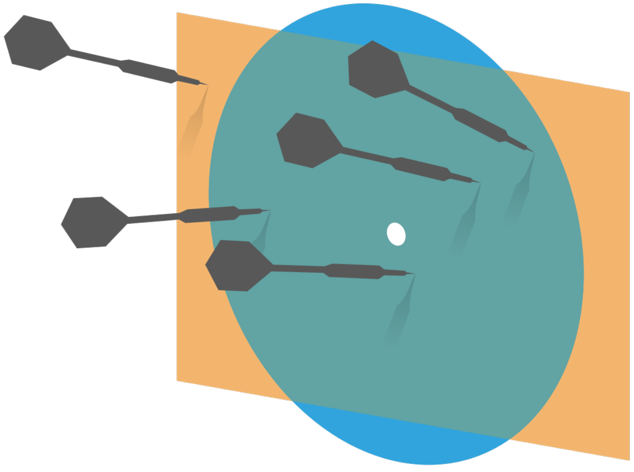
# Probability and Statistics for Computer Science



Credit: wikipedia

"All models are wrong, but some models are useful"--- George Box

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# Last time

- Linear regression
  - The problem
  - The least square solution
  - The training and prediction
  - The R-squared for the evaluation of the fit.

$$y = \beta_0 + \beta_1 x^{(1)} + \beta_2 x^{(2)} \cdots + \xi$$

$$y = X\beta + e$$

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

$$y^P = X\hat{\beta}$$

$$R^2 = \frac{var(X\hat{\beta})}{var(y)}$$

$$y = X\beta + e$$

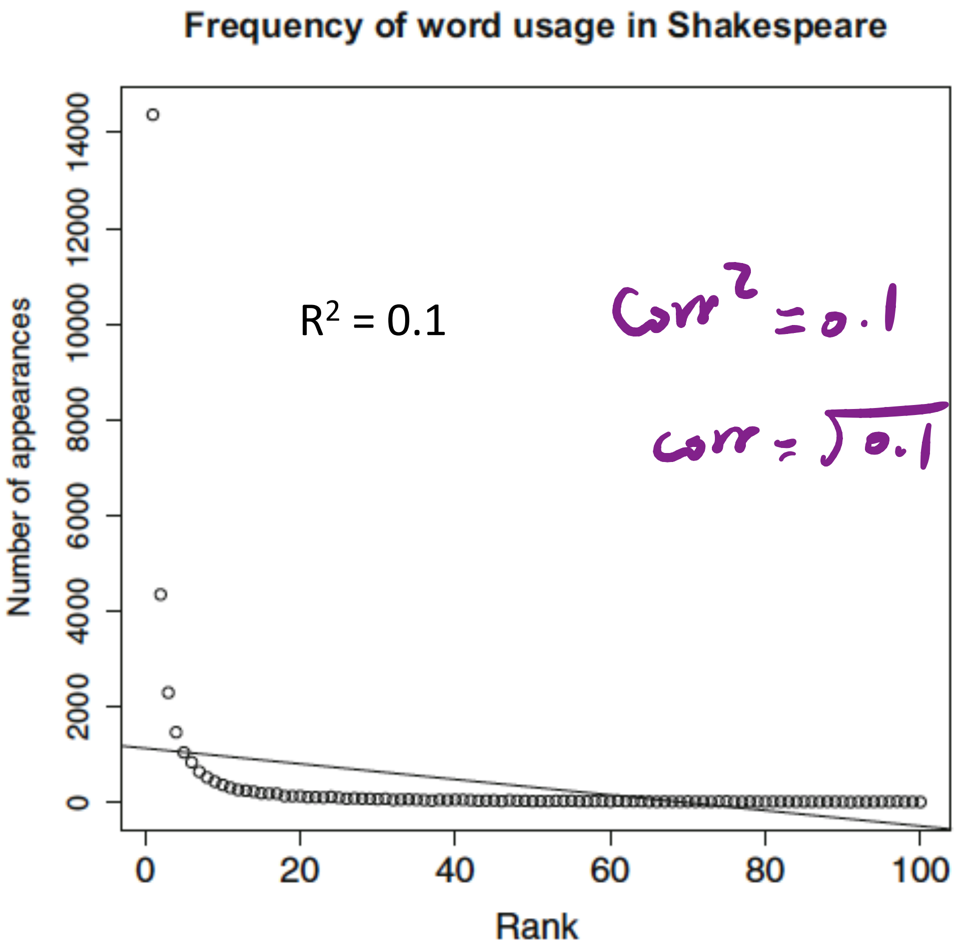
$$X\hat{\beta} \perp e$$

# Objectives

- Linear regression (cont.)
  - Modeling non-linear relationship with linear regression → bigger scope
  - Outliers and over-fitting issues – better
  - Regularized linear regression/Ridge regression
- Nearest neighbor regression

# What if the relationship between variables is non-linear?

- A linear model will not produce a good fit if the dependent variable is **not** linear combination of the explanatory variables



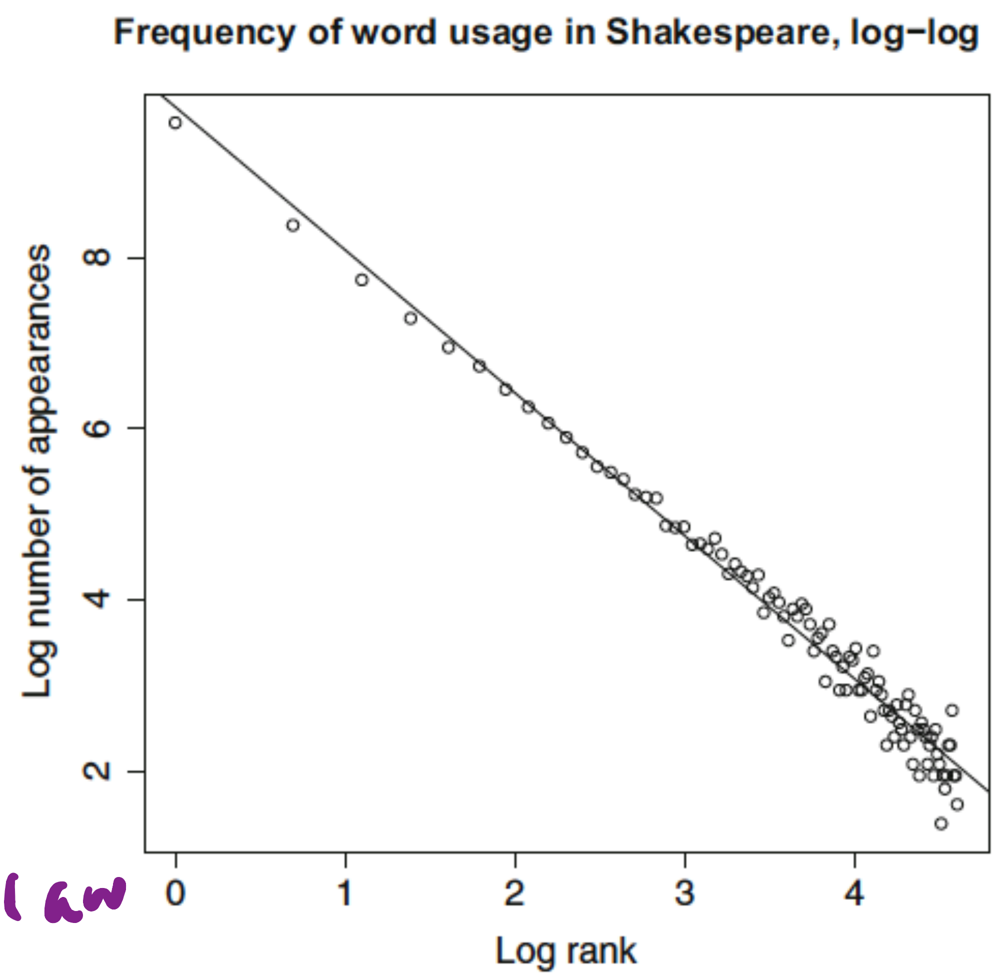
# Transforming variables could allow linear model to model non-linear relationship

- In the word- frequency example, log-transforming both variables would allow a linear model to fit the data well.

$$\log f = \beta_0 + \beta_1 \log r$$

$$f = c \cdot \left(\frac{1}{r}\right)^s$$

Zipf's law



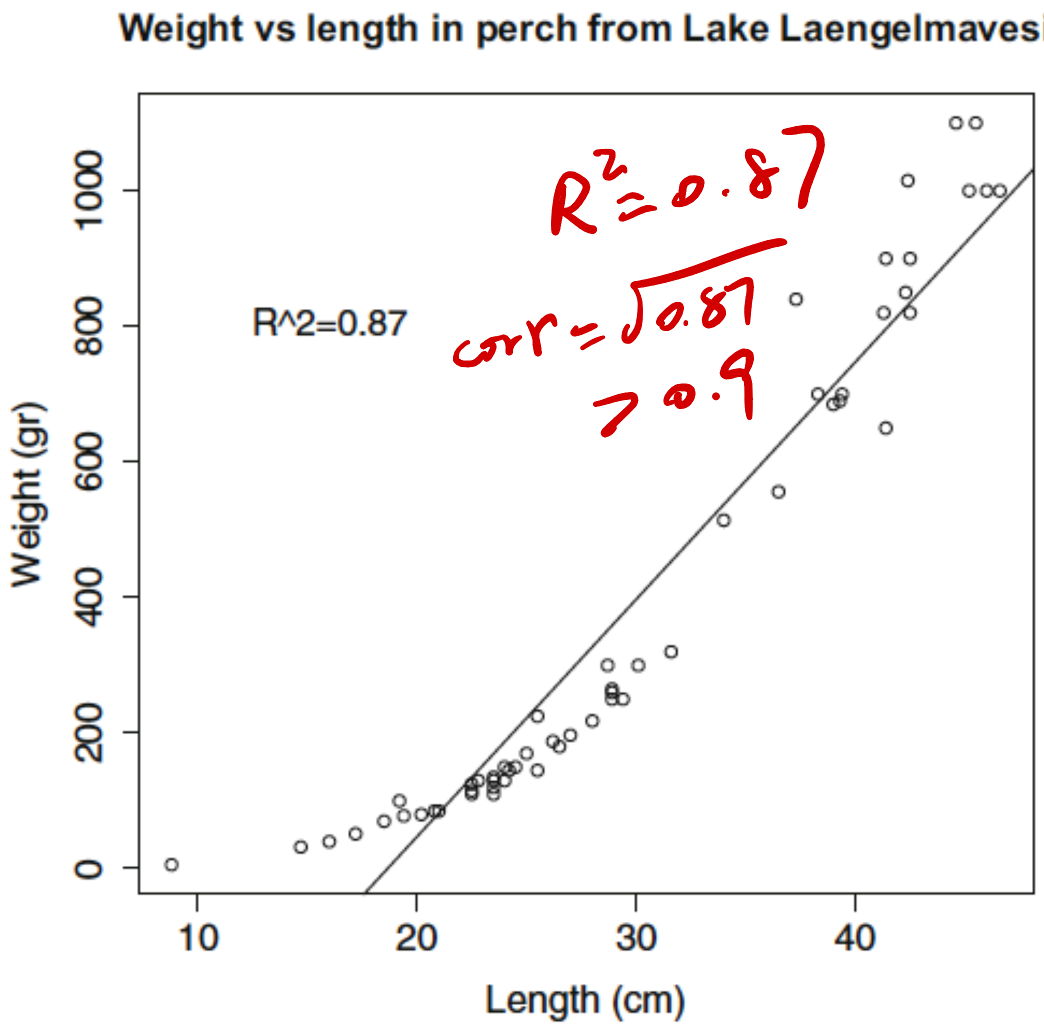
# More example: Data of fish in a Finland lake

- Perch (a kind of fish) in a lake in Finland, 56 data observations
- Variables include: Weight, Length, Height, Width
- In order to illustrate the point, let's model **Weight** as the dependent variable and the **Length** as the explanatory variable.

Yellow Perch

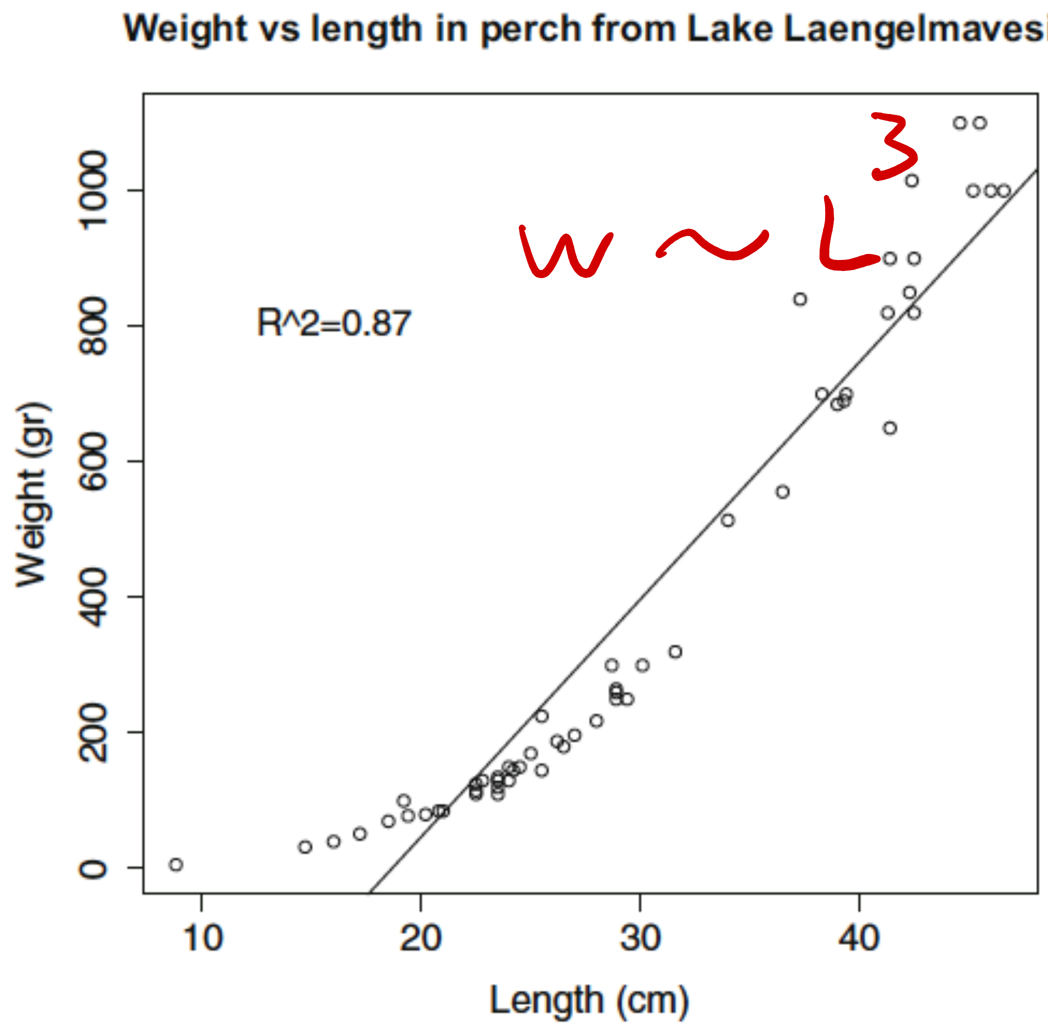
# Is the linear model fine for this data?

A. YES
B. NO

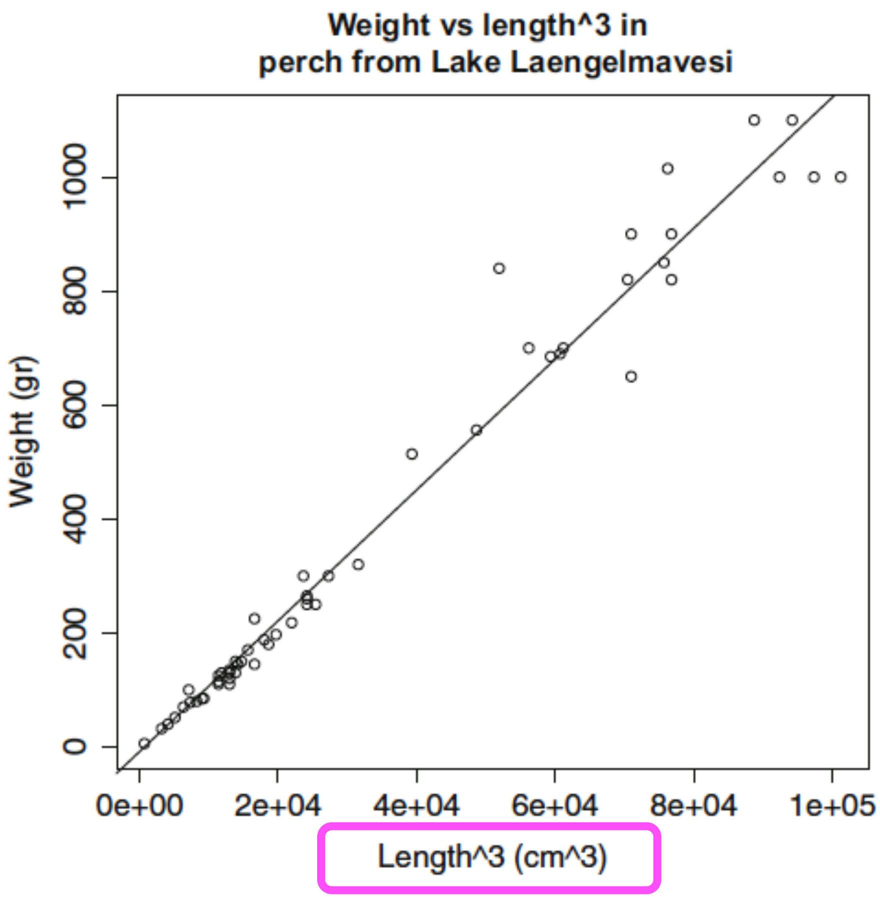


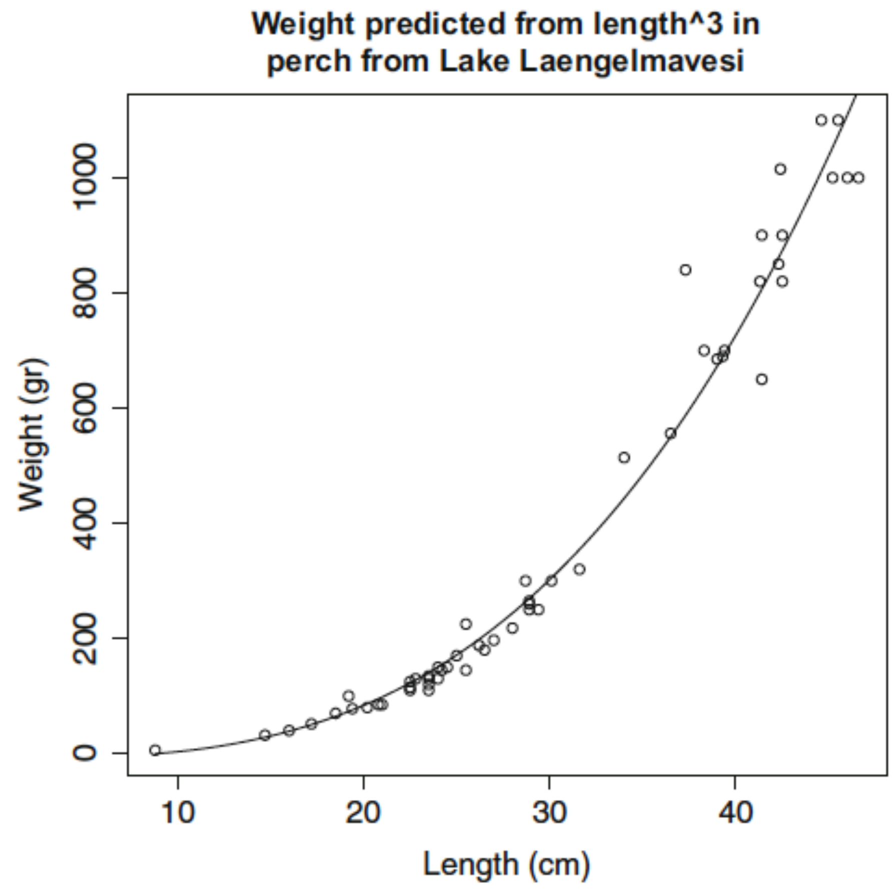
# Is the linear model fine for this data?

- R-squared is 0.87 may suggest the model is OK
- But the trend of the data suggests non-linear relationship
- Intuition tells us length is not linear to weight given fish is 3-dimensional
- We can do better!



# Transforming the explanatory variables



# Q. What are the matrix X and y?

| 1 | $Length^3$ | Weight |
|---|---|---|
| | | |

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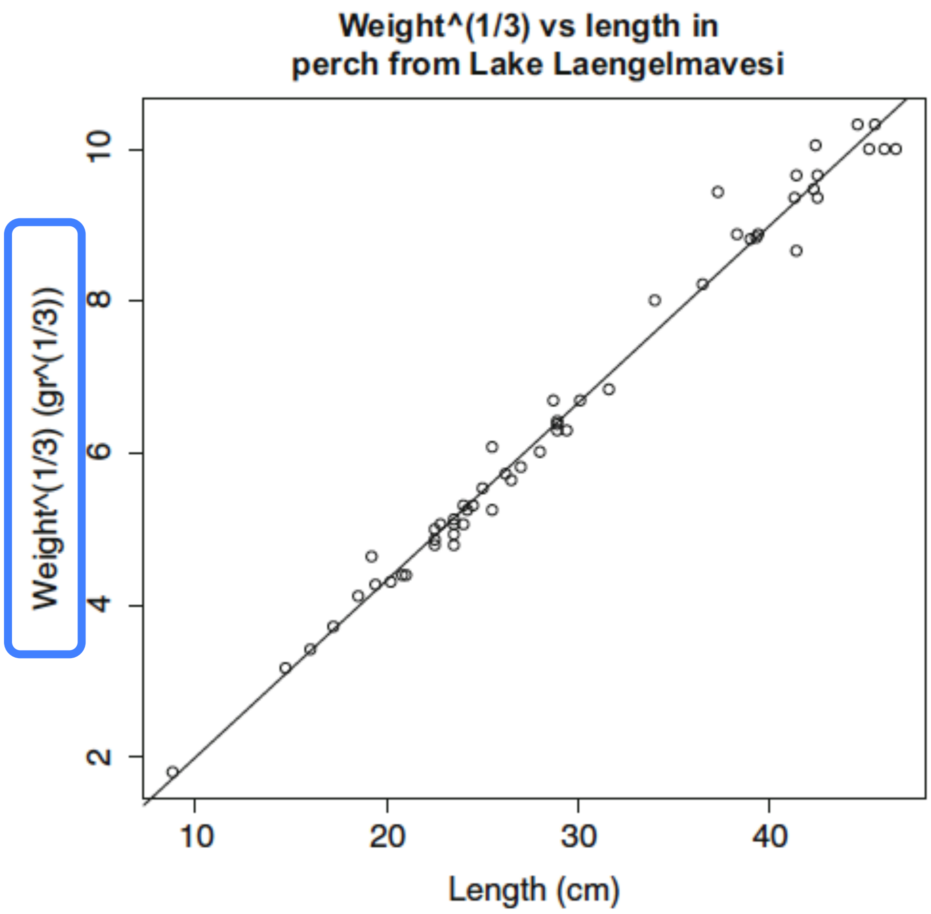
| 1 | Length$^3$ | Weight |
|---|---|---|
| | | |

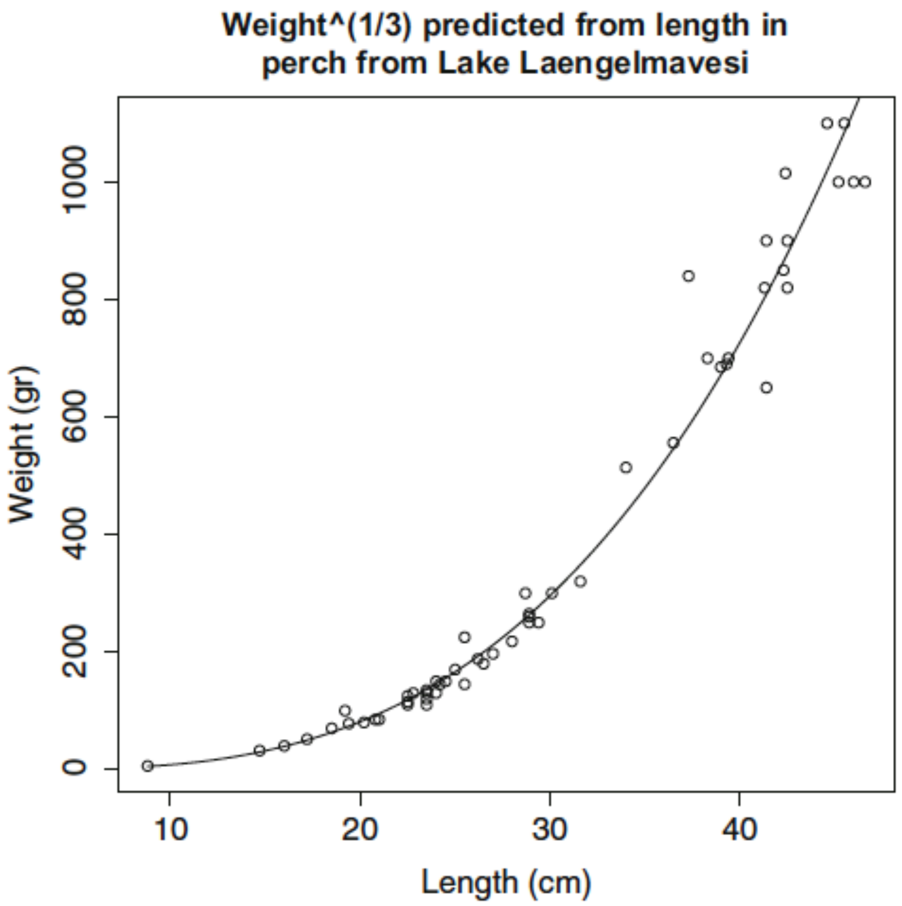
$$X^0 = \begin{array}{cc} & \text{length} \\ \left[\begin{array}{c} 1 \\ 1 \end{array}\right. & \left.\begin{array}{c} 2 \\ 3 \end{array}\right] \end{array}$$

$$\rightarrow X^{new} = \begin{bmatrix} 1 & 8 \\ 1 & 27 \end{bmatrix}$$

$$y = y^0 \quad \text{(as before)}$$

# Transforming the dependent variables



# What is the model now?

$$\sqrt[3]{y} = \beta_0 + \beta_1 x$$

$$y = \beta_0 + \beta_1 x^3$$

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_n x^n$$

# What are the matrix X and y?

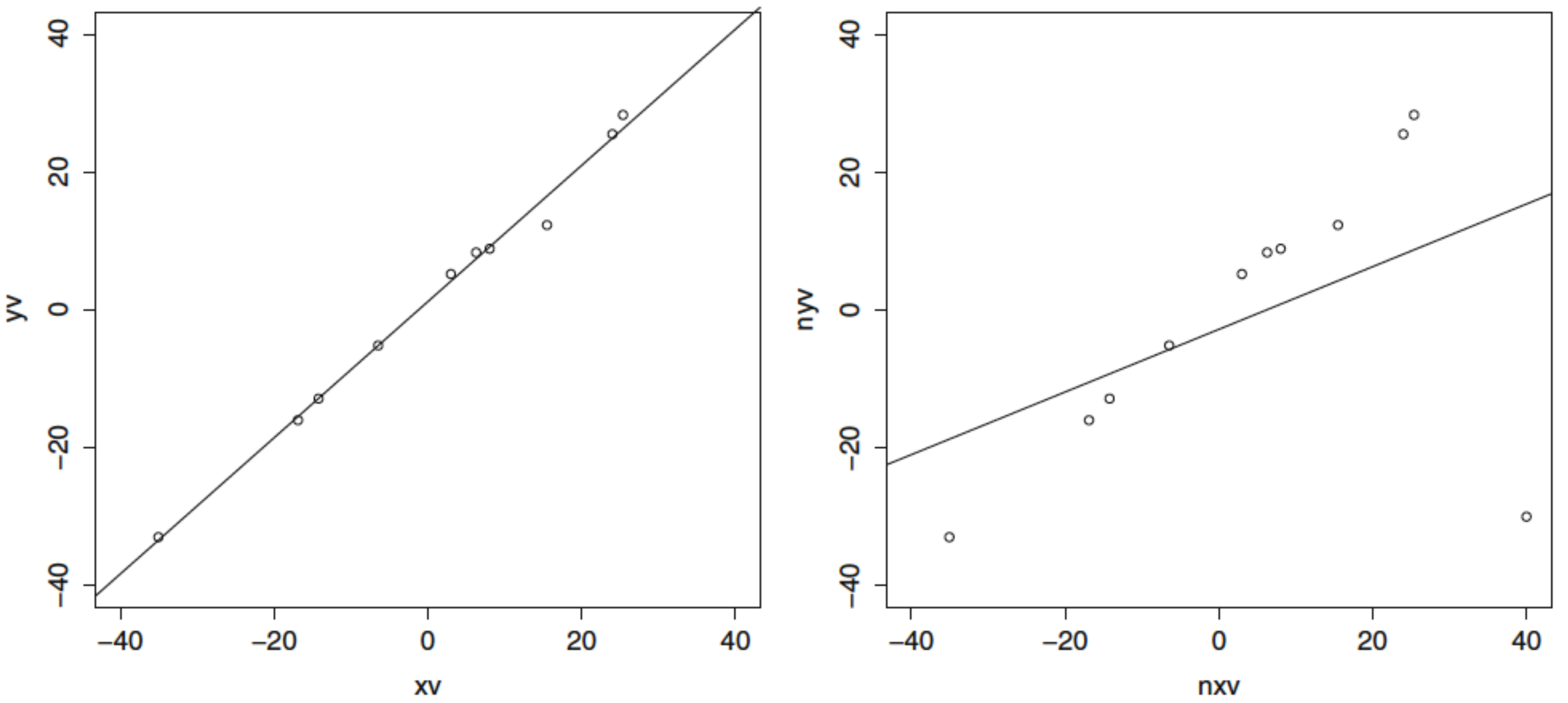
| 1 | Length | $\sqrt[3]{w}$ |
|---|---|---|
| | | |

General form of transformation in Linear Regression

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \cdots$$

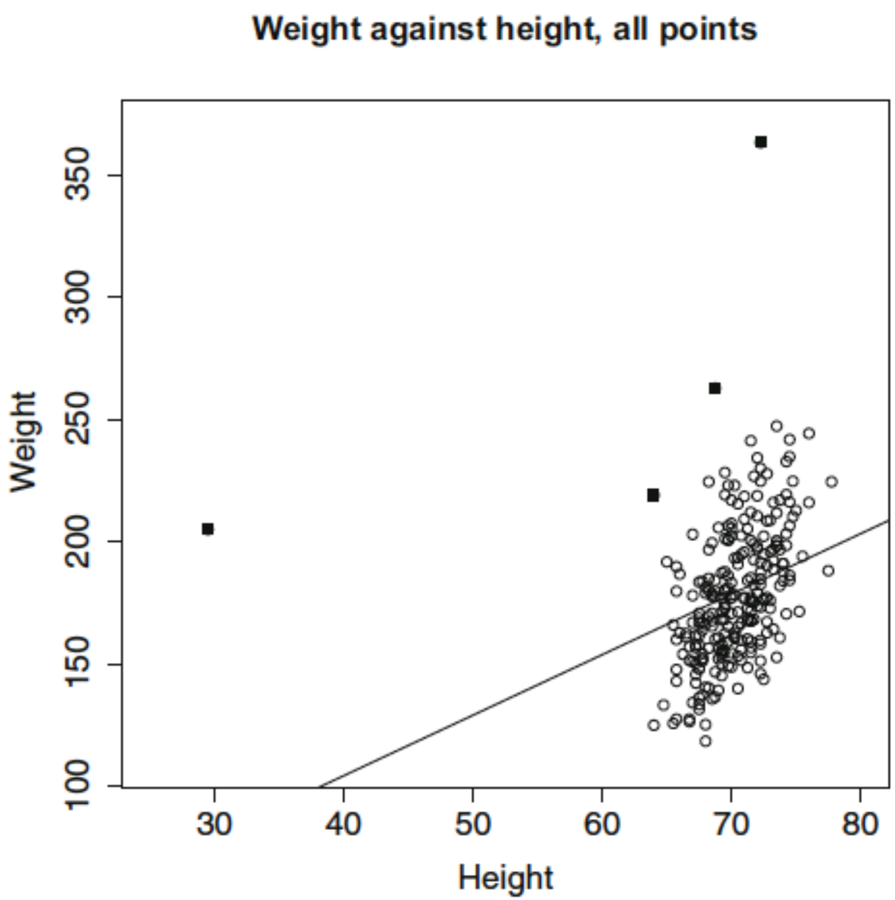
# Effect of outliers on linear regression

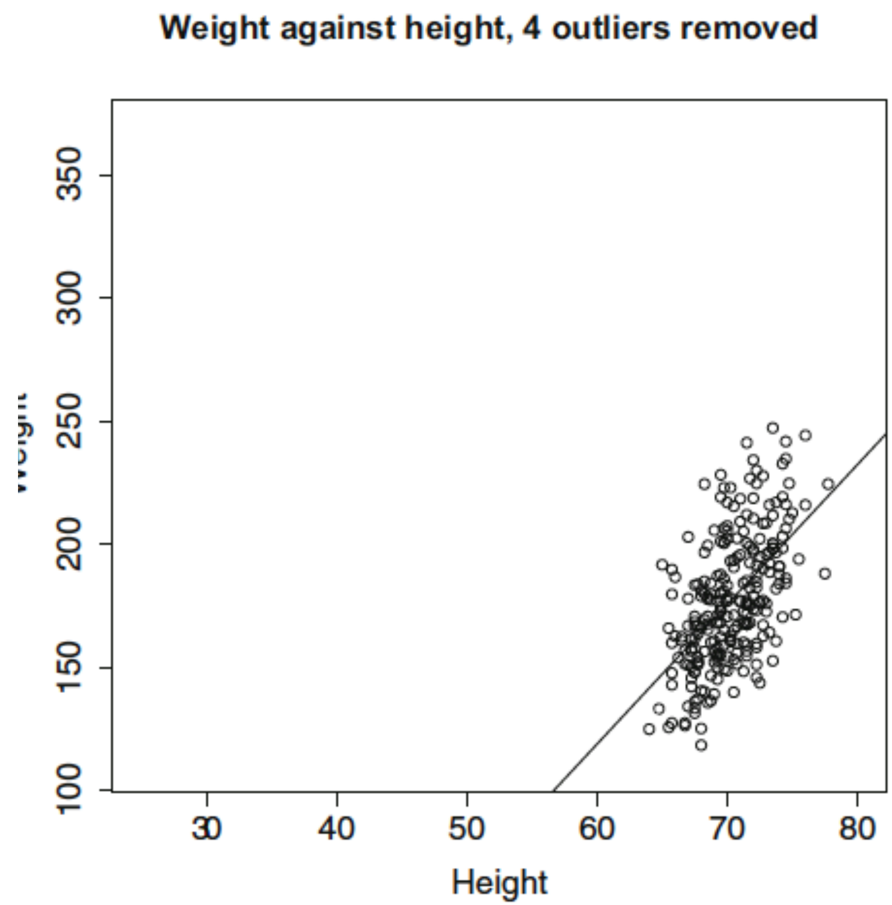
- Linear regression is sensitive to outliers



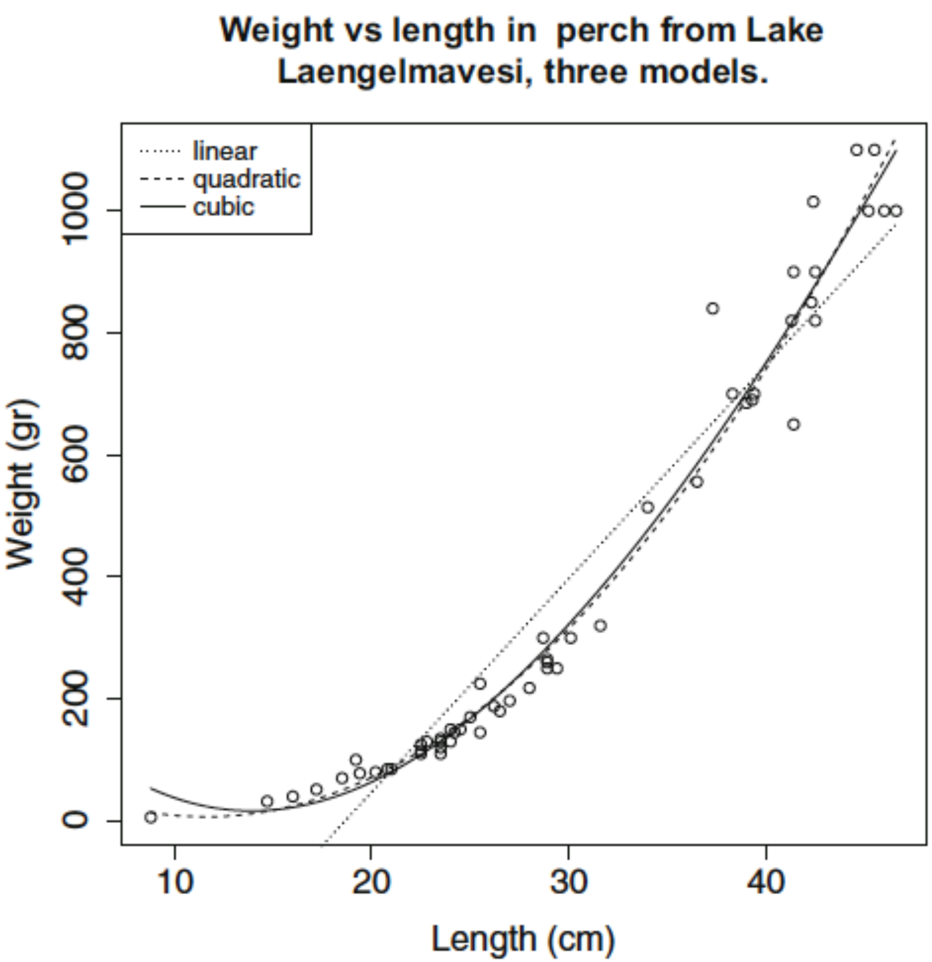
# Effect of outliers: body fat example

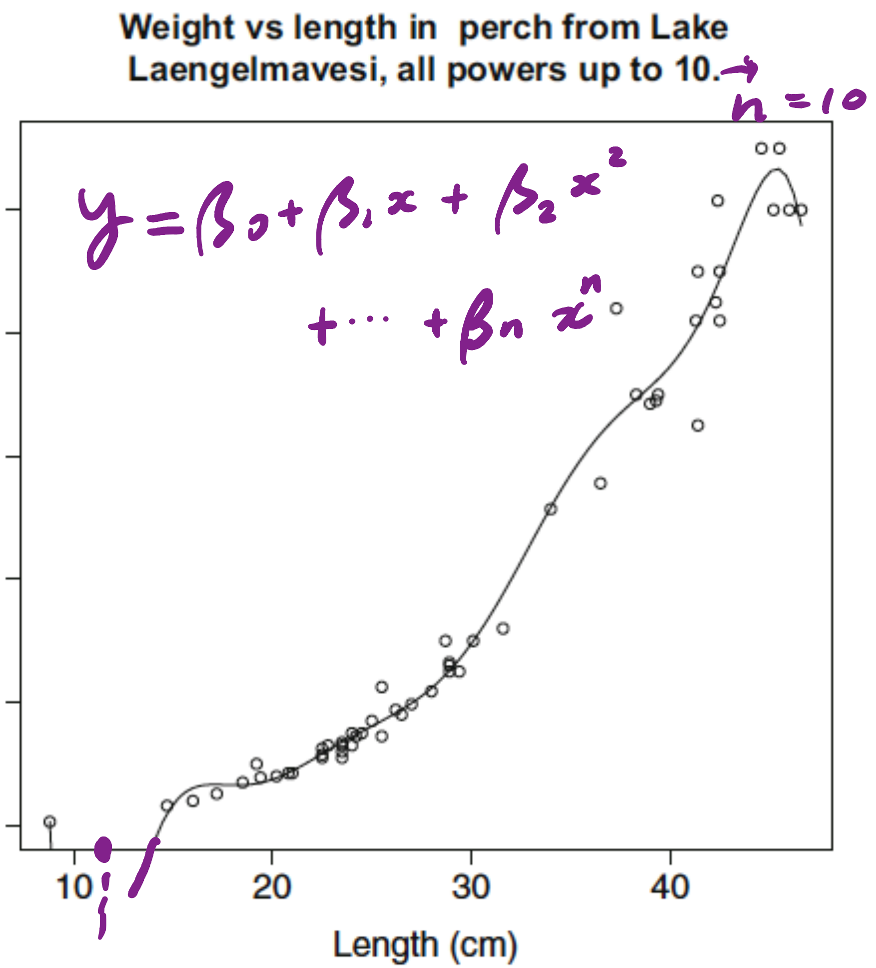
- Linear regression is sensitive to outliers



# Over-fitting issue: example of using too many power transformations



# Avoiding over-fitting

- **Method 1: validation**
  - Use a validation set to choose the transformed explanatory variables
  - The difficulty is the number of combination is exponential in the number of variables.

$x^n$

- **Method 2: regularization**
  - Impose a penalty on complexity of the model during the training
  - Encourage smaller model coefficients
- We can use validation to select regularization parameter λ

$\max(0, 1 - y_i a^T x)$

$+ \text{penalty}$

$\frac{1}{2}\|a\|^2$

# Regularized linear regression

- In ordinary least squares, the cost function is $\|\mathbf{e}\|^2$:

$$\|\mathbf{e}\|^2 = \|\mathbf{y} - X\boldsymbol{\beta}\|^2 = (\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta})$$

$L_2$

- In regularized least squares, we add a penalty with a weight parameter λ (λ>0): regularization parameter

$$\|\mathbf{y} - X\boldsymbol{\beta}\|^2 + \lambda\frac{\|\boldsymbol{\beta}\|^2}{2} = (\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta}) + \lambda\frac{\boldsymbol{\beta}^T\boldsymbol{\beta}}{2}$$

# Training using regularized least squares

- Differentiating the cost function and setting it to zero, one gets:

$X^T X \hat{\beta} = X^T y$

$$(X^T X + \lambda I)\boldsymbol{\beta} - X^T \mathbf{y} = 0$$

least sq. sol.

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

- $(X^T X + \lambda I)$ is always invertible, so the regularized least squares estimation of the coefficients is:

$$\widehat{\boldsymbol{\beta}} = (X^T X + \lambda I)^{-1} X^T \mathbf{y}$$

$y^p = X \hat{\beta}$

# Why is the regularized version always invertible?

Prove: $(X^T X + \lambda I)$ is invertible (λ>0, λ is not the eigenvalue).

positive semi-defi.

$$f^T A f \geq 0$$ $\gamma \to$ eigenvalues

$\gamma_i \geq 0$

positive defi.

$$f^T A f > 0$$

$f \to$ non-zero vector

See Strang Pg 351.

$f^T(X^TX + \lambda I)f > 0$

$= f^T X^T X f + f^T \lambda I f$

$= \underbrace{f^T X^T X f}_{\geq 0} + \lambda \underbrace{f^T f}_{> 0}$

$f^T f \to \|f\|^2 > 0$

$=$

$\lambda > 0$

# Why is the regularized version always invertible?

Prove: $(X^T X + \lambda I)$ is invertible (λ>0, λ is not the eigenvalue).

Energy based definition of **semi-positive definite**:
Given a matrix A and any nonzero vector **f** , we have

$$f^T A f \geq 0$$

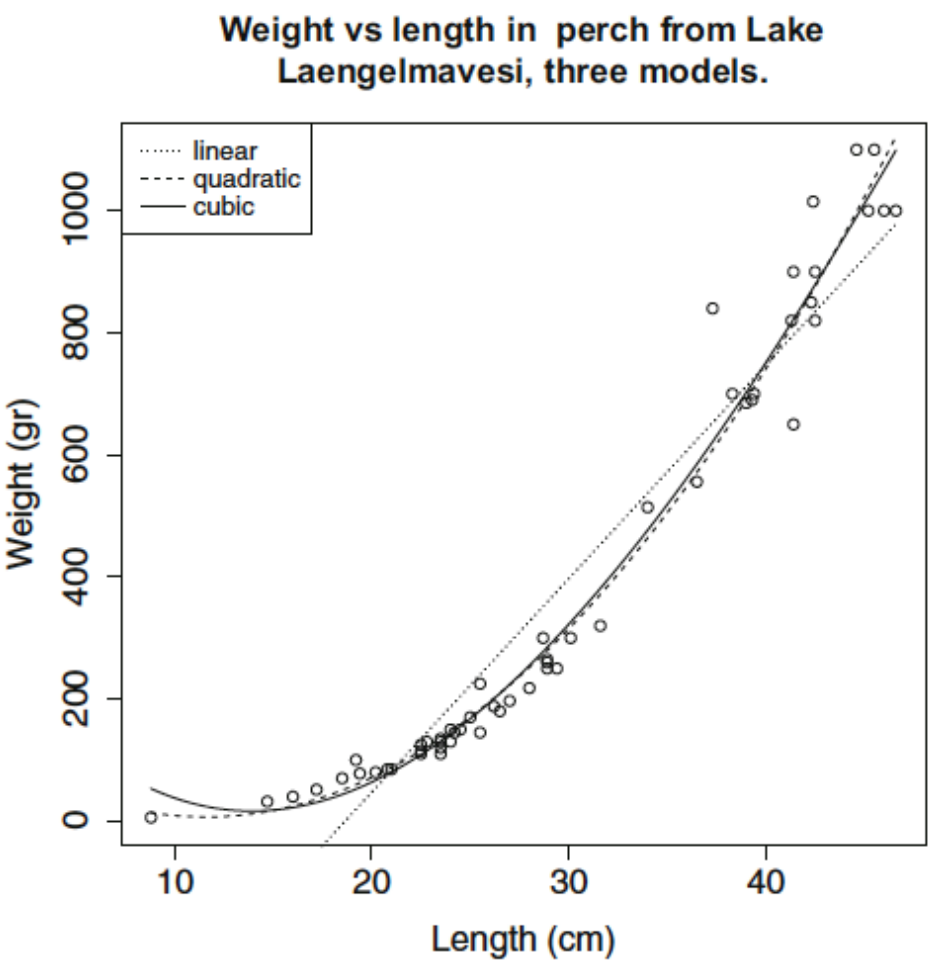
and **positive definite** means

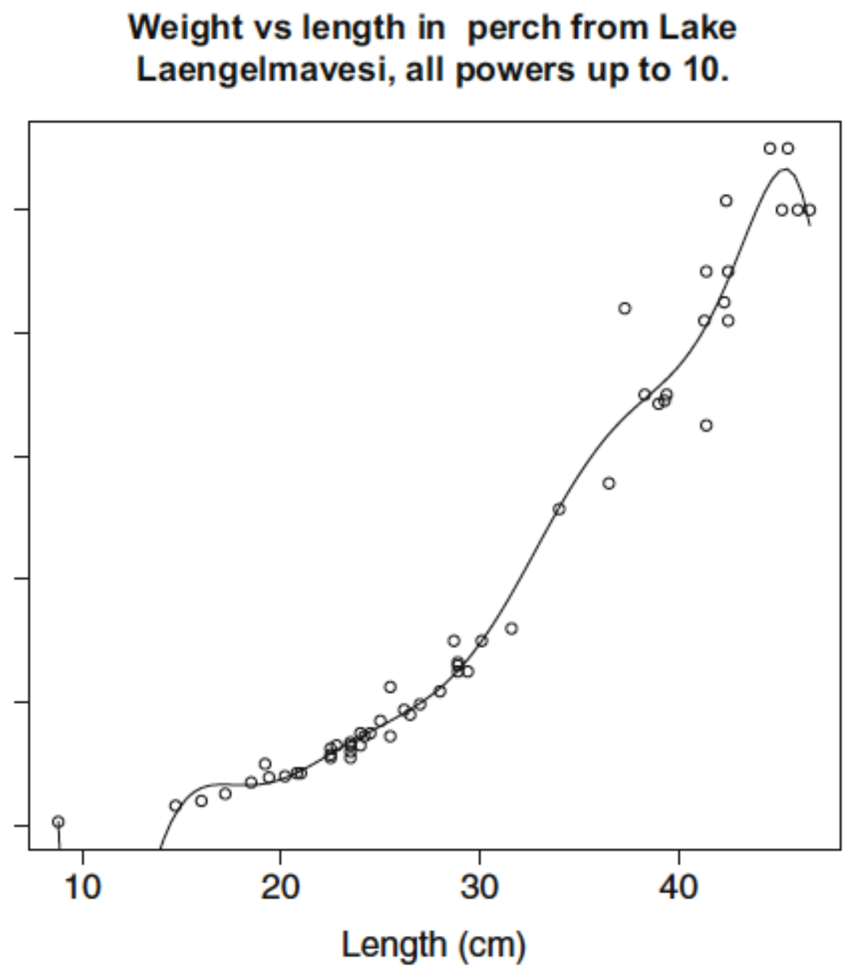
$$f^T A f > 0$$

If A is positive definite, then all eigenvalues of A are positive, then it's invertible

$$
\begin{aligned}
&for\ any\ nonzero\ vector\ f \\
&consider\ f^T(X^T X + \lambda I)f \\
&suppose\ A = X^T X + \lambda I \\
&f^T A f = f^T X^T X f + \lambda f^T f \\
&= f^T X^T X f + \lambda ||f||^2 \\
&given\ X^T X\ is\ semi\ positive\ definite \\
&f^T X^T X f \geq 0 \\
&given\ \lambda > 0 \\
&we\ know\ \lambda ||f||^2 > 0 \\
&\Rightarrow f^T A f > 0
\end{aligned}
$$

# Over-fitting issue: example from using too many power transformations

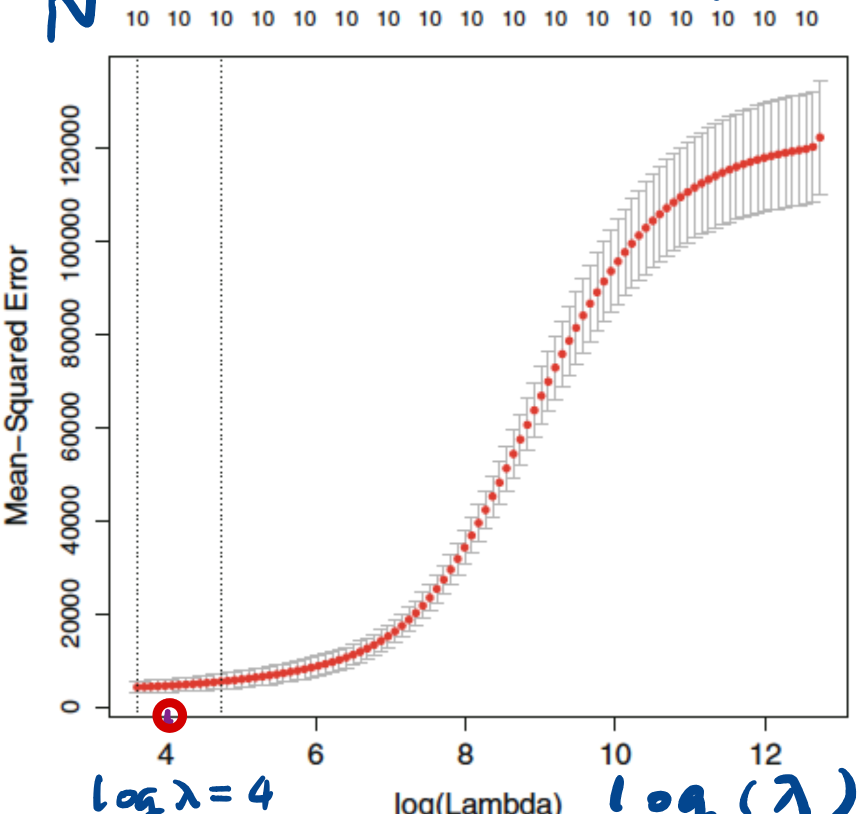


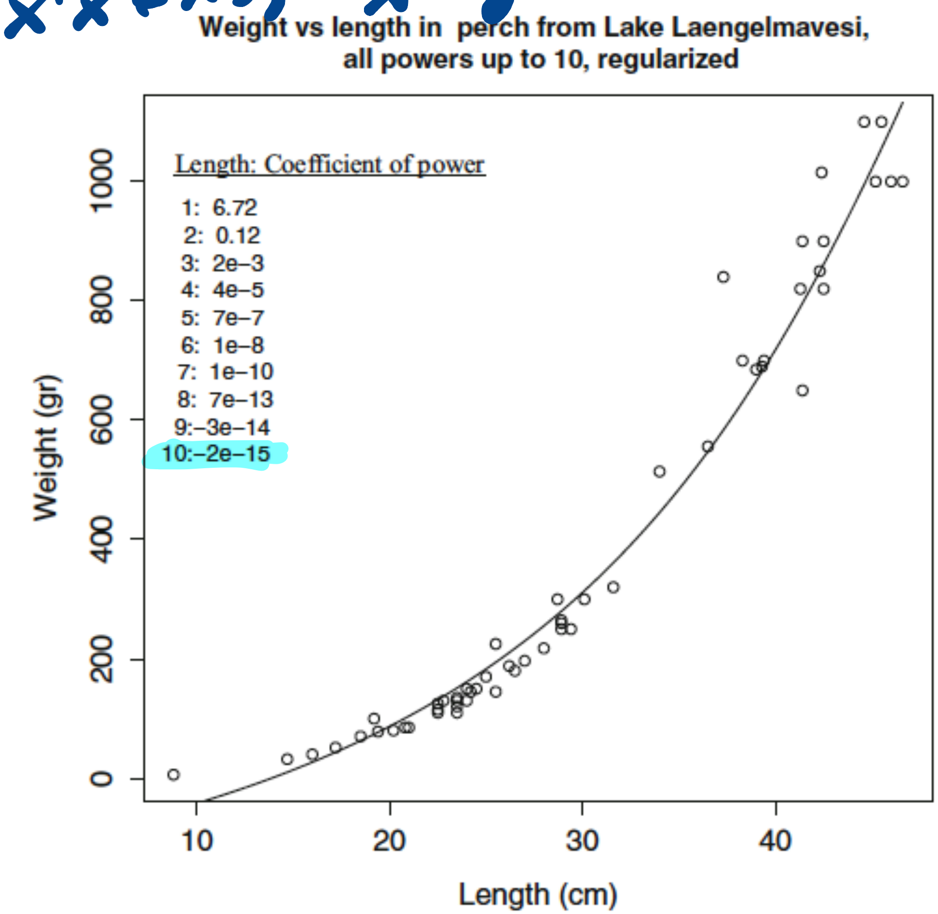



# Choosing lambda using cross-validation

$\frac{\|e\|^2}{N}$

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




$\log \lambda = 4$

$\lambda = e^4$

$\log(\lambda)$

$\lambda > 0$

# Mean Square Error in this model

$$MSE = \frac{e^T e}{N} = \frac{\|y - X\hat{\beta}\|^2}{N}$$

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

$$y^p = X\hat{\beta}$$

# Q. Can we use the R-squared to evaluate the regularized model correctly?

A. YES
B. NO
C. YES and NO

# Q. Can we use the R-squared to evaluate the regularized model correctly?

A. YES

B. NO

C. YES and NO

$X^T X \cdot \hat{\beta} = X^T y$

$e \perp X\hat{\beta}$

$var(y) = var(X\hat{\beta}) + var(e)$

$y = X\beta + e$

$var(y) = var(X^T\hat{\beta}) + var(e) + 2cov(X^T\hat{\beta}, e)$

$(X^T X + \lambda I)\hat{\beta} = X^T y$

$\cancel{e \perp X\hat{\beta}}$

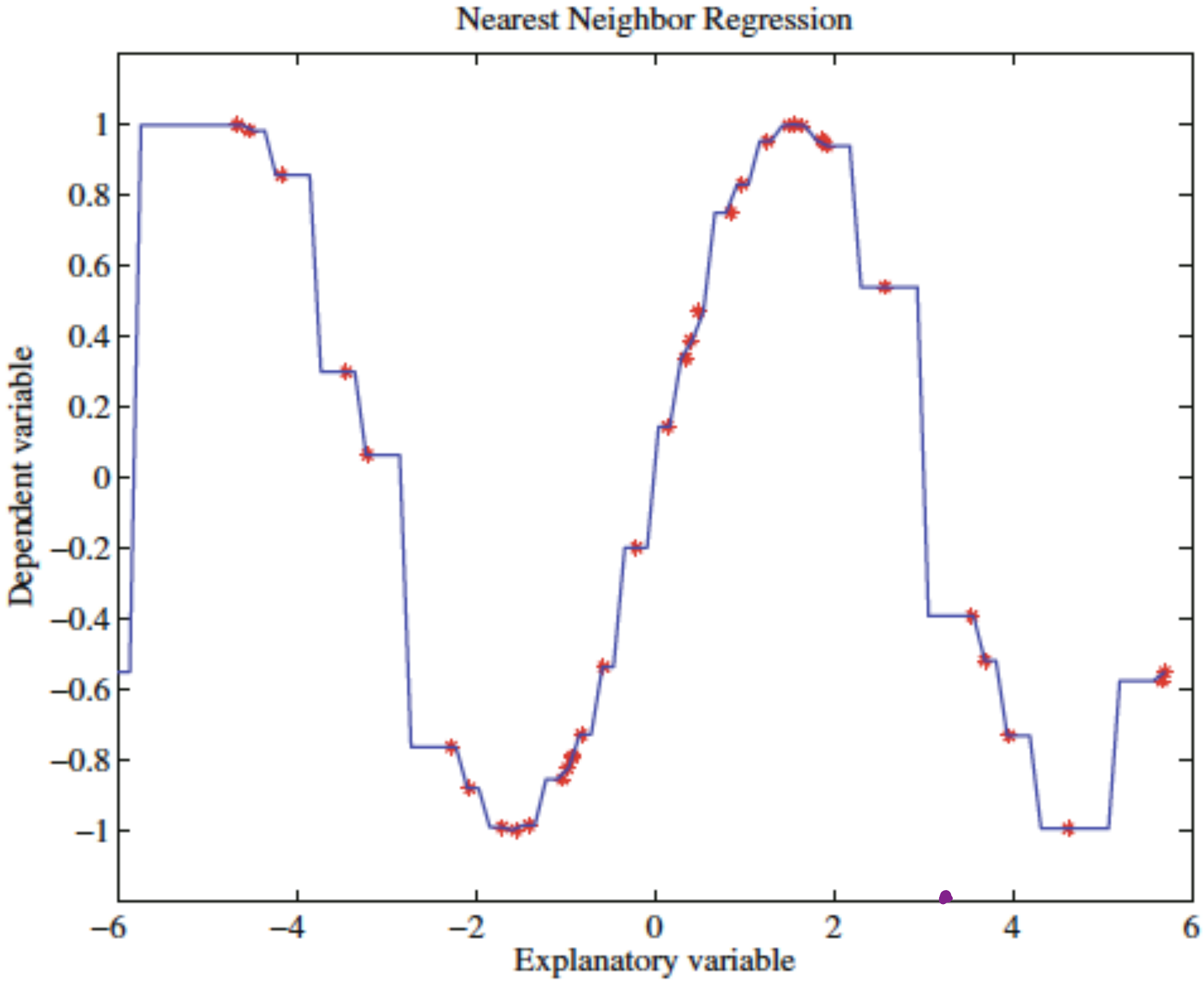
# Nearest neighbor regression

- In addition to linear regression and generalize linear regression models, there are methods such as **Nearest neighbor regression** that do not need much training for the model parameters.
- When there is plenty of data, nearest neighbors regression can be used effectively

# K nearest neighbor regression with k=1

The idea is very similar to k-nearest neighbor classifier, but the regression model predicts numbers

K=1 gives piecewise constant predictions



# K nearest neighbor regression with weights

The goal is to predict $y_0^p$ from $\mathbf{x}_0$ using a training set $\{(\mathbf{x}, y)\}$


- Let $\{(\mathbf{x}_j, \mathbf{y}_j)\}$ be the set of k items in the training data set that are closest to $\mathbf{x}_0$.
- Prediction is the following:

$$\mathbf{y}_0^p = \frac{\sum_j^{k} \mathbf{w}_j \mathbf{y}_j}{\sum_j \mathbf{w}_j}$$

Where $\mathbf{w}_j$ are weights that drop off as $\mathbf{x}_j$ gets further away from $\mathbf{x}_0$.

$w_j \downarrow$ as dist $\uparrow$

$w_j \uparrow$ as dist $\downarrow$

# Choose different weights functions for KNN regression

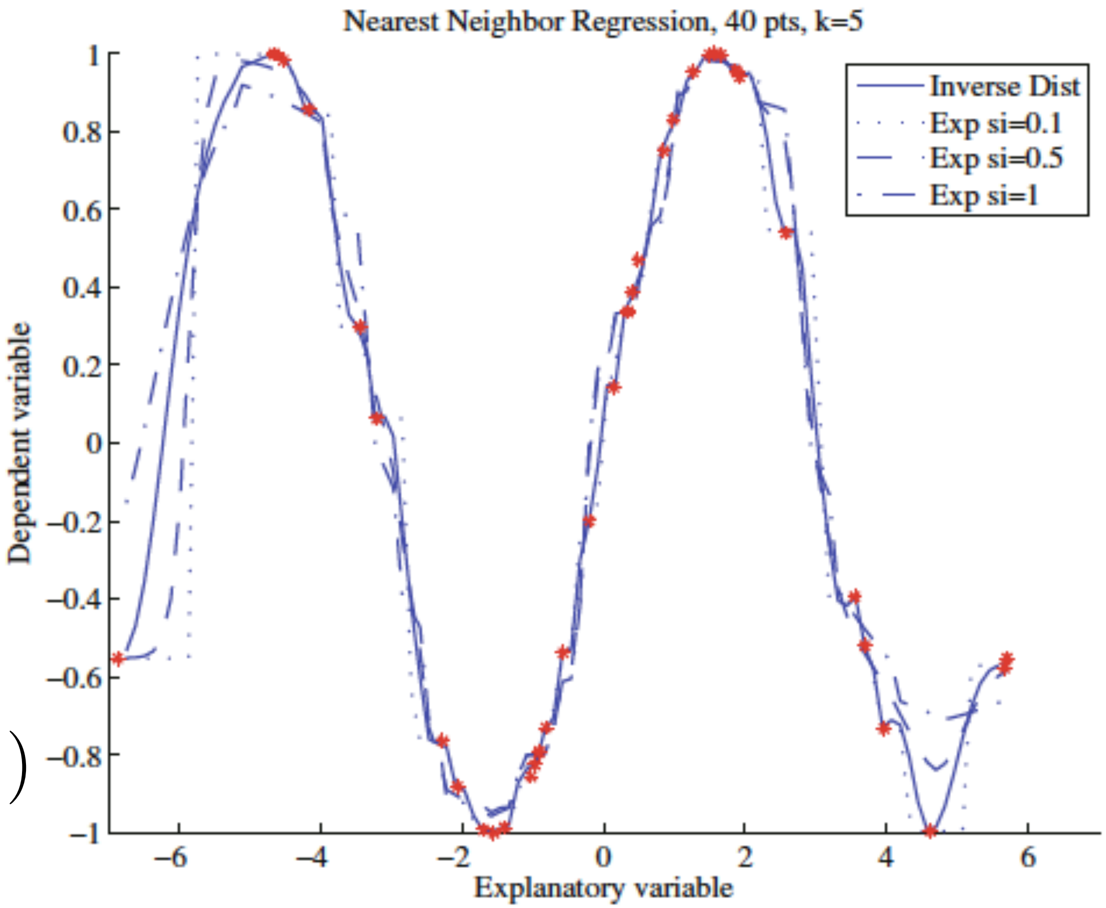
$$\mathbf{y}_0^p = \frac{\sum_j \mathbf{w}_j \mathbf{y}_j}{\sum_j \mathbf{w}_j}$$

- Inverse distance

$$\mathbf{w}_j = \frac{1}{\|\mathbf{x}_0 - \mathbf{x}_j\|}$$

- Exponential function

$$\mathbf{w}_j = exp(-\frac{\|\mathbf{x}_0 - \mathbf{x}_j\|^2}{2\sigma^2})$$



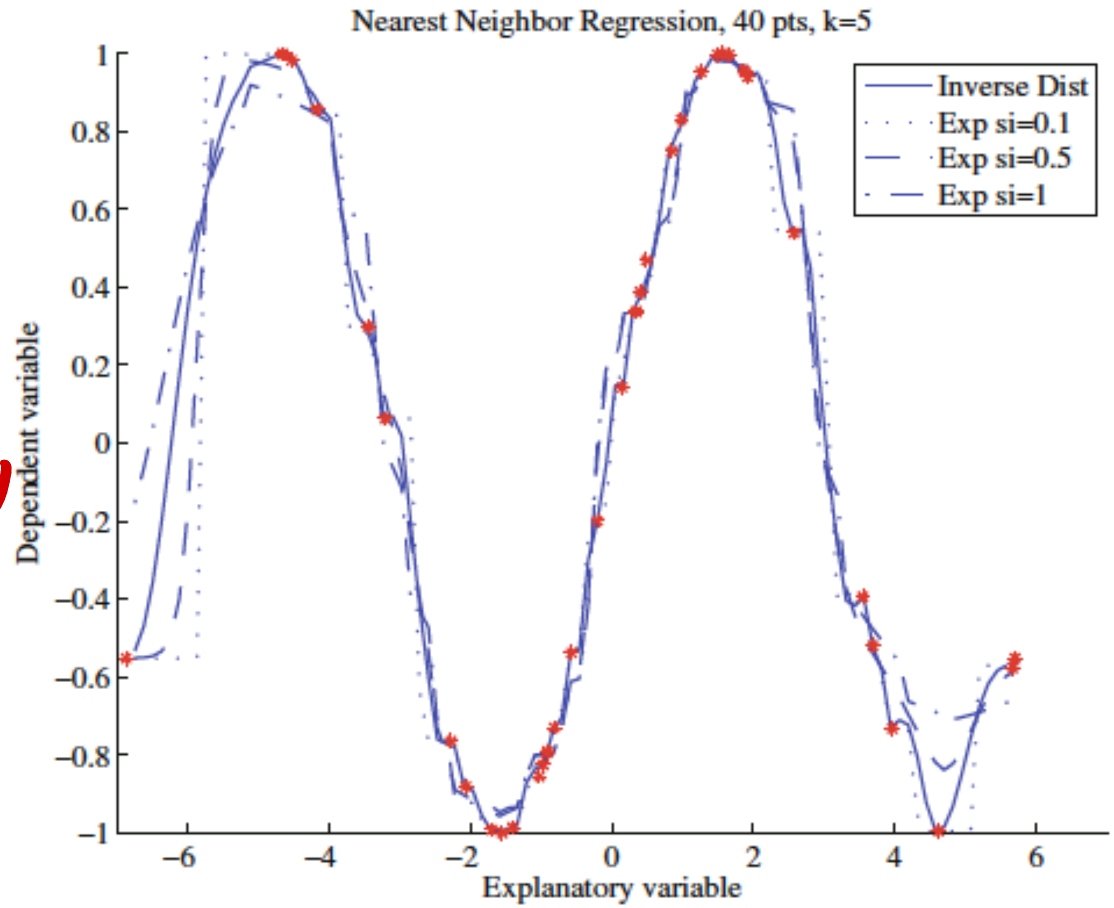
# Evaluation of KNN models

- Which methods do you use to choose K and weight functions?

  A. Cross validation

  B. Evaluation of MSE

  C. Both A and B



# The Pros and Cons of K nearest neighbor regression

- Pros:
  - The method is very intuitive and simple
  - You can predict more than numbers as long as you can define a similarity measure.
- Cons
  - The method doesn't work well for very high dimensional data
  - The model depends on the scale of the data

| Fruit | y |
| --- | --- |
| Apple | 5 |
| pear | 6 |
| banana | 5.5 |

# Assignments

- Finish Chapter 13 of the textbook
- Week 13 module including the quiz
- Next time: Curse of Dimension, clustering

# Additional References

- Robert V. Hogg, Elliot A. Tanis and Dale L. Zimmerman. "Probability and Statistical Inference"
- Kelvin Murphy, "Machine learning, A Probabilistic perspective"

# See you next time

*See You!*