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Statistical Methods in AI (CS7.403)

Lecture-5: k-Nearest Neighbours, Linear Regression

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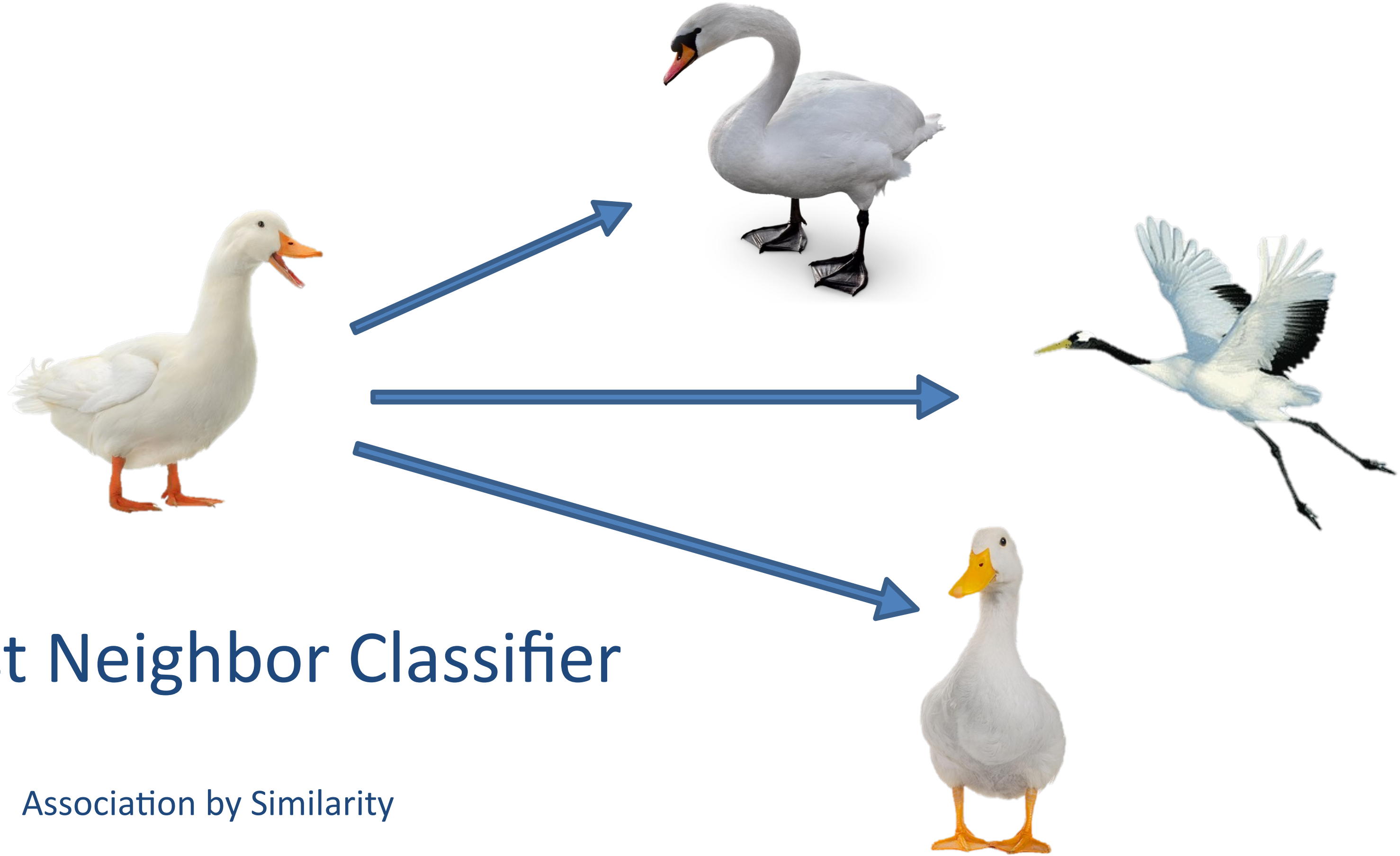
- F1-macro (HM) v/s F1-macro (scikit-learn)

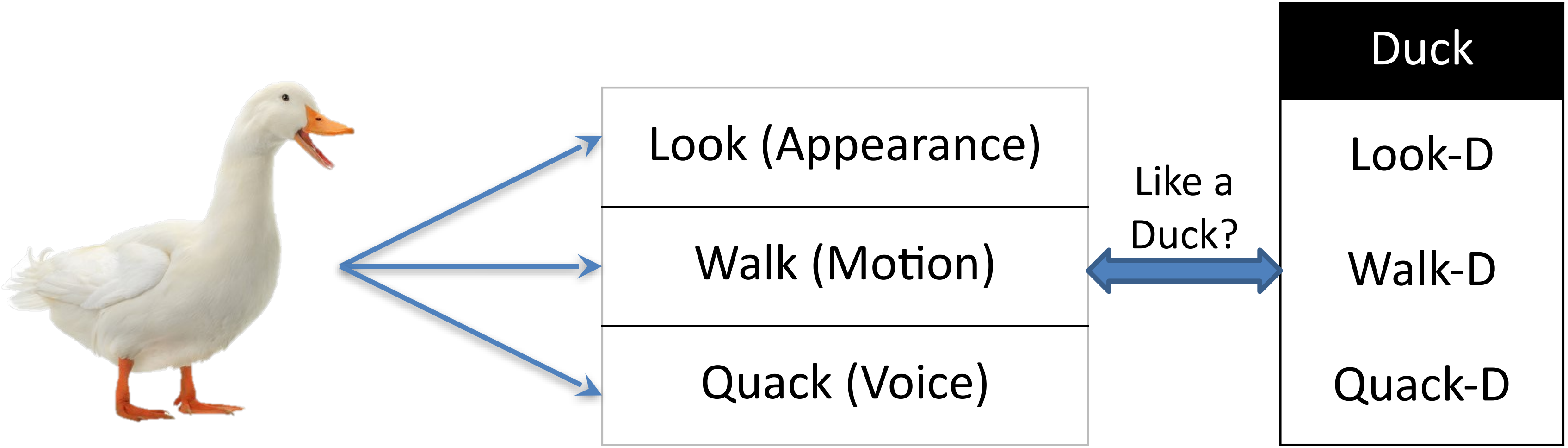
Nearest Neighbor Classifier



Association by Similarity

How do we compare?

If it looks like a duck, walks like a duck and quacks like a duck,



- Find distance to feature vectors of known classes

Nearest Neighbor Classifier

- Assign label of that sample which is nearest to the test sample

X_{test} :

[30.9, 15.1, 1.32]

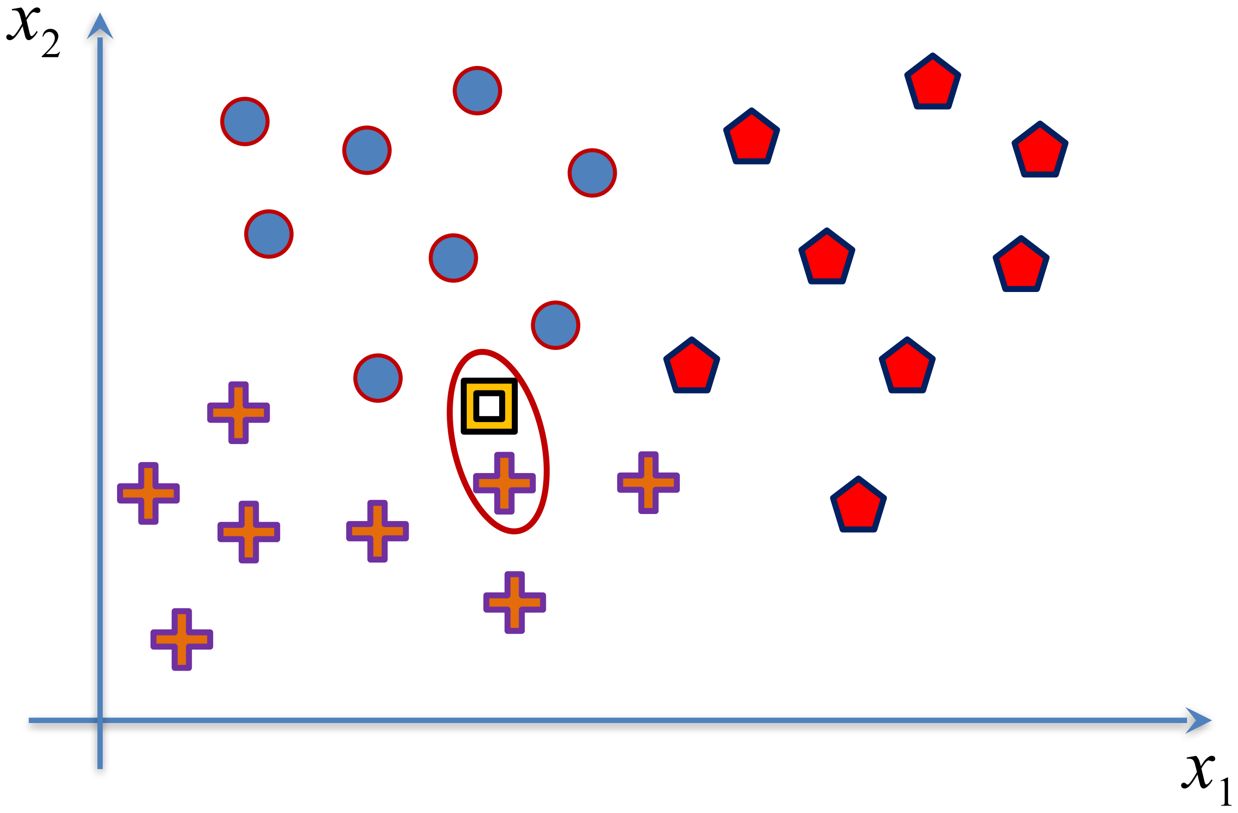
The test sample is a Duck

Training Samples

Distance	Feature Vector	Label
$\boxed{1.30}$	X_1 [32.1, 14.6, 1.42]	$\boxed{\text{Duck}}$
5.78	X_2 [25.3, 16.3, 2.11]	Swan
13.54	X_3 [42.2, 7.7, 0.38]	Crane
4.71	X_4 [26.7, 17.1, 2.04]	Swan
15.21	X_5 [44.1, 7.6, 0.32]	Crane
3.04	X_6 [31.4, 12.1, 1.29]	Duck
13.58	X_7 [41.9, 7.2, 0.35]	Crane

Visualization in Feature Space

- The nearest train sample is a +.
- We assign the test sample to the + class.



The 1-NN Classification Algorithm

Problem

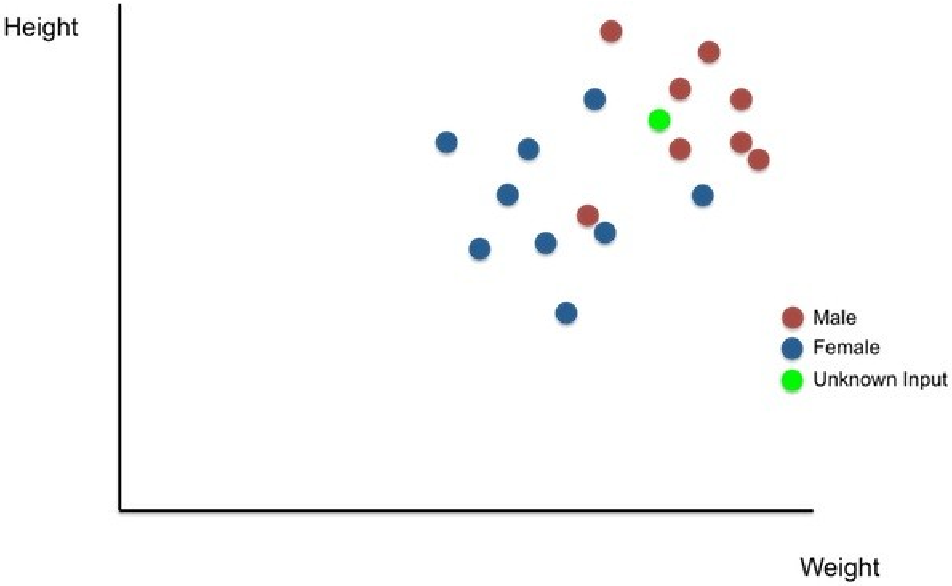
- Given:
  - A set of training ***n*** training samples: $(\mathbf{x}_i, y_i)$
  - A test sample: $\mathbf{x}_t$
- Find:
  - label($\mathbf{x}_t$)

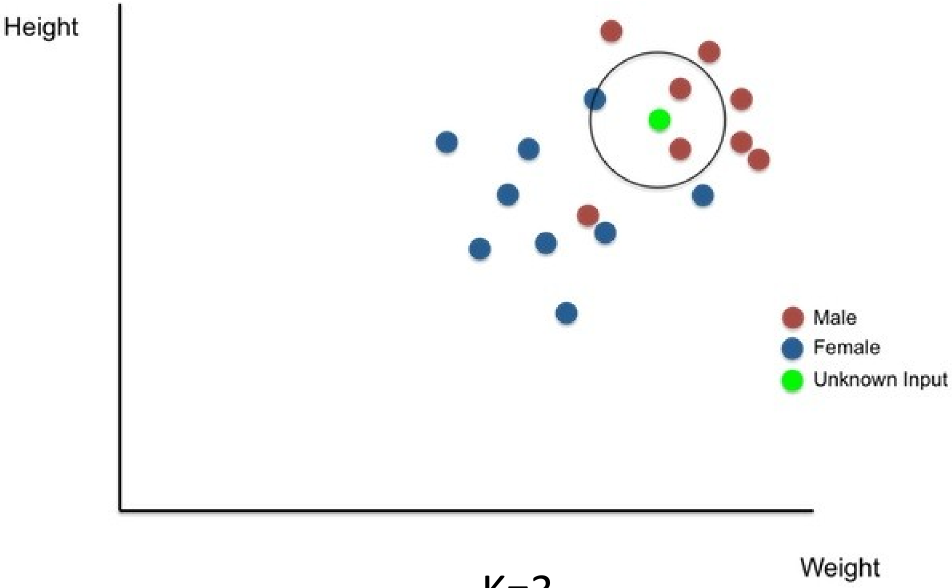
Algorithm

```
def 1NN_Classifier(X_train,x_t,dist_metric):

 minDist = sys.float_info.max
 for (x_i,y_i) in {X_train}:
    dist = Dist(x_i, x_t,dist_metric)
    if (dist < minDist):
            minDist = dist
            nearest = y_i
 return nearest
```

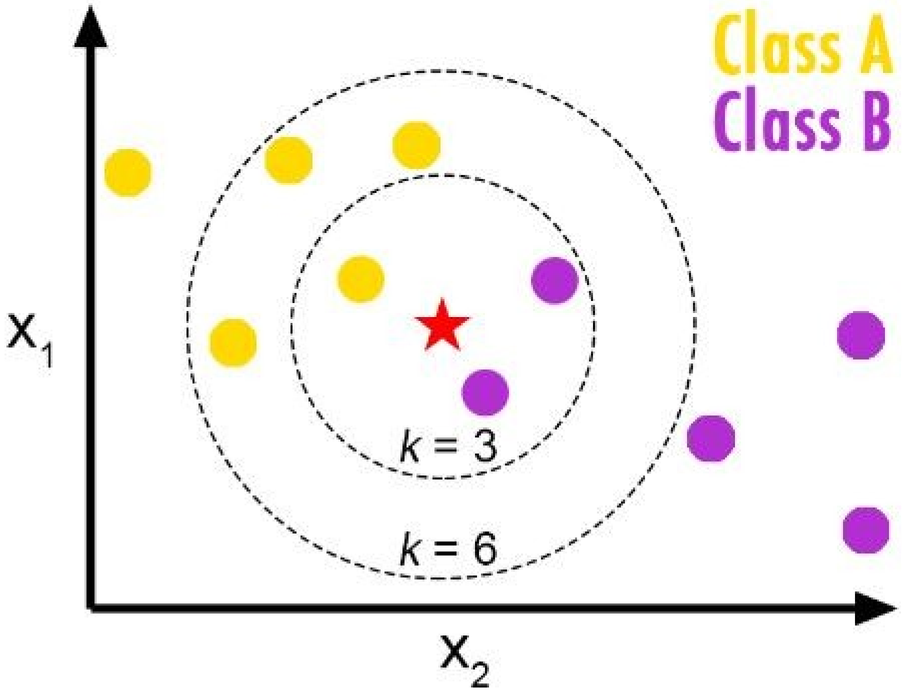
k-nearest neighbor classifier





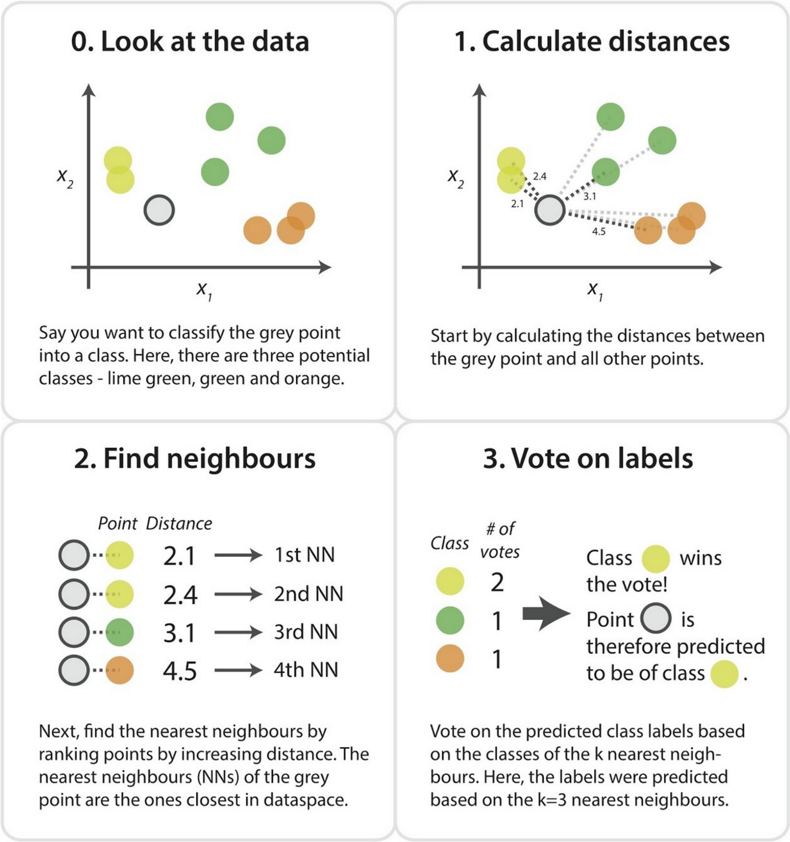
K=3

k-nearest neighbor classifier



K is usually an odd number

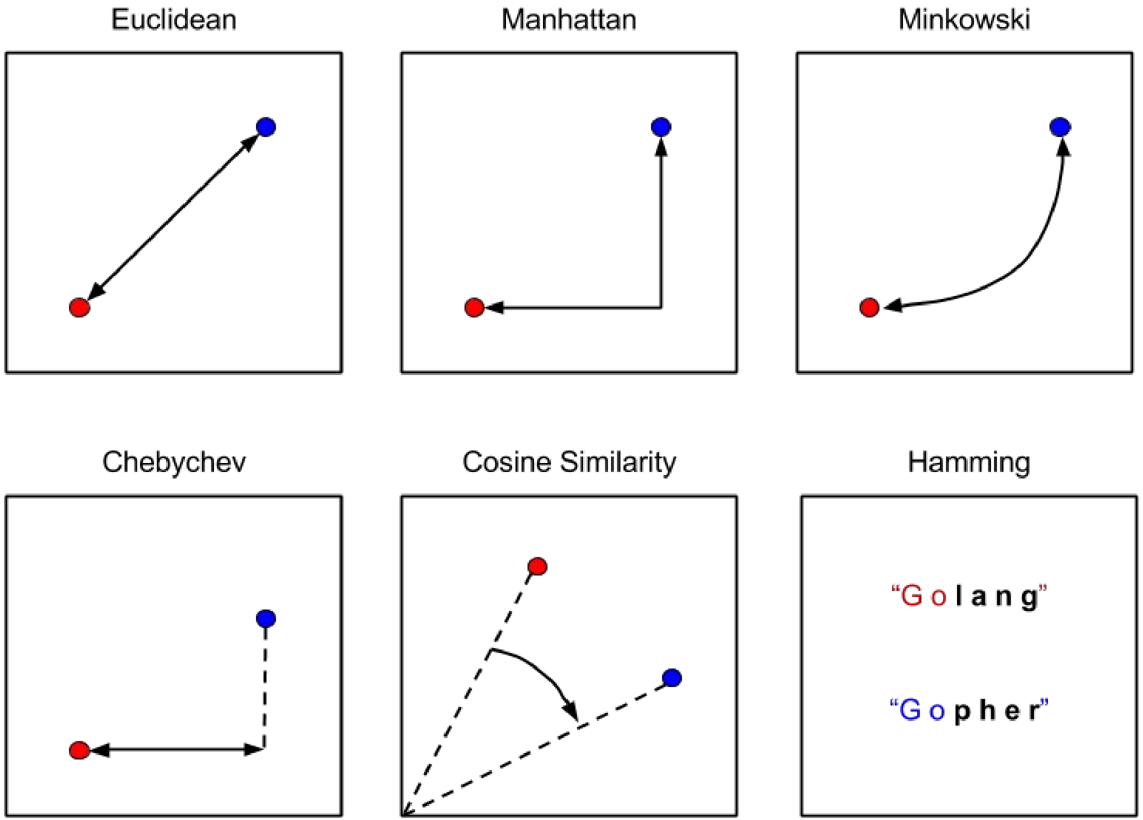
k-NN algorithm in pictures



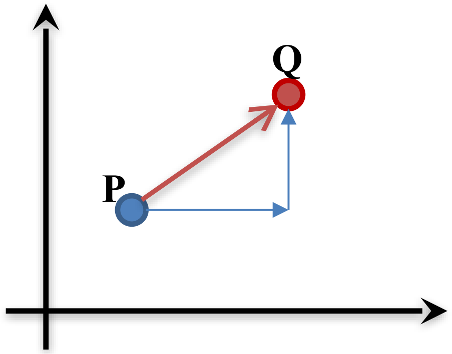
Complexity of k-NN

- Training
  - Time:
  - Space:
- Testing
  - Time:
  - Space:

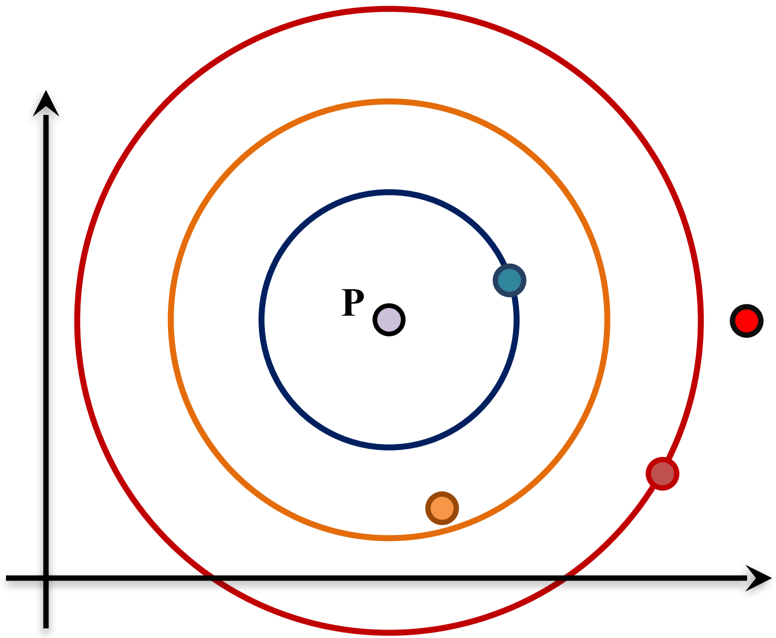
Distance measures



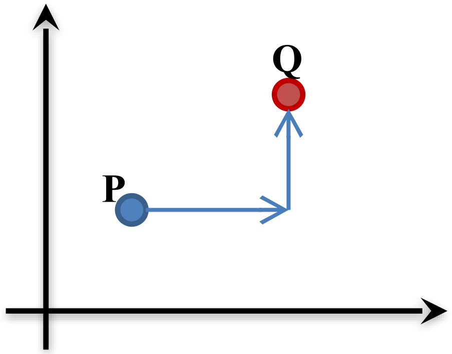
Euclidean Distance [L2]

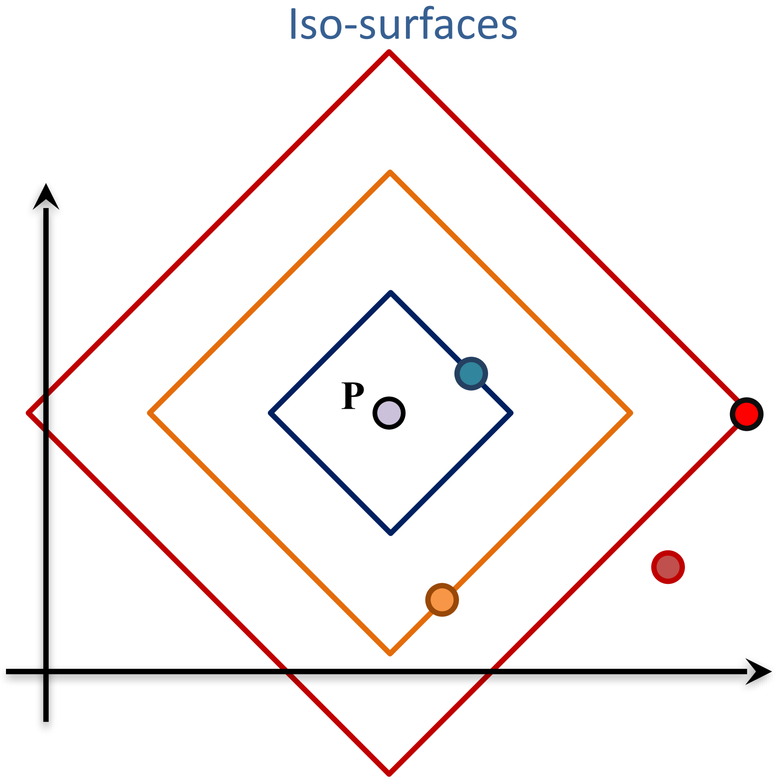


Iso-surfaces

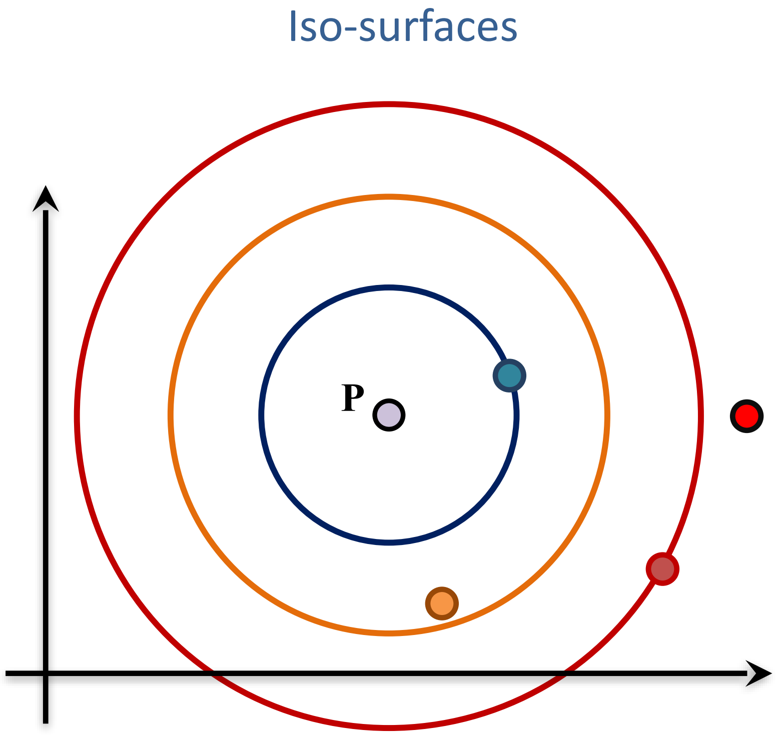


Manhattan Distance [L1]

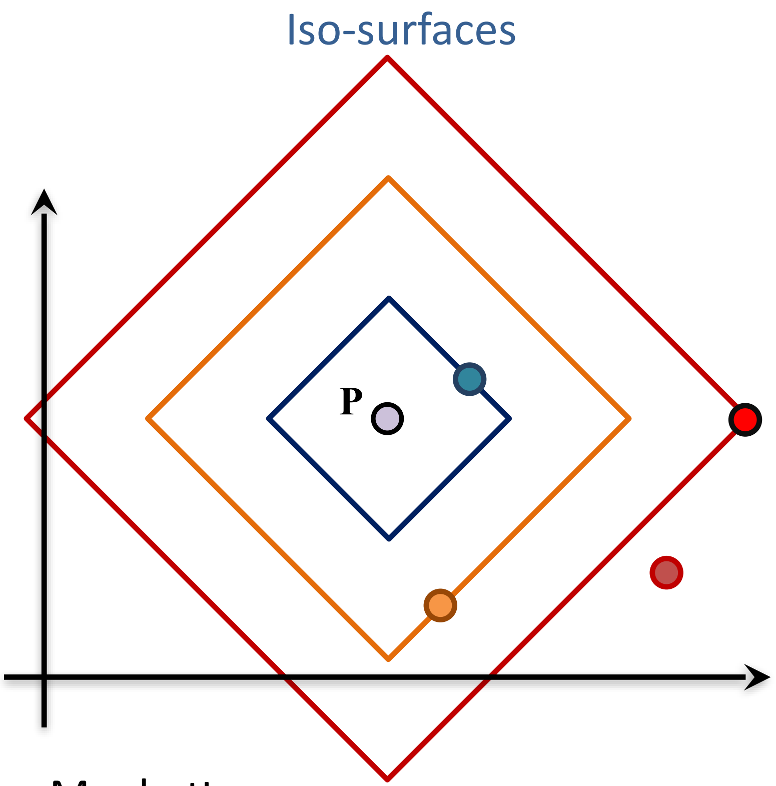




Distance measure can affect k-NN classification

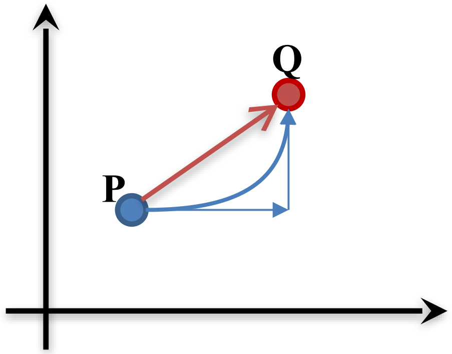


Euclidean



Manhattan

Minkowski Dist.



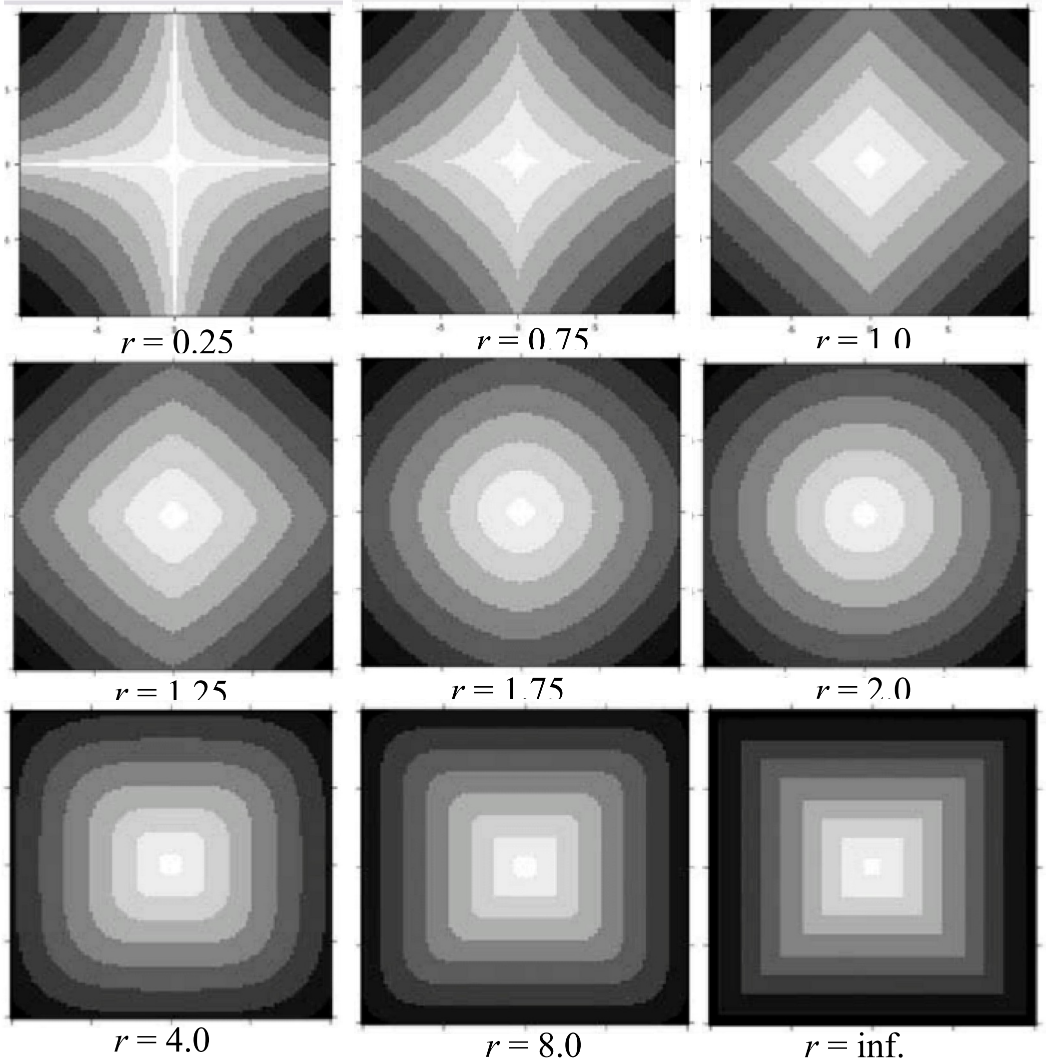
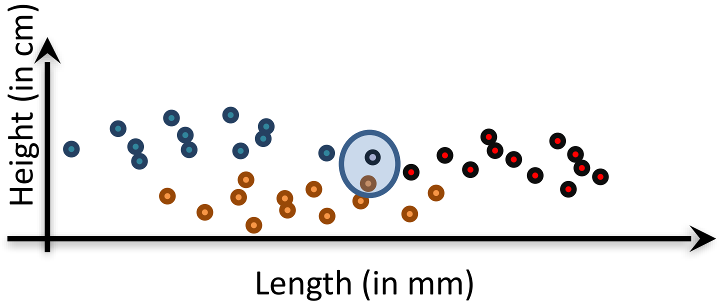
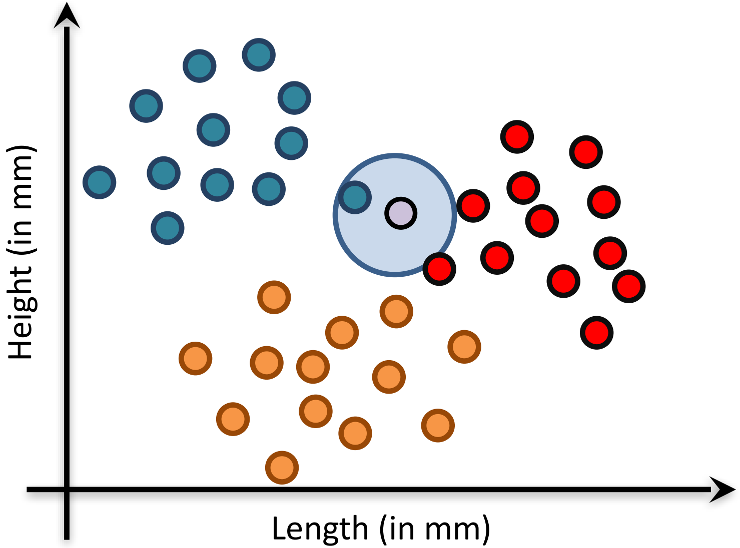


Fig. by Lu et al., "The Minkowski Approach for Choosing the Distance Metric in Geographically Weighted Regression"

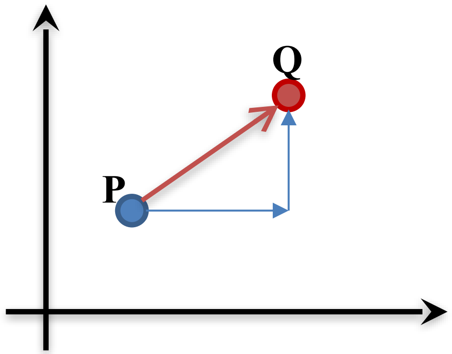
Note: Feature Normalization

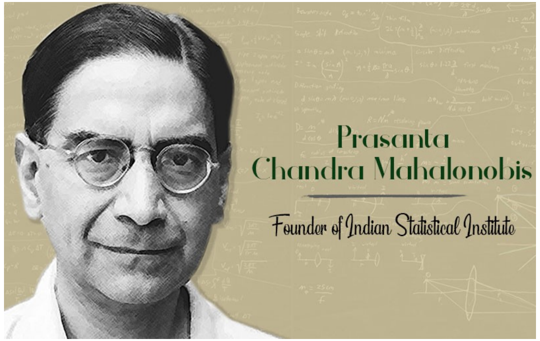
- If different features have different variances
  - Some features will dominate distance computation
  - Normalization can reduce this feature bias



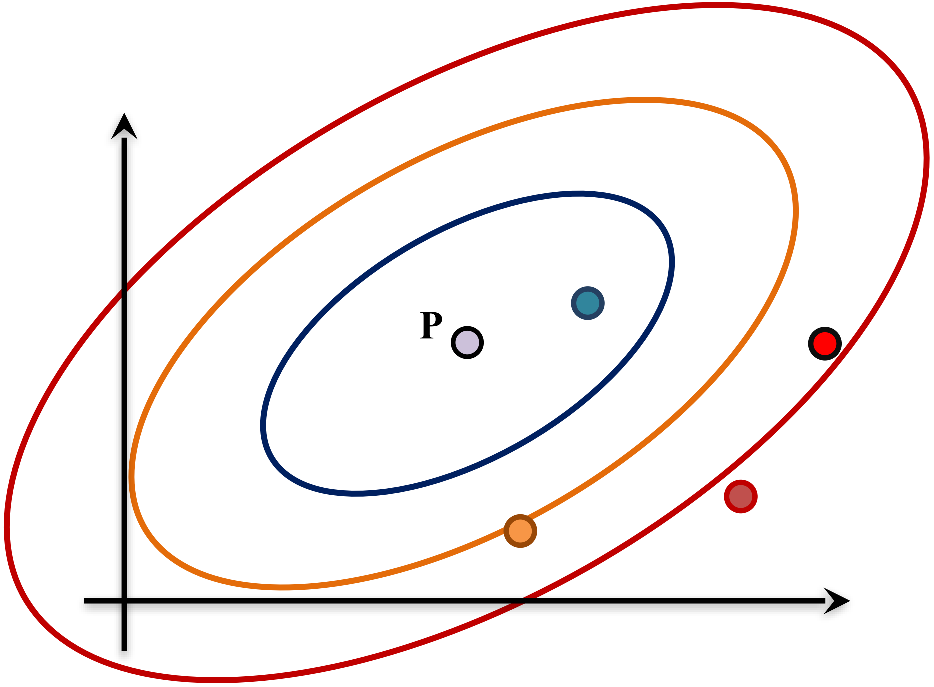


Mahalanobis Distance



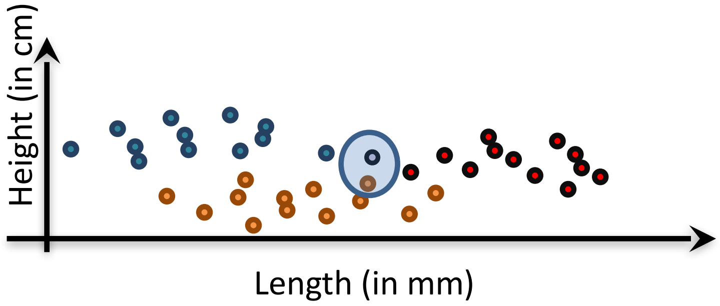


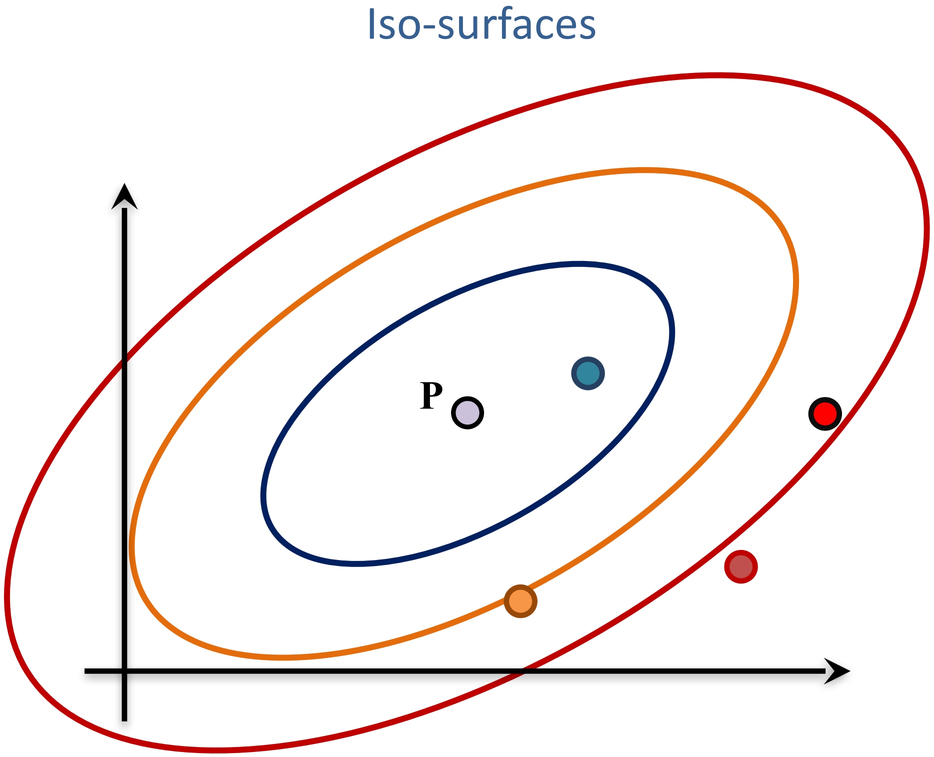
Iso-surfaces



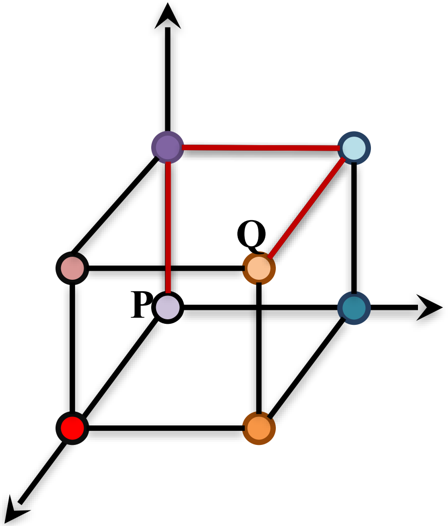
https://www.getbengal.com/details/the-indian-statistical-institute-in-kolkata-was-founded-by-the-father-of-indian-statistics-pc--mahalanobis-getbengal-story

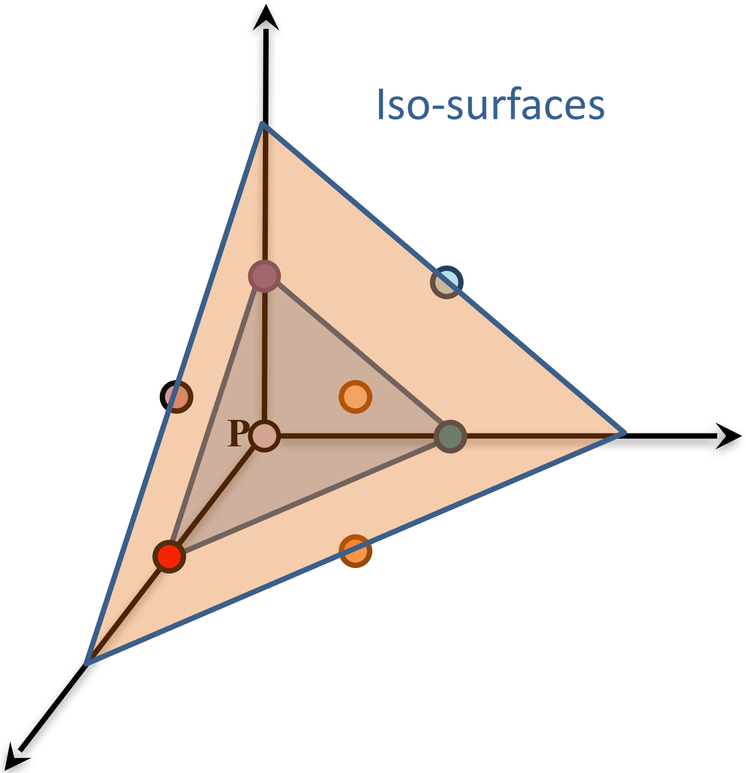
Mahalanobis Distance





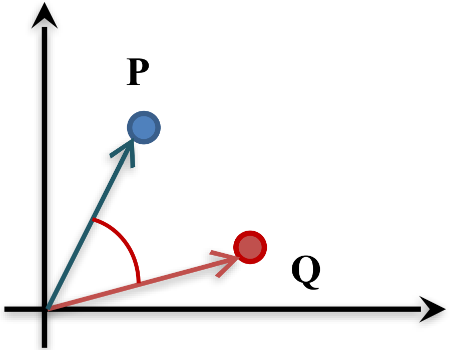
Hamming Distance



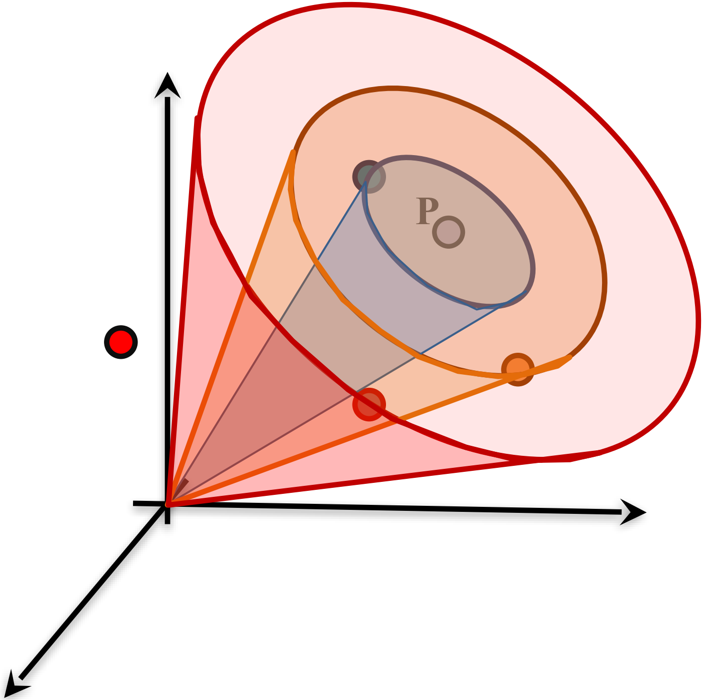


0	1	1	0	1	1	0
0	0	1	0	1	0	0

Cosine Distance



Iso-surfaces

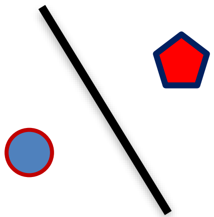


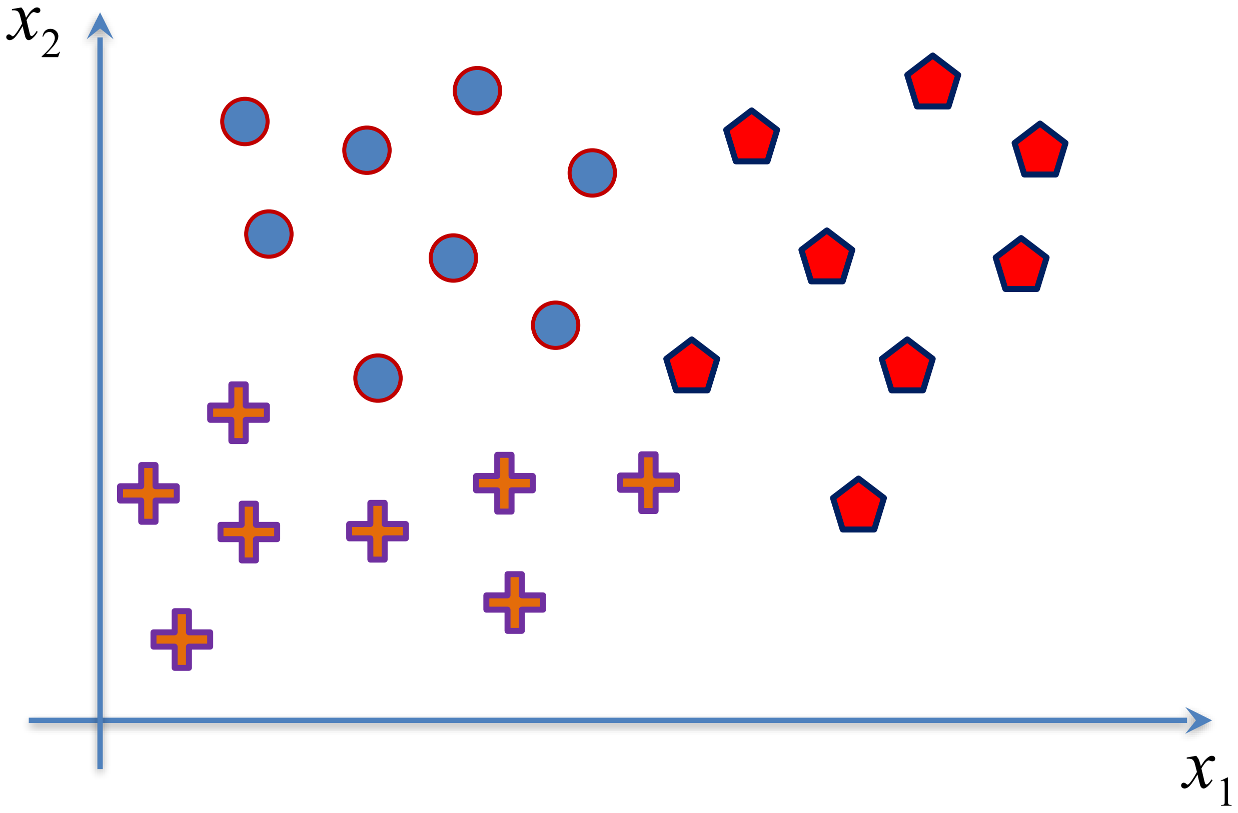
Summary of Distances

- Distance Metrics decide Neighborhoods
- Need not be a ”metric”
  - Jaccard Distance
  - Edit Distance
- Feature vectors need not be of same length
- Selection of metric depends on the nature of feature vector

Class Boundaries

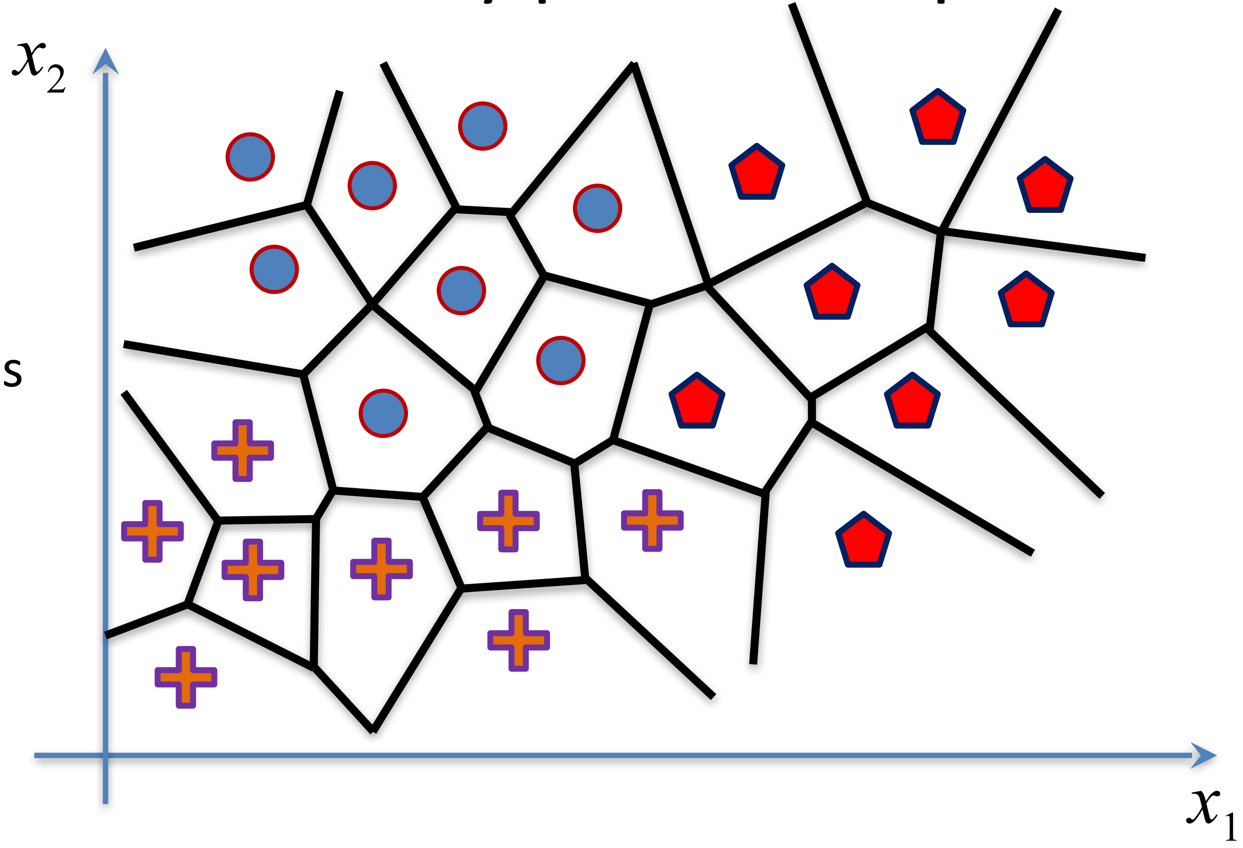
- Partition the feature space
- Consider 2 samples





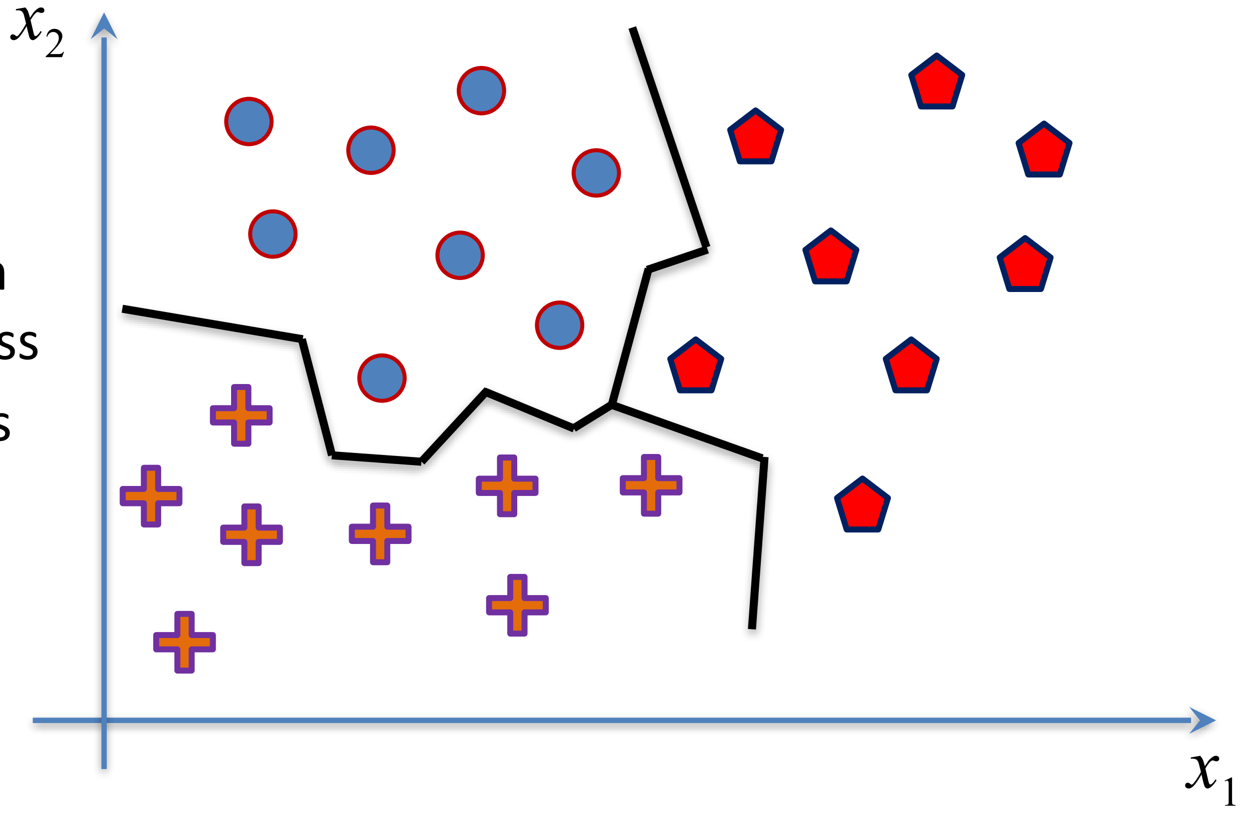
Boundaries between every pair of samples

- Voronoi Tessellation
- We can ignore boundaries between samples of same class

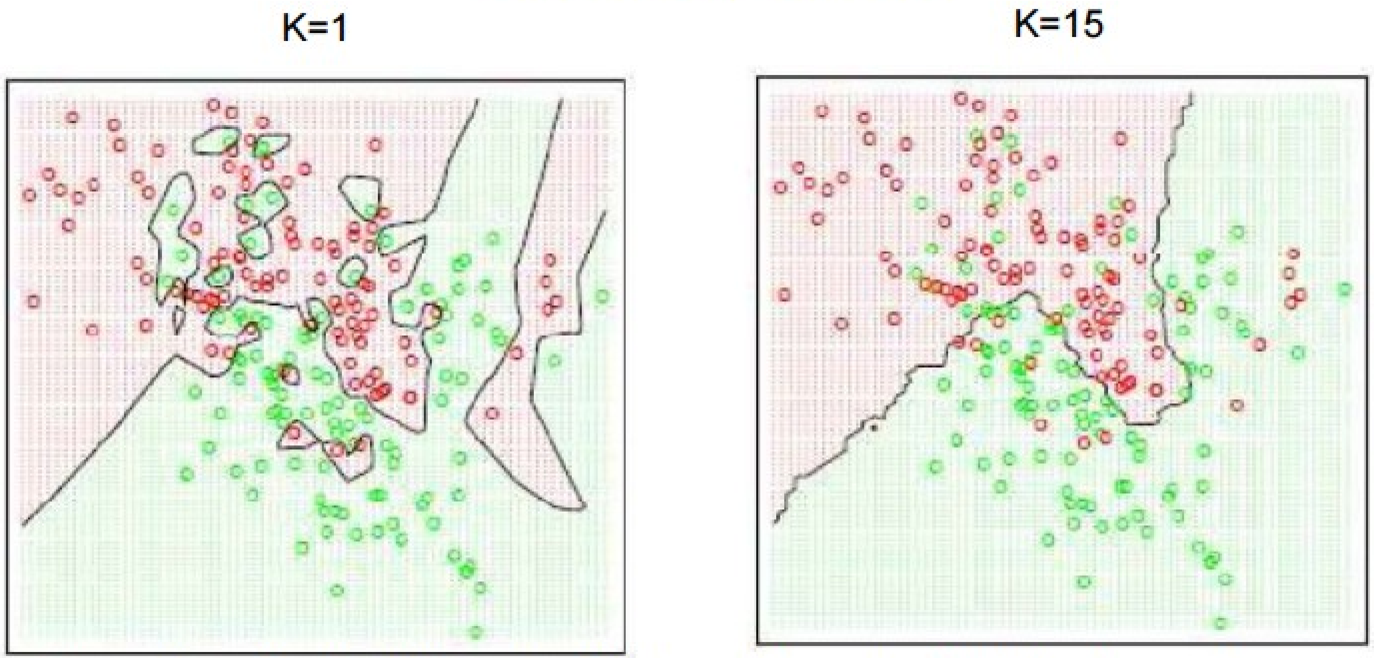


Boundaries between every pair of samples

- Voronoi Tessellation
- We can ignore boundaries between samples of same class
- Decision Boundary is piece-wise Linear

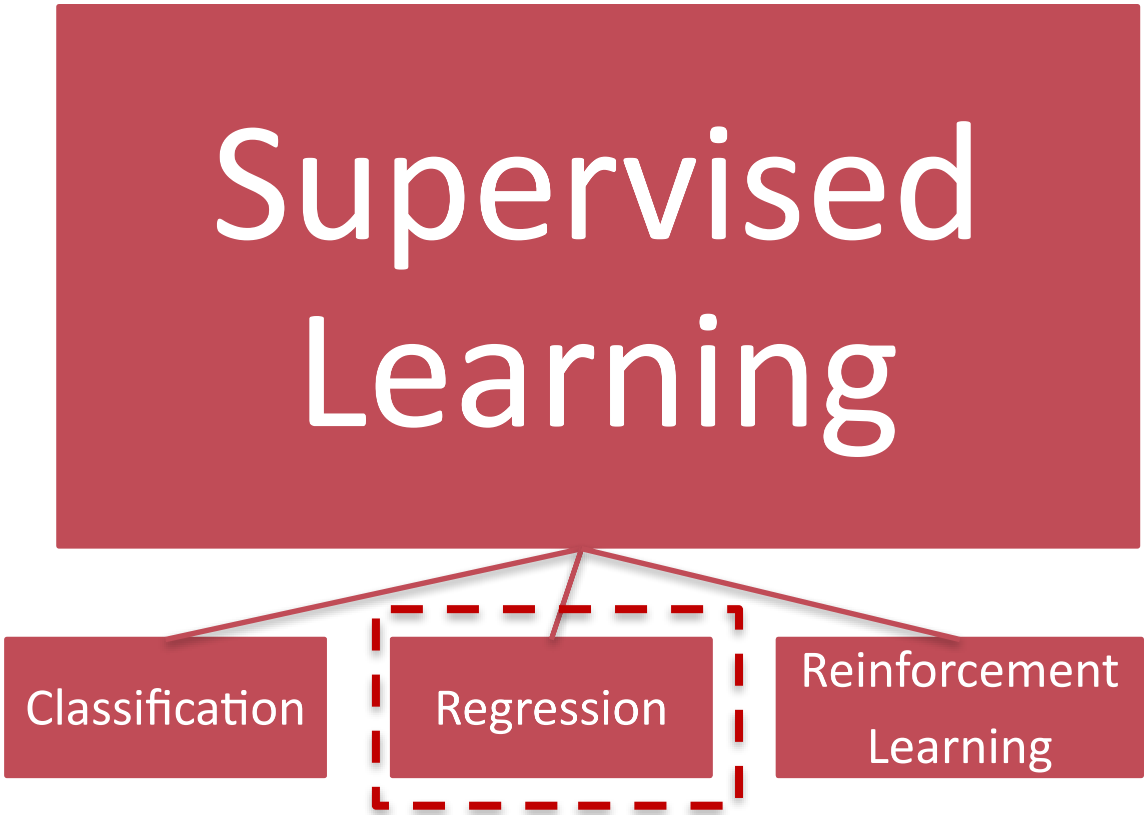


Effect of K



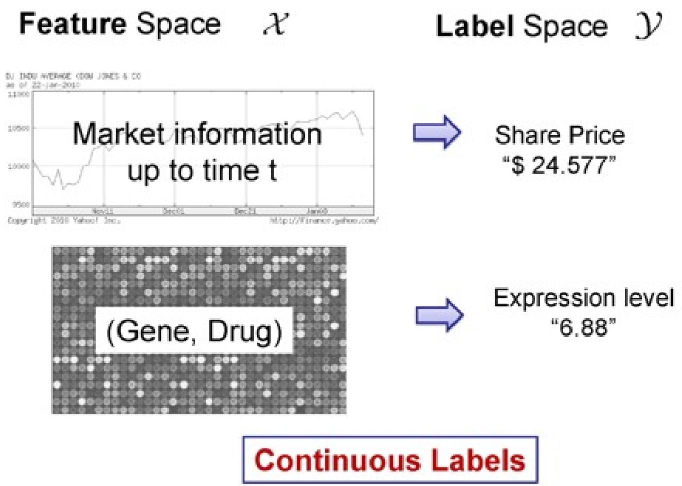
Figures from Hastie, Tibshirani and Friedman (Elements of Statistical Learning)

Larger k produces smoother boundary effect and can reduce the impact of class label noise.


Supervised Learning
Classification
Regression
Reinforcement Learning

Regression model

- Regression model
  - Explanatory variables: **independent** variables
  - Variables to be explained : **dependent** variables



Examples

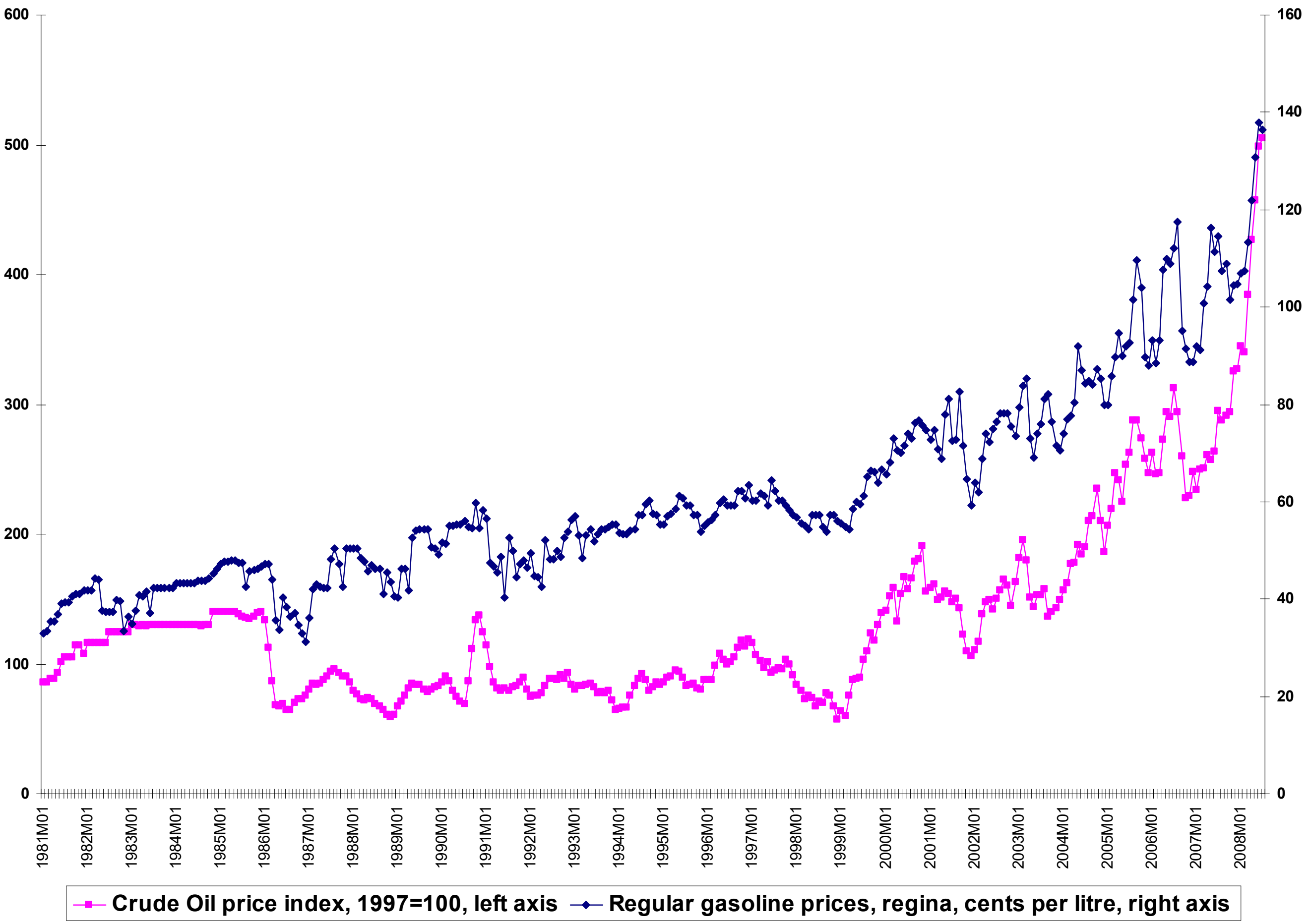
- Independent variable: Price of crude oil
- Dependent variable: Retail price of petrol

- Independent variables: hours of work, education, occupation, sex, age, years of experience etc.
- Dependent variable: Employment income

- Independent variables: Area of house, Population Density
- Dependent variable: Rent or Price of house

- Price of a product and quantity produced or sold:
  - Quantity sold affected by price. Dependent variable is quantity of product sold – independent variable is price.

  - Price affected by quantity offered for sale. Dependent variable is price – independent variable is quantity sold.



Source: CANSIM II Database (Vector v1576530 and v735048 respectively)

Linear Regression Model

- 1. Relationship Between Variables Is a Linear Function

Y-Intercept

Slope

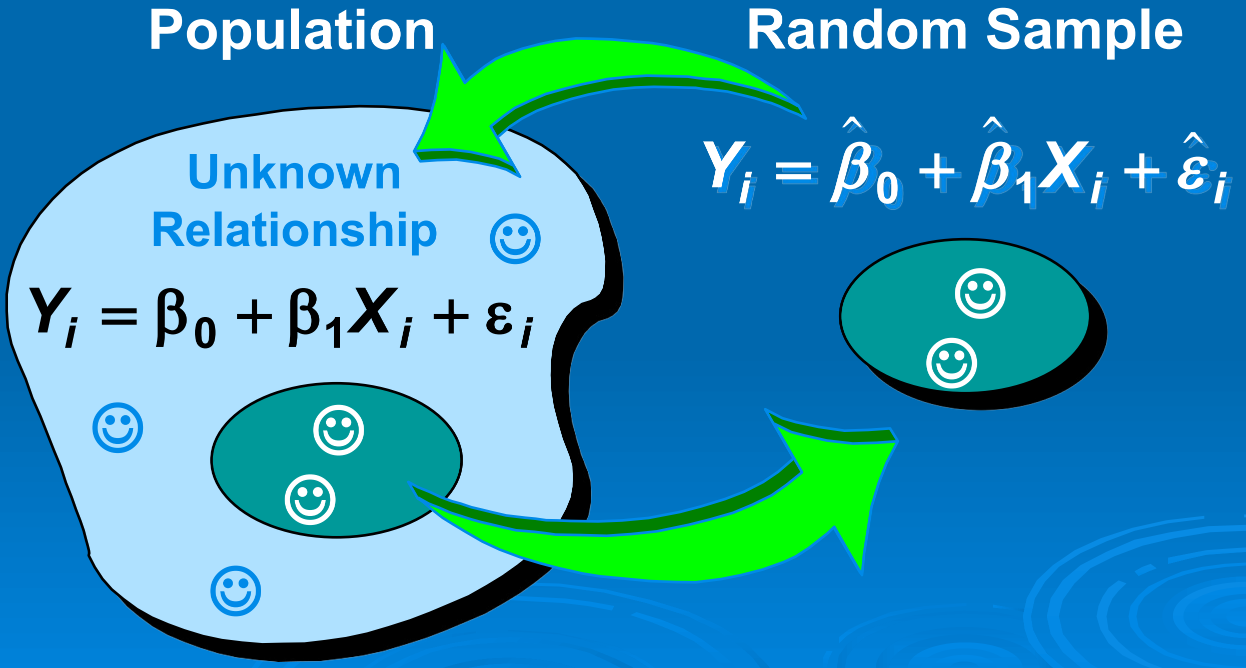
Random Error

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

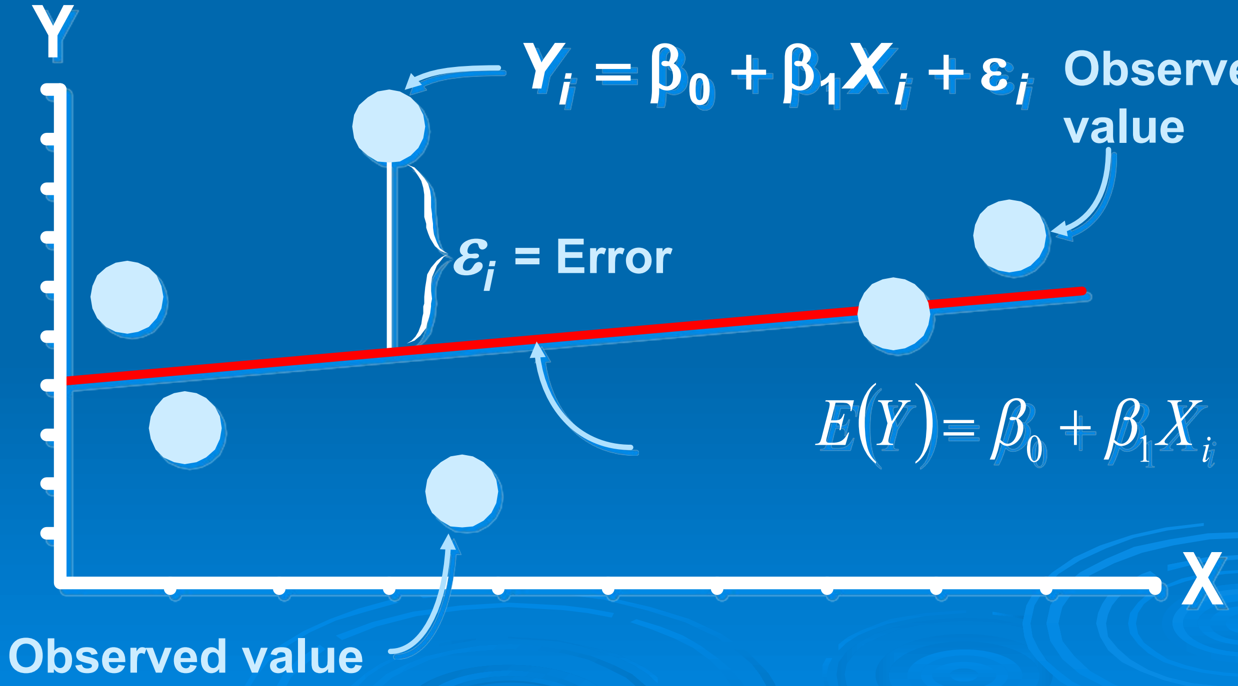
Dependent (Response) Variable (e.g. Salary)

Independent (Explanatory) Variable (e.g. Yrs of experience)

Population & Sample Regression Models



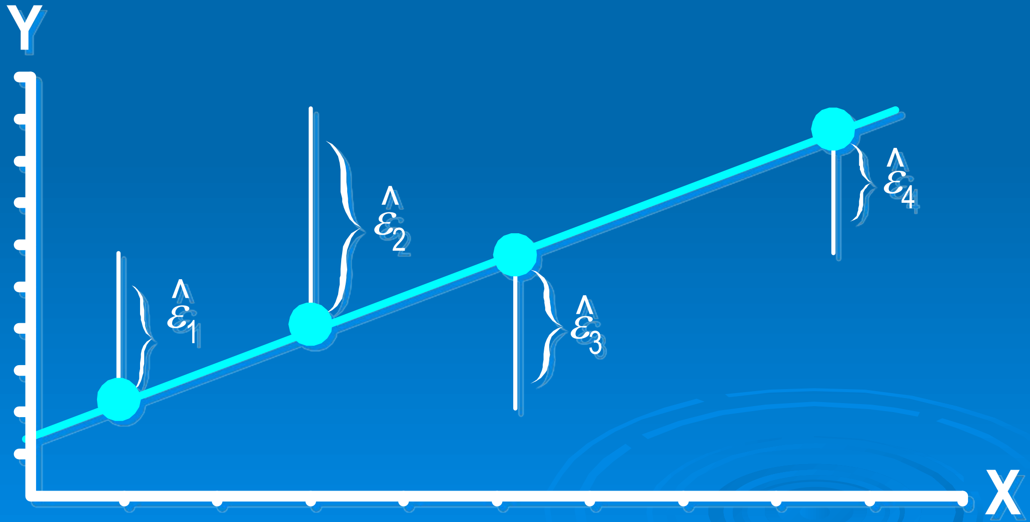
Linear Regression Model



Estimating Parameters: Least Squares Method

Least Squares

- 1. ‘Best Fit’ Means Difference Between Actual Y Values & Predicted Y Values Are a Minimum. *But* Positive Differences Offset Negative ones

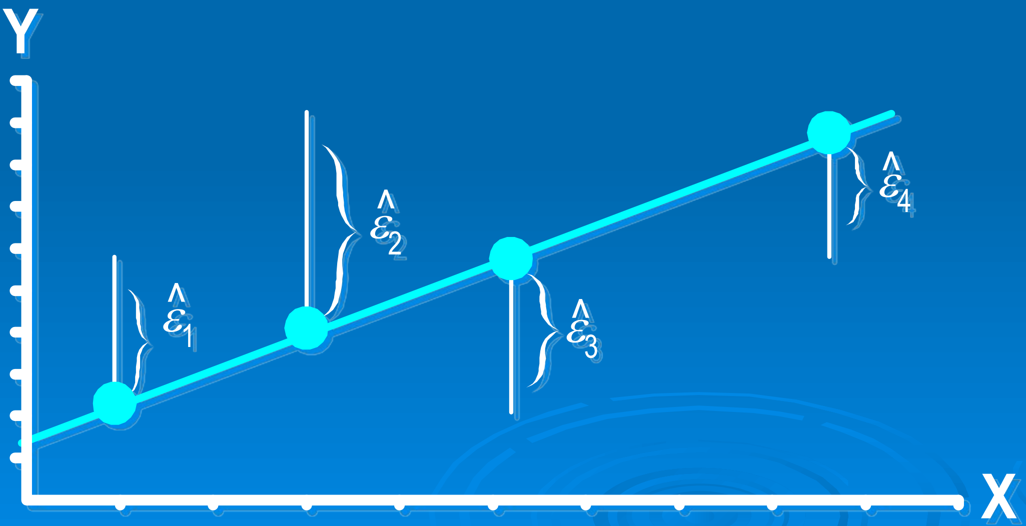


$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

$$E(Y) = \beta_0 + \beta_1 X_i$$

Least Squares

- 1. 'Best Fit' Means Difference Between Actual Y Values & Predicted Y Values is a Minimum. *But* Positive Differences Offset Negative ones. So square errors!



$$\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2 = \sum_{i=1}^{n}\hat{\varepsilon}_i^2$$

$$\mathbf{Y}_i = \beta_0 + \beta_1 \mathbf{X}_i + \varepsilon_i$$

$$E(Y) = \beta_0 + \beta_1 X_i$$

Least Squares

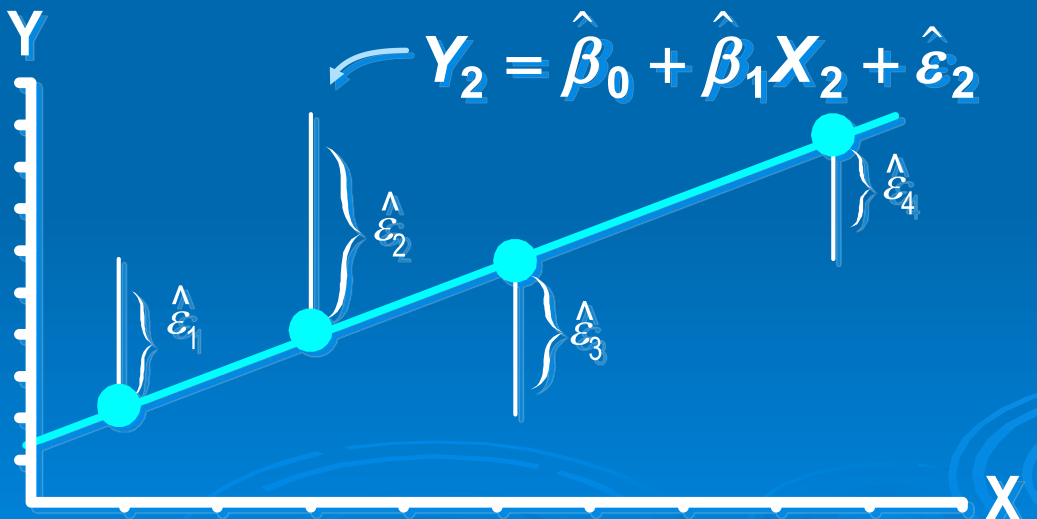
- 1. 'Best Fit' Means Difference Between Actual Y Values & Predicted Y Values Are a Minimum. *But* Positive Differences Off-Set Negative. So square errors!

$$\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2 = \sum_{i=1}^{n}\hat{\varepsilon}_i^2$$

- 2. LS Minimizes the Sum of the Squared Differences (errors) (SSE)

Least Squares Graphically

LS minimizes $\sum_{i=1}^{n} \hat{\varepsilon}_i^2 = \hat{\varepsilon}_1^2 + \hat{\varepsilon}_2^2 + \hat{\varepsilon}_3^2 + \hat{\varepsilon}_4^2$



Derivation of Parameters (1)

Least Squares (L-S):

Minimize squared error

$$\sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \beta_1 x_i \right)^2$$

Derivation of Parameters (1)

Least Squares (L-S):

Minimize squared error

$$\sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \beta_1 x_i \right)^2$$

$$0 = \frac{\partial \sum \varepsilon_i^2}{\partial \beta_0} = \frac{\partial \sum \left(y_i - \beta_0 - \beta_1 x_i \right)^2}{\partial \beta_0}$$

$$= -2\left(n\bar{y} - n\beta_0 - n\beta_1 \bar{x} \right)$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

Derivation of Parameters (1)

Least Squares (L-S):

Minimize squared error

$$0 = \frac{\partial \sum \varepsilon_i^2}{\partial \beta_1} = \frac{\partial \sum \left(y_i - \beta_0 - \beta_1 x_i\right)^2}{\partial \beta_1}$$

$$= -2 \sum x_i \left(y_i - \beta_0 - \beta_1 x_i\right)$$

$$= -2 \sum x_i \left(y_i - \overline{y} + \beta_1 \overline{x} - \beta_1 x_i\right)$$

$$\beta_1 \sum x_i \left(x_i - \overline{x}\right) = \sum x_i \left(y_i - \overline{y}\right)$$

$$\beta_1 \sum \left(x_i - \overline{x}\right)\left(x_i - \overline{x}\right) = \sum \left(x_i - \overline{x}\right)\left(y_i - \overline{y}\right)$$

$$\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}}$$

Coefficient Equations

Prediction equation

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

Sample slope

$$\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}} = \frac{\sum (x_i - \overline{x})(y_i - \overline{y})}{\sum (x_i - \overline{x})^2}$$

Sample Y - intercept

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}$$

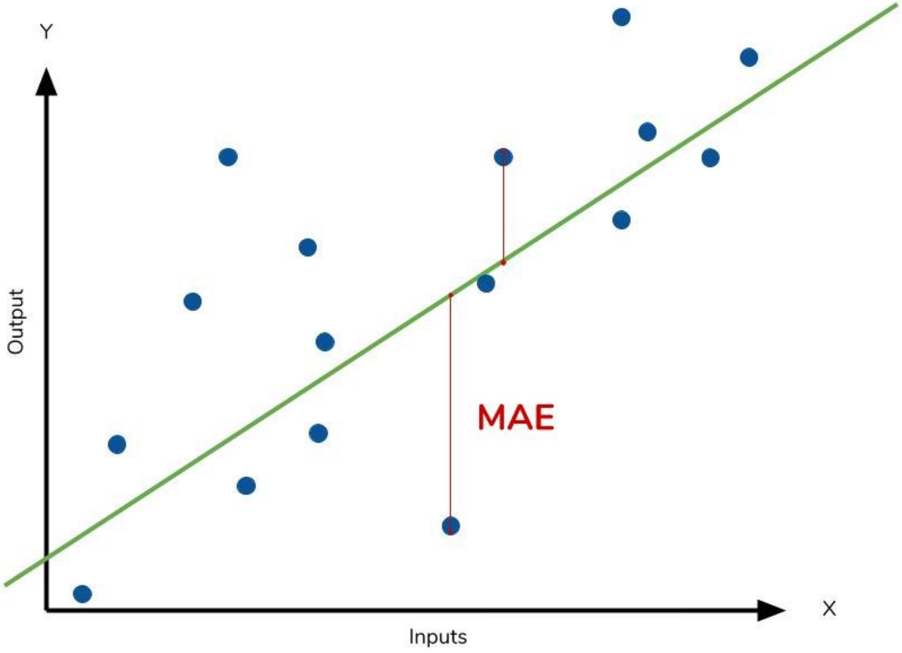
Regression – Error measures

Divide by the total number of data points

Predicted output value

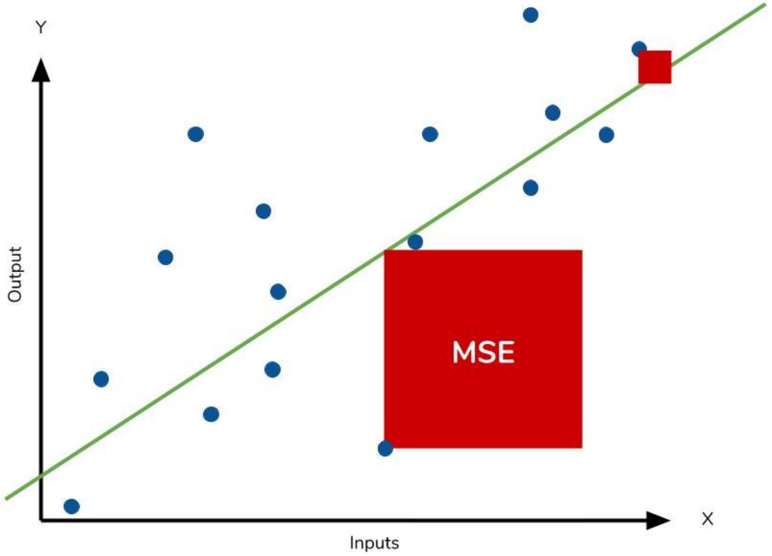
Actual output value

$$MAE = \boxed{\frac{1}{n}} \underset{\text{Sum of}}{\sum} \underbrace{\left| \boxed{y} - \boxed{\hat{y}} \right|}_{\text{The absolute value of the residual}}$$

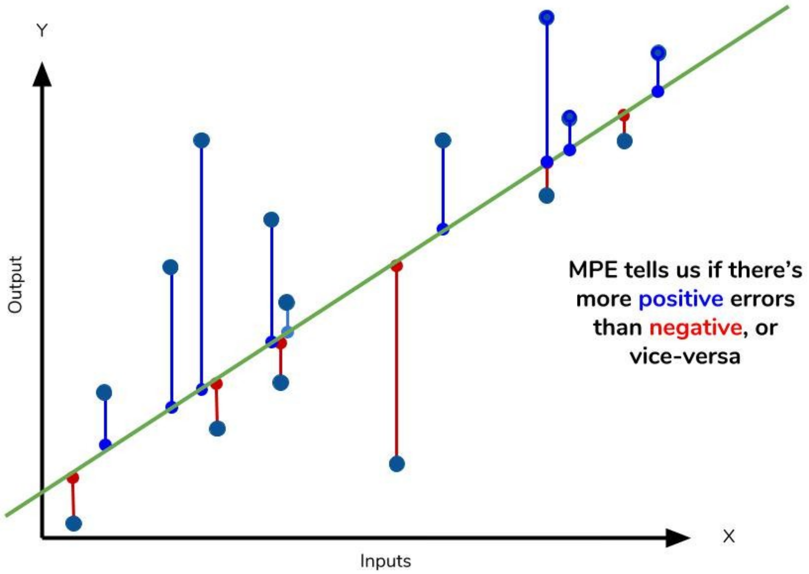


Regression – Error measures

$$MSE = \frac{1}{n}\Sigma\underbrace{\left(y - \widehat{y}\right)}_{\text{The square of the difference between actual and predicted}}^{2}$$



$$MPE = \frac{100\%}{n} \Sigma \left(\frac{y - \widehat{y}}{y} \right)$$



Linear Regression – Matrix Form

Consider the model

$$Y = X\beta + \epsilon$$

where $Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}$ $\quad X = \begin{pmatrix} 1 & X_{11} & X_{12} & \dots & X_{1p} \\ 1 & X_{21} & X_{22} & \dots & X_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \dots & X_{np} \end{pmatrix}$ $\quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$ $\quad \epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$

Linear Regression – Matrix Form

Consider the model

$$Y = X\beta + \epsilon$$

where $Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}$ $X = \begin{pmatrix} 1 & X_{11} & X_{12} & \dots & X_{1p} \\ 1 & X_{21} & X_{22} & \dots & X_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \dots & X_{np} \end{pmatrix}$ $\beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$ $\epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$

Then using matrix calculus we find that the least squares estimate for β is given by

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

Hence, the least squares regression line is $\hat{Y} = X\hat{\beta}$.

Influence Matrix

Linear Regression – Matrix Form - Issues

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

Hence, the least squares regression line is $\hat{Y} = X\hat{\beta}$.

- N samples, p-dimensional (what if p > N ?)
- Complexity of matrix inversion (what if N very large ?)
- Collinearity

Gradient Descent

$$\hat{y} = \beta_0 + \beta_1 \mathbf{x}$$

$$\begin{aligned} \boxed{\mathcal{L}(\mathbf{w})} &= \mathcal{L}(\beta_0, \beta_1) \\ &= \frac{1}{n}\sum_{i=1}^{n}(\hat{y} - y)^2 \end{aligned}$$

1. Initialize the parametersto some random values.
2. Update the parameters using gradient descent rule

3. Repeat 2 until is close to 0

Gradient Descent

1. Initialize the parameters to some random values.
2. Update the parameters using gradient descent rule

3. Repeat 2 until is close to 0

$$\hat{y} = \beta_0 + \beta_1 \mathbf{x}$$

$$\mathcal{L}(\beta_0, \beta_1)$$

$$= \frac{1}{n}\sum_{i=1}^{n}(\hat{y} - y)^2$$

$$= \frac{1}{n}\sum_{i=1}^{n}(\beta_0 + \beta_1 \mathbf{x} - y)^2$$

$$\implies \frac{\partial \mathcal{L}}{\partial \beta_0} = \frac{1}{n}\sum_{i=1}^{n} 2(\beta_0 + \beta_1 \mathbf{x} - y)$$

$$\implies \frac{\partial \mathcal{L}}{\partial \beta_1} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}(\beta_0 + \beta_1 \mathbf{x} - y)$$

Gradient Descent

1. Initialize the parameters to some random values.
2. Update the parameters using gradient descent rule

3. Repeat 2 until is close to 0

$$\mathbf{w} = [\beta_0 \;\; \beta_1]$$

$$\hat{y} = \beta_0 + \beta_1 \mathbf{x}$$

$$\begin{aligned}
\mathcal{L}(\mathbf{w}) &= \mathcal{L}(\beta_0, \beta_1) \\
&= \frac{1}{n}\sum_{i=1}^{n}(\hat{y} - y)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}(\beta_0 + \beta_1 \mathbf{x} - y)^2
\end{aligned}$$

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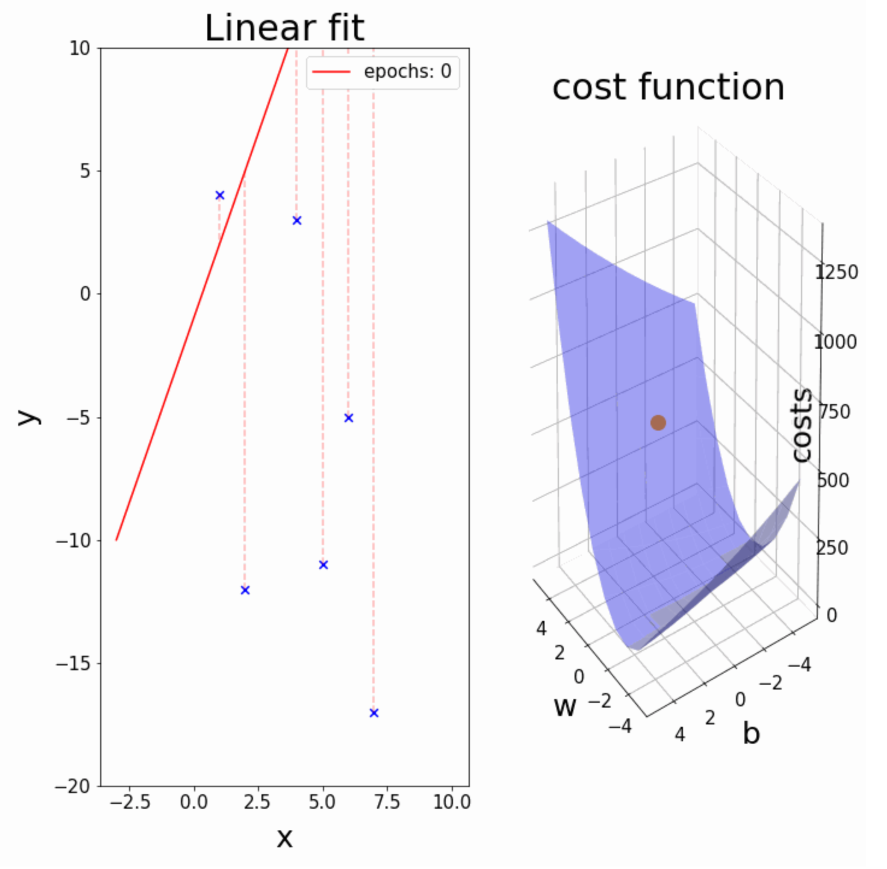

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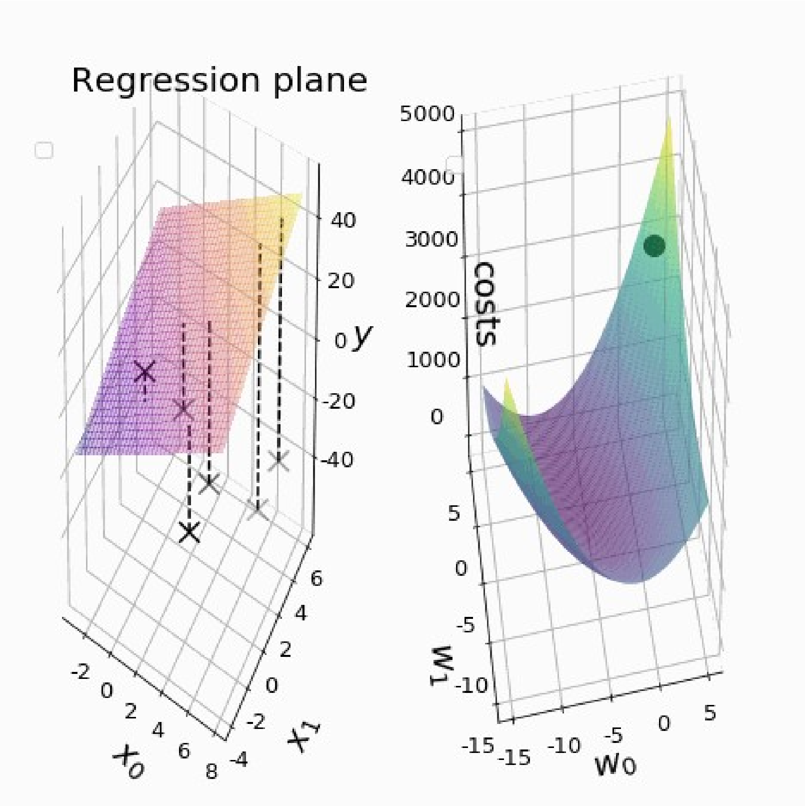


Linear Regression

- Linear Regression → Linear in coefficients and NOT variables

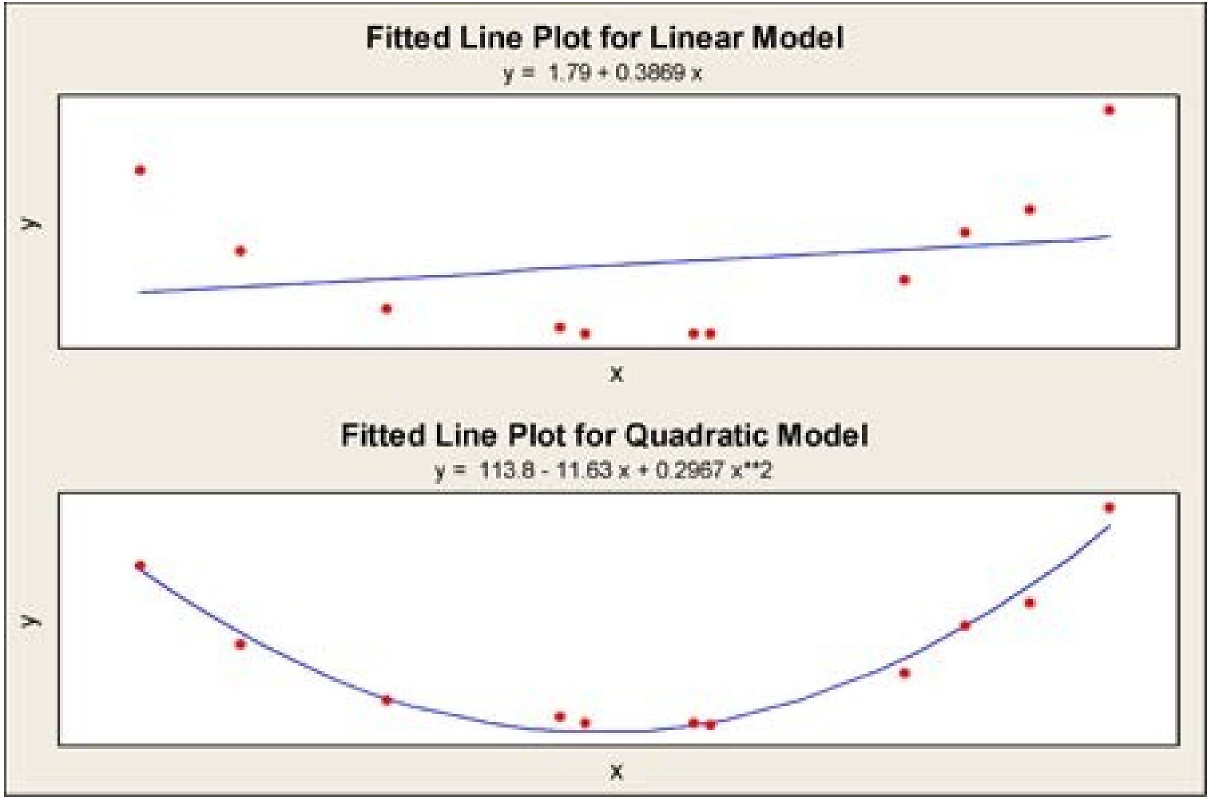
- A second-order model (quadratic model):

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$$

- β_1: Linear effect parameter.
- β_2: Quadratic effect parameter.

kth order polynomial model in one variable

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_k x^k + \epsilon$$



Fitted Line Plot for Linear Model
y = 1.79 + 0.3869 x
y
x
Fitted Line Plot for Quadratic Model
y = 113.8 - 11.63 x + 0.2967 x**2
y
x

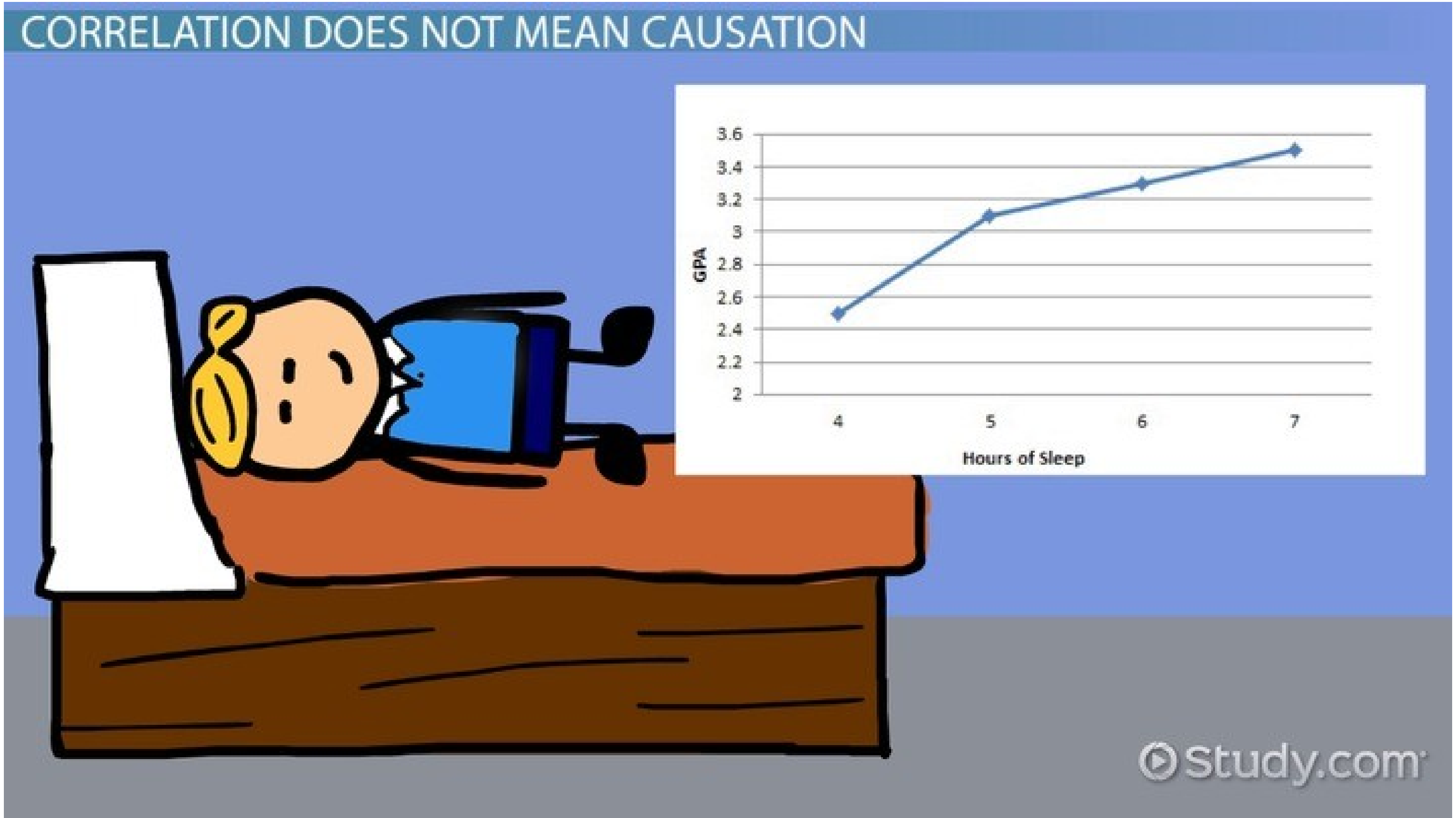
A quadratic polynomial regression function

$$Y_i = \beta_0 + \beta_1 X_i + \beta_{11} X_i^2 + \varepsilon_i$$

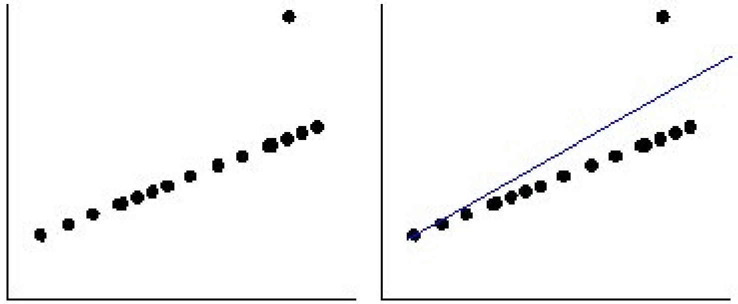
where:

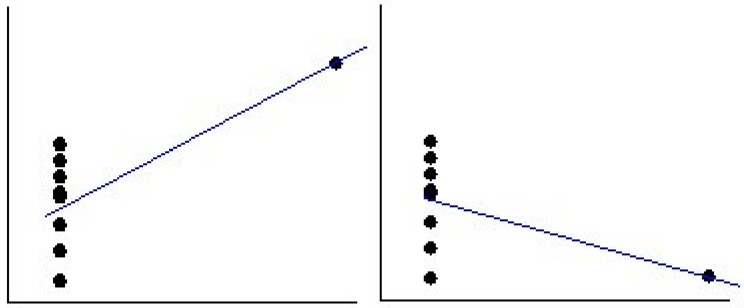
- Y_i = amount of immunoglobin in blood (mg)
- X_i = maximal oxygen uptake (ml/kg)
- typical assumptions about error terms ("INE")

Careful: X may not be causing y !

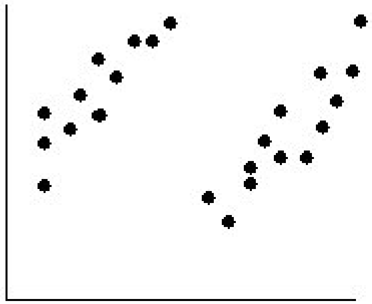


Linear Regression – Outliers





Linear Regression is problematic in many other cases



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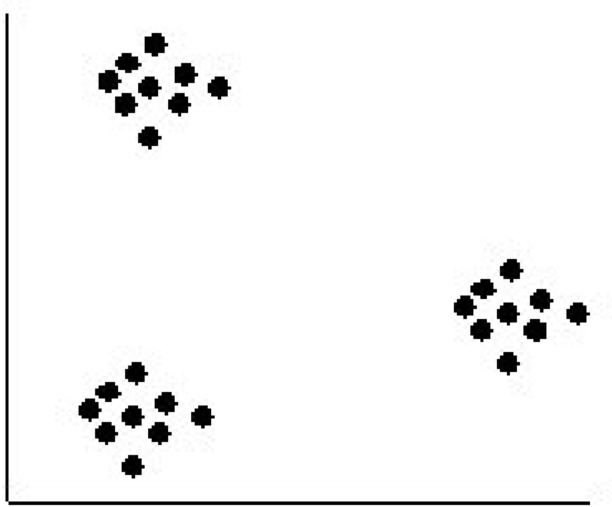

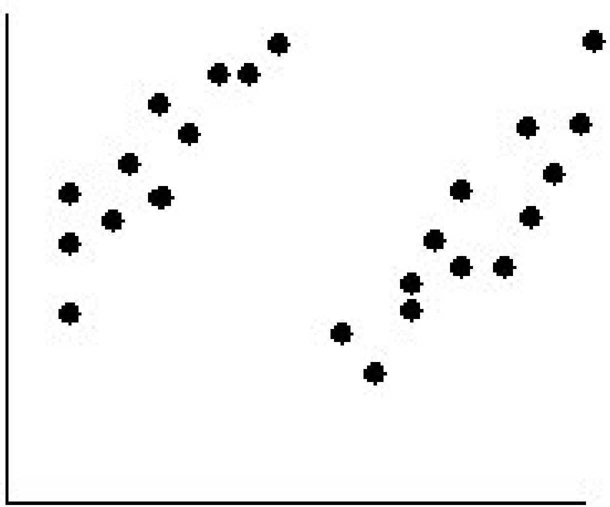

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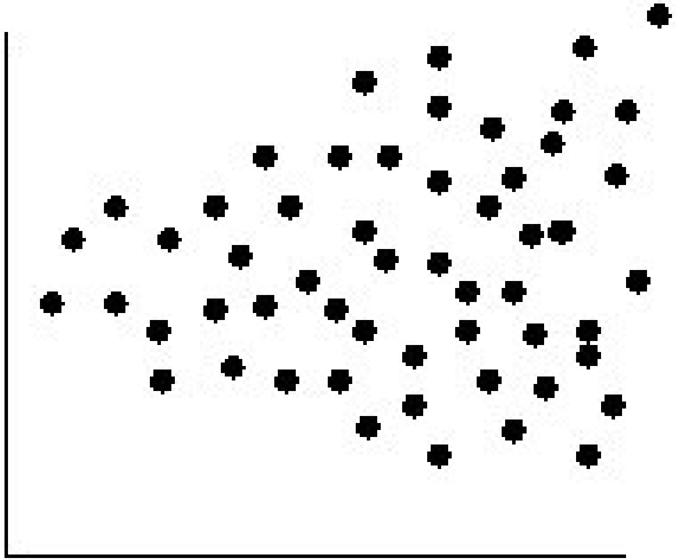

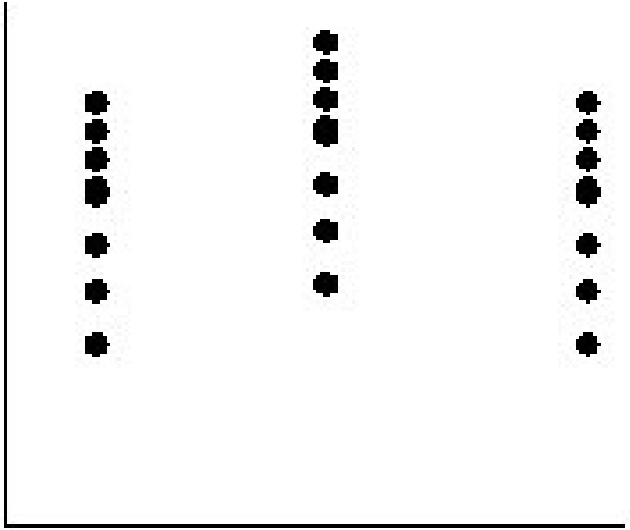

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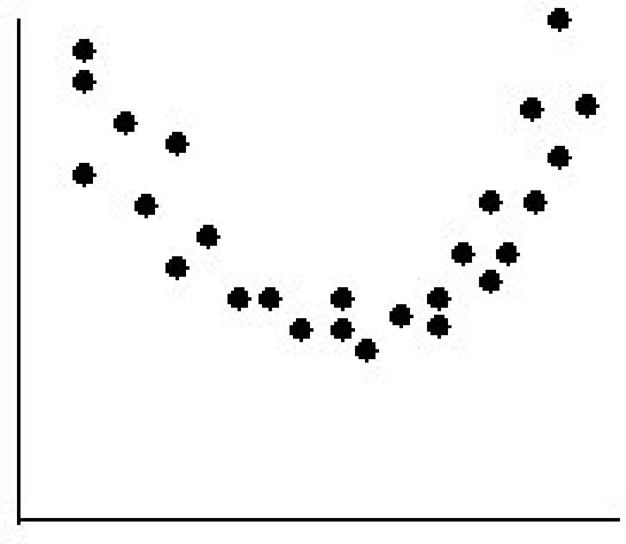
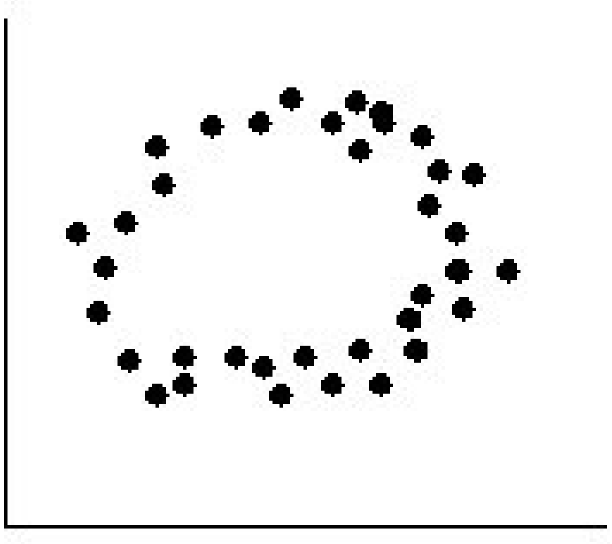
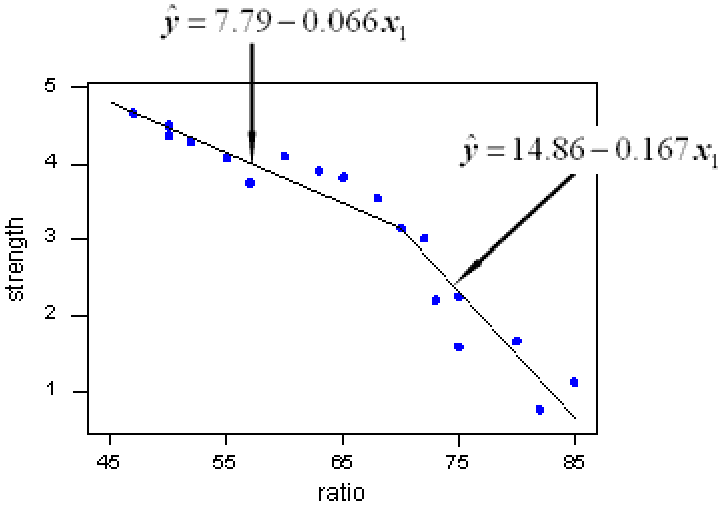
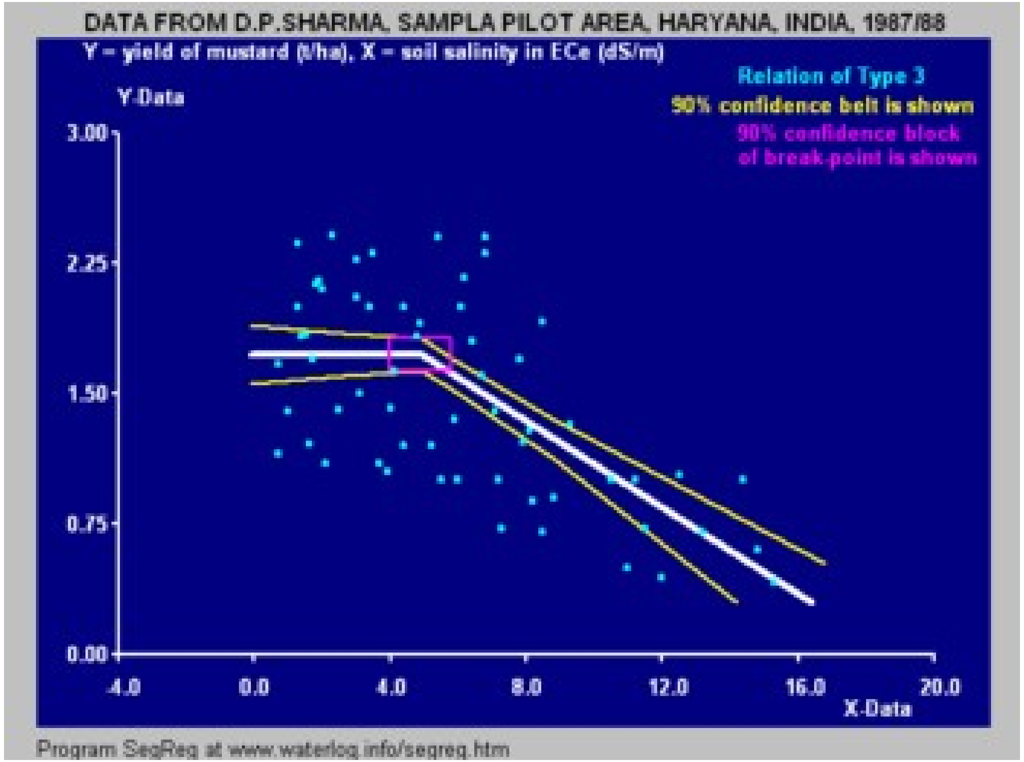




Piecewise Linear Regression





Also ref: Multivariate Adaptive Regression Splines (MARS)

Bivariate and multivariate models

Bivariate or simple regression model

(Education) $x \longrightarrow y$ (Income)

Multivariate or multiple regression model

(Education) x_1

(Gender) x_2

(Experience) x_3

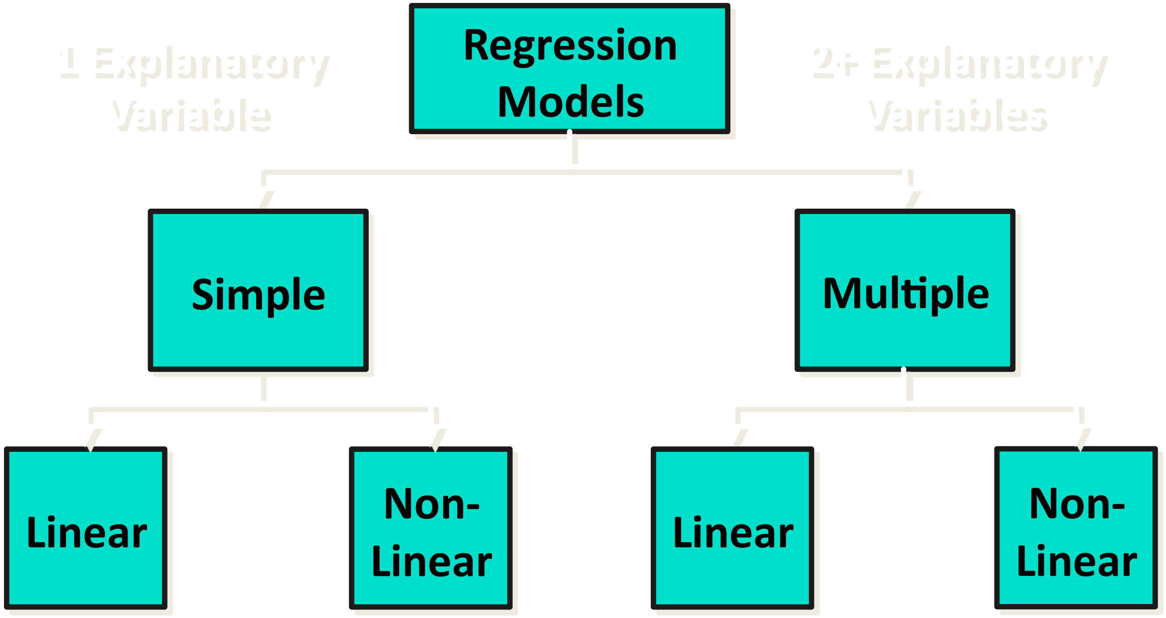
(Age) x_4

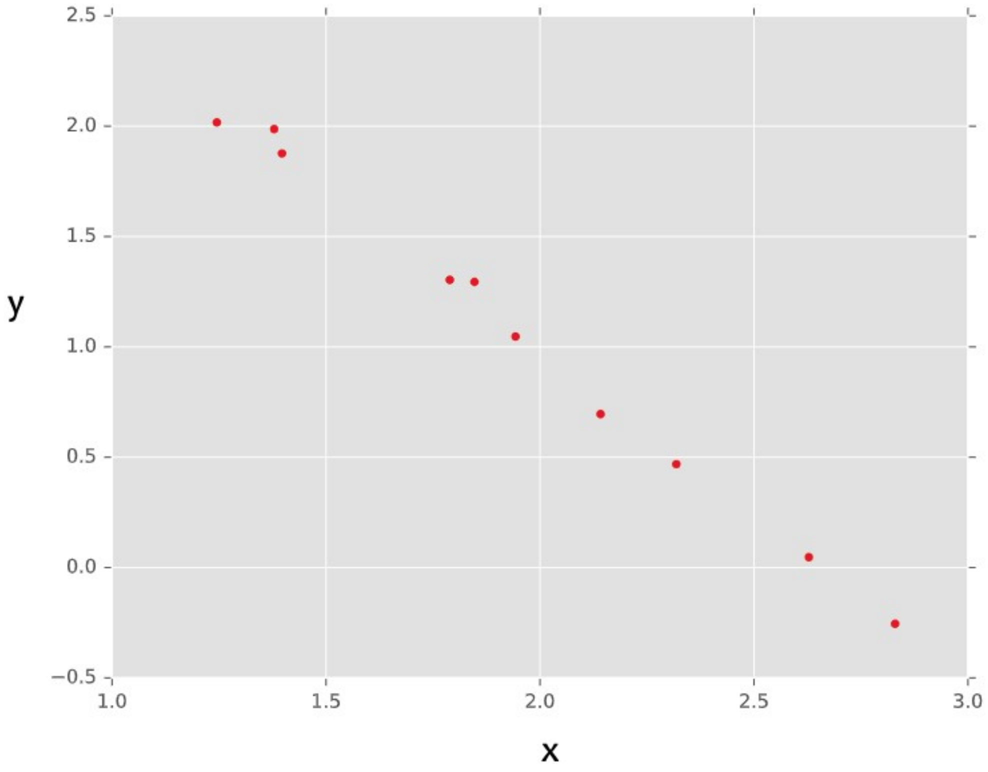
y (Income)

Model with simultaneous relationship

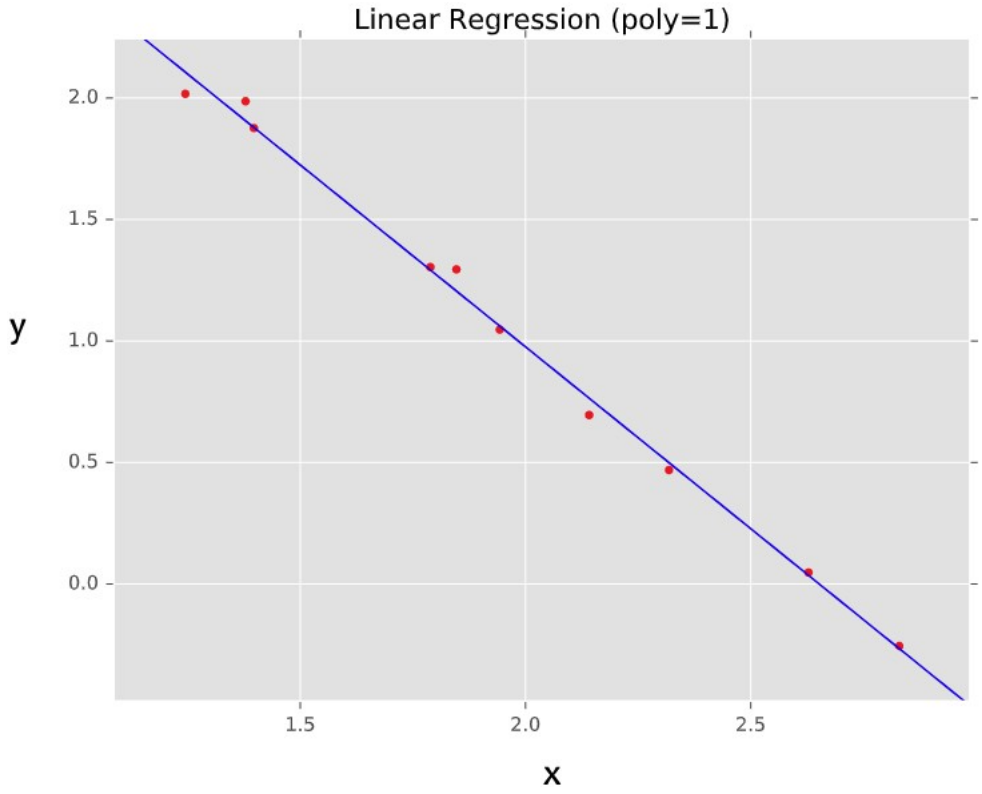
Price of wheat $\longleftrightarrow$ Quantity of wheat produced

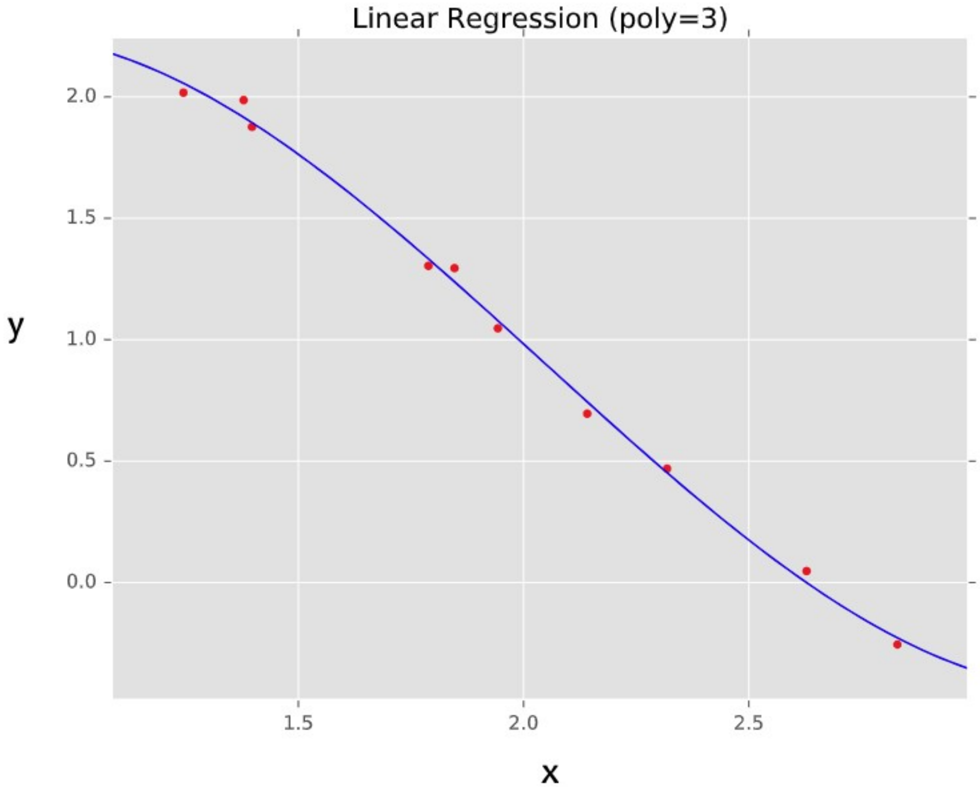
Types of
Regression Models

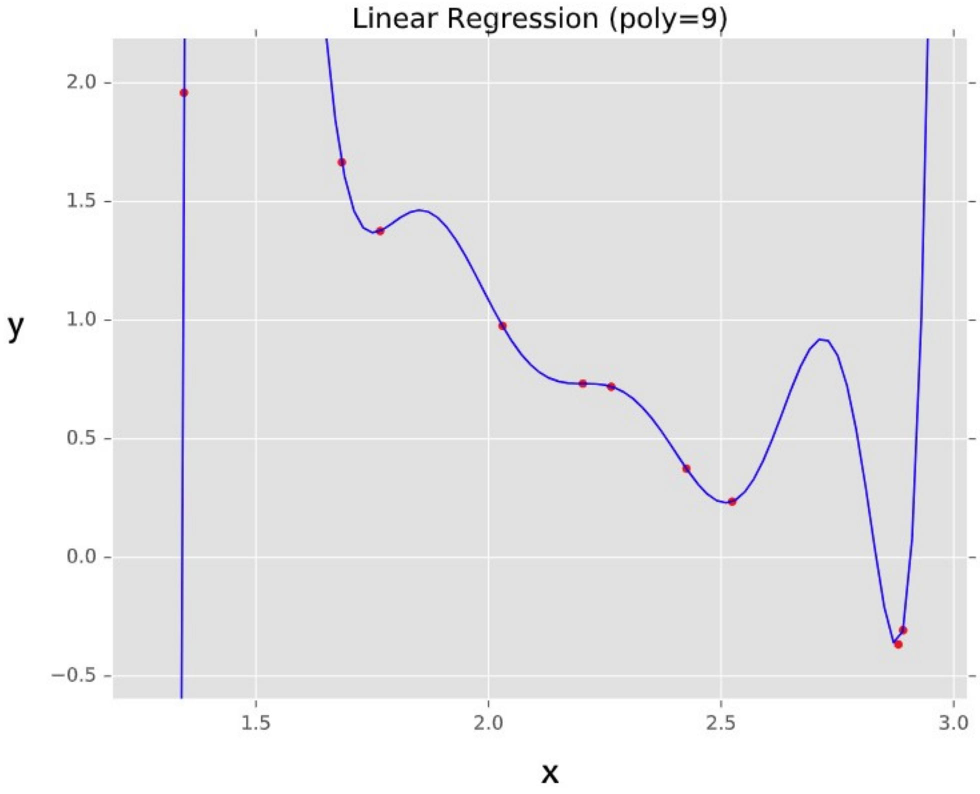




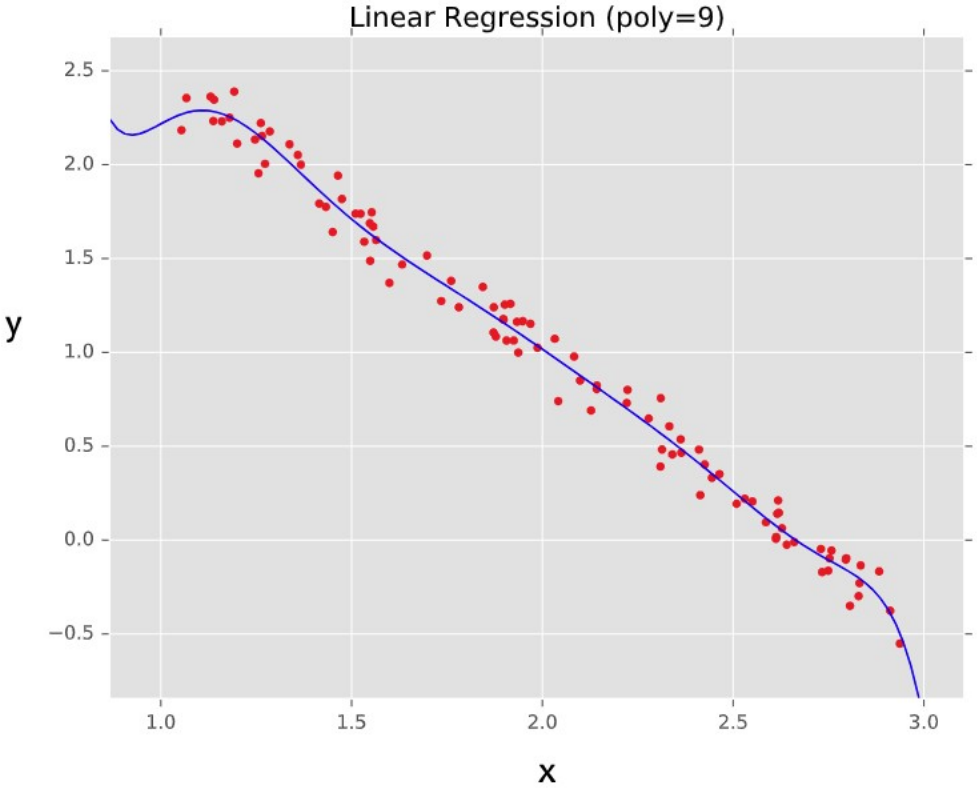
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
1.0
1.5
2.0
2.5
3.0
y
x


Linear Regression (poly=1)
y
x
2.0
1.5
1.0
0.5
0.0
1.5
2.0
2.5


Linear Regression (poly=3)
2.0
1.5
1.0
0.5
0.0
y
1.5
2.0
2.5
x


Linear Regression (poly=9)
y
x
2.0
1.5
1.0
0.5
0.0
−0.5
1.5
2.0
2.5
3.0

Test Time



Overfitting

The example shows:

- perfect fit on **in sample (training)** data

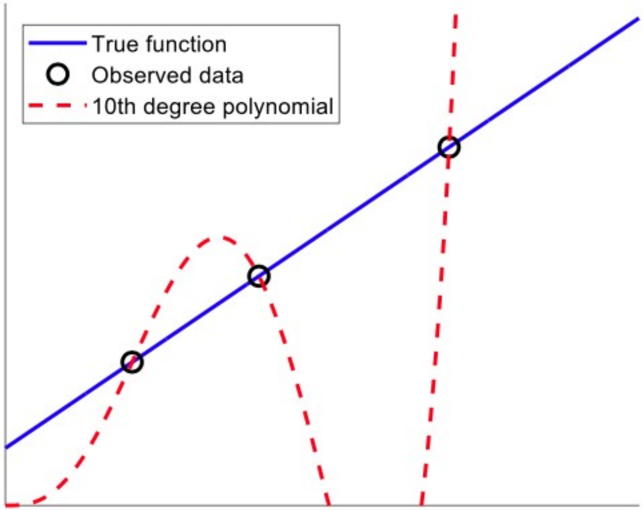
$$\downarrow$$

$$E_{in} = 0$$

- low fit on **out of sample (test)** data

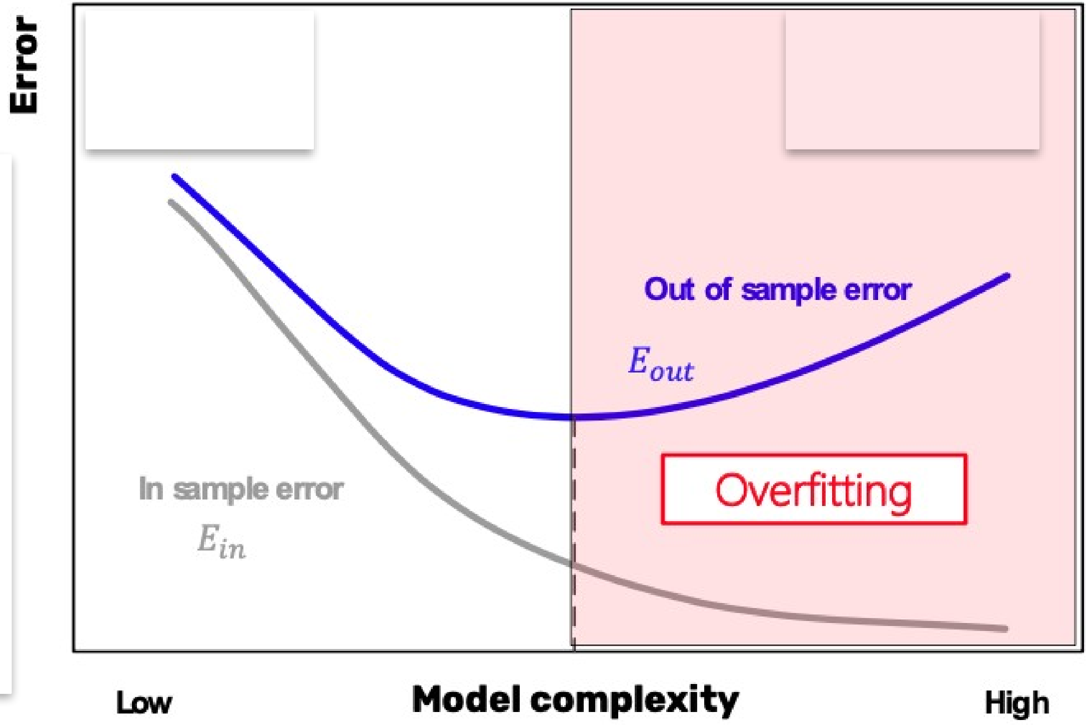
$$\downarrow$$

E_{out} **huge**



Overfitting vs. model complexity

We talk of **overfitting** when decreasing E_{in} leads to increasing E_{out}



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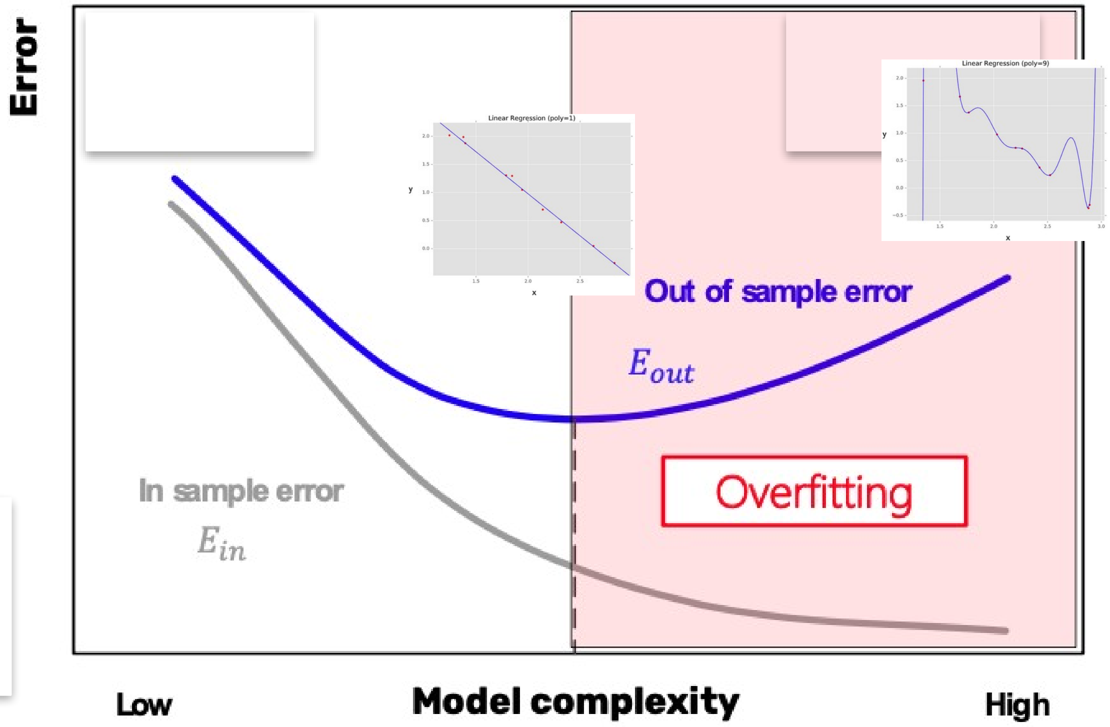
Major source of failure for machine learning systems

Overfitting leads to bad generalization



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Major source of failure for machine learning systems

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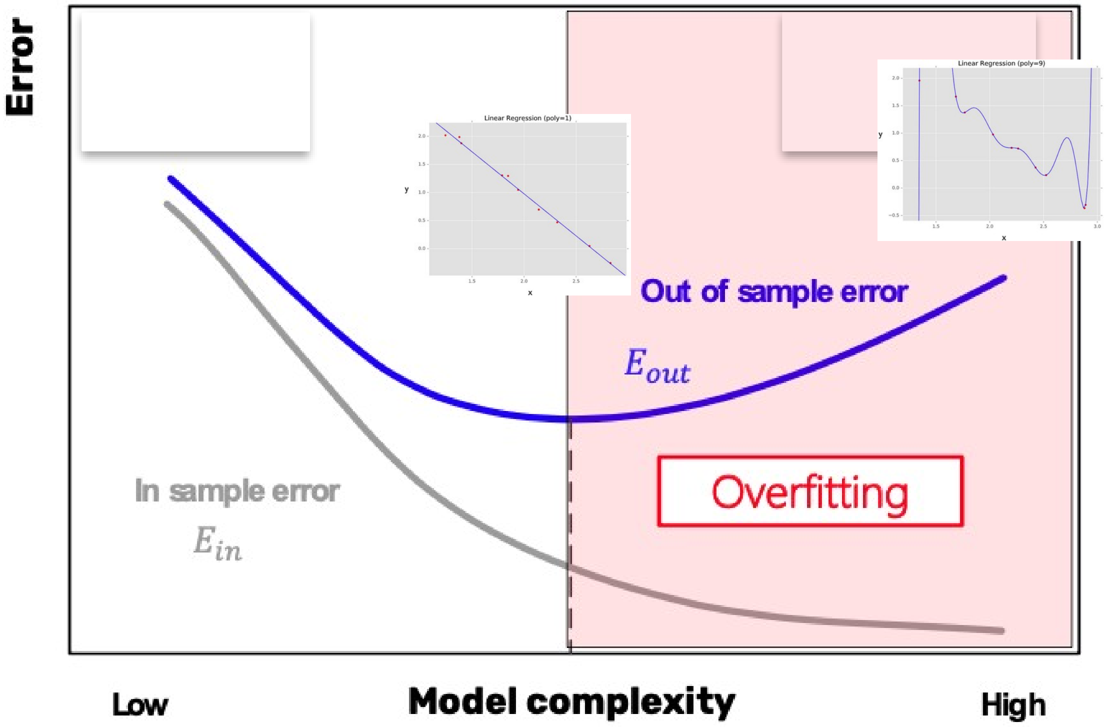
A model can exhibit bad generalization even if it does not overfit



A cure for overfitting

Regularization is the first line of defense against overfitting

We have seen that **complex models** are more prone to overfitting

- This is because they are more powerful, and thus they can fit the noise

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- However, if we stick only to simple models, we may not end up with a satisfying approximation of the target function $f(\cdot)$

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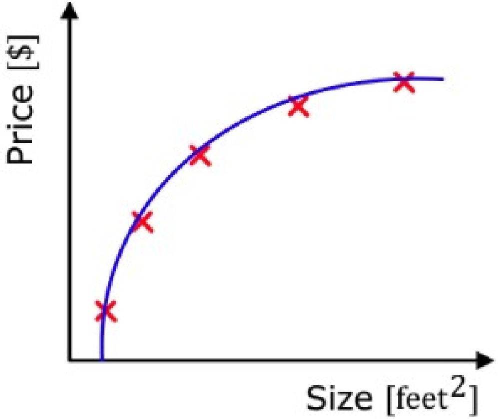
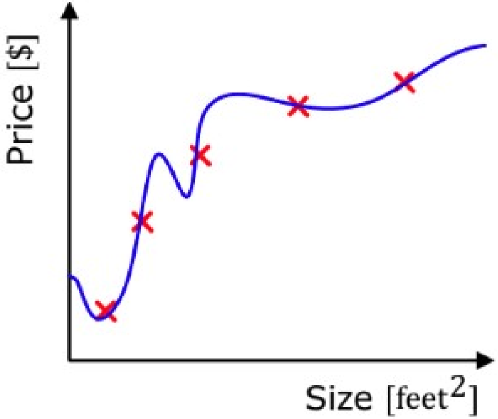
*How can we retain the benefits of **both** worlds?*

A cure for overfitting

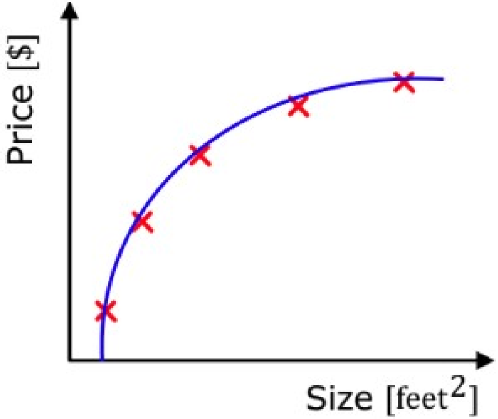


$\mathcal{H}_1\colon y = \theta_0 + \theta_1\varphi + \theta_2\varphi^2$

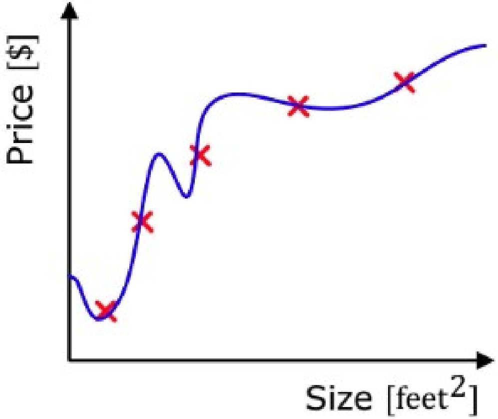


$\mathcal{H}_2\colon y = \theta_0 + \theta_1\varphi + \theta_2\varphi^2 + \theta_3\varphi^3 + \theta_4\varphi^4$

A cure for overfitting



$\mathcal{H}_1$: $y = \theta_0 + \theta_1\varphi + \theta_2\varphi^2$



$\mathcal{H}_2$: $y = \theta_0 + \theta_1\varphi + \theta_2\varphi^2 + \theta_3\varphi^3 + \theta_4\varphi^4$

We can «recover» the model $\mathcal{H}_1$ from the model $\mathcal{H}_2$ by **imposing** $\theta_3 = \theta_4 = 0$

This can be done by minimizing, along with $J(\boldsymbol{\theta})$, also the value of the parameters θ_3, θ_4

Regularization

$h(\cdot)$ is some function that represents our model

More generally, instead of minimizing the in-sample error E_{in} (i.e. the cost function $J(\boldsymbol{\theta})$), minimize the **augmented error:**

For simplicity, suppose $J(\boldsymbol{\theta})$ as squared error function

$$\boxed{E_{aug}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\big(y(i) - h(\boldsymbol{\varphi}(i);\boldsymbol{\theta})\big)^2 + \lambda \cdot \sum_{j=0}^{d-1}(\theta_j)^2}$$

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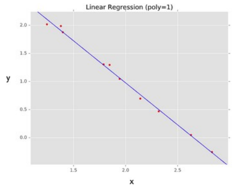
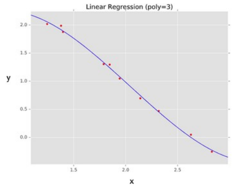
- The term $\Omega = \sum_{j=0}^{d-1}\left(\theta_j\right)^2$ is called **regularizer**

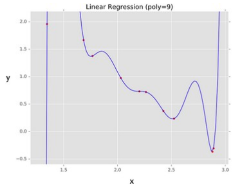
- The term λ (**regularization hyper-parameter**) weights the importance of minimizing $J(\boldsymbol{\theta})$, with respect to minimizing Ω

Polynomial Coefficients

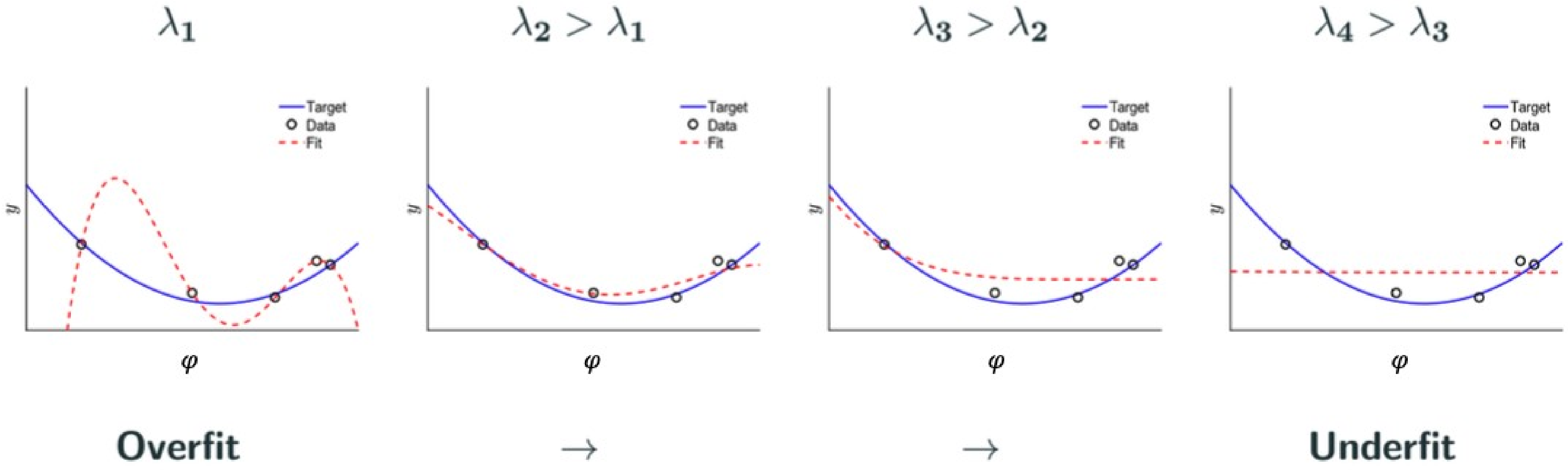
	$M=0$	$M=1$	$M=3$	$M=9$
θ_0	0.19	0.82	0.31	0.35
θ_1		-1.27	7.99	232.37
θ_2			-25.43	-5321.83
θ_3			17.37	48568.31
θ_4				-231639.30
θ_5				640042.26
θ_6				-1061800.52
θ_7				1042400.18
θ_8				-557682.99
θ_9				125201.43







Effect of λ



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Choice of the regularizer

There are many choices of possible regularizers. The most used ones are:

- L_2 **regularizer:** also called **Ridge** regression $\Omega(\boldsymbol{\theta}) = \sum_{j=0}^{d-1} \left(\theta_j\right)^2 = \boldsymbol{\theta}^\top \boldsymbol{\theta} = \|\boldsymbol{\theta}\|_2^2$
- L_1 **regularizer:** also called **Lasso** regression $\Omega(\boldsymbol{\theta}) = \sum_{j=0}^{d-1} \left|\theta_j\right| = \|\boldsymbol{\theta}\|_1$
- **Elastic-net regularizer:** $\Omega(\boldsymbol{\theta}) = \sum_{j=0}^{d-1} \beta \left(\theta_j\right)^2 + (1-\beta) \sum_{j=0}^{d-1} \left|\theta_j\right|$

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The different regularizers behaves differently:

- The ridge penalty tends to shrink all coefficients to a **lower value**
- The lasso penalty tends to set more coefficients **exactly to zero**
- The elastic-net penalty is a compromise between ridge and lasso, with the β value controlling the two contributions