + \lambda \left\|\mathbf{w}\right\|_{p=2} \xrightarrow{\lambda=1} \mathbf{w} = \begin{bmatrix} -0.0707 & -5.3544 & -3.7368 & 0.0495 & -0.0800 & 1.0119 \end{bmatrix}^T$$

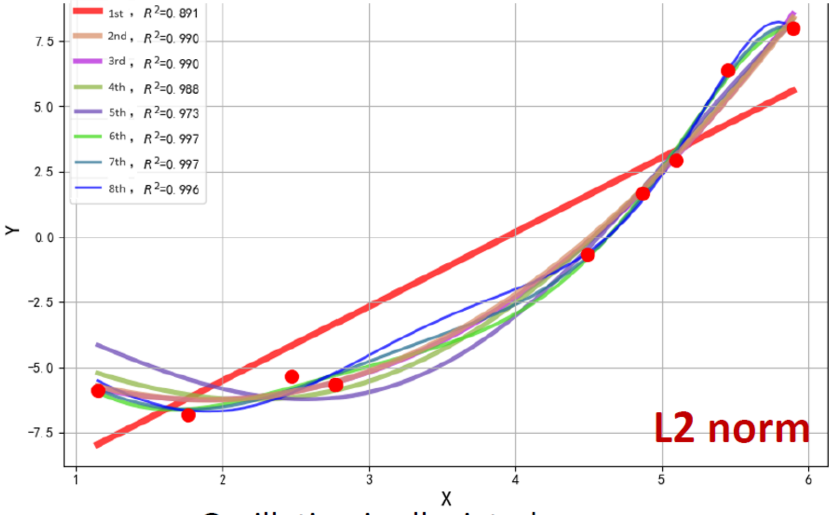




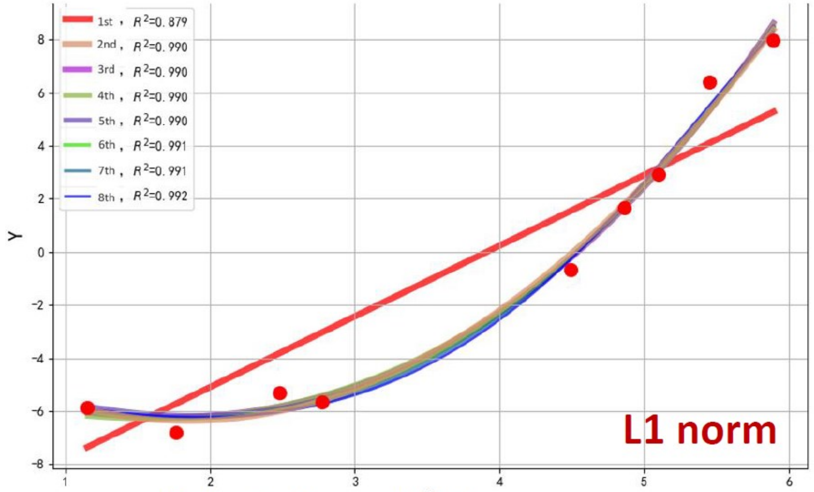
Example: Comparison of Regularization



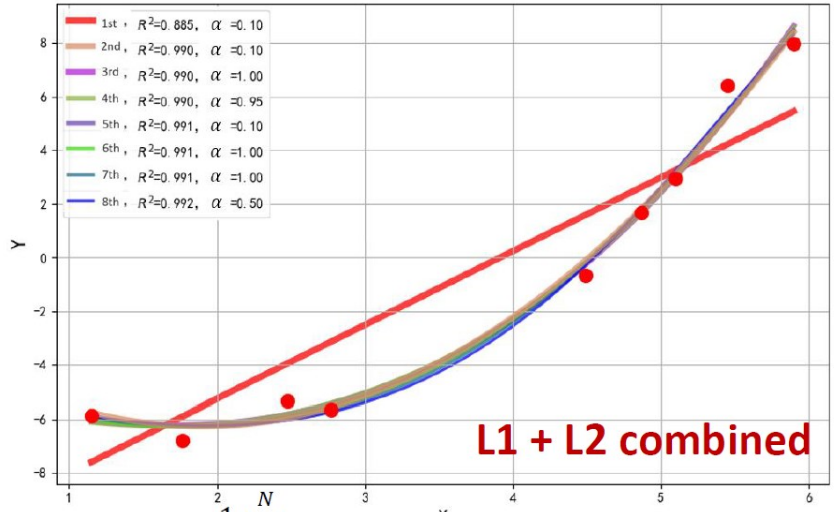
Overfitting. **Without regularization**



Oscillation is alleviated.



Fitting is clean with L1 norm.



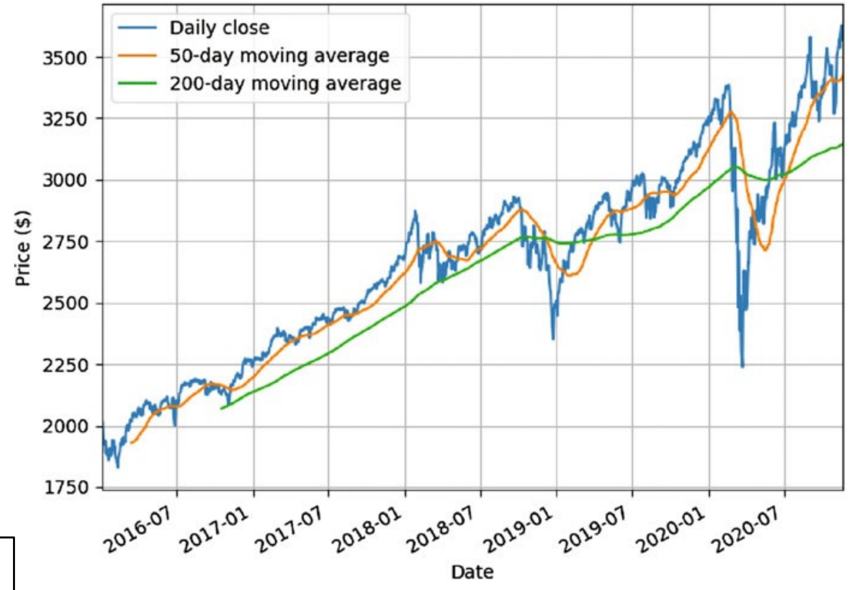
$$c(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N}(y_{n*} - y_n)^2 + \lambda(\alpha||\boldsymbol{\omega}||_1 + (1-\alpha)||\boldsymbol{\omega}||_2^2)$$

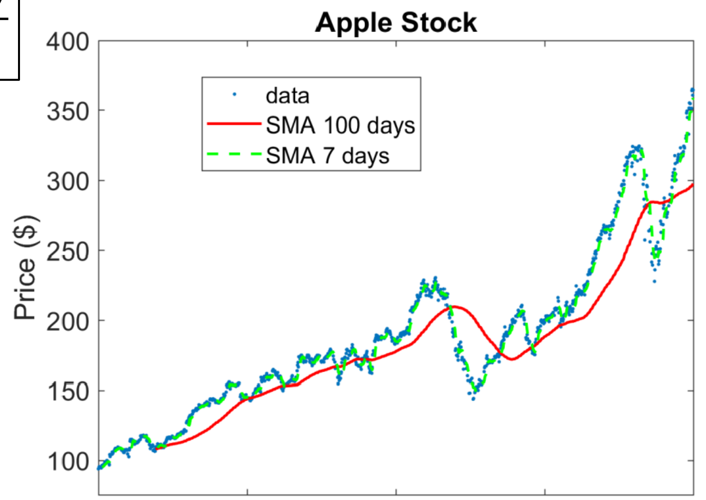
Nonlinear Regression: Moving Average

- good method to smooth out data and mute the effects of spikes in the data
  - analyzing trends with stock prices in order to smooth out the effects of day to day movement of the stock price (volatile or downturn)
  - 200-day can also act as a “floor” or lower limit—buying opportunities exist when the price drops down to that level or below
- Simple Moving Average (SMA)

$$\mathrm{SMA} = \frac{\sum \left(P_c + P_{c-1} + \cdots + P_{c-k}\right)}{k}$$

  - sum of the stock price for the previous k amount of days divided by k
- appearance of being off of the original data
  - at the average of the independent variable instead of at the extent





Python code: Fig.3.20

```
#!pip install yfinance
import yfinance as yf
#import pandas_datareader.data as web

start = '2016-01-01'
#df2 = web.DataReader('^GSPC', 'yahoo',start)
df2 = yf.download('^GSPC', start=start)
df2.to_csv('gspc.csv')
df2['Close'].plot()
df2['Close'].rolling(50).mean().plot()
df2['Close'].rolling(200).mean().plot()
plt.legend(['Daily close','50-day moving average','200-
day moving average'])
plt.ylabel('Price ($)')
plt.grid()
plt.show()
```

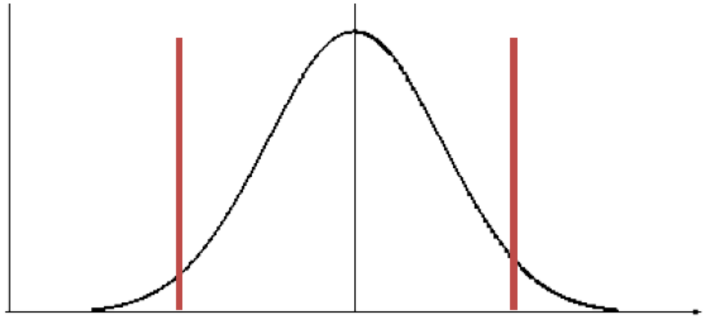
Nonlinear Regression: Moving Least Squares

- So far, we have considered all our data of equal importance. However, we might want to place more weight on certain data points for a variety of reasons including:
  - Emphasize data points closer to our point of interest
  - Minimize fitting towards outliers
- weight function results in a localized point-by-point least square fit instead of a global least squares fit
  - weighting functions move so that the regression is always being done with a few of the data points

$$c(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \theta(x_n)\left(y_n^*(\mathbf{w}) - y_n\right)^2$$

$\theta = 1$: regular least squares

Typical weighting function



Example: Apple Stock

- Original 252 data points
- MLS: only 45 evenly spaced points
- cubic spline with a coverage radius of 3

Linear regression (one line through all data)

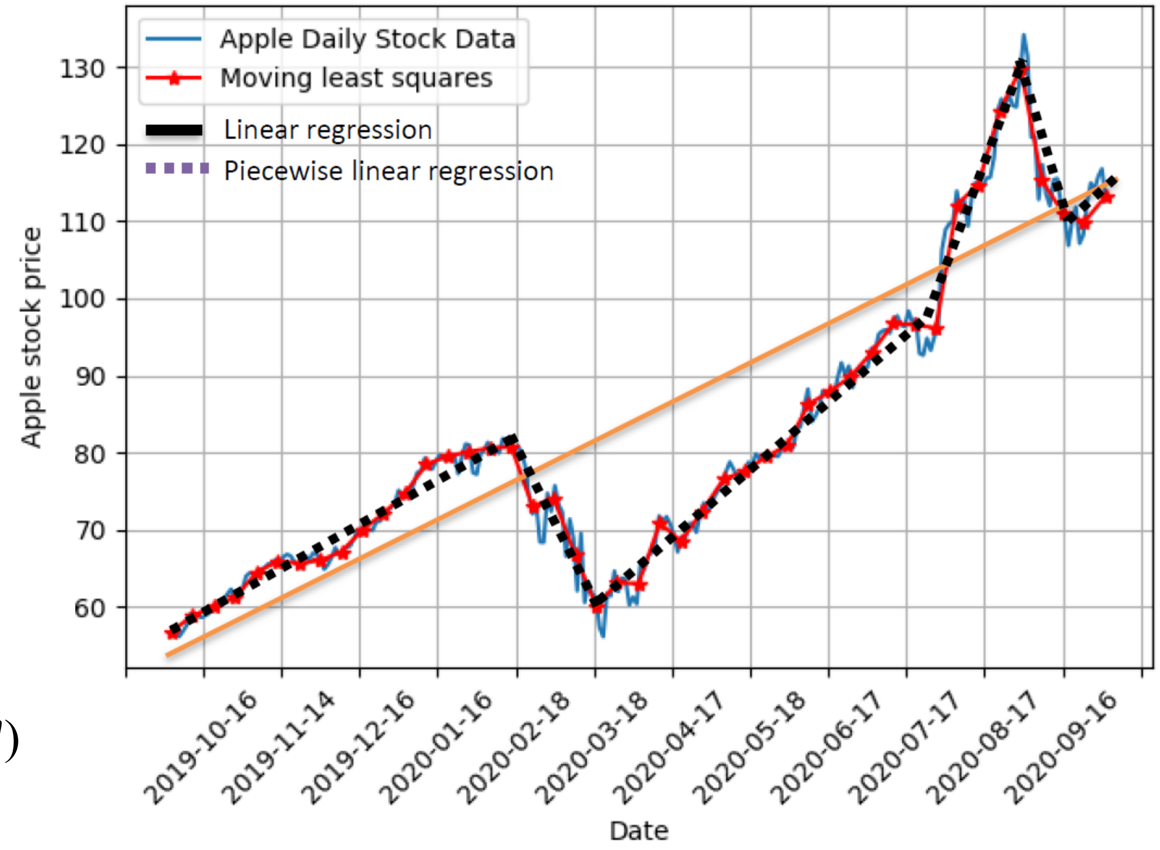
$$c(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(y_n^* - y_n\right)^2$$

Piecewise Linear regression (multiple lines through data)

$$c(\mathbf{w}) = \frac{1}{N_1}\sum_{n=1}^{N_1}\left(y_n^* - y_n\right)^2 + \frac{1}{N_2}\sum_{m=1}^{N_2}\left(y_m^* - y_m\right)^2 + \cdots$$

Weighted regression ("bend" line through data using "weight")

$$c(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\theta(x_n)\left(y_n^* - y_n\right)^2$$



1) Local influence only choose a few points at a time
2) Often use a bell-shaped curve: focus on center point, taper down at edges

Moving Least Squares (MLS) Approximation

$$y_n^* = \mathbf{p}(x_n)^T \mathbf{w}(x) = \left[1, x_n, x_n^{\ 2}, \ldots, x_n^{\ d-1}, x_n^{\ d}\right] \begin{bmatrix} w_0(x) \\ w_1(x) \\ \vdots \\ w_d(x) \end{bmatrix} = \mathbf{p}(\mathbf{x})^T \mathbf{w}(\mathbf{x})$$

$$c(\mathbf{w}(\mathbf{x})) = \sum_{n=1}^{N} \theta(\mathbf{x}-\mathbf{x}_n)\left(\mathbf{p}(\mathbf{x}_n)^T \mathbf{w}(\mathbf{x}) - y_n\right)^2$$

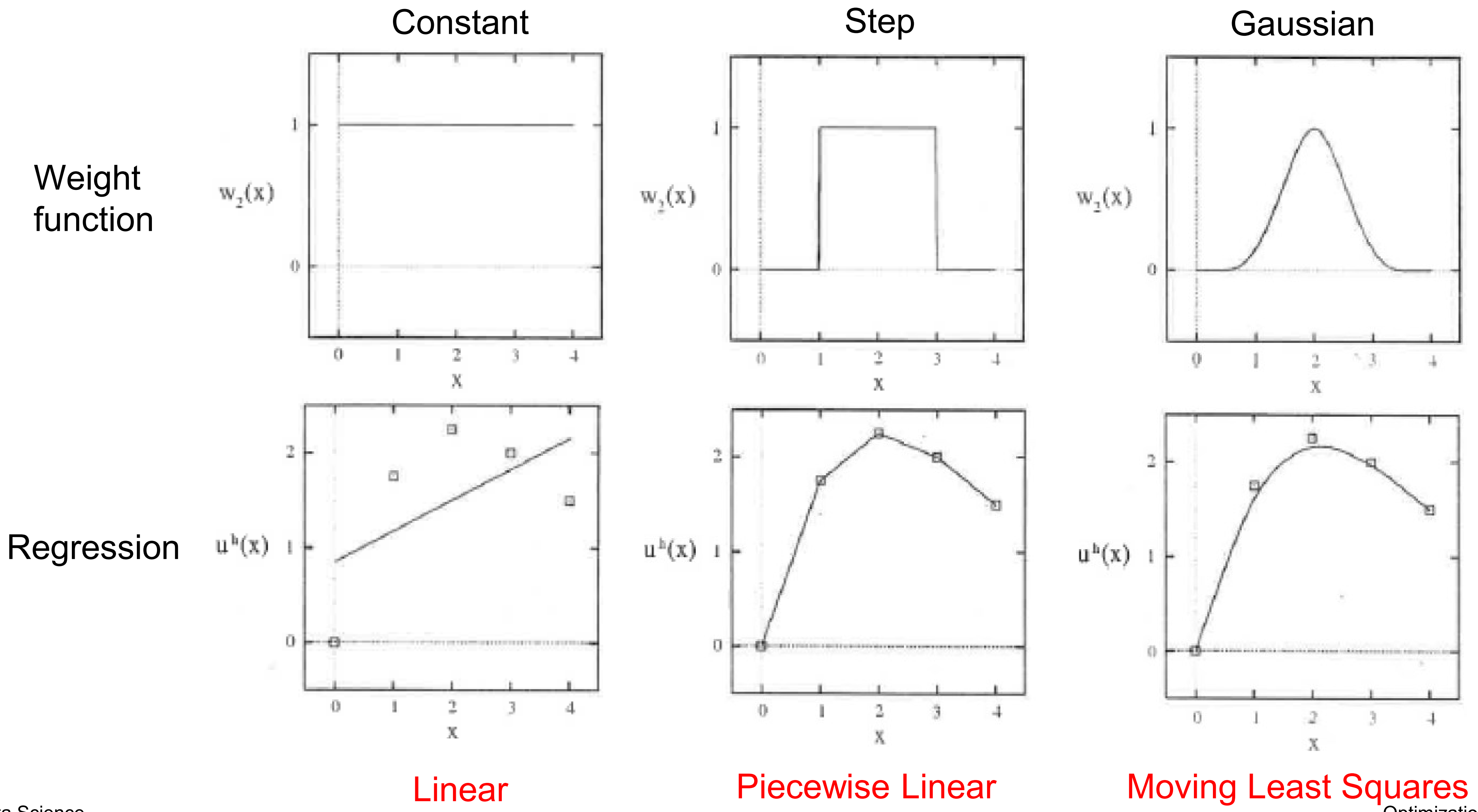
$$\frac{\partial c}{\partial \mathbf{w}(\mathbf{x})} = \sum_{n=1}^{N} \theta(\mathbf{x}-\mathbf{x}_n)\left(\mathbf{p}(\mathbf{x}_n)^T \mathbf{w}(\mathbf{x}) - y_n\right)\mathbf{p}(\mathbf{x}_n) = 0$$

$$\underbrace{\sum_{n=1}^{N} \theta(\mathbf{x}-\mathbf{x}_n)\mathbf{p}(\mathbf{x}_n)\mathbf{p}(\mathbf{x}_n)^T}_{\mathbf{A}(\mathbf{x})} \mathbf{w}(\mathbf{x}) = \underbrace{\sum_{n=1}^{N} \theta(\mathbf{x}-\mathbf{x}_n)\mathbf{p}(\mathbf{x}_n)}_{\mathbf{B}_n(\mathbf{x})}\mathbf{y} \rightarrow \mathbf{w}(\mathbf{x}) = \mathbf{A}(\mathbf{x})^{-1}\mathbf{B}(\mathbf{x})\mathbf{y}$$

$$y_n^* = \mathbf{p}(\mathbf{x})^T \mathbf{w}(\mathbf{x}) = \underbrace{\mathbf{p}(\mathbf{x})^T \mathbf{A}(\mathbf{x})^{-1}\mathbf{B}_n(\mathbf{x})}_{\phi_n(\mathbf{x})}\mathbf{y} = \sum_{n=1}^{N} \phi_n(\mathbf{x})\, y_n$$

y_n^* : reduced order MLS approximation

Moving Least Squares: Weighting Function Effect



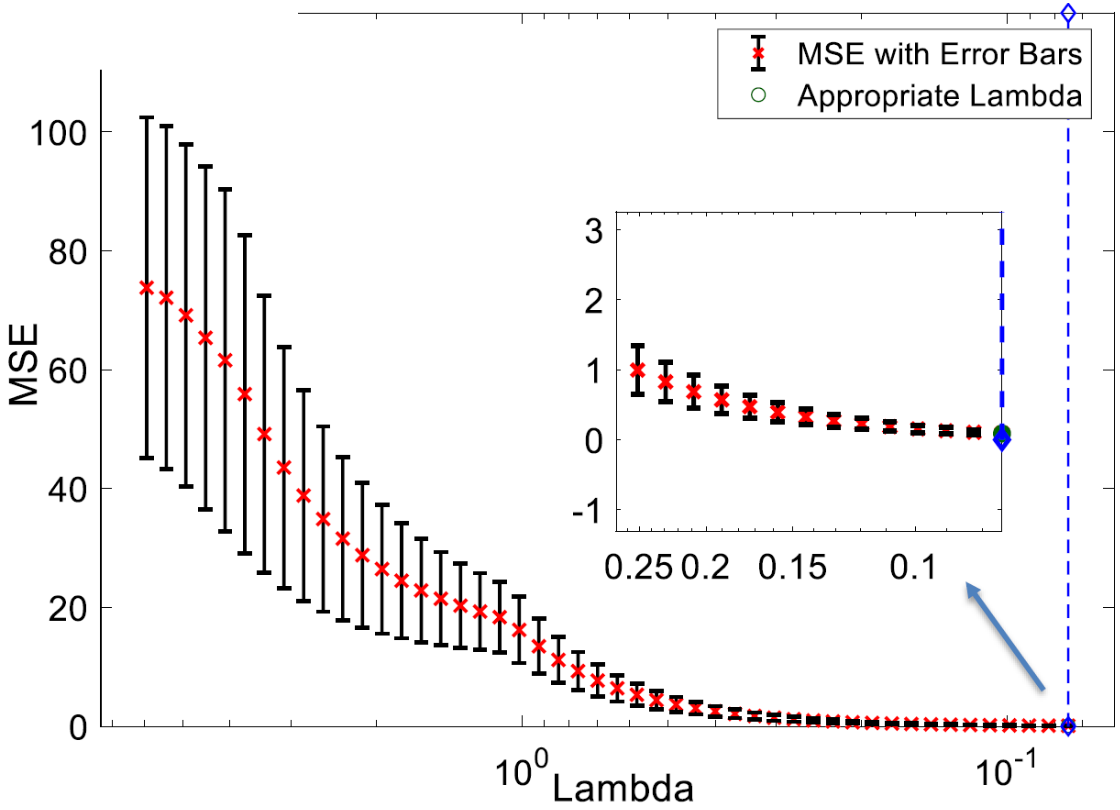
K-fold Cross Validation (1)

- rotation estimation or out-of-sample testing
  - assess how the results of a statistical analysis will generalize to an independent data set
- can remove bias in choosing training and test set and improve model confidence
  - Step 1: Divide the original data set into equal K folds (parts).
  - Step 2: Use one part as the test set and the rest as the training sets.
  - Step 3: Train model and calculate mean square error (MSE) on test set.
  - Step 4: Repeat steps 2 and 3 K times each time using a different section as the test set.
  - Step 5: The average accuracy is taken as the final model accuracy.

	Data				
	Fold 1	Fold 2	Fold 3	…	Fold 10
Set 1	**Test**	Train	Train	Train	Train
Set 2	Train	**Test**	Train	Train	Train
Set 3	Train	Train	**Test**	Train	Train
…	Train	Train	Train	**Test**	Train
Set 10	Train	Train	Train	Train	**Test**

K-fold Cross Validation (2)

- For each regularization parameter λ, K-fold cross-validation can be used to find MSE of data.
- By comparing result of K-fold cross-validation, appropriate λ can be found.



Matlab Code: Fig.3.30 (1)

```
%% L1 and L2 norm regression example
%% Generation of data
clc
clear
x0 = -2:0.05:2; % 81 linearly spaced x coordinates are spaced between interval [-2,2]
n = length(x0); % The total number of data points (81)
x1 = x0+randn(1,n)*0.05; % x+epsilon1
x2 = x0+randn(1,n)*0.05; % x+epsilon2
x3 = x0+randn(1,n)*0.05; % x+epsilon3
x = [x1.^5;x0.^4;x0.^3;x2.^2;x3;ones(1,n)]';
weights = [1;0;0;-4;-5;0]; % Weights
y = x*weights; % Simulated data y = x^5 - 4*x^2 - 5*x


%% Regressions
[b_lasso,fitinfo] = lasso(x, y,'CV',10); % L1 norm regularized regression
lam = fitinfo.Index1SE; % Index of appropriate Lambda
b_lasso_opt = b_lasso(:,lam) % Weights for L1 norm regularized regression
lambda = 1; % Set lambda equals to 1 for L2 norm regularized regression (You can also find an appropriate Lambda yourself)
b_ridge = (x'*x+lambda*eye(size(x,2)))^-1*x'*y % Weights for L2 norm regularized regression (Has analytical solution)


b_ols = polyfit (x1',y,5) % Weights for non regularized regression (Ordinary Least Squares)
```

Matlab Code: Fig.3.30 (2)

```
xplot = [x0.^5;x0.^4;x0.^3;x0.^2;x0;ones(1,n)]';
y_lasso = xplot*b_lasso_opt ; % L1 norm regression result
y_ols = xplot*b_ols'; % Non regularized regression result
y_ridge = xplot*b_ridge ; % L2 norm regression result


%% Plots
plot(x0,y,'bo') % Plot of origin data
hold on
plot(x0,y_lasso,'LineWidth',1) % Plot of L1 norm regression
hold on
plot(x0,y_ridge,'LineWidth',1) % Plot of L2 norm regression
hold on
plot(x0,y_ols,'LineWidth',1) % Plot of non regularized regression
ylabel('Y','fontsize',20)
xlabel('X','fontsize',20)
legendset = legend('Original data','L1 norm regression','L2 norm regression','No regularization','location','southeast')
set(gca,'FontSize',20);
lassoPlot(b_lasso,fitinfo,'PlotType','CV'); % Cross validated MSE
legend('show') % Show legend
```

Homework #2: Regression

- (1) Perform Multivariate Linear Regression on baseball data
  - (OBP, SLG) vs. RS
  - Compare the results from Python and Matlab

- (2) Perform non-linear regression without any regularization, and with L1 and L2 regularization.

$$y = \frac{1}{4}e^{x} - \frac{1}{8}\sin x - \cos x + 0.1x^{3}$$

  - Generate your training data with Gaussian noise and compare the performance with true data.
  - Show how changing the penalty parameter can affect your prediction.