S&DS 265 / 565

Introductory Machine Learning

Some Context and Concepts

Thursday, September 9

Yale

Logistics

- Recordings posted to Canvas under Media Library
- Assignment 1 posted on Tuesday
- Quiz 0 available on Canvas at noon today, for 24 hours
- Check Canvas / EdD for office hours

Plan for Today

- Continue Python elements
- Basics of classification, regression, overfitting
- Linear regression example

Some Terminology

- supervised vs. unsupervised
- classification vs. regression
- prediction vs. inference

Supervised Learning vs. Unsupervised Learning

Supervised learning:

- Given a set of (x, y), learn to predict y using x.
- e.g.
  - Predicting whether a loan will default based on customer characteristics

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Unsupervised learning:

- Given a set of x, learn underlying structure or relationships of x.
- e.g.
  - Identifying market segments with similar spending patterns.

Classification vs. Regression

The `Income` dataset:

Education	Seniority	Income
21.58621	113.1034	99.91717
18.27586	119.3103	92.57913
12.06897	100.6897	34.67873
17.03448	187.5862	78.70281
19.93103	20.0000	68.00992
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Information for 30 *simulated individuals*.

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Regression: Model income based on other characteristics.

Classification: Model whether someone will earn above the median income based on other characteristics.

Inference vs. Prediction

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Prediction: accurately predict Y for new observations

Inference: explain the underlying relationship between Y and X

Example: Handwritten Digit Recognition

- Data: images of handwritten digits (grayscale pixel values)
- Classify images as digits 0 to 9.

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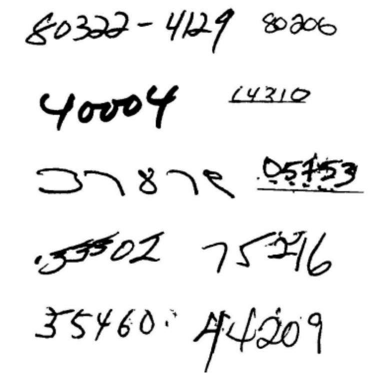

Regression Example

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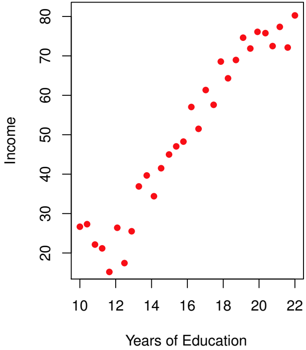

Quantitative response Y

Predictors $X = (X_1, \ldots, X_p)$

Assume the relationship can be expressed by:

$$Y = f(X) + \epsilon,$$

where f is a fixed, unknown function and ϵ is error term.

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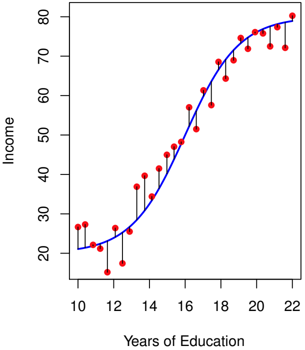

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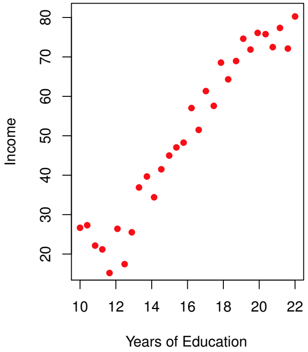
Regression Example

Back to regression with $p = 1$:



$$Y = f(X) + \epsilon$$

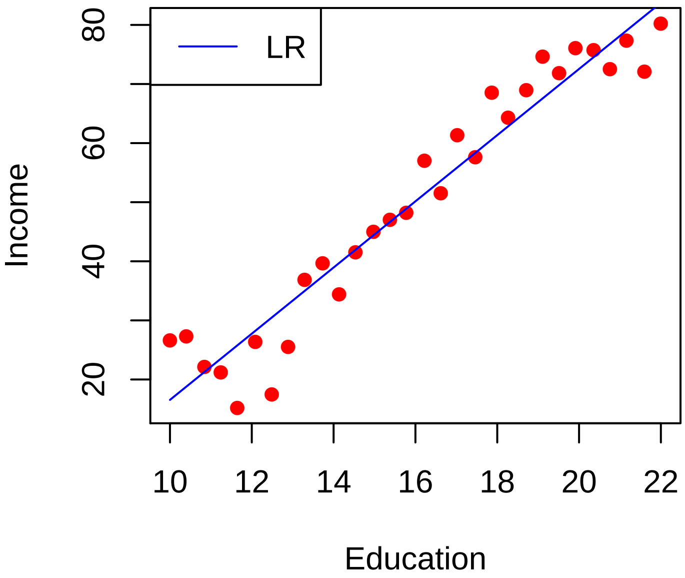
Modeling:

Use a procedure to get $\widehat{f}$. Derive estimates $\widehat{Y} = \widehat{f}(X)$.

Possible Regression Approaches

- linear regression
  - Fitting a straight line through the data.
- k-nearest neighbors regression
  - Average together the y_i for x_i close to x

Possible Regression Approaches



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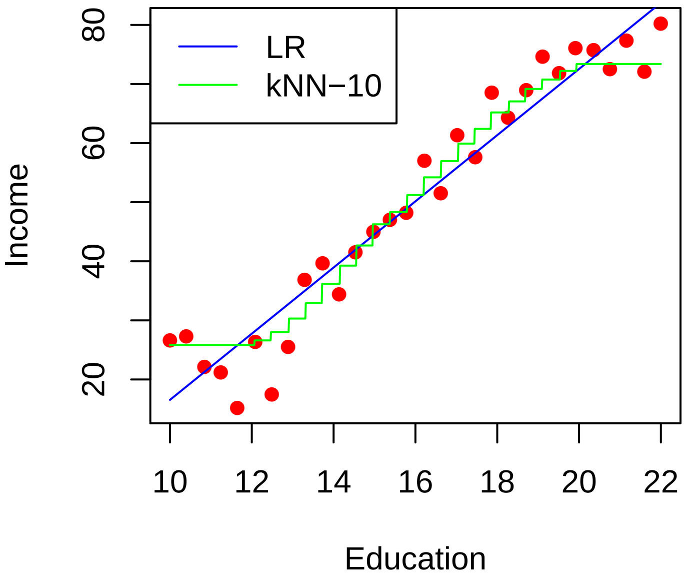

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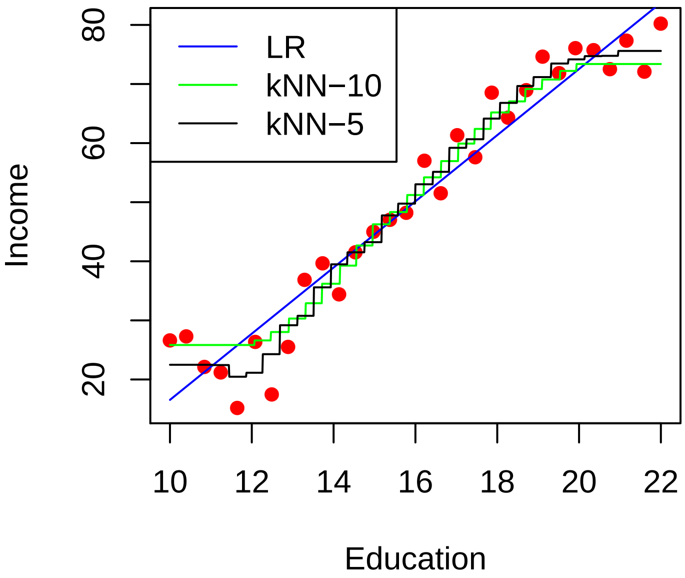

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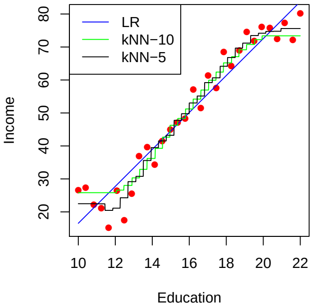

Measuring performance via **Mean Squared Error**

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \widehat{f}(x_i))^2$$

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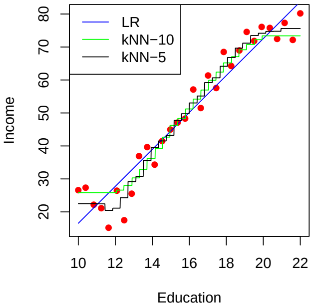

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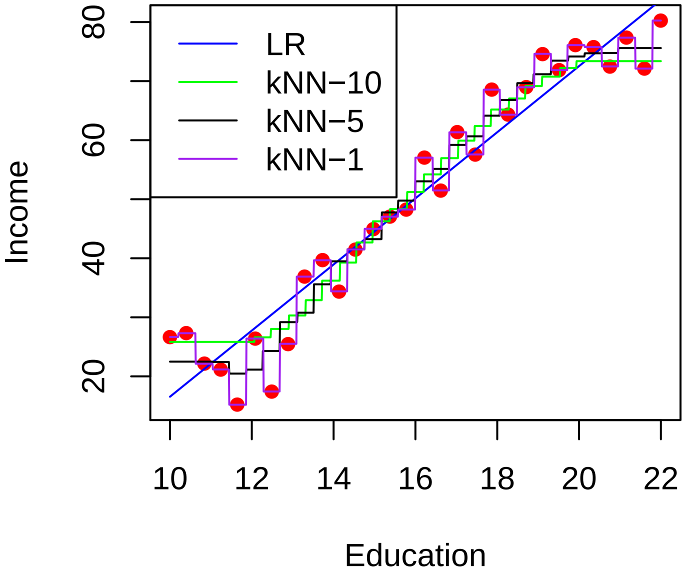
MSEs for three methods:

Linear Regression	29.829
k-Nearest Neighbors (k=10)	23.519
k-Nearest Neighbors (k=5)	16.21

A k-nearest neighbors model with $k = 5$ achieves lowest error. Is it the best?


LR
kNN−10
kNN−5
kNN−1
Income
Education
20
40
60
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22

Training MSE vs. Test MSE

MSE in the previous table, **training MSE**, was computed based on data used in fitting the model.

We are more interested in **test MSE** computed on *unseen data*.

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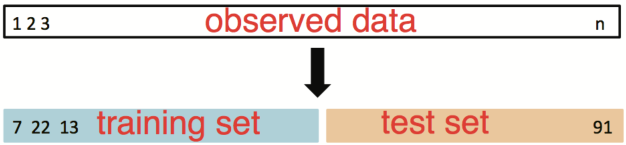
We can randomly split our data into a test set and a training set.



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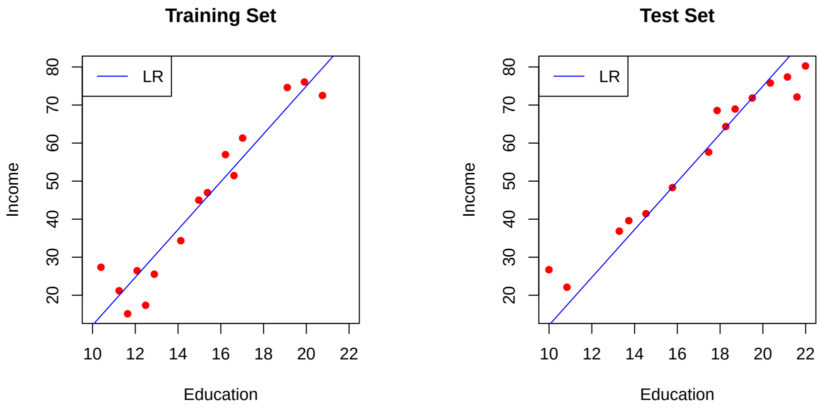

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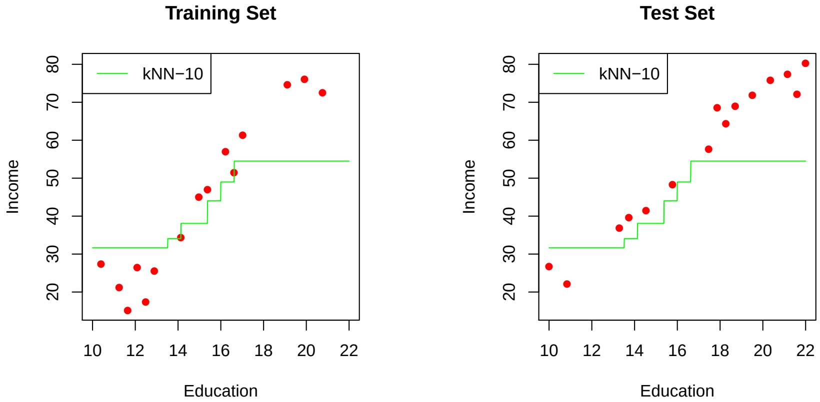

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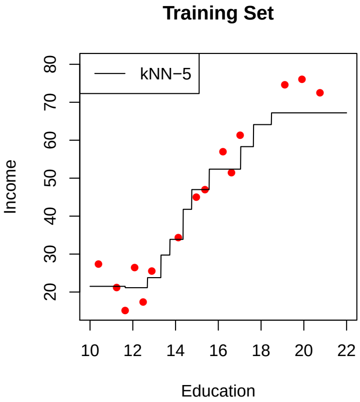

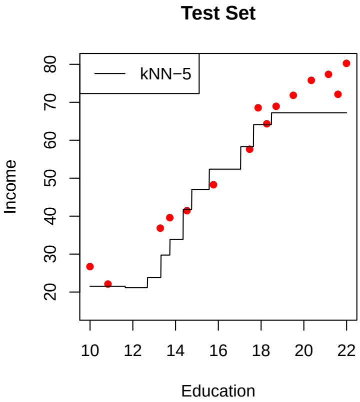

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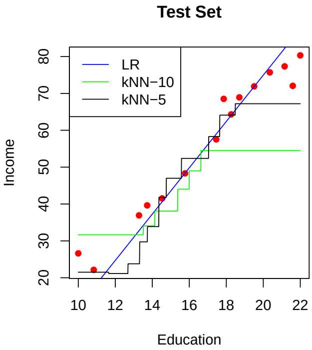

Compute MSE on the test set:

$$MSE = \frac{1}{n}\sum(y_i - \widehat{f}(x_i))^2$$

Linear Regression	37.807
k-Nearest Neighbors (k=10)	197.809
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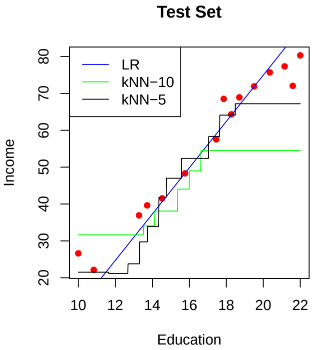

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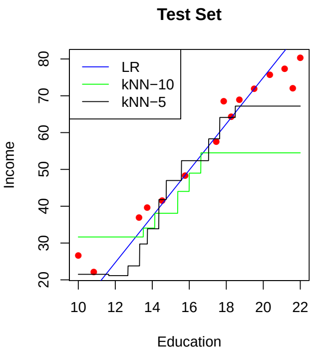

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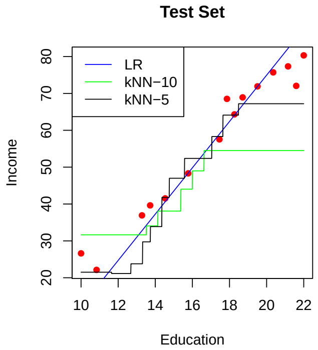

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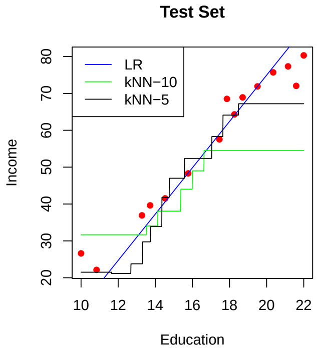

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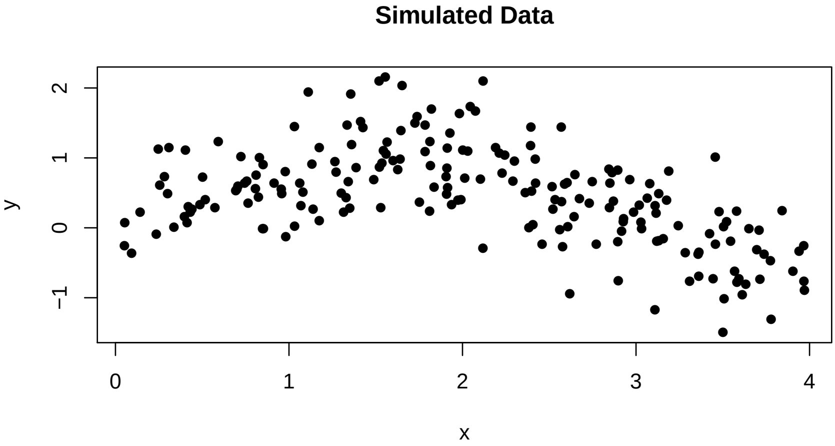

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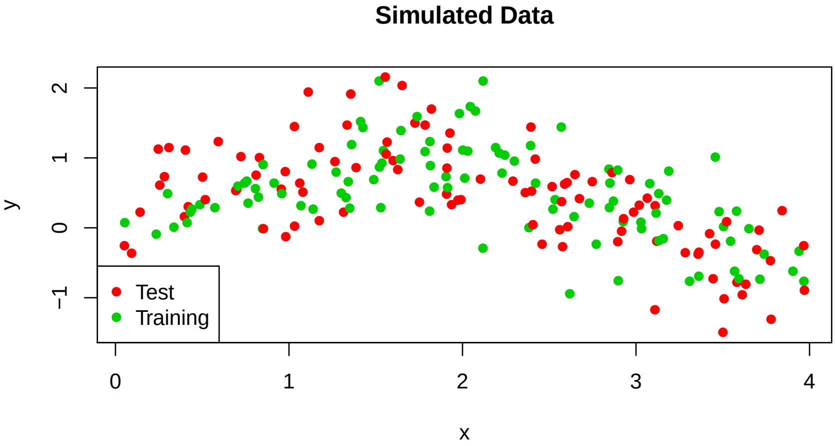

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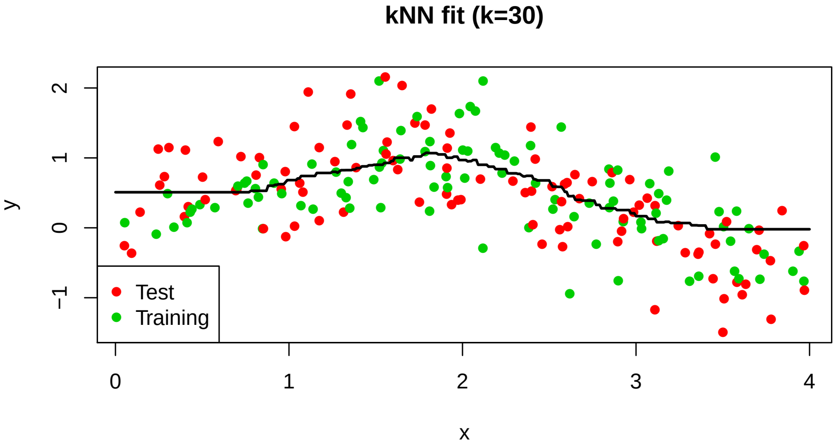

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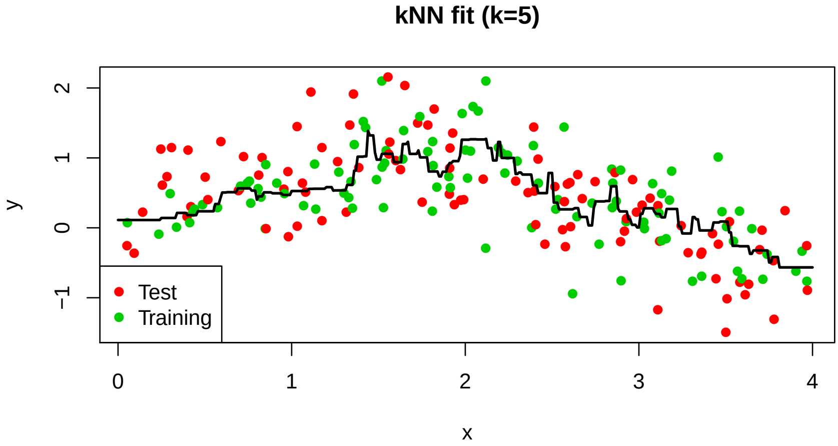
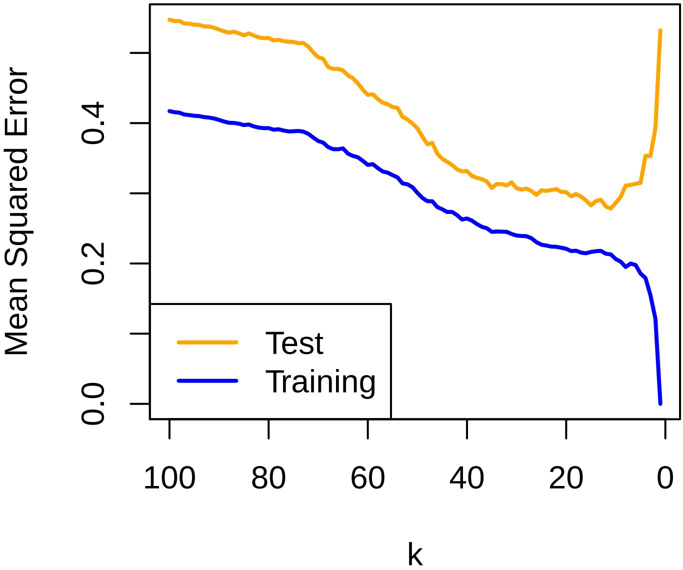


Overfitting via k-Nearest Neighbors



Summary

- Two cultures: model based and prediction based
- Prediction based approaches are sometimes not interpretable
- Overfitting is easy with very flexible models and algorithms

Next week: Linear regression and classification