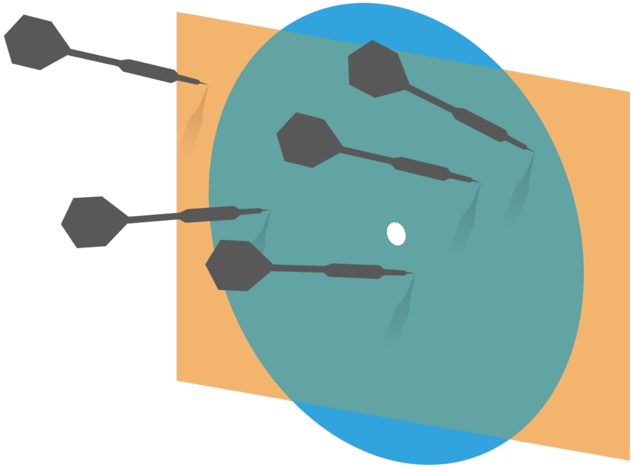
Probability and Statistics for Computer Science



Credit: wikipedia

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

Hongye Liu, Teaching Assistant Prof, CS361, UIUC, 11.27.2021

Last time

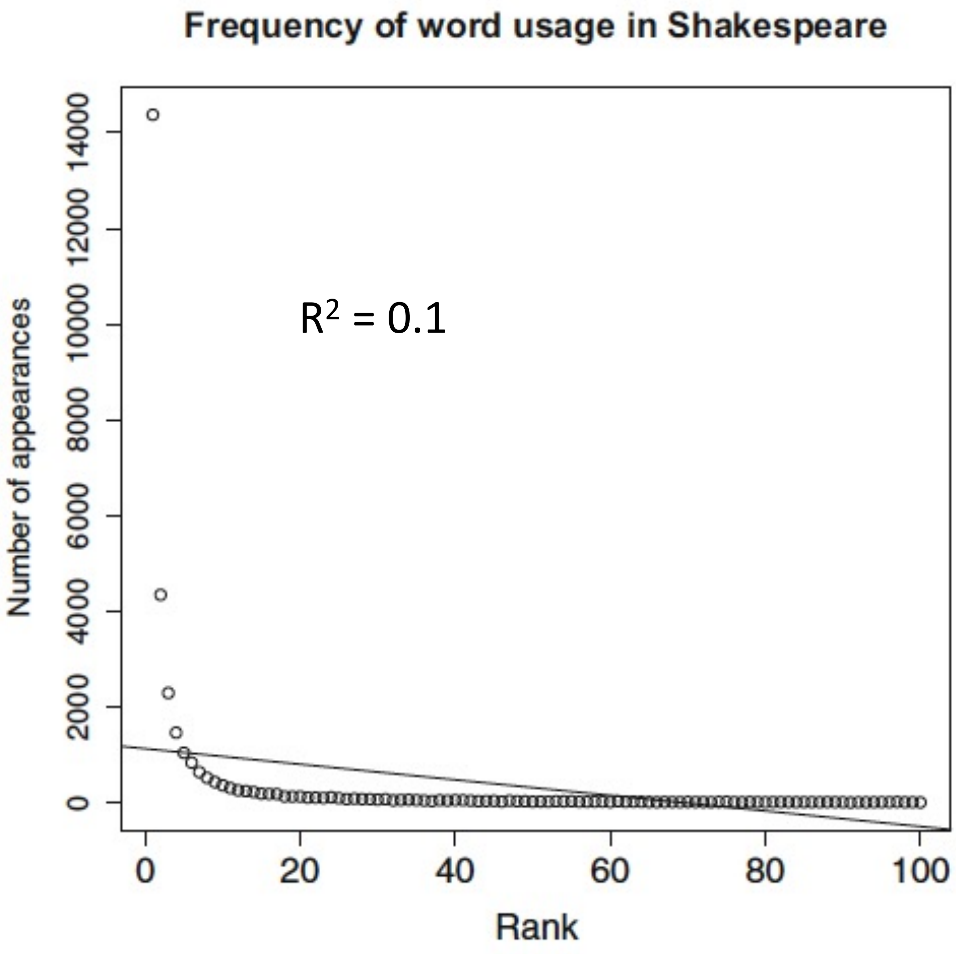
- Linear regression
  - The problem
  - The least square solution
  - The training and prediction
  - The R-squared for the evaluation of the fit.

Objectives

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

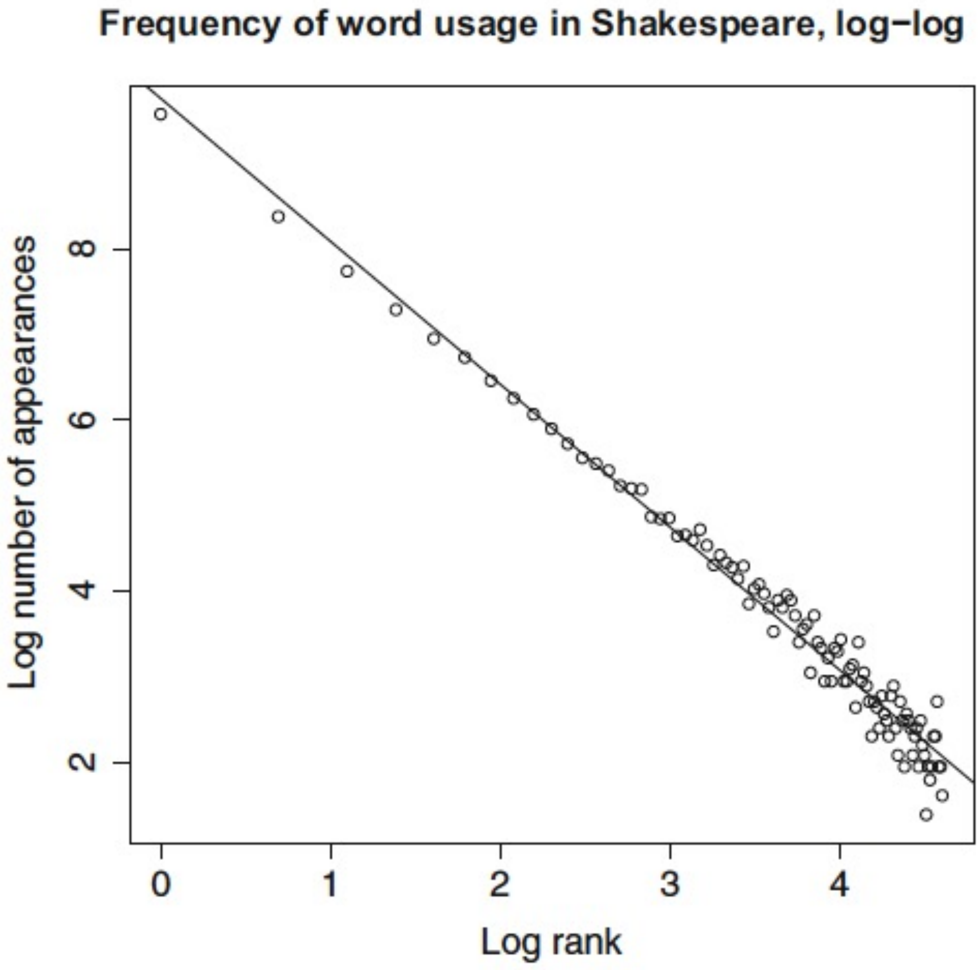
What if the relationship between variables is non-linear?

- 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.



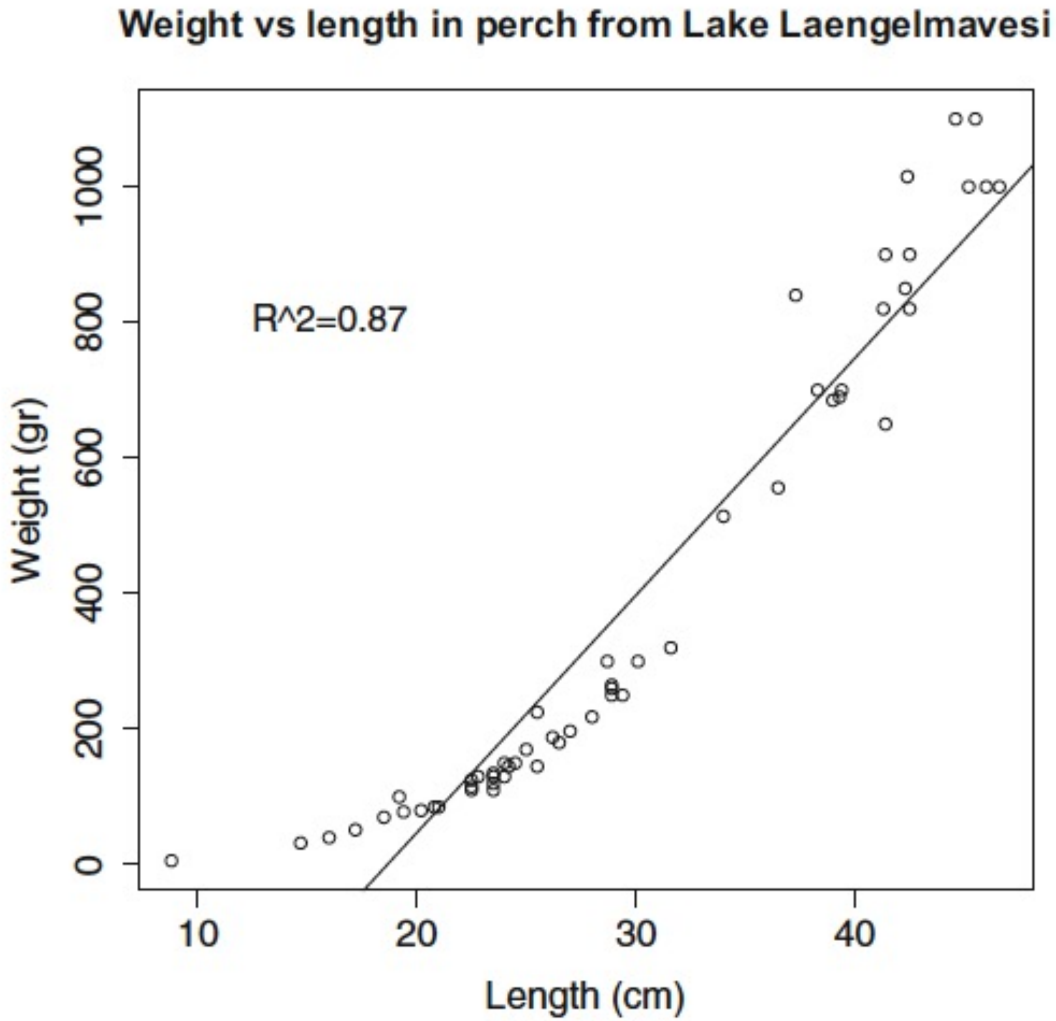
More example: Data of fish in a Finland lake

- 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

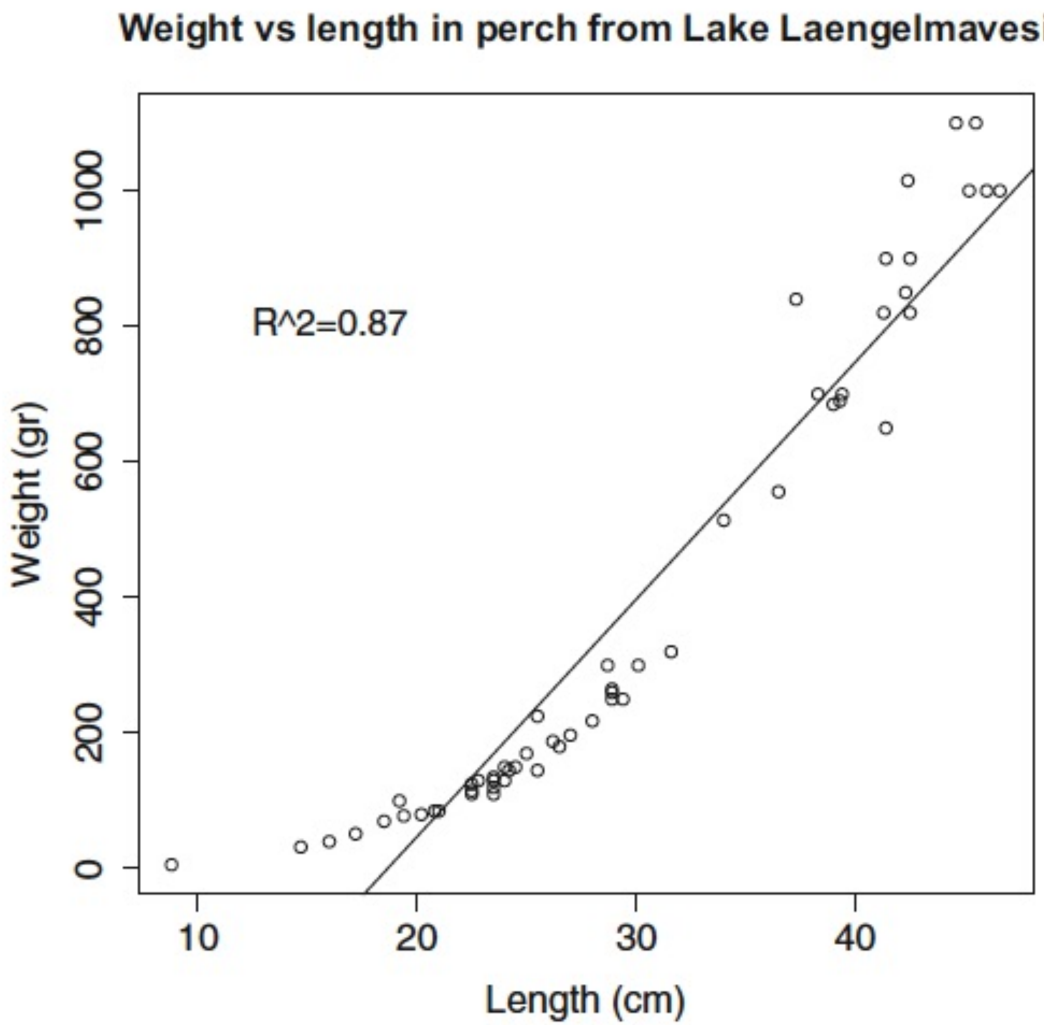
Is the linear model fine for this data?

A. YES
B. NO

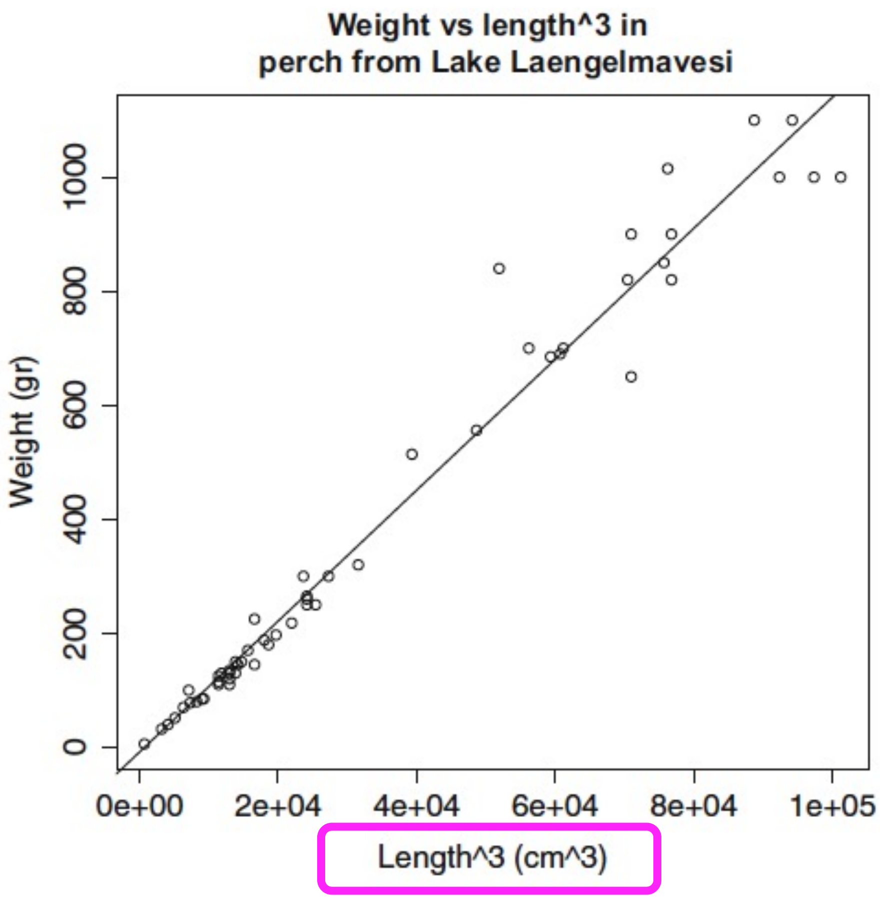


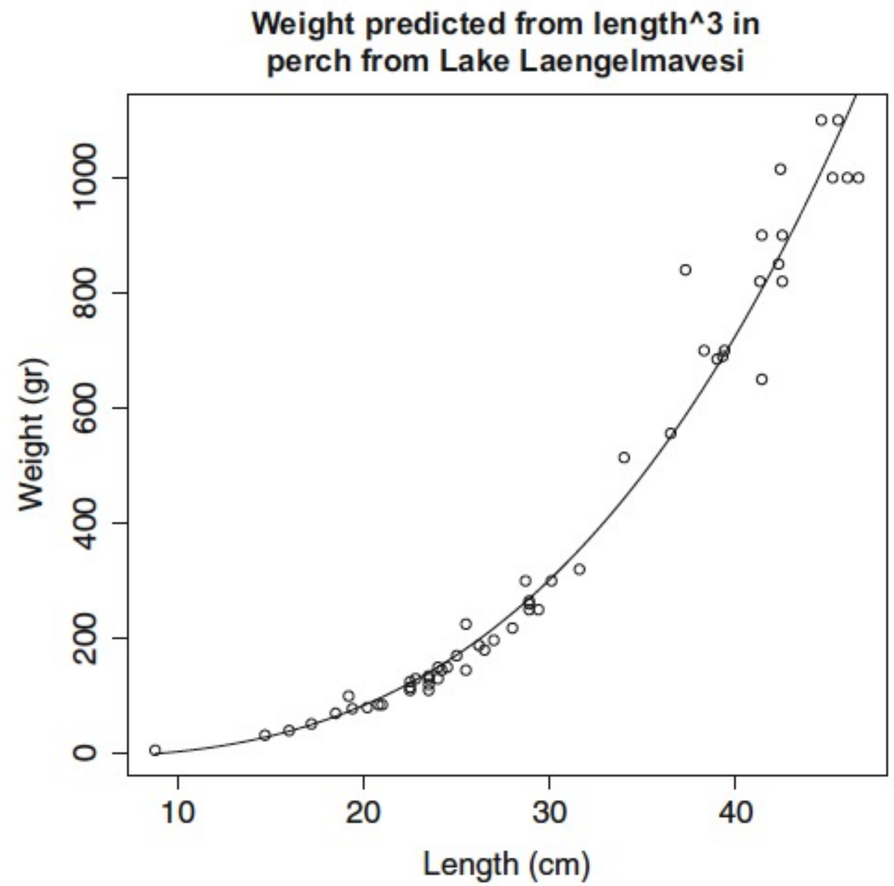
Is the linear model fine for this data?

- 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

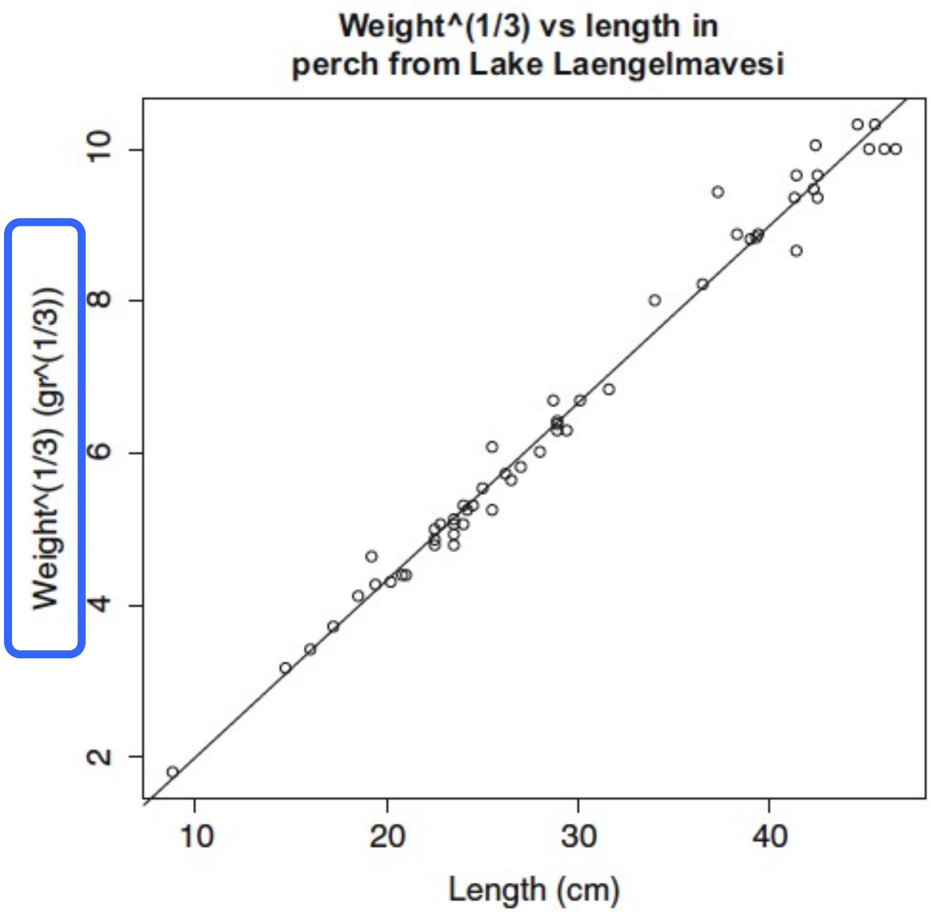


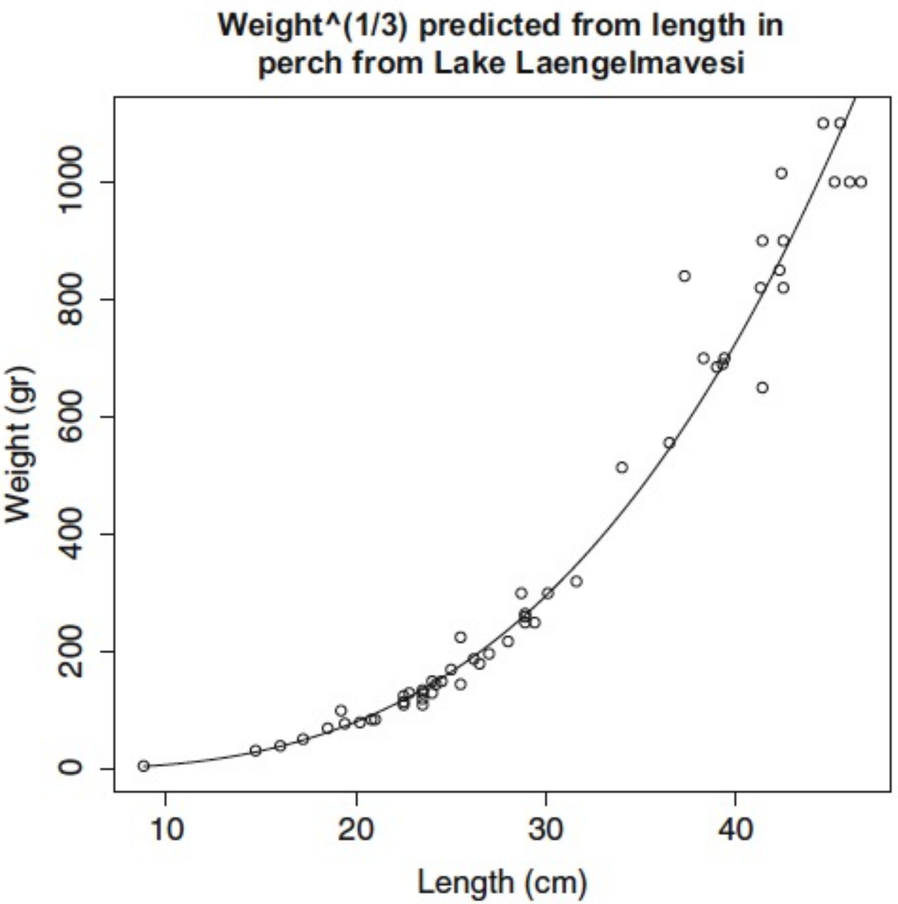


Q. What are the matrix X and y?

1	$Length^3$	Weight

Transforming the dependent variables





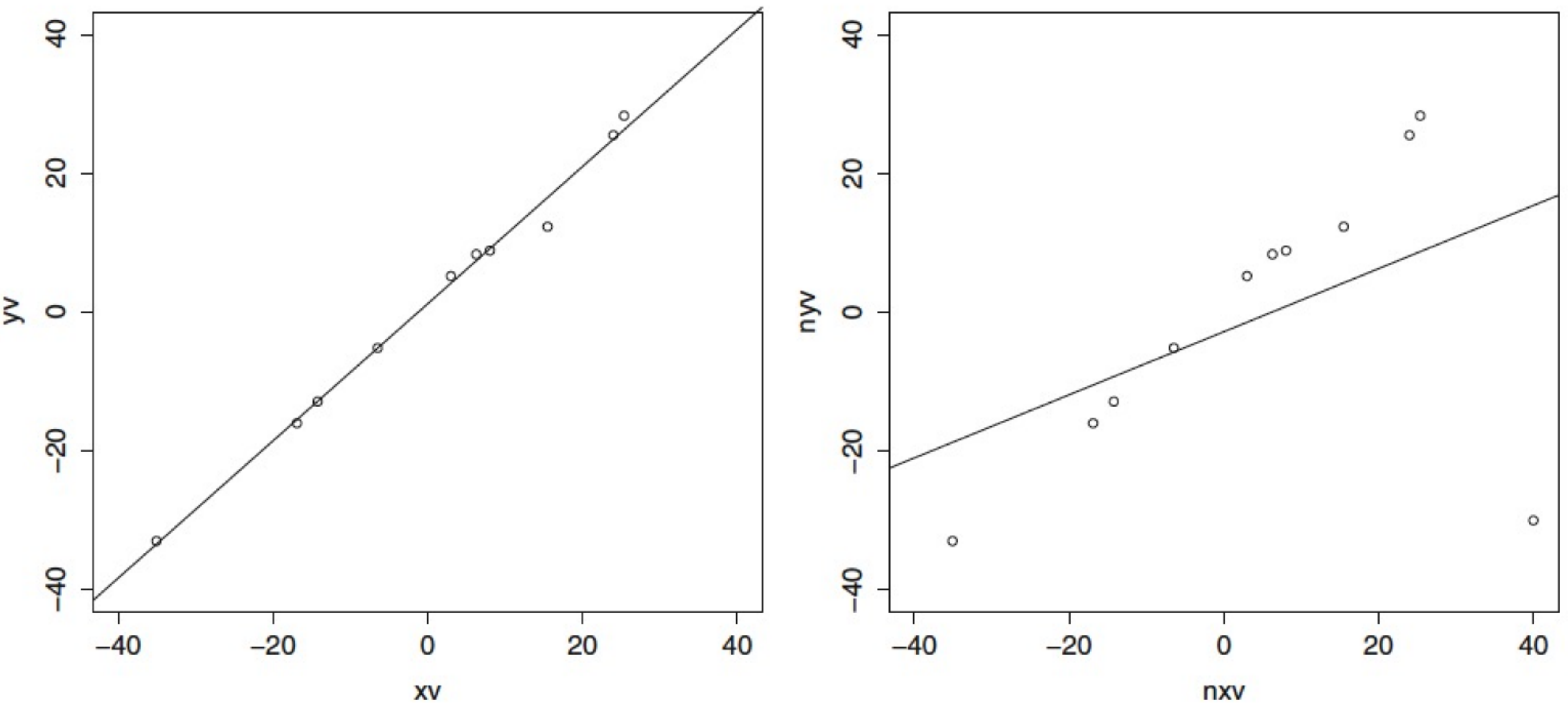
What is the model now?

What are the matrix X and y?

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

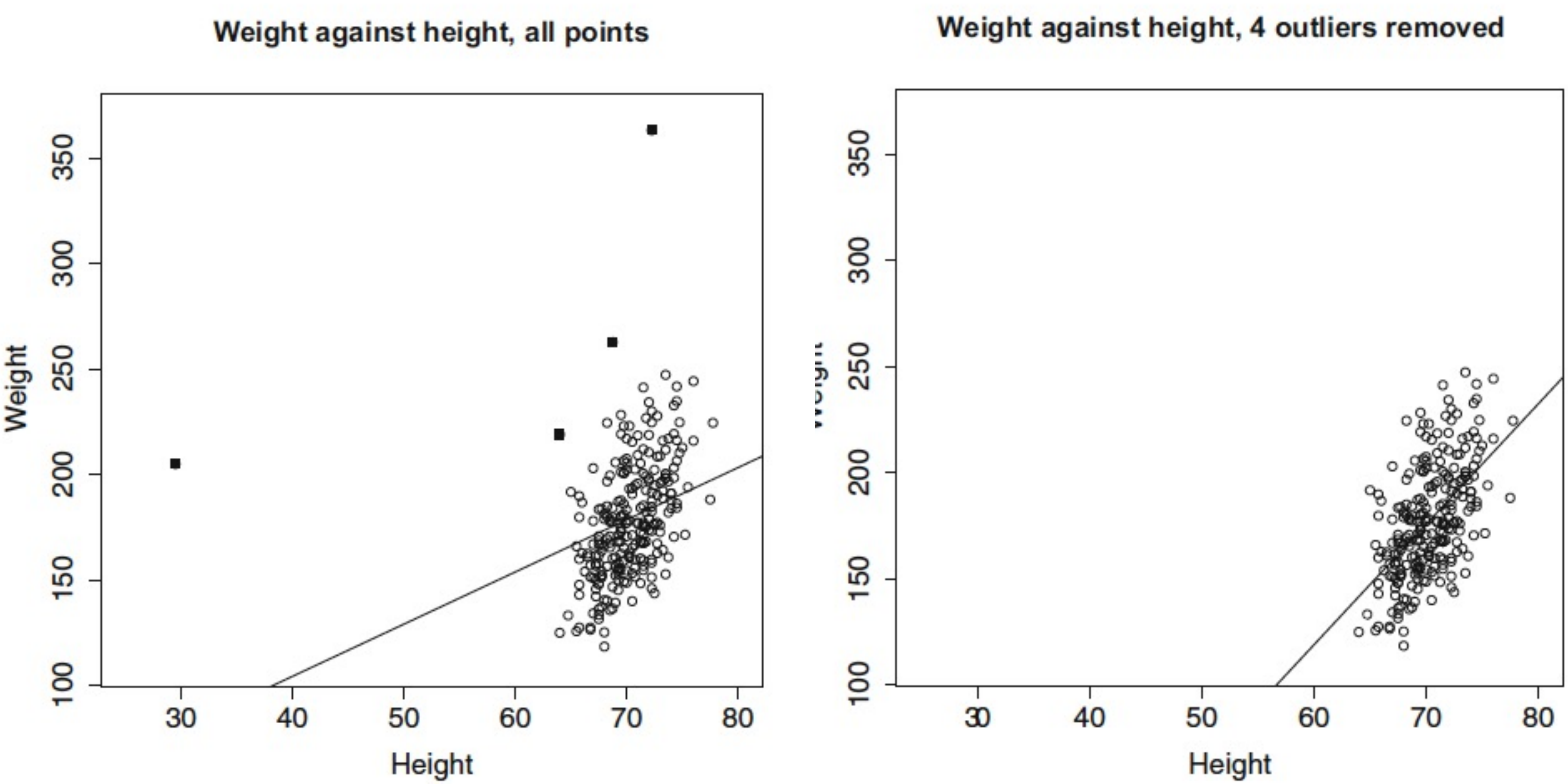
Effect of outliers on linear regression

- Linear regression is sensitive to outliers

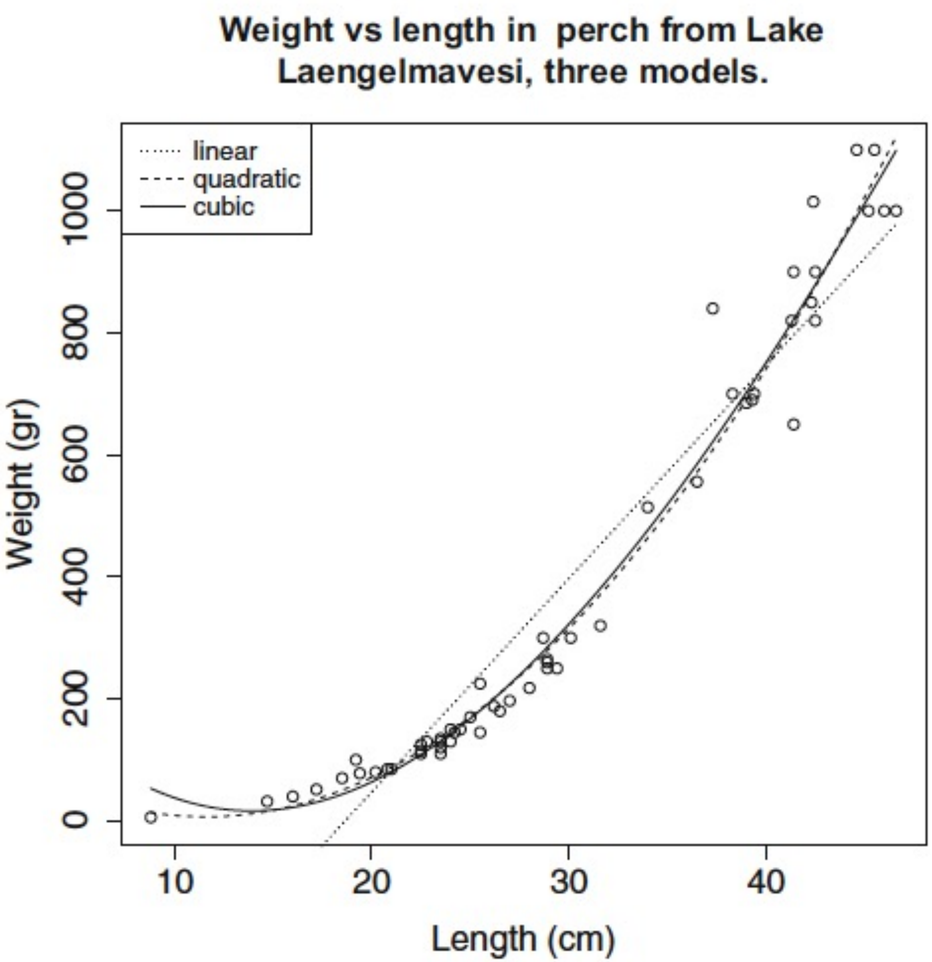


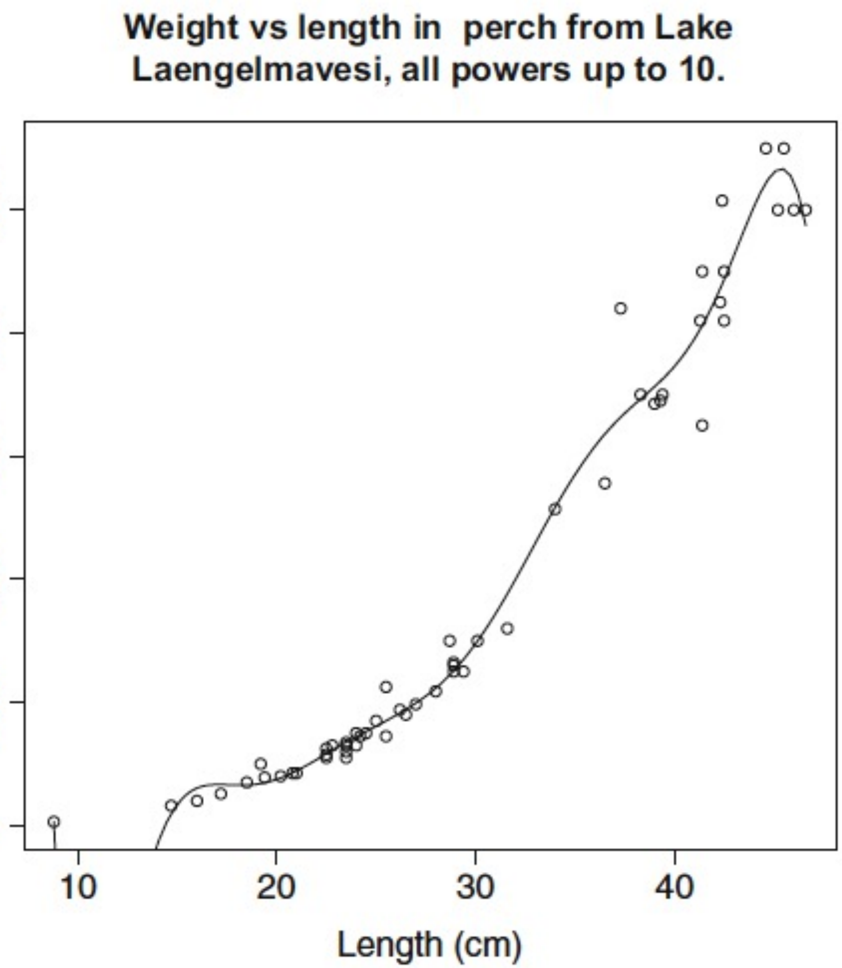
Effect of outliers: body fat example

- 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.
- **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

Regularized linear regression

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

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

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

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

Training using regularized least squares

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

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

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

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

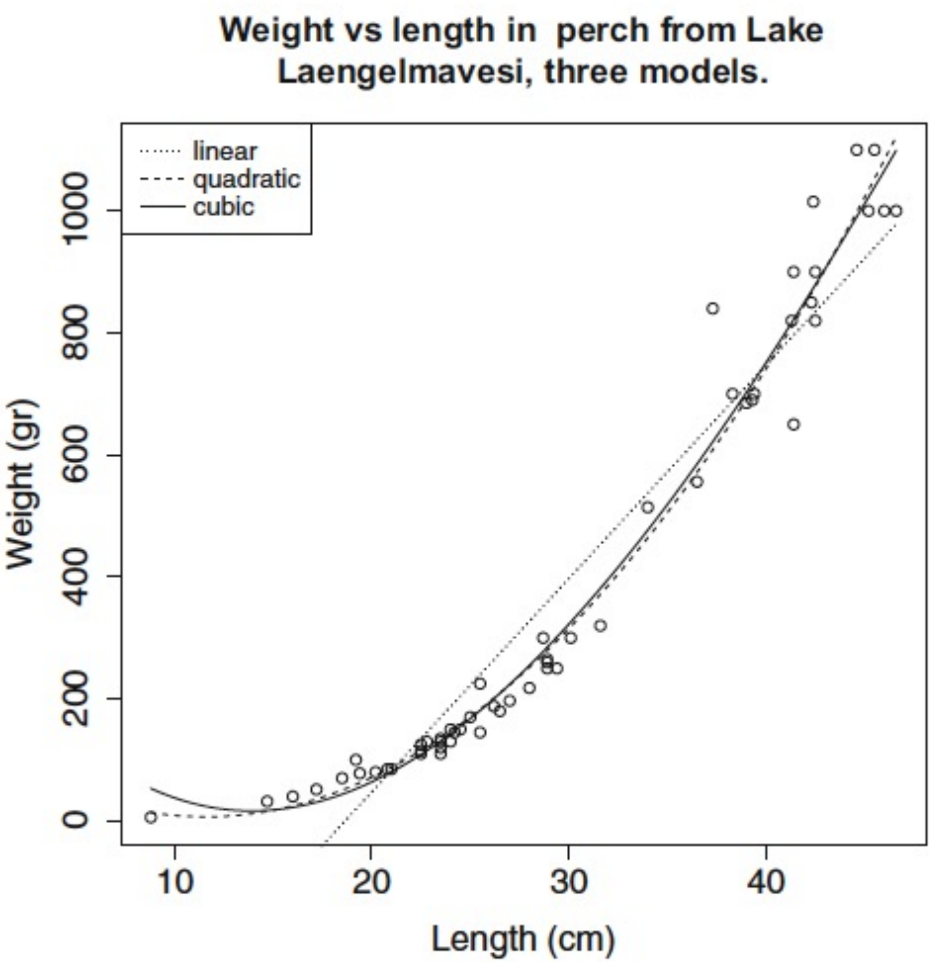
Why is the regularized version always invertible?

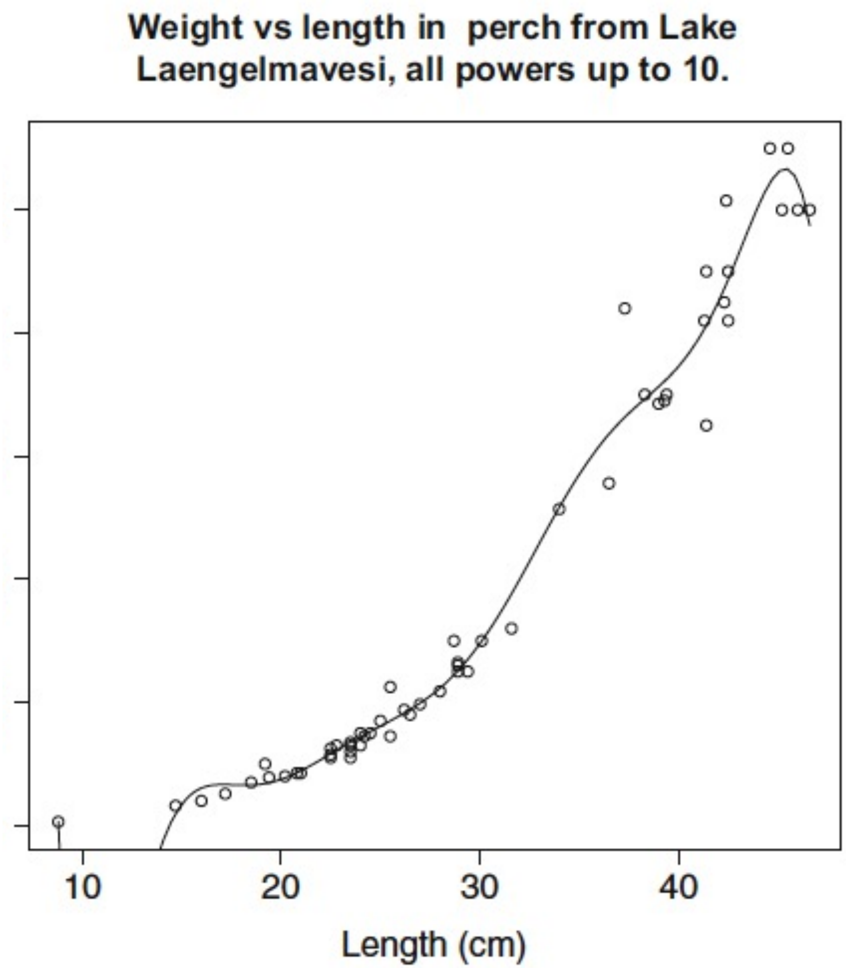
Prove: $(X^T X + \lambda I)$ is invertible (λ>0, λ is not the eigenvalue).

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

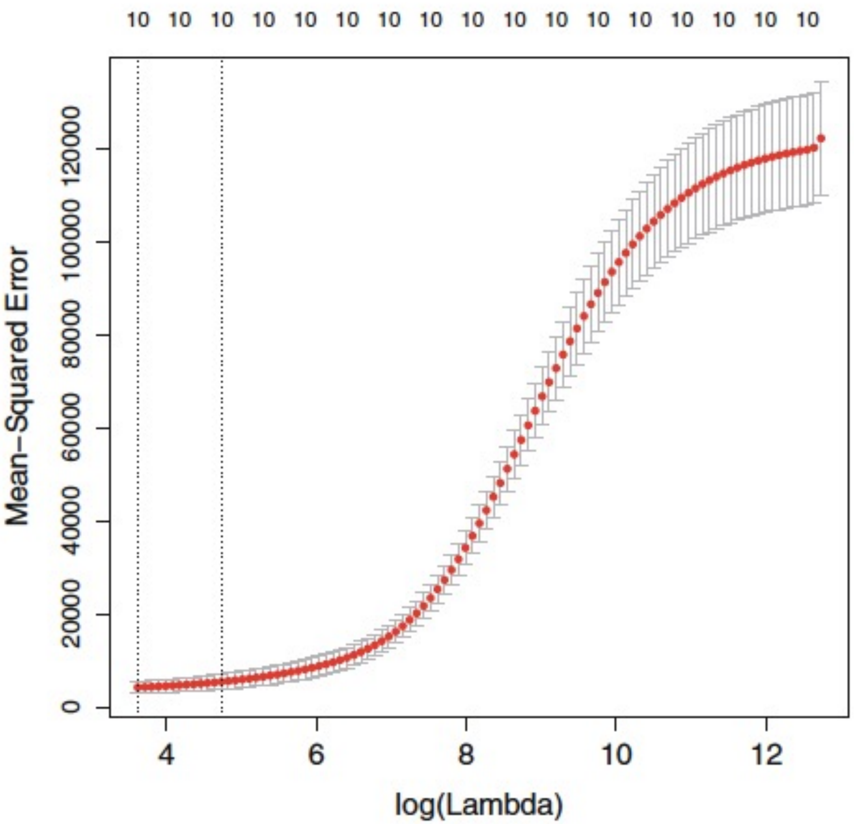
$$f^T A f > 0$$

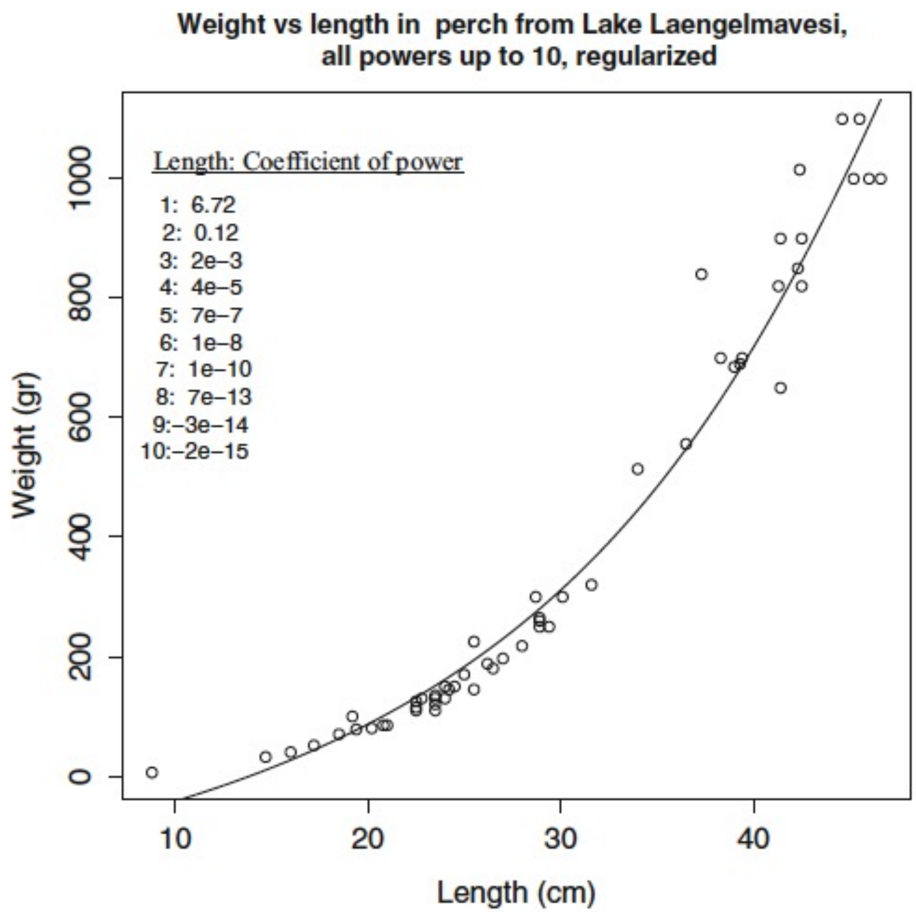
Over-fitting issue: example from using too many power transformations





Choosing lambda using cross-validation





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

A. YES
B. NO
C. YES and NO

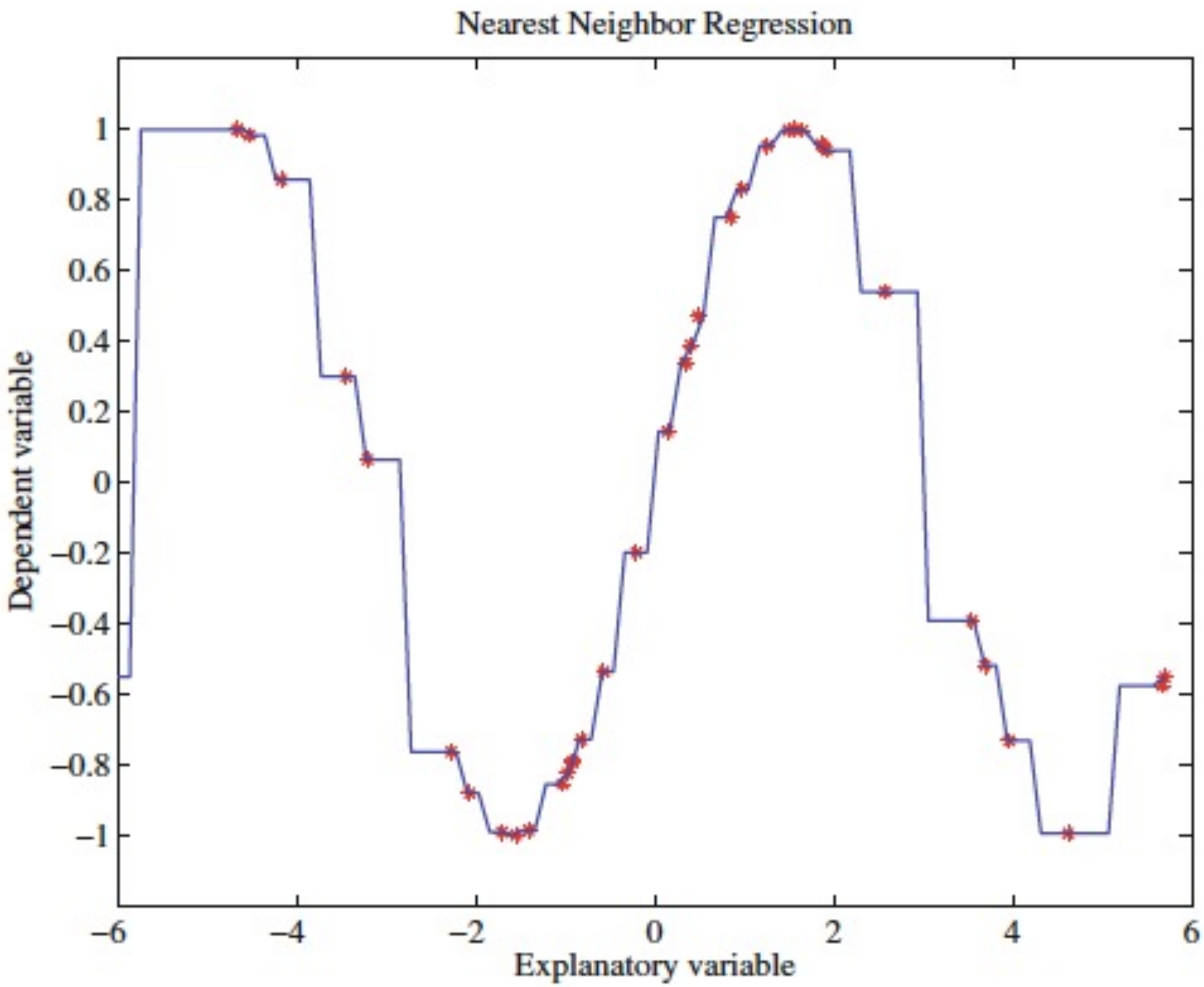
Nearest neighbor regression

- 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:

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

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

Choose different weights functions for KNN regression

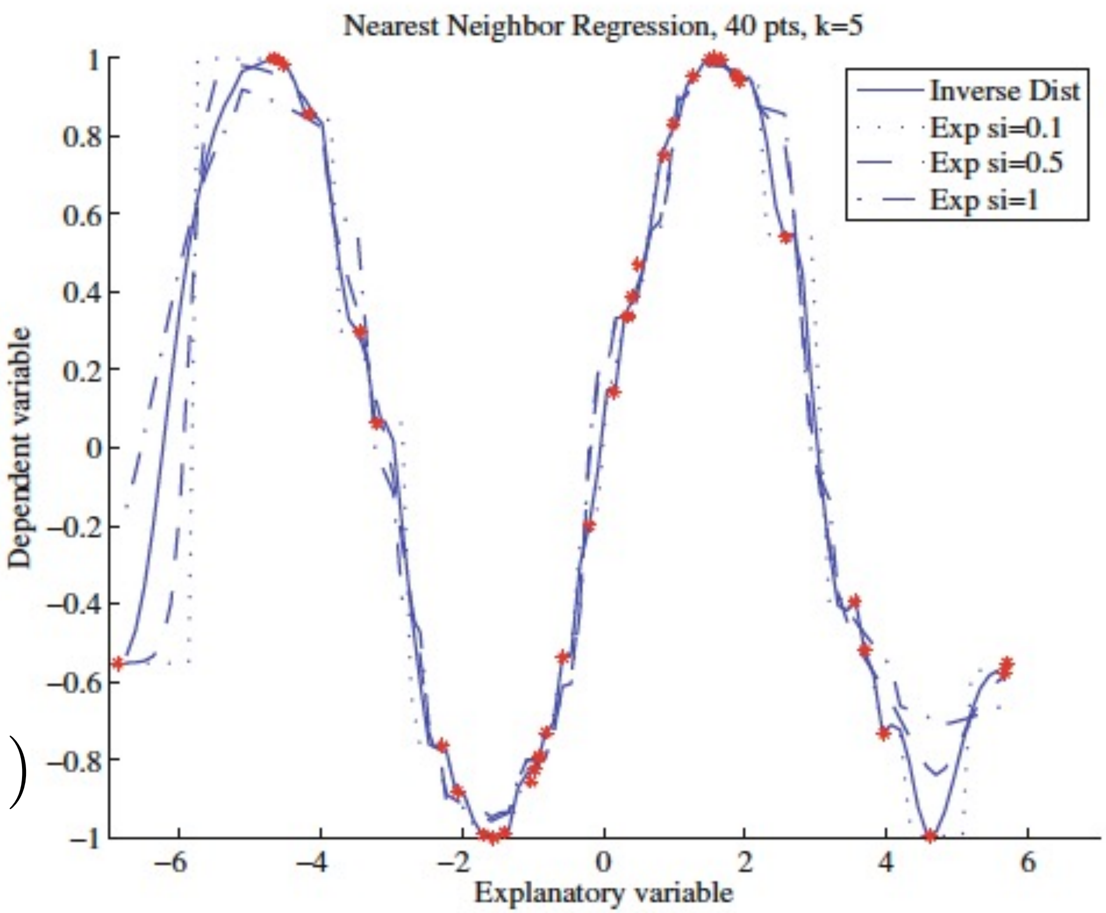
$$\mathbf{y}_0^p = \frac{\sum_j \mathbf{w}_j \mathbf{y}_j}{\sum_j \mathbf{w}_j}$$

- Inverse distance

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

- Exponential function

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



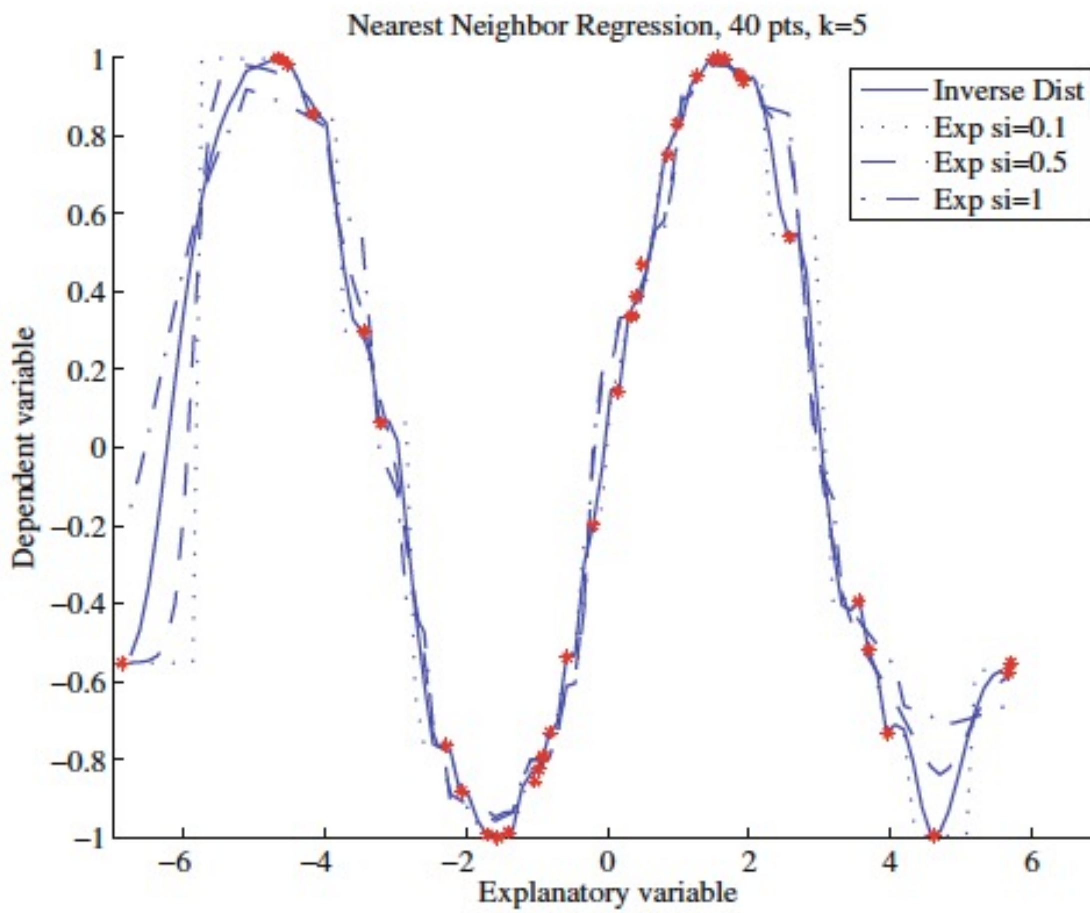
Evaluation of KNN models

- 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

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!