Regression

IE500 Data Mining

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What is Regression?

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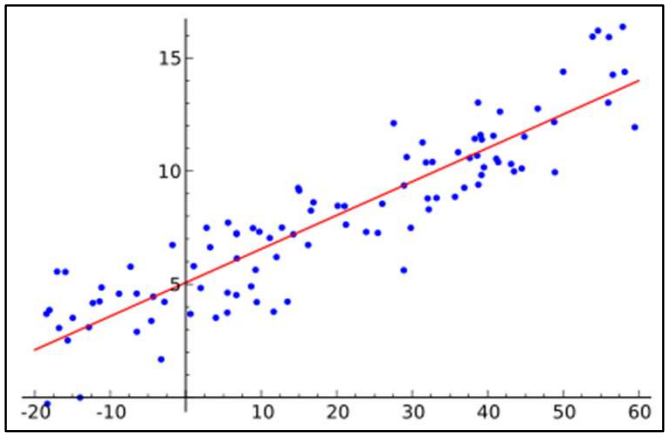
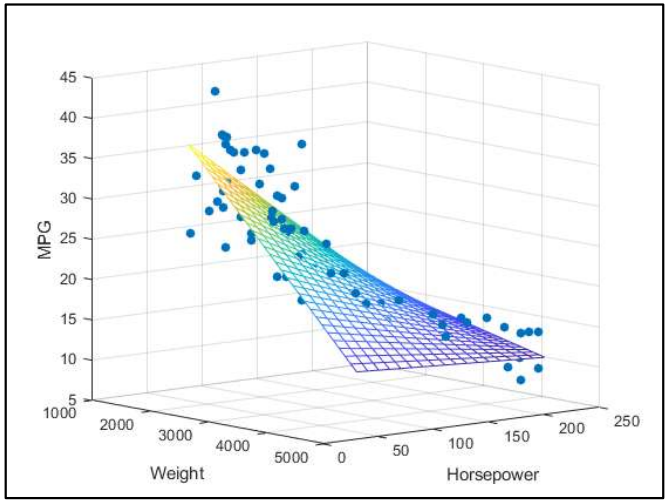
- Goal: **predict a numerical value** from a possibly infinite set of possible values
- The predicted variable is called **dependent and is denoted $\hat{y}$**
- The other variables are called **explanatory variables or independent variables** denoted $X = x_1, x_2, \ldots, x_n$





The Regression Problem

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- Examples
  - Weather Forecasting
    - Dependent: wind speed
    - Explanatory variables: temperature, humidity, air pressure change
  - House Market
    - Dependent: price of a house
    - Explanatory variables: rooms, distance to public transport, size of garden
- Regression vs. Classification
  - Classification
    - Algorithm “knows” all possible labels, e.g. yes/no, low/medium/high
    - All labels appear in the training data
    - The prediction is always one of those labels
  - Regression
    - Algorithm “knows” some possible values, e.g., 18°C and 21°C
    - Prediction may also be a value not in the training data, e.g., 20°C

Regression Model Learning and Application

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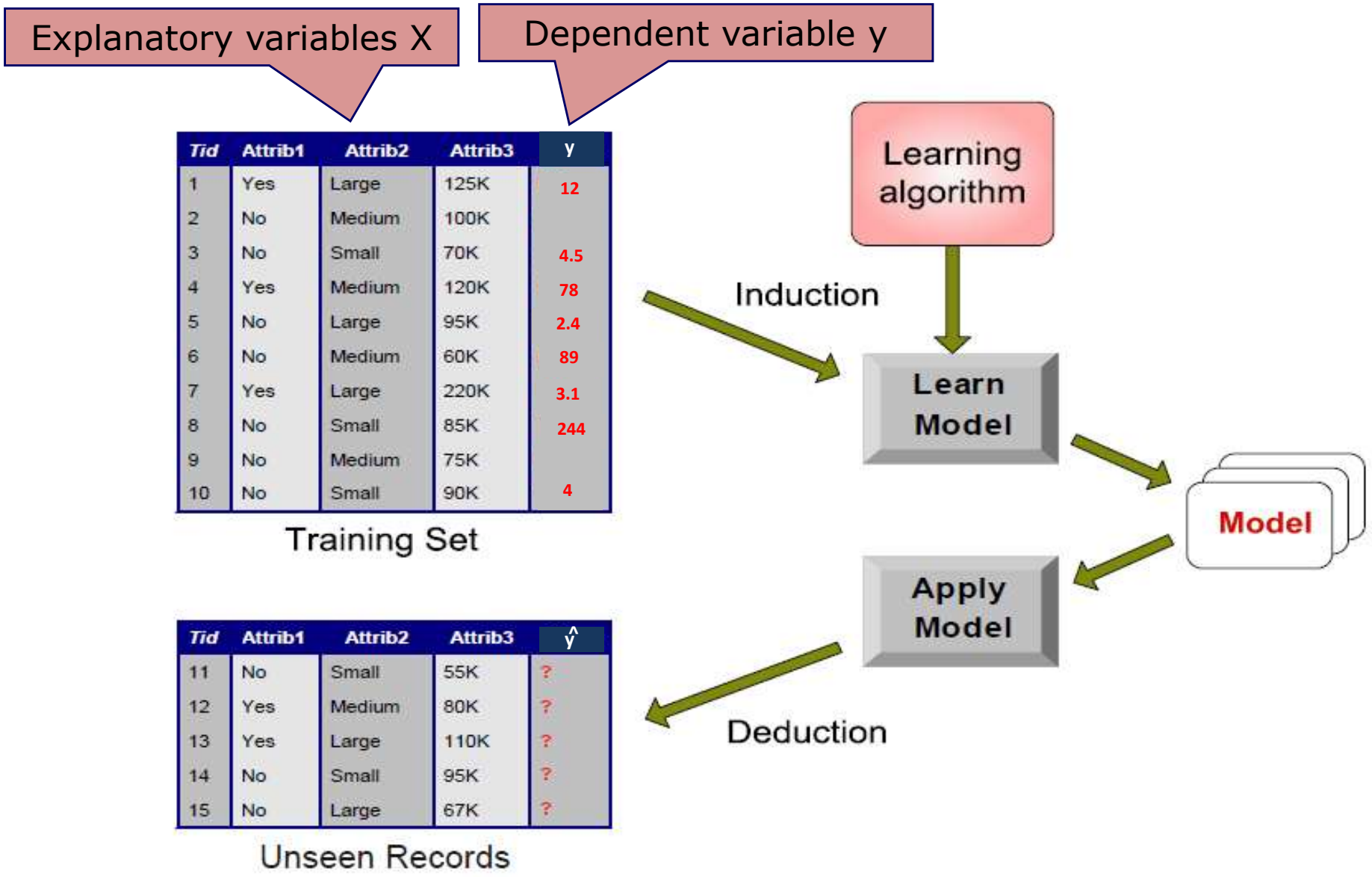

Outline

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1. KNN for Regression
2. Model Evaluation
3. Regression Trees
4. Linear Regression
5. Polynomial Regression
6. Local Regression
7. ANNs for Regression
8. The Bias/Variance-Tradeoff

1. K-Nearest-Neighbors Regression

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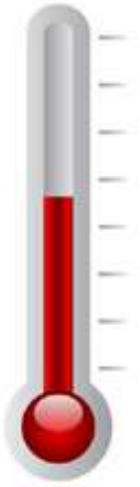
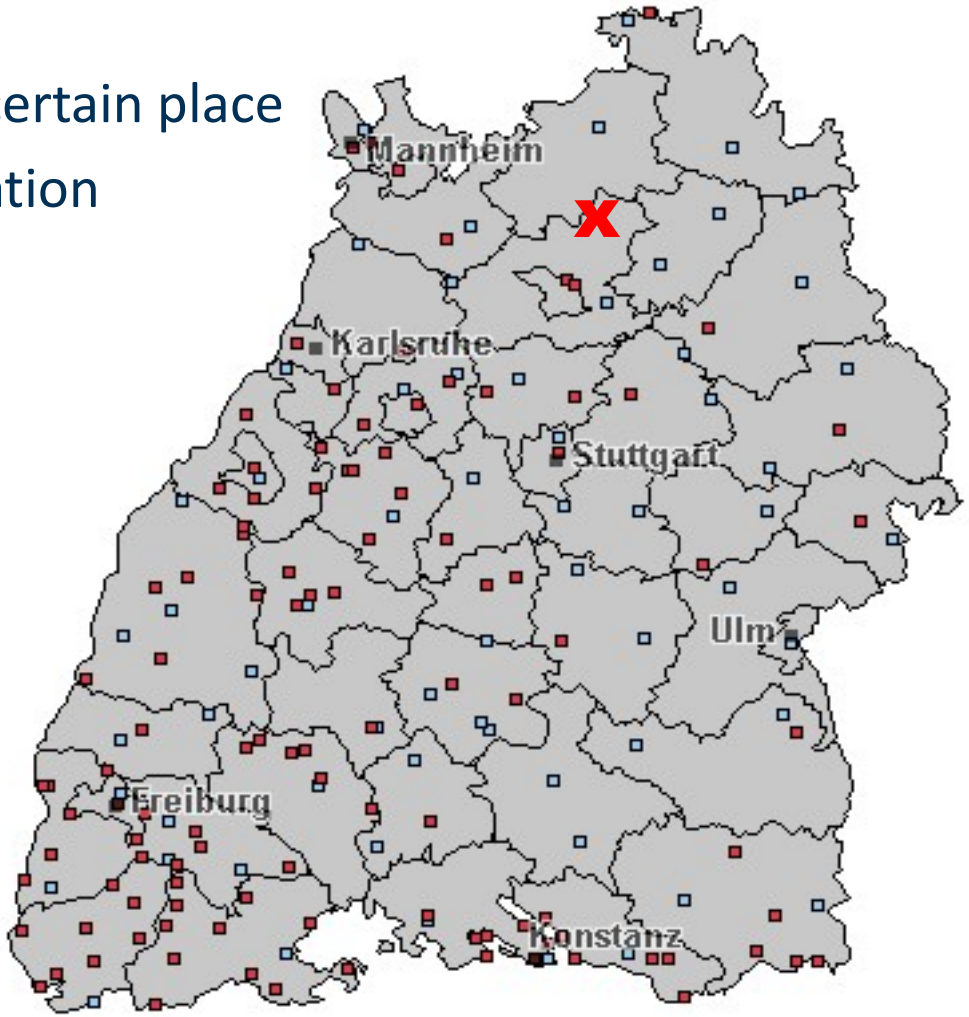
- Problem
  - Predict the **temperature** in a certain place
  - Where there is no weather station
  - How could you do that?

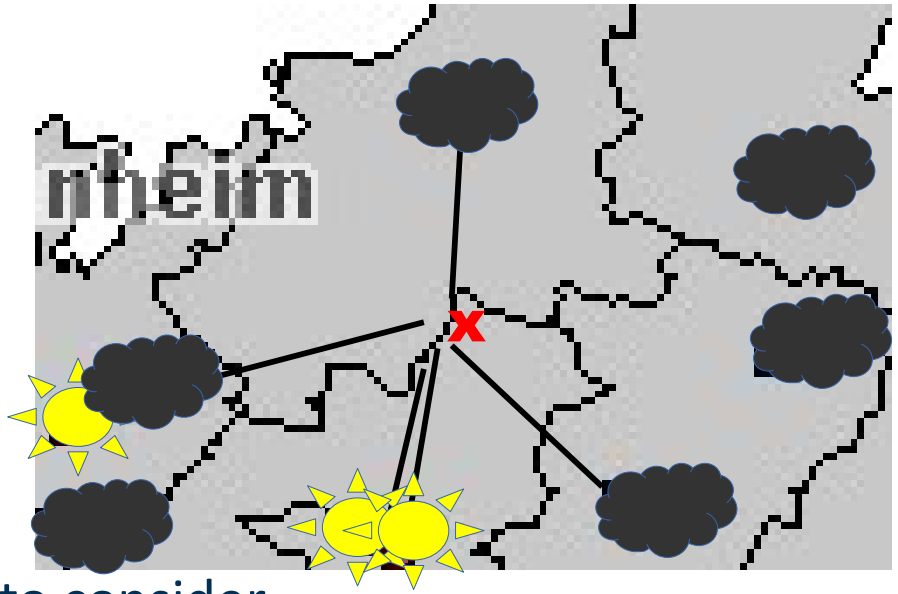


? °C



Recap: K-Nearest-Neighbors Classification

- Idea: **Vote of the nearest stations**
- Example:
  - 3x cloudy
  - 2x sunny
  - Result: cloudy
- Approach is called
  - “k nearest neighbors”
  - where k is the number of neighbors to consider
  - in the example: k=5
  - in the example: “near” denotes geographical proximity



K-Nearest-Neighbors Regression

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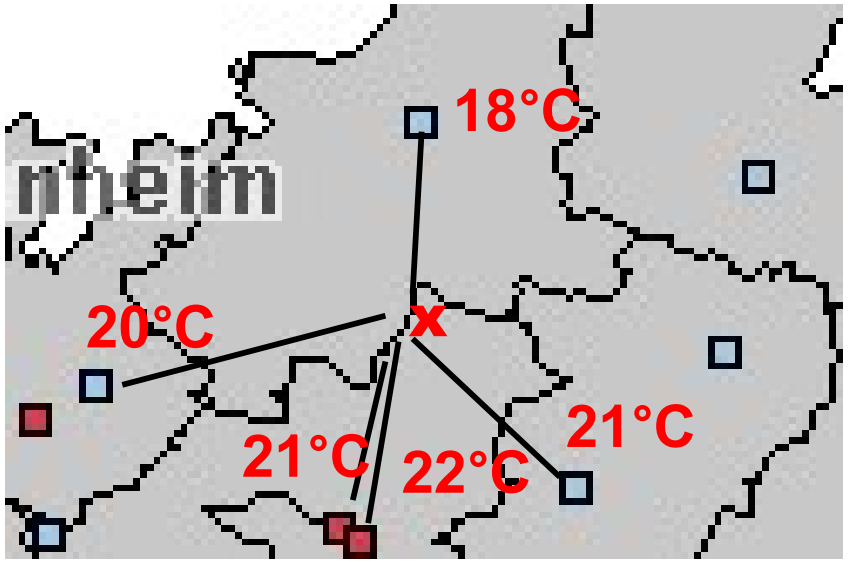
- Idea: **Use the numeric average of the nearest stations**
- Example:
  - 18°C, 20°C, 21°C, 22°C, 21°C
- Compute the average
  - again: k=5
  - average = (18+20+21+22+21) / 5
  - prediction: $\hat{y}$ = 20.4°C



- Can also be weighted by the distance to the nearest neighbors

K-NN Regression in Python

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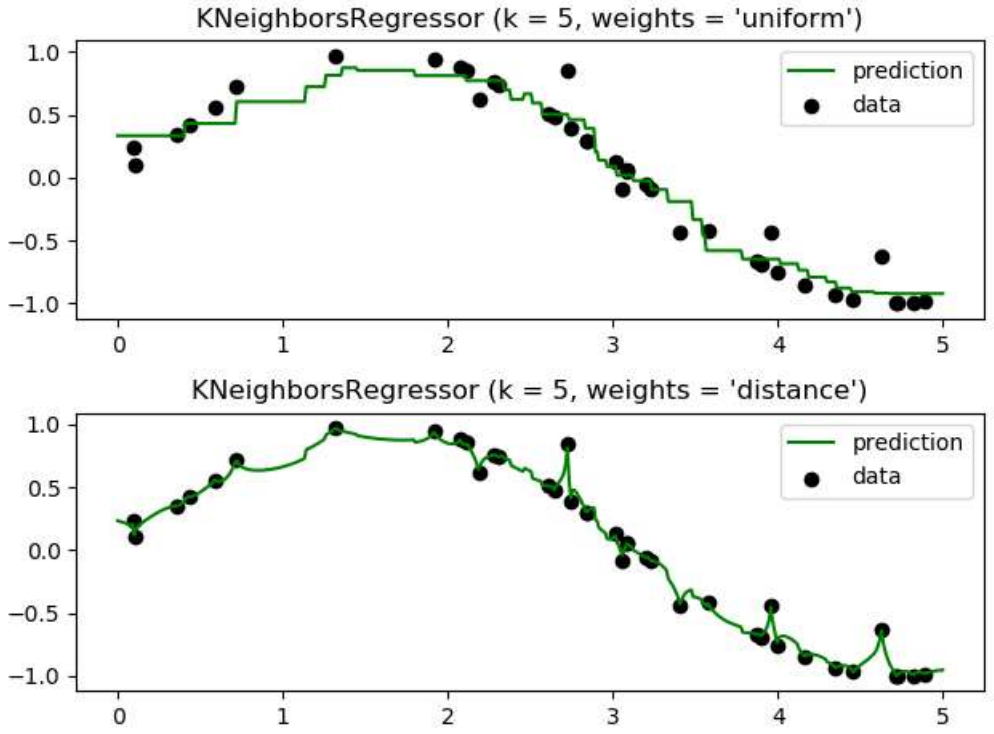
Python

```python
from sklearn.neighbors import KNeighborsRegressor

# Create and fit a KNN regressor
estimator = KNeighborsRegressor(n_neighbors=15)
estimator.fit(training_set_X, training_dependent_y)

# Make predictions for unseen examples
y_hat = estimator.predict(test_set_X)
```



2. Model Evaluation

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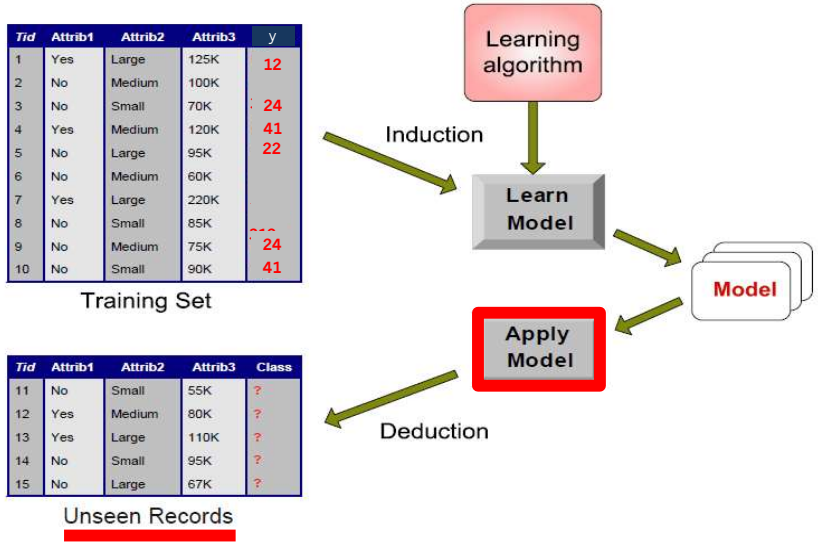
Central Question:

How good is a model at predicting the dependent variable for unseen records?

(generalization performance)



3.1 Methods for Model Evaluation

- How to obtain reliable estimates?

3.2 Metrics for Model Evaluation

- How to measure the performance of a regression model?

2.1 Methods for Model Evaluation

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- The same considerations apply as for classification:
- Cross validation: 10-fold (90% for training, 10% for testing in each iteration)
- Nested cross-validation for hyperparameter selection
  - uses inner cross validation to select best hyperparameter values
  - uses outer cross validation to estimate generalization error of models learned using best hyperparameter values

Python

```python
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import cross_val_score
from sklearn.neighbors import KNeighborsRegressor

# Create KNN regressor
estimator_knn = KNeighborsRegressor()

# Specify the hyperparameter values for the search
grid = {"n_neighbors": range(1,20)}

# Create the grid search estimator for model selection
estimator_gs = GridSearchCV(estimator_knn, grid, cv=5, scoring='neg_mean_squared_error')

# Run nested cross-validation for model evaluation
mse_cv = cross_val_score(estimator_gs, X, y, cv=5, scoring='neg_mean_squared_error')
```

2.2 Evaluation Metrics

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- **Mean Absolute Error (MAE)** computes the average deviation between **predicted value $\hat{y}_i$** and the **actual value y_i**

$$MAE = \frac{1}{n}\sum_{i=1}^{n} |\hat{y}_i - y_i|$$

Same scale as the domain
e.g. temperature

- **Mean Squared Error (MSE)** places more emphasis on larger deviations

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

- **Root Mean Squared Error (RMSE)** has similar scale as MAE and places more emphasis on larger deviations

$$RMSE = \sqrt{MSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}$$

Same scale as the domain
e.g. temperature

Evaluation Metrics

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- **R Squared** (also called **Coefficient of Determination**)
  - measures the proportion of variance (of y) that has been explained by the independent variables X in the model
  - best possible score is 1.0, lower values are worse
  - $R^2 = 1$: Perfect model as total variation of y can be completely explained from X

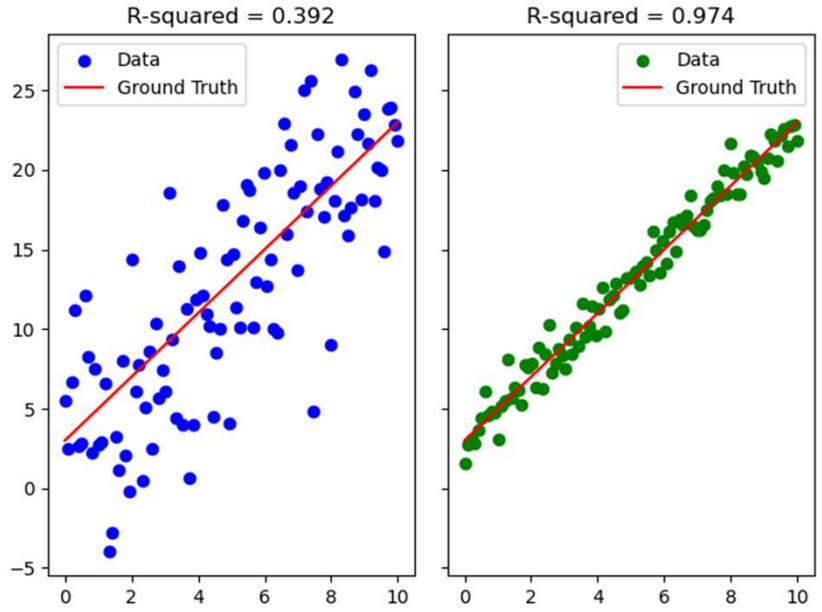
$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

sum of squares of residuals

total sum of squares

Model predicting the mean, will have $R^2 = 0$

$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$



3. Regression Trees

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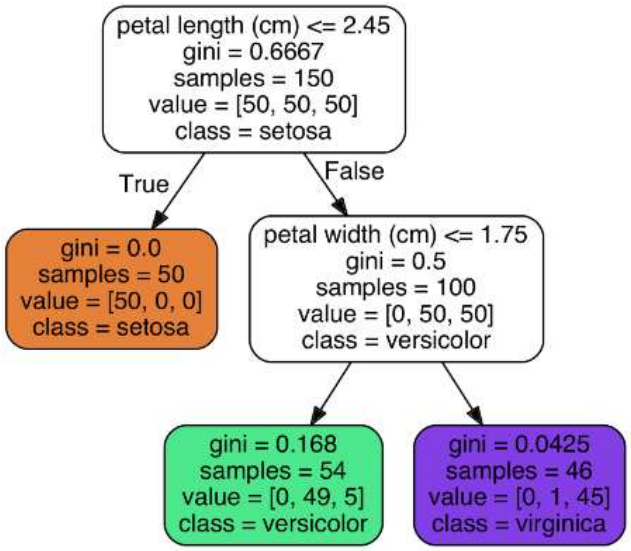
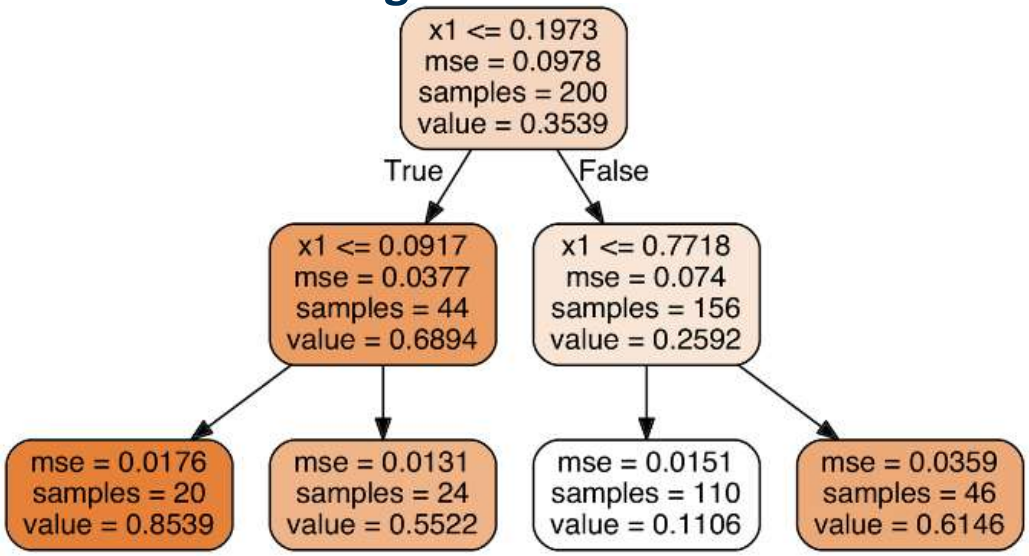
- The basic idea of how to learn and apply decision trees can also be used for regression
- Differences:
  1. Splits are selected by maximizing the MSE reduction (not GINI)
  2. Prediction is average value of the training examples in a specific leaf

Decision Tree



Regression Tree



Regression Trees

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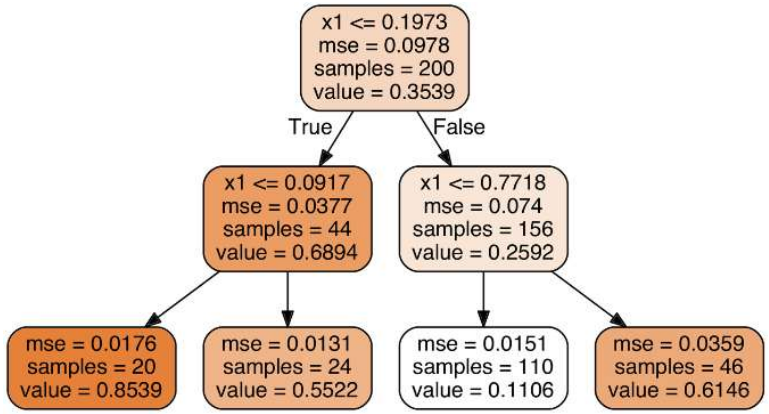
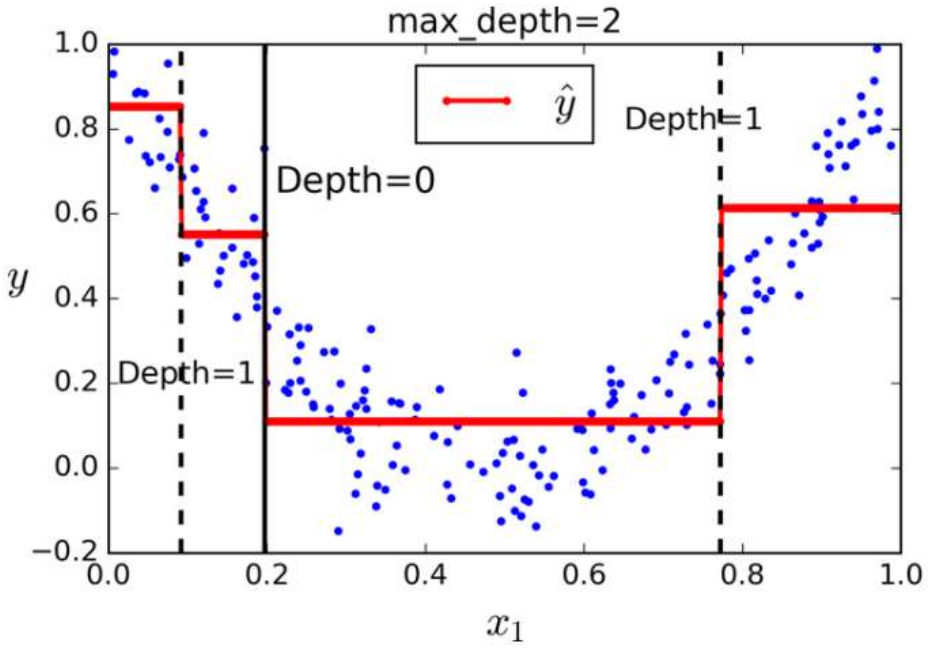
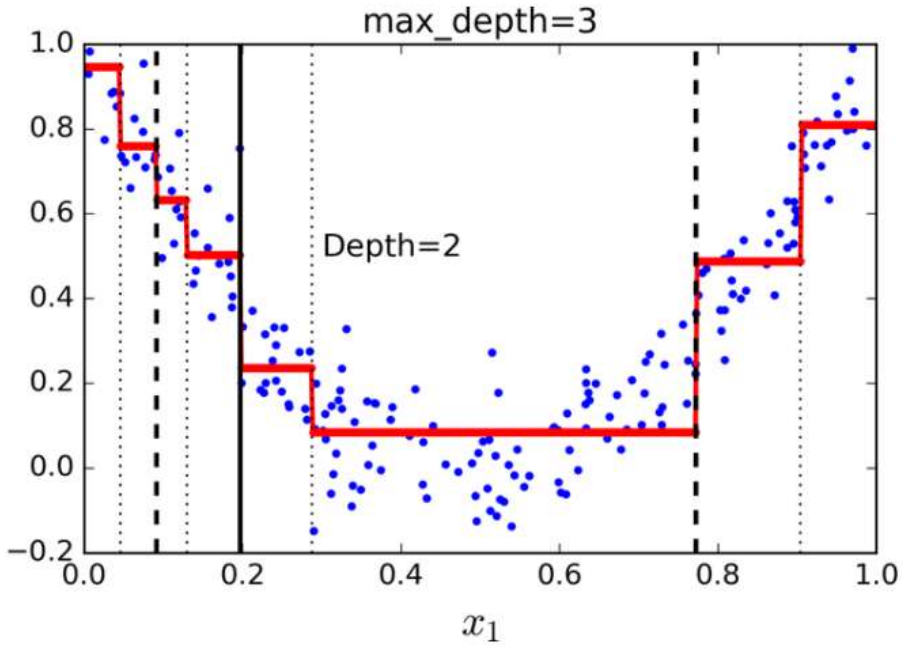
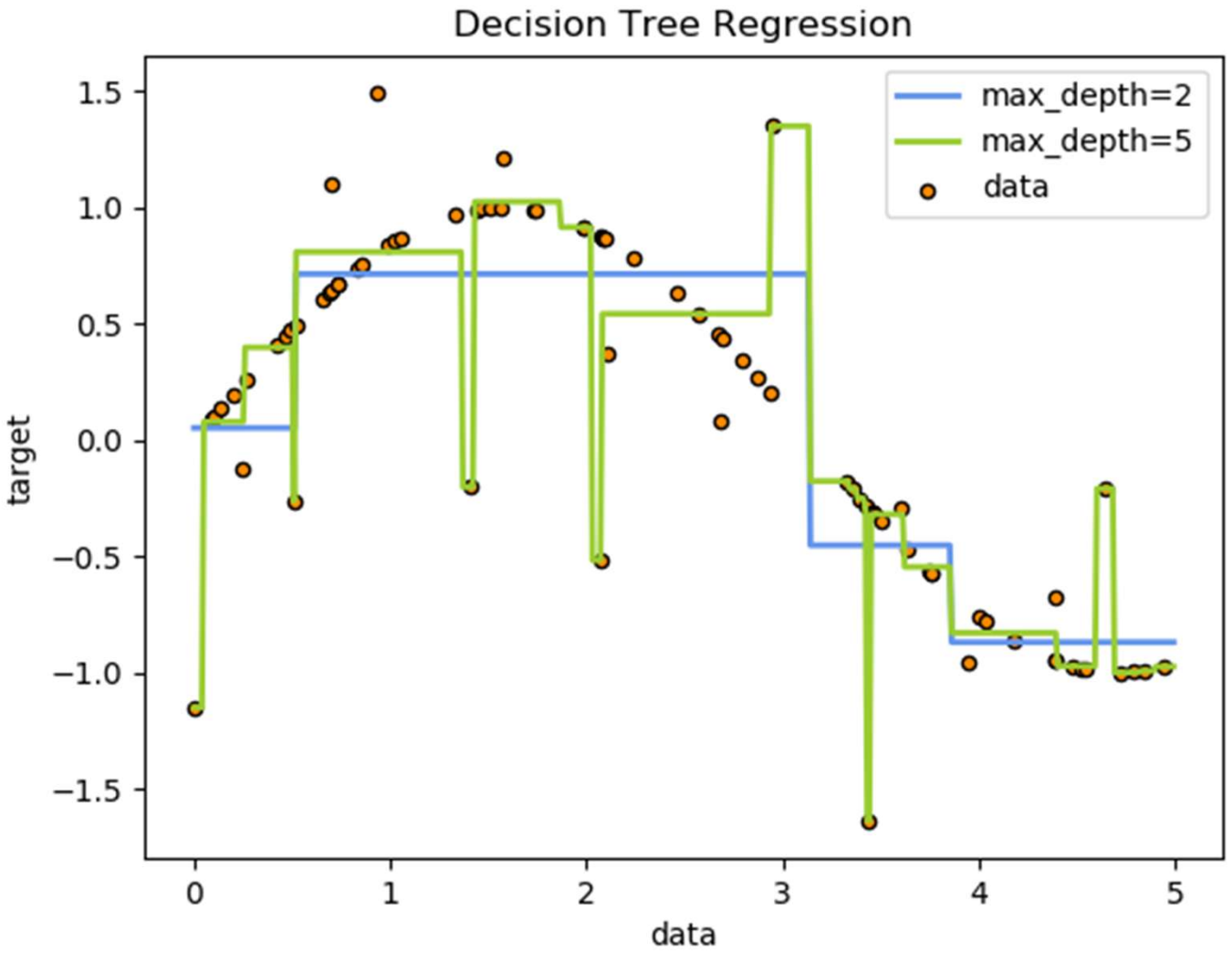
- Pre-pruning parameters determine how closely the tree fits the training data
  - E.g. max_depth parameter
- Resulting model: piecewise constant function







Overfitted Regression Tree



The learning algorithm uses the available tree depth to model the most extreme outliers

4. Linear Regression

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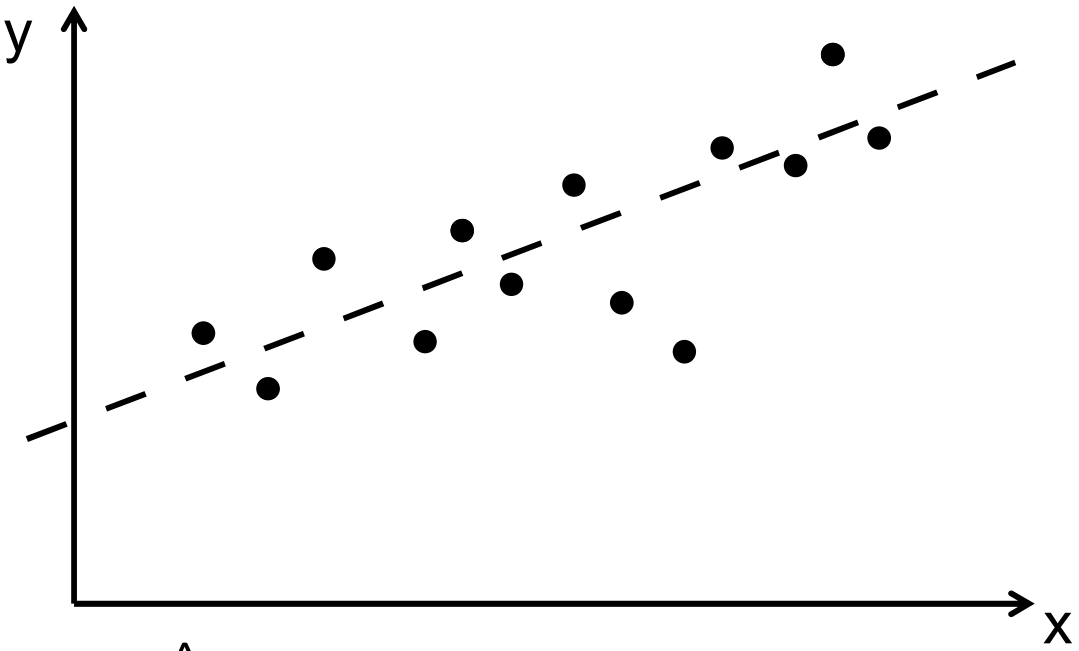
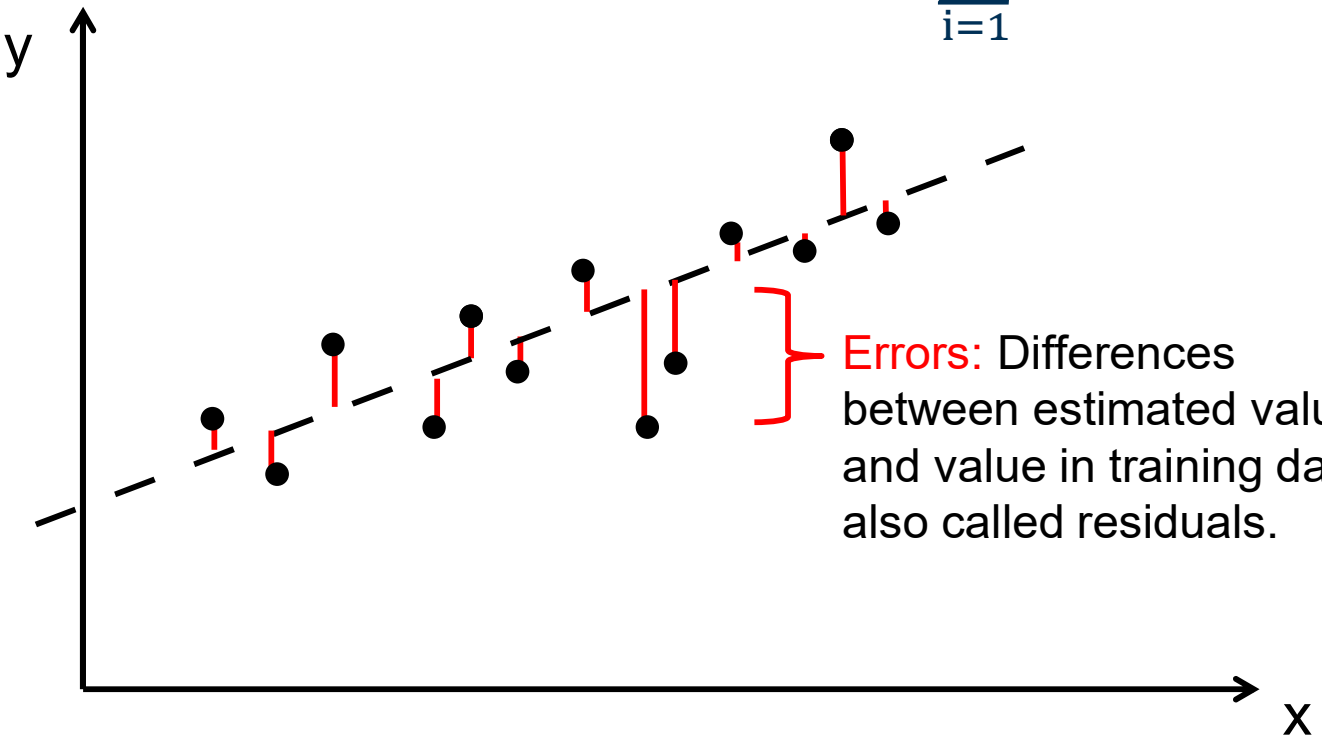
- Assumption: The target variable $\hat{y}$ is (approximately) linearly dependent on explanatory variables X
  - For visualization: we use one variable x (simple linear regression)
  - In reality: vector $X = x_1, x_2, \ldots, x_n$ (multiple linear regression)



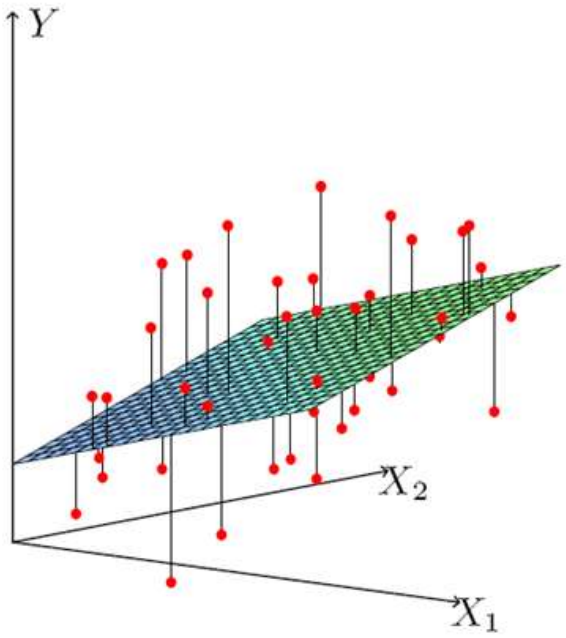
Fitting a Regression Function

Least-Squares Approach: Find the weight vector $W = (w_0, w_1, .., w_n)$ that minimizes the sum of squared error (SSE) over all training examples

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



Errors: Differences between estimated value and value in training data, also called residuals.

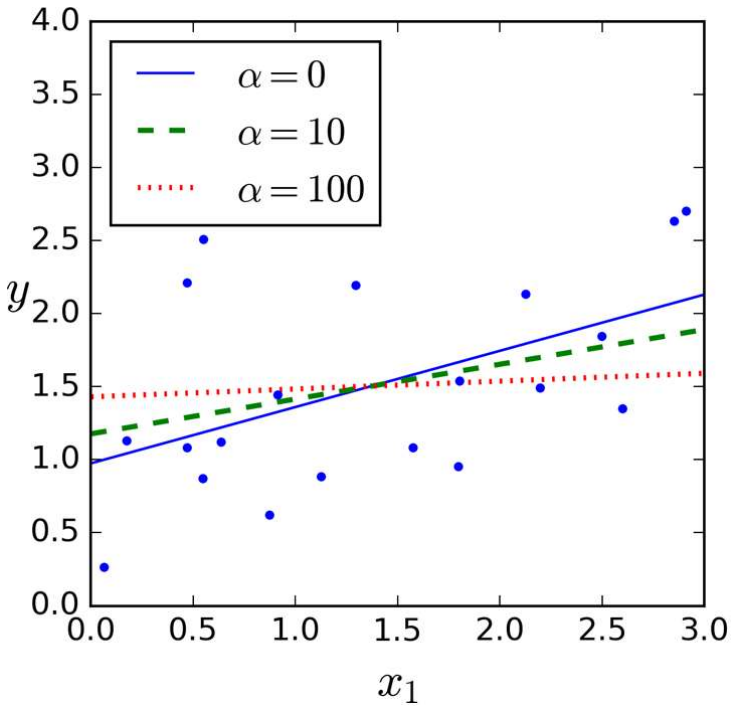


Ridge Regularization

- Variation of least squares approach which tries to avoid overfitting by keeping the weights W small
- Ridge regression cost function to minimize

$$C(W) = MSE(W) + \alpha \sum_{i=1}^{n} w_i^2$$

  - α = 0 : Normal least squares regression
  - α = 100 : Strongly regularized flat curve



Feature Selection

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- Question: Do all explanatory variables X help to explain y or is only a subset of the variables useful?
- Problem 1: Highly correlated variables (e.g. height in cm and inch)
  - weights are meaningless and one variable should be removed for the better interpretability of the weights
- Problem 2: Insignificant variables (e.g. the weather for stock prices)
  - uncorrelated variables get w=0 or relatively small weights assigned
  - Question for variables having small weights: Is the variable still useful or did it get the weight by chance due to biased training data?
  - Answer: Statistical test with null-hypothesis "w=0 as variable is insignificant"
    - **t-stat:** number of standard deviations that w is away from 0
      - high t-stat ➔ Variable is significant as it is unlikely that weight is assigned by chance
    - **p-value:** Probability of wrongly rejecting the hull-hypothesis
      - p-value close to zero ➔ variable is significant
  - See: James, Witten, et al.: An Introduction to Statistical Learning. Chapter 3.1.2

Interpolation vs. Extrapolation

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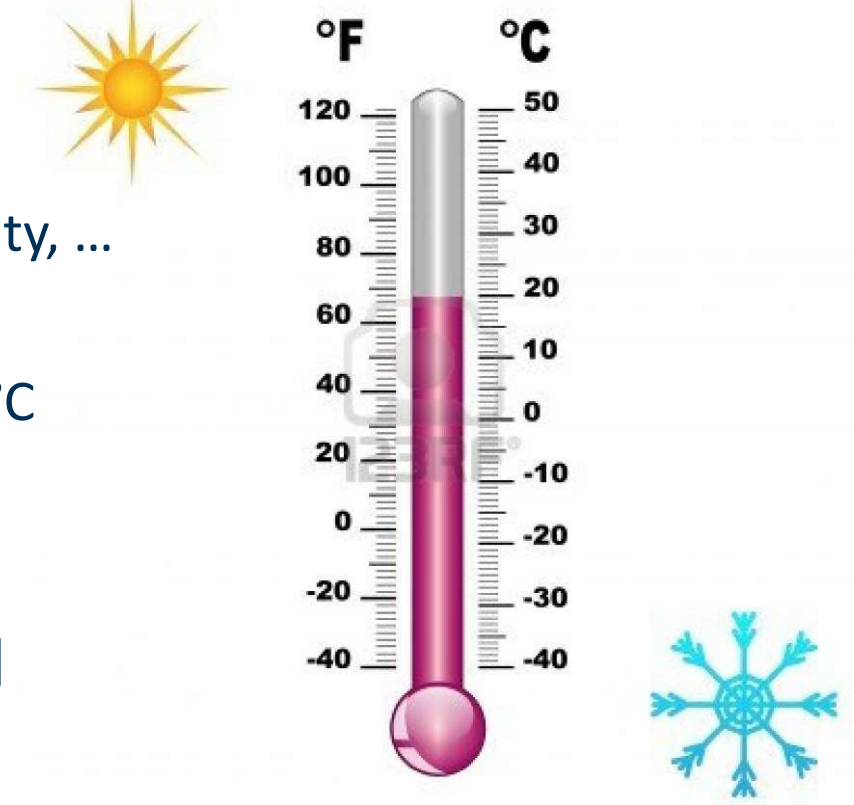
- Training data:
  - Weather observations for current day
  - E.g., temperature, wind speed, humidity, …
  - Target: temperature on the next day
  - Training values between -15°C and 32°C
- Interpolating regression
  - Only predicts values **from the training interval** [-15°C,32°C]
- Extrapolating regression
  - May also predict values ***outside*** **of this interval**



Interpolation vs. Extrapolation

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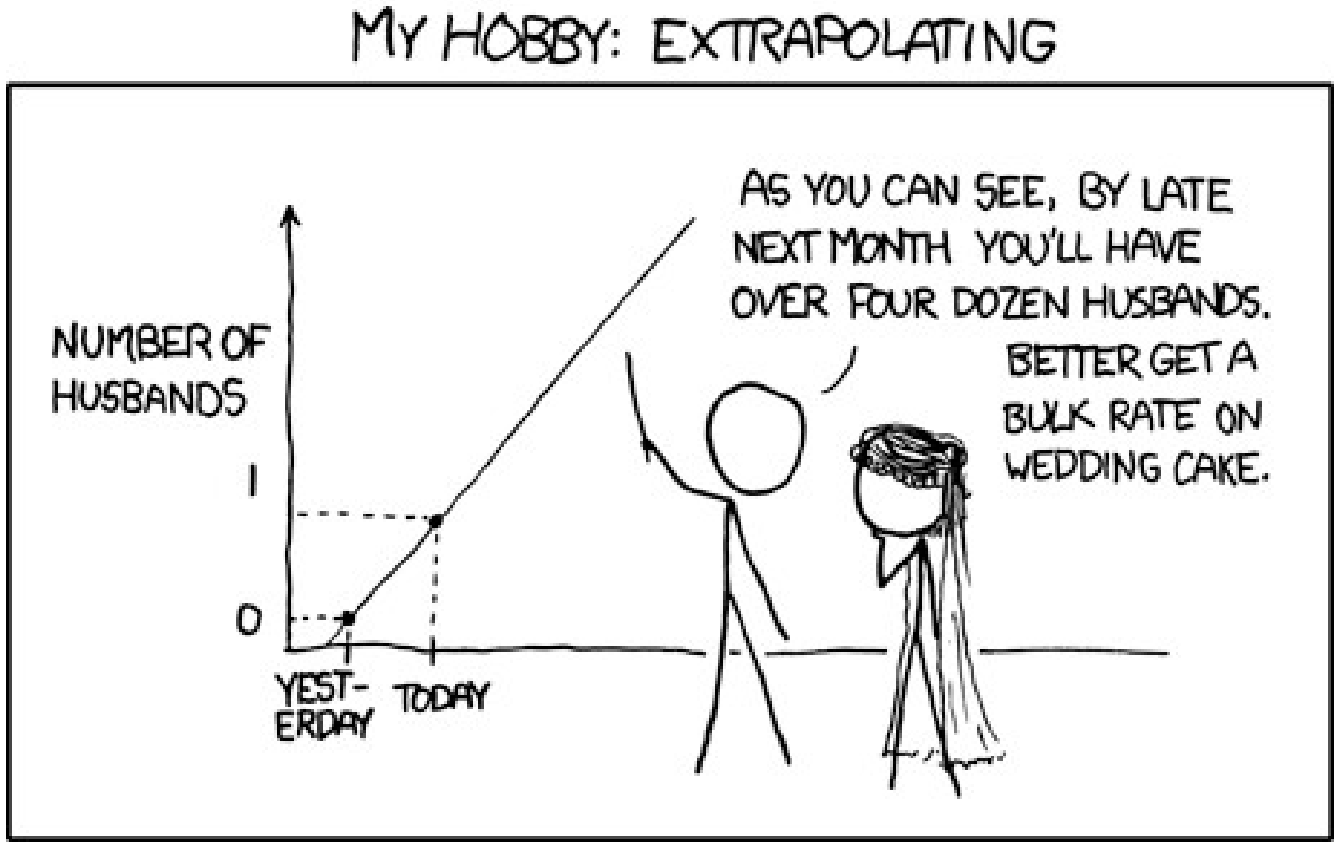
- Interpolating regression is regarded as “safe”
  - i.e., only reasonable/realistic values are predicted



http://xkcd.com/605/

Interpolation vs. Extrapolation

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- Sometimes, however, extrapolation is interesting
  - how far will the sea level have risen by 2050?
  - how much will the temperature rise in my nuclear power plant?

http://i1.ytimg.com/vi/FVfiujbGLfM/hqdefault.jpg

Linear Regression vs. K-NN Regression

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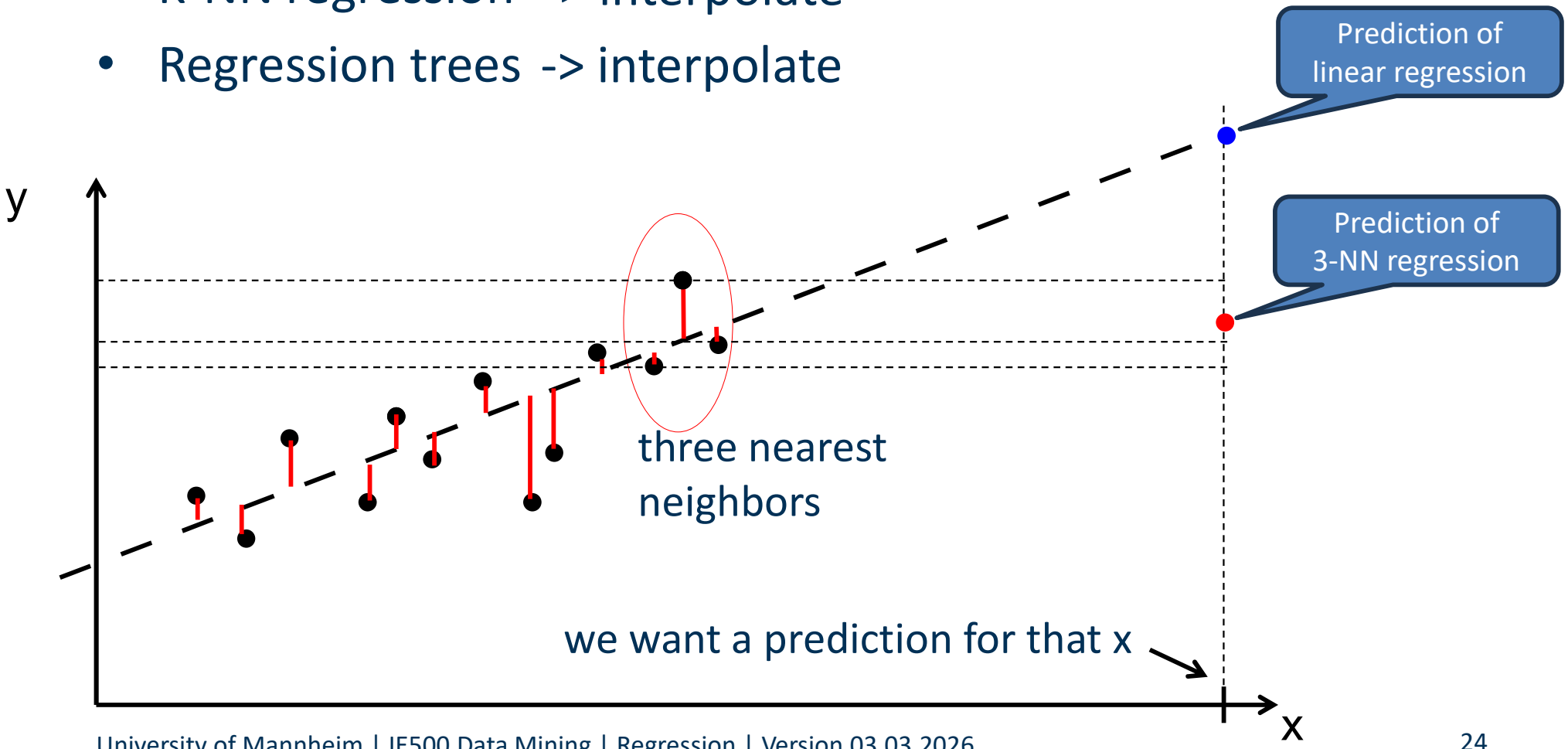
- Linear regression -> extrapolates
- K-NN regression -> interpolate
- Regression trees -> interpolate



Prediction Baseline

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- For classification:
  We predicted the most frequent label as baseline

- For regression: We either use as baseline
  - mean value or
  - median or

Linear Regression Examples

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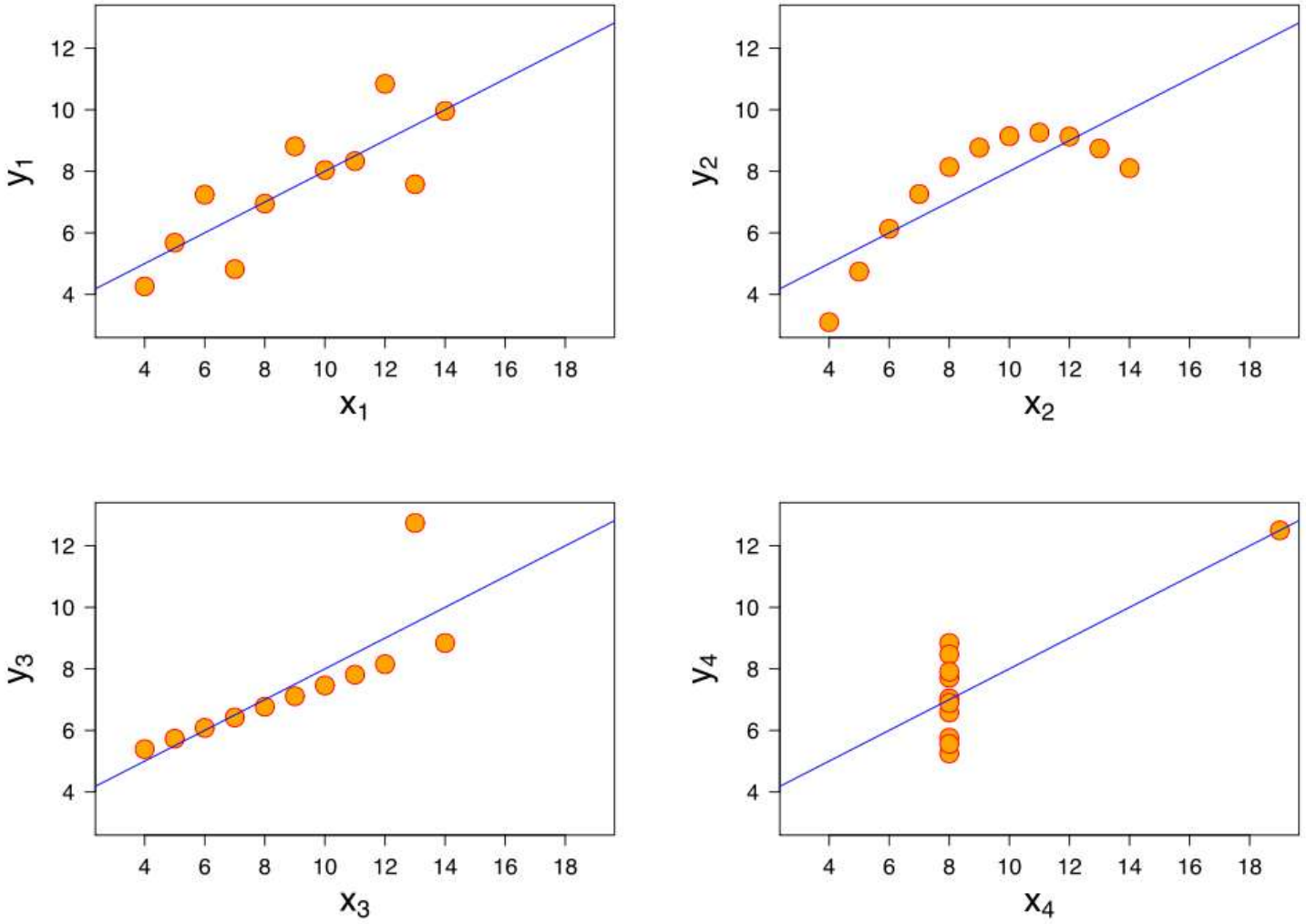
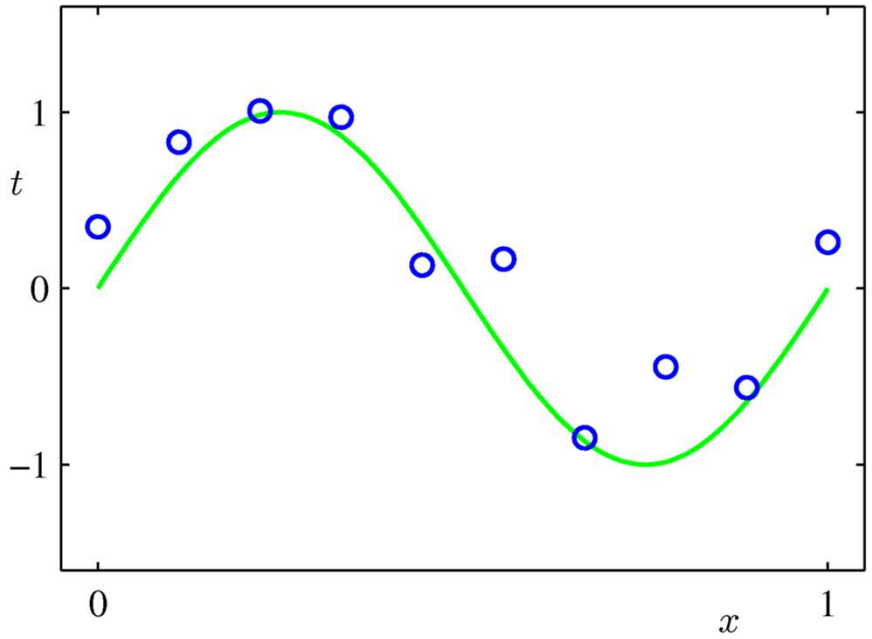


…but what about non-linear Problems?



- One possibility is to apply transformations to the explanatory variables X within the regression function
  - e.g. log, exp, square root, square, etc.
  - polynomial transformation $y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$
- This allows linear regression techniques to model complex non-linear relationships in the data.

Polynomial Regression

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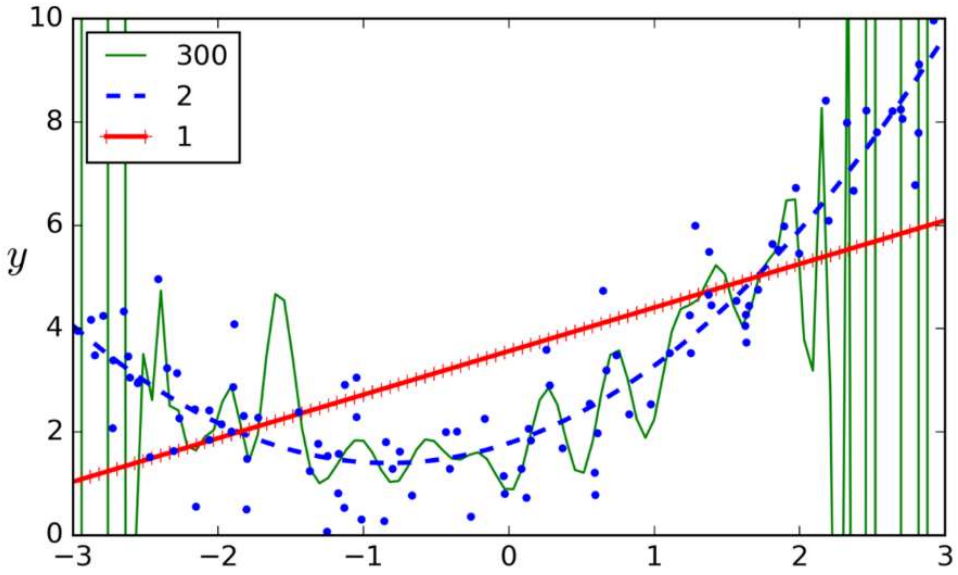
$$\hat{y}(x, \boldsymbol{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_d x^d = \sum_{j=0}^{d} w_j x^j$$

- widely used extension of linear regression
- can also be fitted using the least squares method
- has tendency to over-fit training data for large degrees d
- Workarounds:
  - decrease d
  - increase amount of training data



Polynomial Regression in Python

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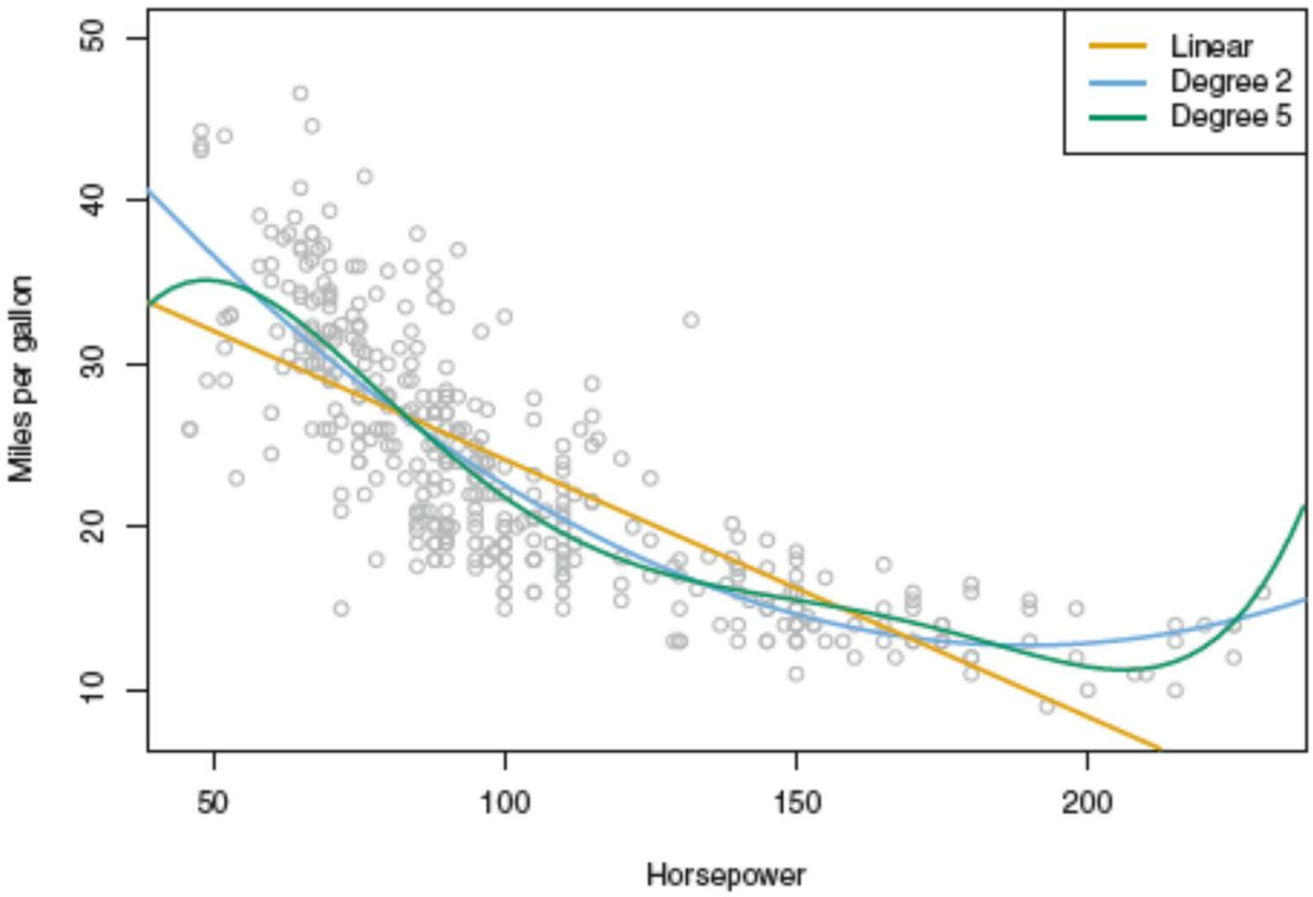
Python

```python
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression

poly_features = PolynomialFeatures(degree=2, include_bias=False).fit_transform(X, y)
estimator = LinearRegression()
estimator.fit(poly_features, y)
```

Polynomial Regression Overfitting Training Data



Overfitting often happens in **sparse regions**

- left and right side of green line
- workaround: Local regression

6. Local Regression

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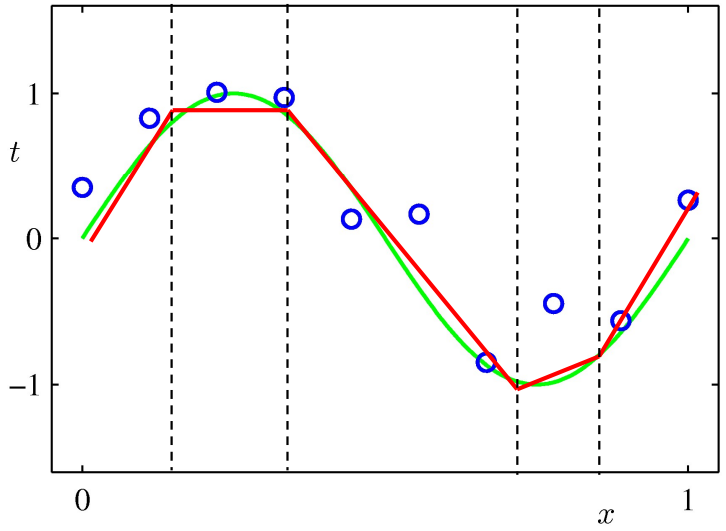
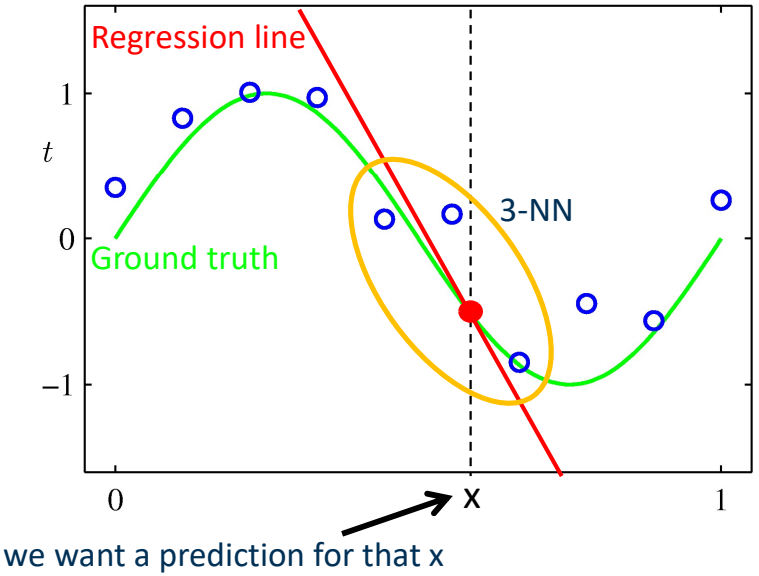
- Assumption: non-linear problems are approximately linear in local areas
- Idea:
  - use linear regression locally
  - only for the data point at hand (lazy learning)



Local Regression

- A combination of **k nearest neighbors** and **linear regression**
- Given a data point for prediction
  1. retrieve the k nearest neighbors
  2. learn a regression model using those neighbors
  3. use the learned model to predict y value



Discussion of Local Regression

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- Advantage: fits non-linear models well
  - good local approximation
  - often better than pure k-NN

- Disadvantage
  - slow at runtime
  - as for each test example:
    1. find k nearest neighbors
    2. learn a local model
    3. use local model for prediction

7. Artificial Neural Networks (ANNs) for Regression

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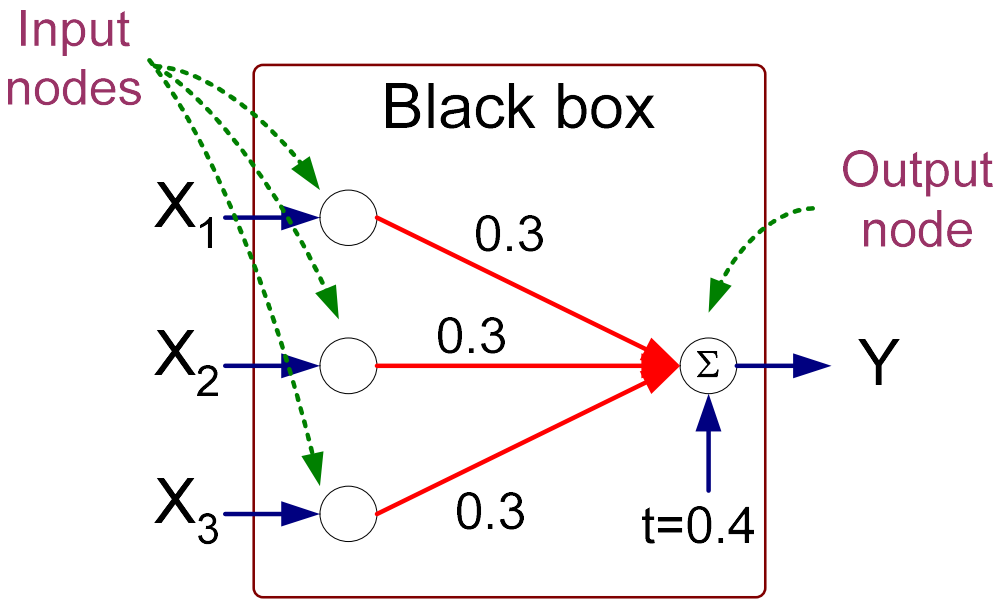
- **Recap**: How did we use ANNs for classification?

X_1	X_2	X_3	Y
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	0
0	1	0	0
0	1	1	1
0	0	0	0



$$Y = I(0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4 > 0)$$

$$\text{Where } I(z) = \begin{cases} 1 \text{ if } z \text{ is true} \\ 0 \text{ otherwise} \end{cases}$$

Artificial Neural Networks (ANNs) for Regression

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- The function $I(z)$ was used to separate the two classes:

$$Y = I(0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4 > 0\ )$$

$$\text{Where } I(z) = \begin{cases} 1\ if\ z\ is\ true \\ 0\ otherwise \end{cases}$$

- However, we may simply use the inner formula to predict a numerical value (between 0 and 1):

$$\hat{Y} = 0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4$$

ANNs for Regression

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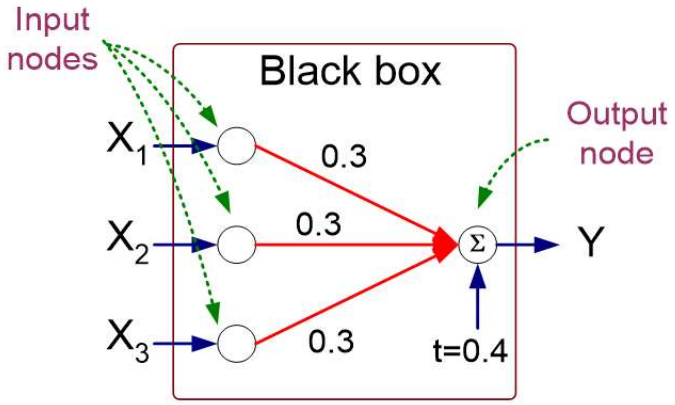
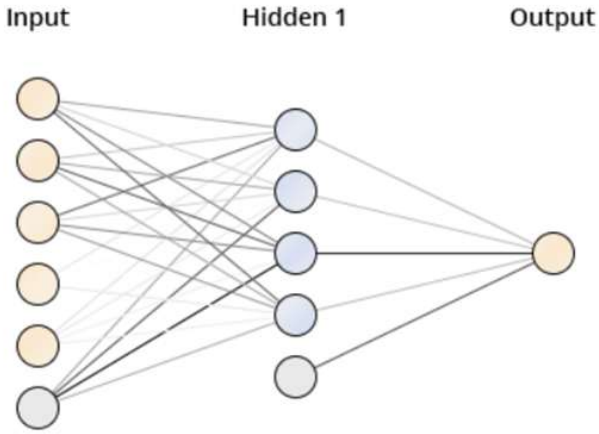
- Given that our formula is of the form

$$\hat{Y} = 0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4$$



- we can learn only linear models
  - i.e., the target variable is a linear combination the input variables
- More complex regression problems can be handled by using multiple hidden layers
  - this allows for approximating **arbitrary functions**
- Deep ANNs take this idea further by
  - employing millions of neurons
  - arranging them into specific network topologies
  - see Gemulla: Machine Learning + Deep Learning



- If you use ANNs be cautions about overfitting!

The Bias/Variance-Tradeoff

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- We want to learn regression as well as classification models that generalize well to **unseen data**
- The generalization error of any model can be understood as a sum of three errors:
  - **Bias**: Part of the generalization error due to wrong model complexity
    - Simple model (e.g. linear regression) used for complex real-world phenomena
    - Model thus **underfits** the training and test data
  - **Variance**: Part of the generalization error due to a model's excessive sensitivity to small variations in the training data
    - Models with high degree of freedom/flexibility (like polynomial regression models or deep trees) are likely to **overfit** the training data
  - **Irreducible Error**: Error due to noisiness of the data itself
    - To reduce this part of the error the training data needs to be cleansed (by removing outliers – only in training, fixing broken sensors)

8. The Bias/Variance-Tradeoff

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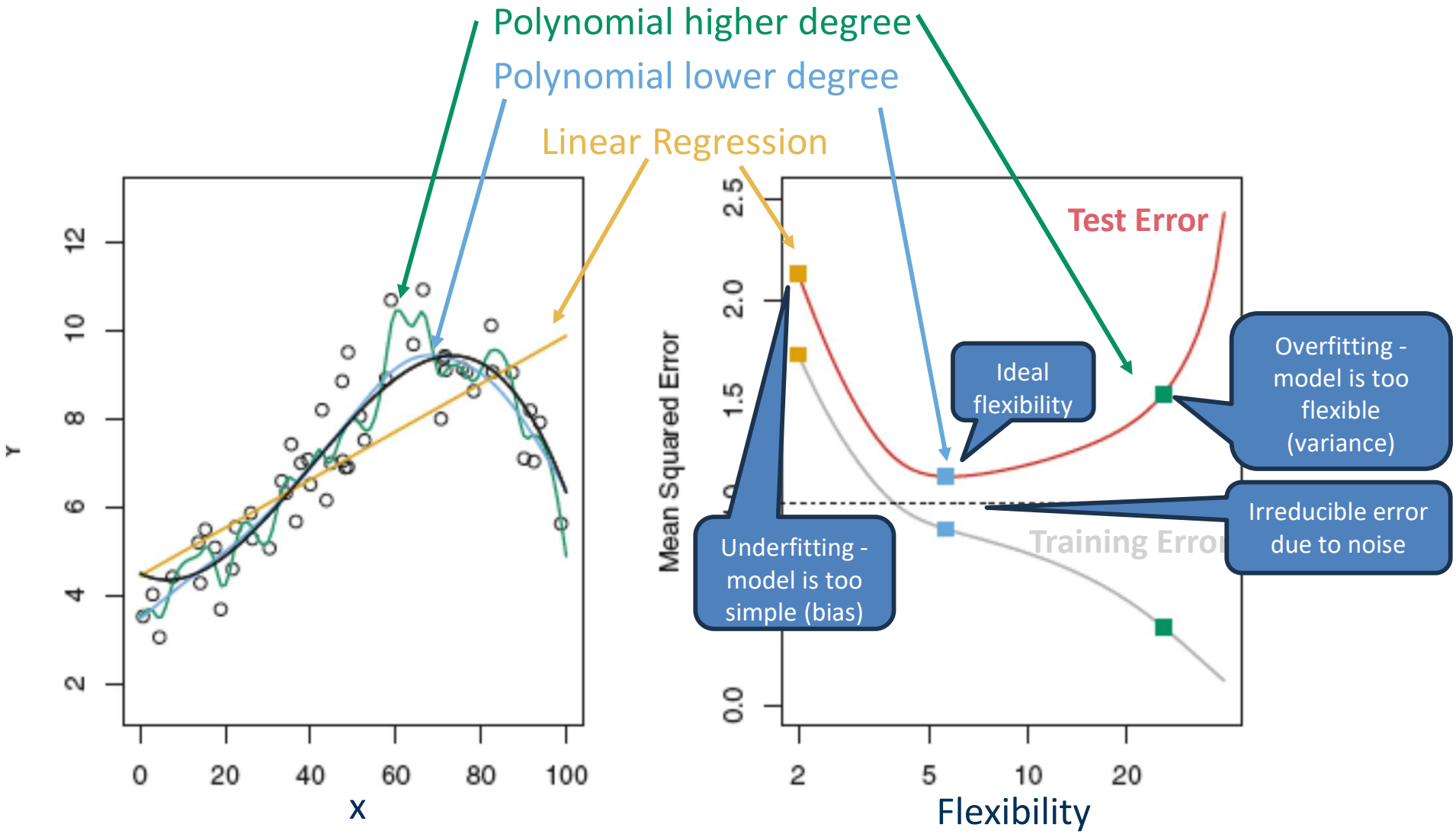
- Three models with different flexibility trying to fit a function



Learning Method and Hyperparameter Selection

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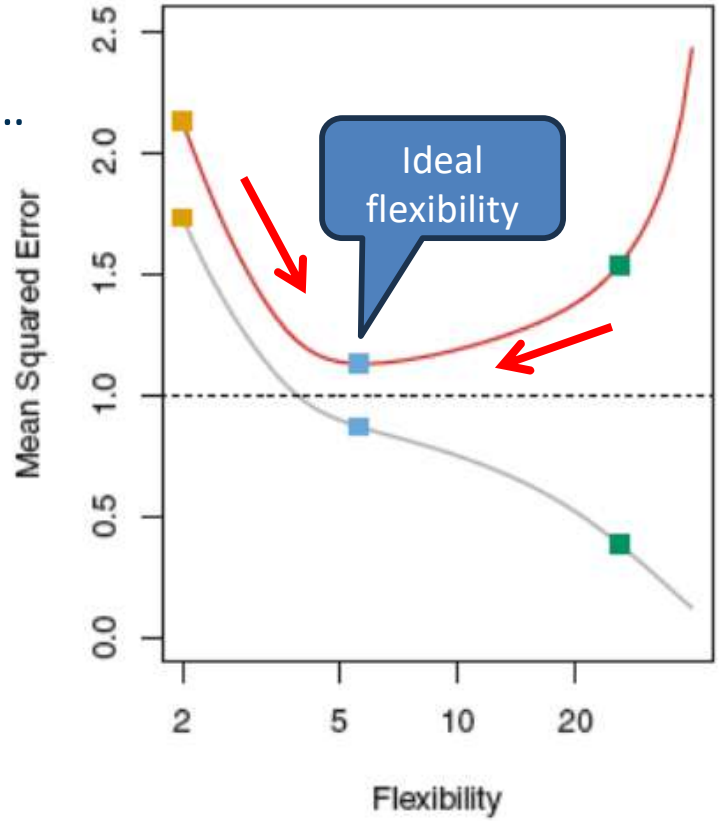
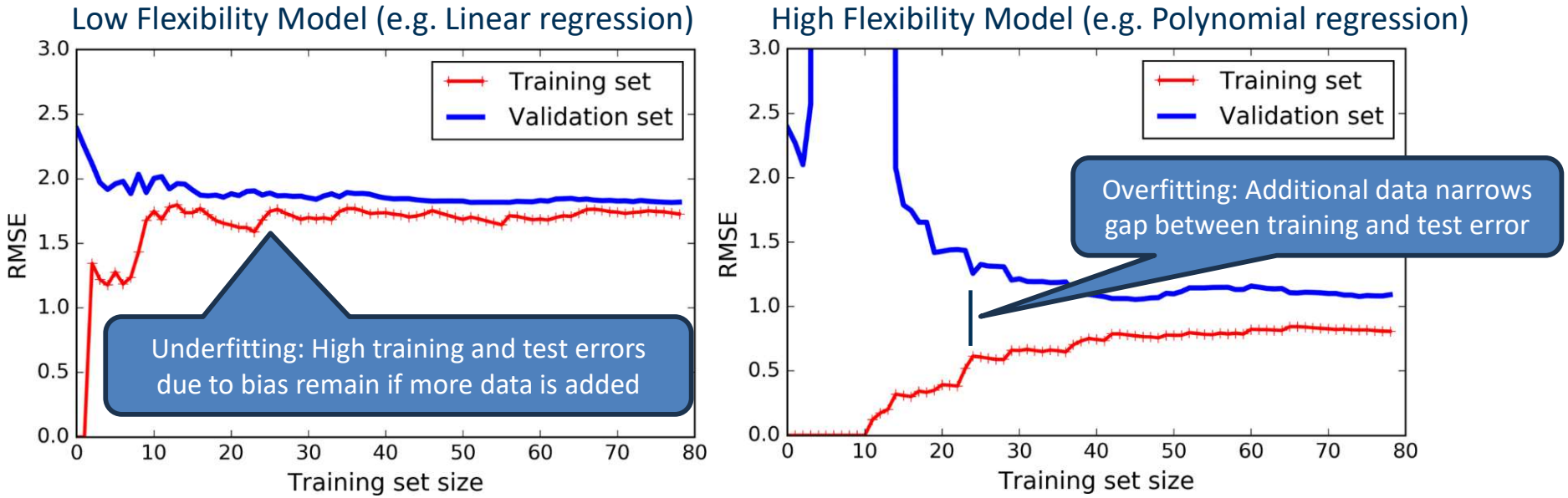
- We try to find the **ideal flexibility** (bias/variance-tradeoff) by
  - testing different learning methods
    - linear regression, polynomial regression, …
    - decision Trees, ANNs, Naïve Bayes, …
  - testing different hyperparameters
    - degree of polynomial, ridge
    - max depth of tree, min examples branch
    - number of hidden layers of ANN
- But we have **three more options**:
  - increase the amount of training data
  - increase the interestingness of the data by including more corner cases
  - cleanse the training data



Learning Curves for Under- and Overfitting Models

- Visualize the training error and test error for **different training set sizes**



  - For overfitting models, the gap between training and test error can often be narrowed by adding more training data
  - Thus, having more training data also allows us to use models having a higher flexibility, e.g. Deep Learning

Summary

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- Regression
  - predict numerical values instead of classes
- Model evaluation
  - metrics: (root) mean squared error, R squared
- Methods
  - K nearest neighbors, regression trees
  - linear regression, ridge regression
  - polynomial regression, local regression
  - artificial neural networks for regression
- For good performance on unseen data
  - choose learning method having the right flexibility (bias/variance-tradeoff)
  - use large quantities of interesting training data

Online Lectures

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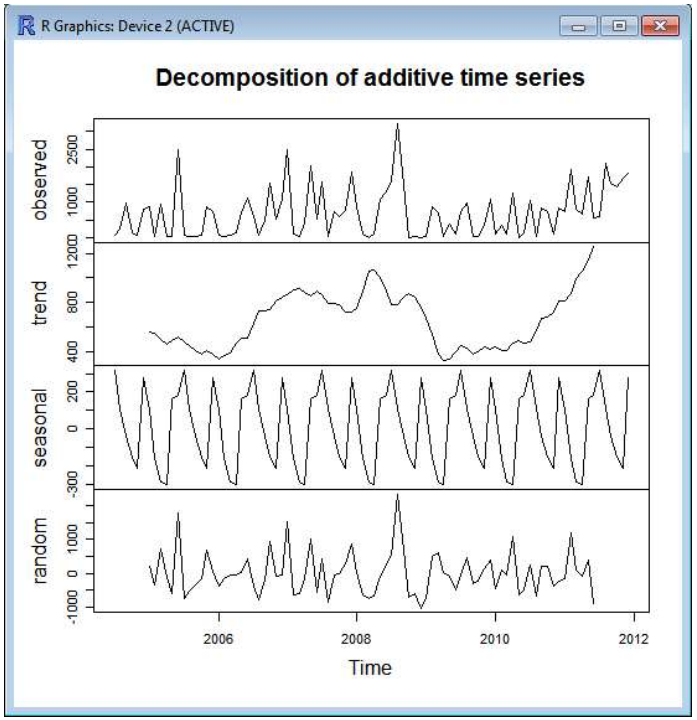
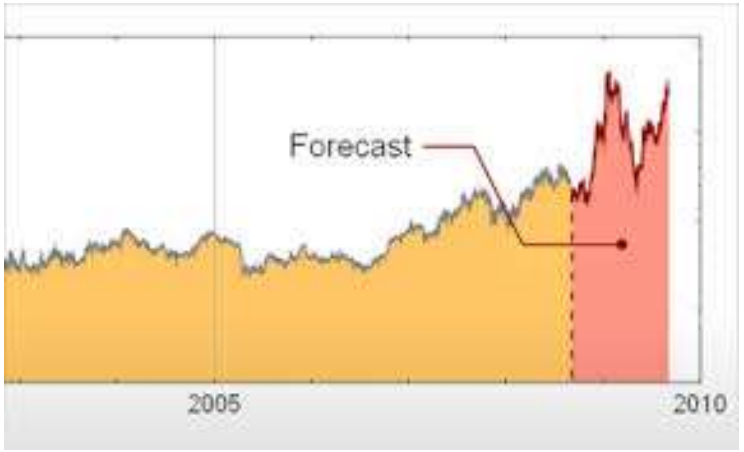
- This week additional material is about Time Series

Week	Wednesday (Offline Lecture, Room A5, B243)	Online Lecture (see Ilias Course)
11.02.2026	Introduction to Data Mining (PDF, 4 MB)	Nearest Centroids
18.02.2026	Classification 1 (PDF, 3 MB)	Ensembles
25.02.2026	Classification 2	Comparing Classifiers
04.03.2026	Regression	Time Series
11.03.2026	Preprocessing	Multi Modal Data
18.03.2026	Clustering and Anomalies	Hierarchical Clustering





Literature for this Slideset

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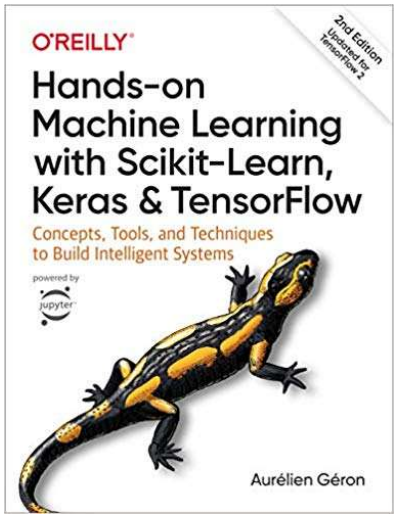
- Solving practical regression tasks using Python:
  - Geron: Hands-on Machine Learning - Chapter 4



- Sophisticated coverage of regression including theoretical background
  - James, Witten, et al.:
    An Introduction to Statistical Learning
    Chapters 3, 7, 8