UNIVERSITY OF MANNHEIM

Data Mining

Regression

Outline

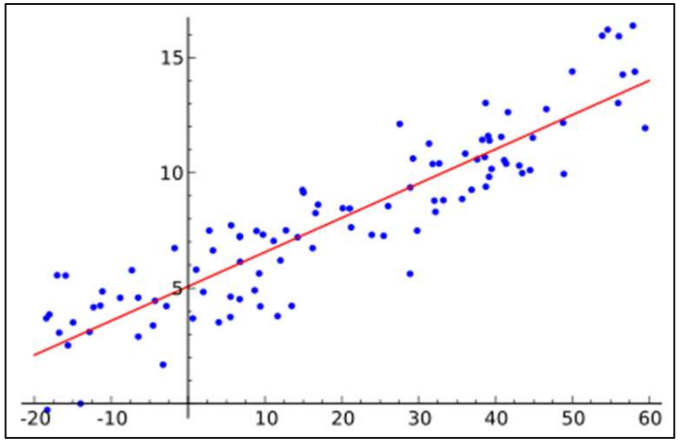
1. What is Regression?
2. KNN for Regression
3. Model Evaluation
4. Regression Trees
5. Linear Regression
6. Polynominal Regression
7. Local Regression
8. ANNs for Regression
9. Time Series Forecasting
10. The Bias/Variance-Tradeoff

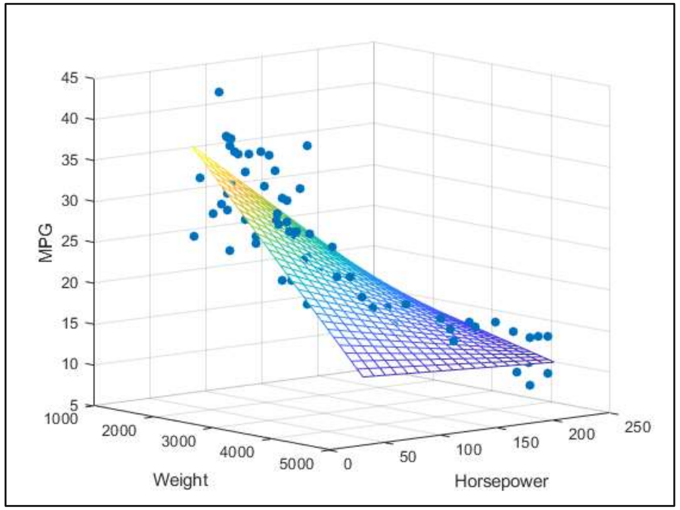
1. What is Regression?

– Goal: Predict the value of a continuous variable based on the values of other variables assuming a linear or nonlinear model of dependency
  - The predicted variable is called dependent and is denoted $\hat{y}$
  - The other variables are called explanatory variables or independent variables denoted $X = x_1, x_2, \ldots, x_n$

– Approach: Given training examples (X_i, y_i) learn a model f to predict $\hat{y}$ from X_{unseen}

– Difference to classification: The predicted attribute is continuous, while classification is used to predict nominal class attributes





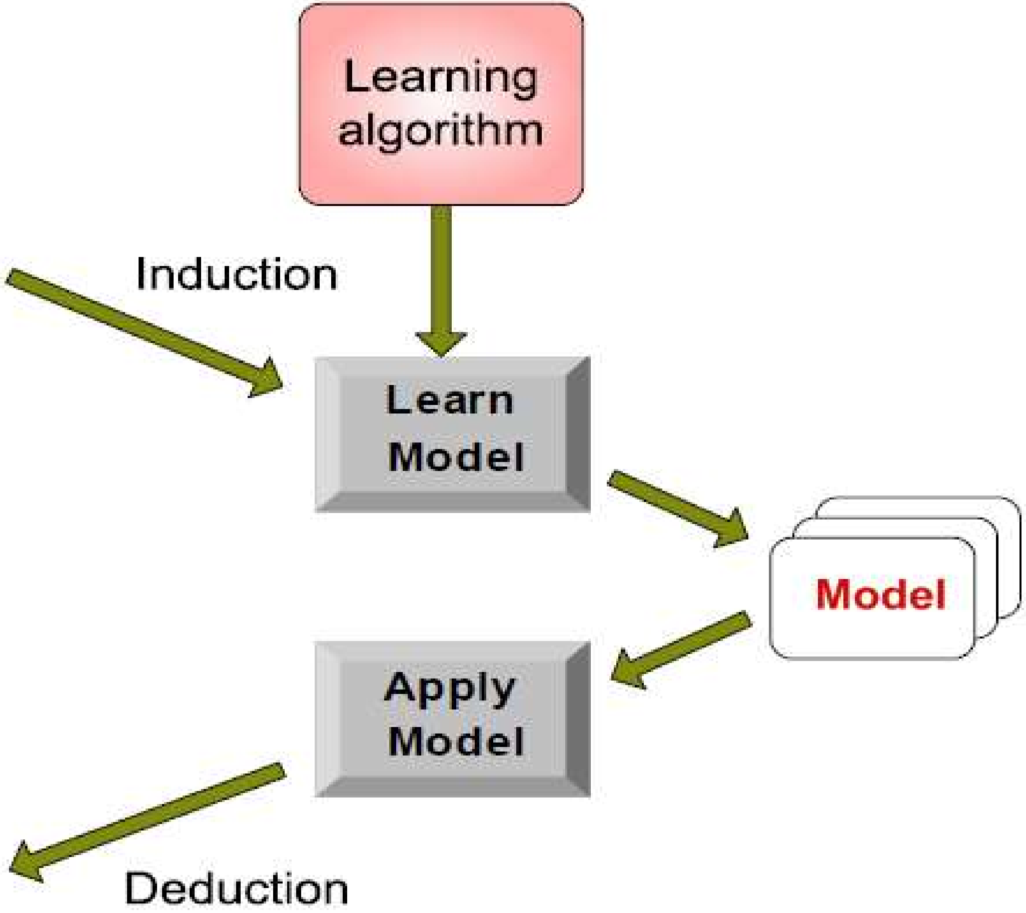
Regression Model Learning and Application

Explanatory variables X

Dependent variable y

Tid	Attrib1	Attrib2	Attrib3	y
1	Yes	Large	125K	12
2	No	Medium	100K	194
3	No	Small	70K	4.5
4	Yes	Medium	120K	78
5	No	Large	95K	2.4
6	No	Medium	60K	89
7	Yes	Large	220K	3.1
8	No	Small	85K	244
9	No	Medium	75K	669
10	No	Small	90K	4

Training Set

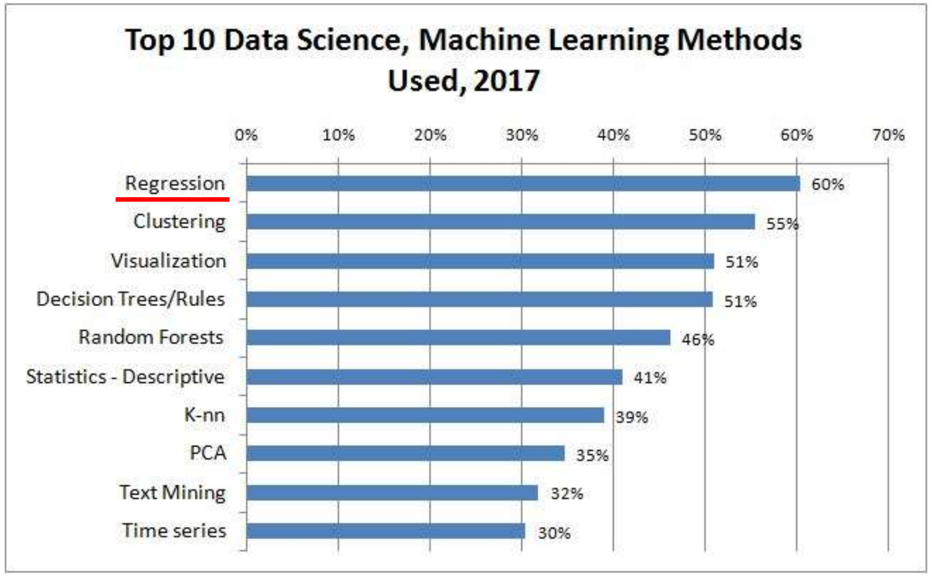


Tid	Attrib1	Attrib2	Attrib3	$\hat{y}$
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Unseen Records

Application Examples

– Weather Forecasting
  - dependent: wind speed
  - explanatory variables: temperature, humidity, air pressure change
– Gasoline Consumption
  - dependent: MPG (miles per gallon)
  - explanatory variables: weight of car, horse power, type of engine
– House Market
  - dependent: price of a house
  - explanatory variables: rooms, distance to public transport, size of garden
– Stock Market
  - dependent: price of a stock
  - explanatory variables: company profit, sector outlook, month of year, mood of investors



Source: KDnuggets online poll, 732 votes

Regression Techniques

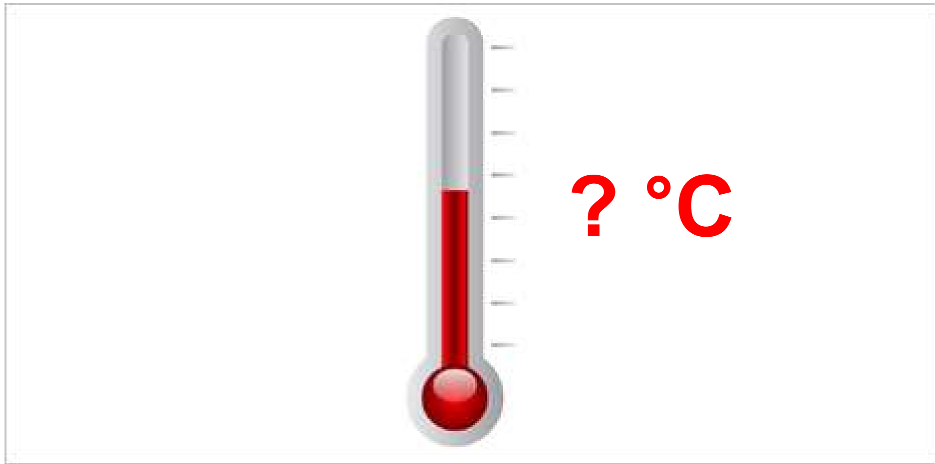
1. Linear Regression
2. Polynomial Regression
3. Local Regression
4. K-Nearest-Neighbors Regression
5. Regression Trees
6. Artificial Neural Networks
7. Deep Neural Networks
8. Component Models of Time Series

…

2. K-Nearest-Neighbors Regression

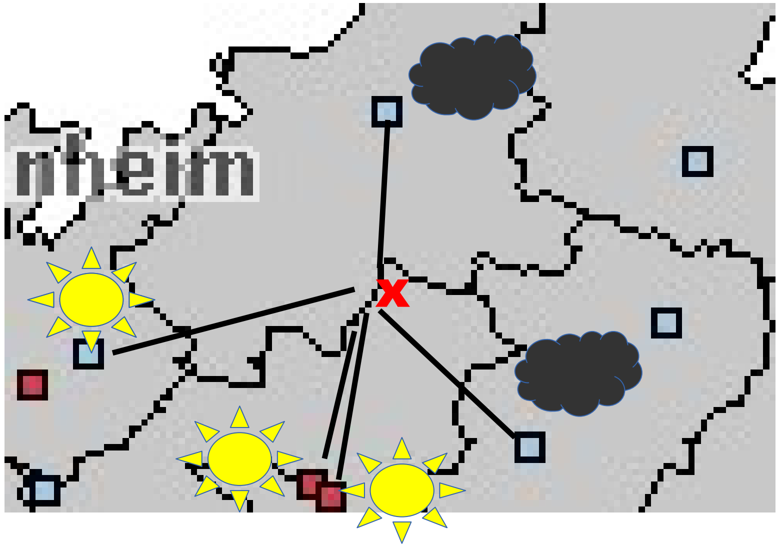
Problem

- predict the temperature in a certain place
- where there is no weather station
- how could you do that?



Recap: K-Nearest-Neighbors Classification

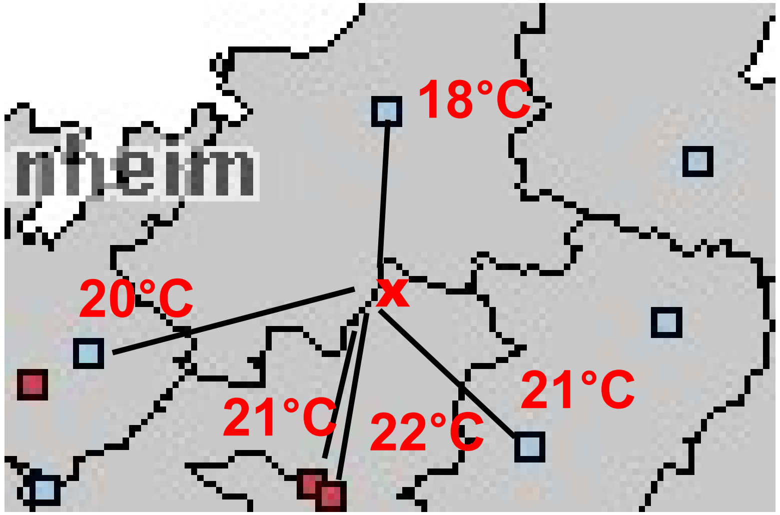
- Idea: Vote of the nearest stations
- Example:
  - 3x sunny
  - 2x cloudy
  - Result: sunny



- 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

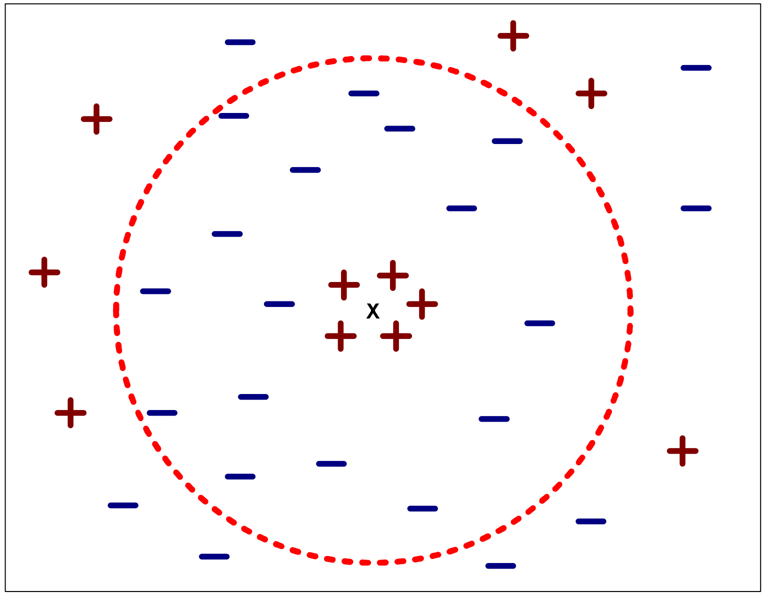
K-Nearest-Neighbors Regression

- 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



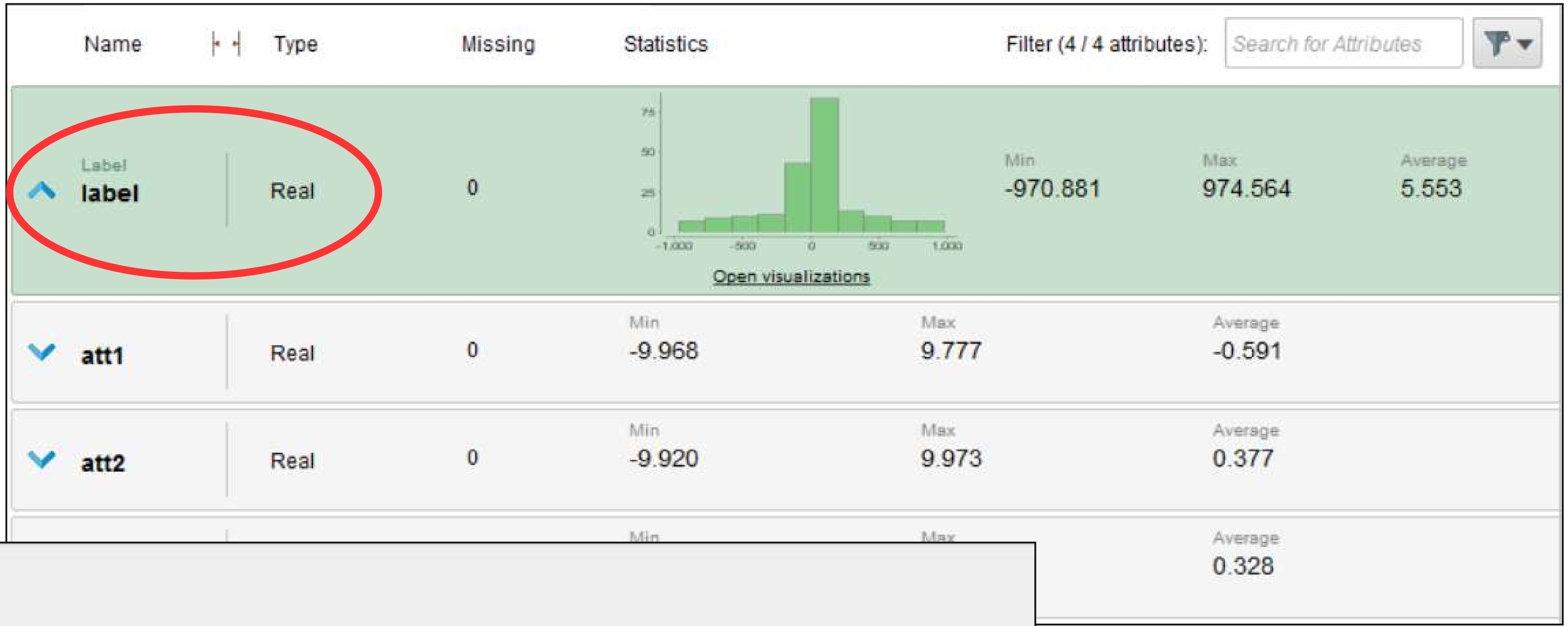
Choosing a Good Value for K

- All considerations from KNN classification also apply to KNN regression
  - If k is too small, the result is sensitive to noise points
  - If k is too large, local patterns may be averaged out
- Rule of thumb: Test k values between 1 and 20



K-Nearest-Neighbor Regression in RapidMiner and Python

RapidMiner



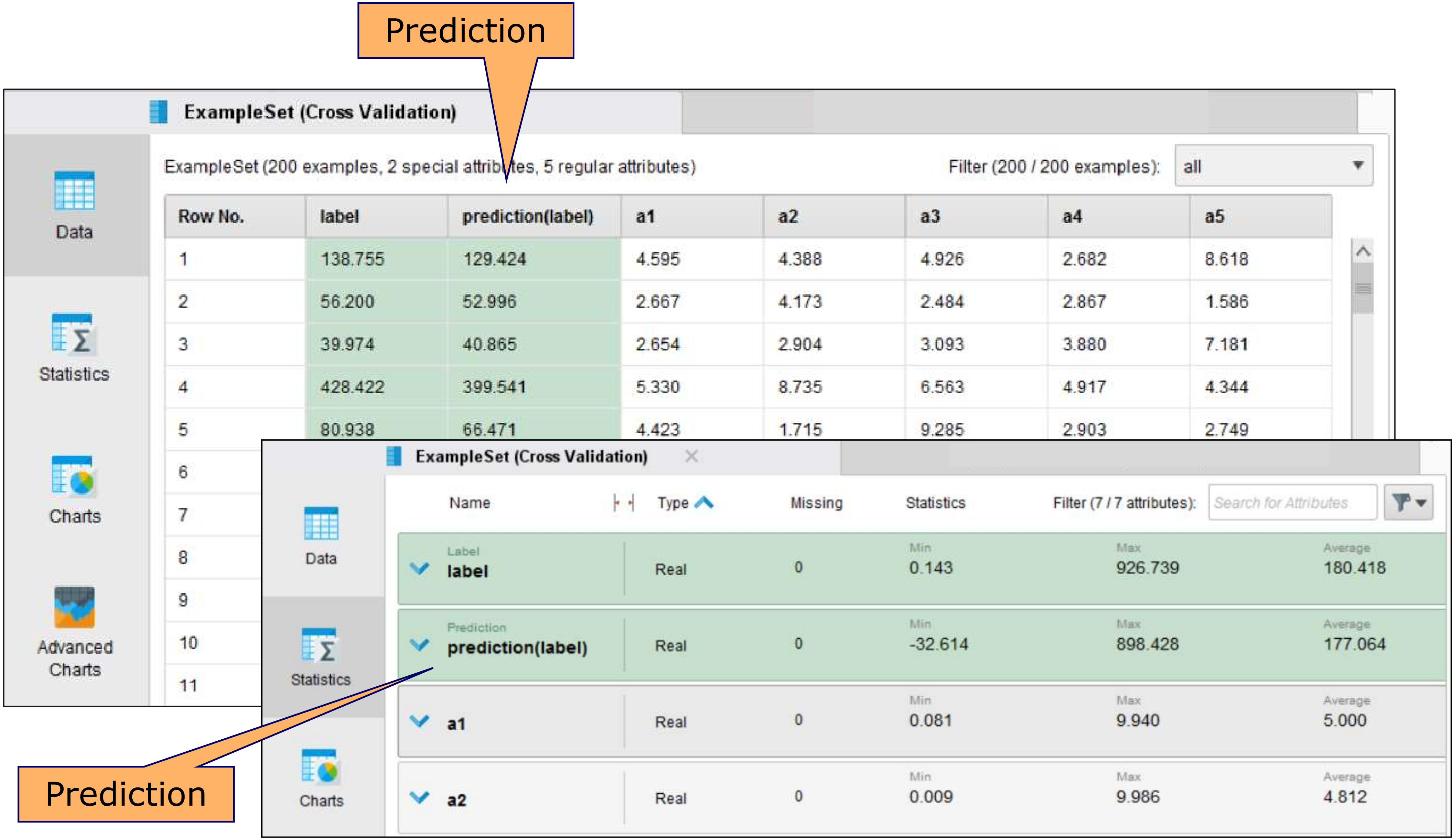
Python

```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)
```

Numeric Predictions are Added to the Dataset



Row No.	label	prediction(label)	a1	a2	a3	a4	a5
1	138.755	129.424	4.595	4.388	4.926	2.682	8.618
2	56.200	52.996	2.667	4.173	2.484	2.867	1.586
3	39.974	40.865	2.654	2.904	3.093	3.880	7.181
4	428.422	399.541	5.330	8.735	6.563	4.917	4.344
5	80.938	66.471	4.423	1.715	9.285	2.903	2.749
6							
7							
8							
9							
10							
11							

ExampleSet (Cross Validation)

Filter (7 / 7 attributes): Search for Attributes

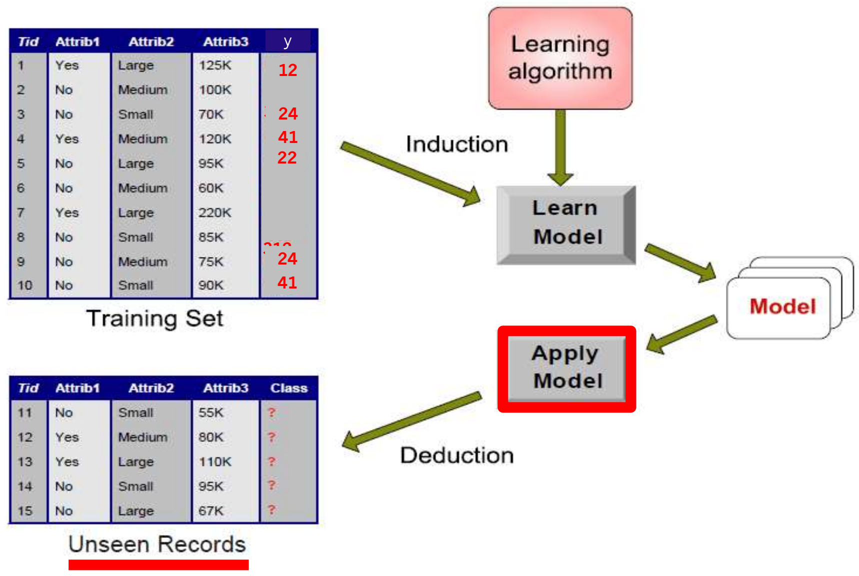
Name	Type	Missing	Min	Max	Average
Label: label	Real	0	0.143	926.739	180.418
Prediction: prediction(label)	Real	0	-32.614	898.428	177.064
a1	Real	0	0.081	9.940	5.000
a2	Real	0	0.009	9.986	4.812

3. Model Evaluation

Central Question:

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

(generalization performance)



3.1 Methods for Model Evaluation

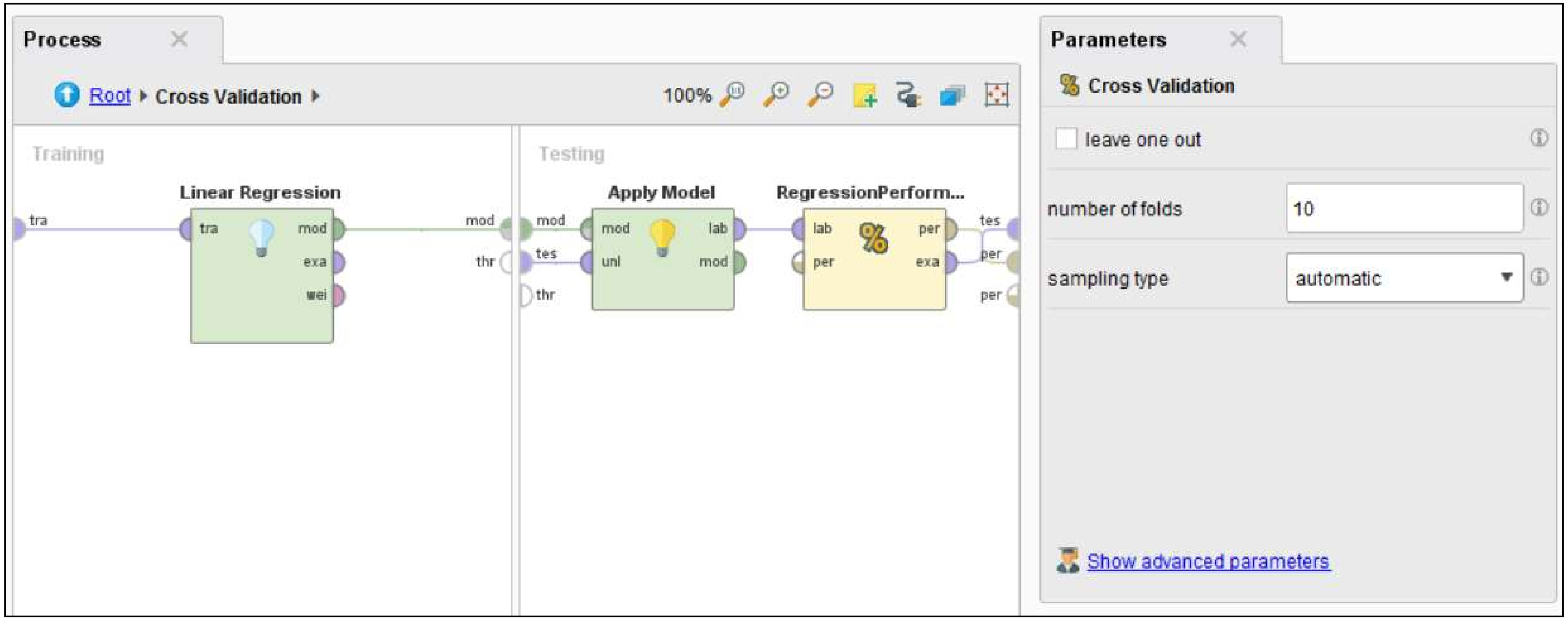
- How to obtain reliable estimates?

3.2 Metrics for Model Evaluation

- How to measure the performance of a regression model?

3.1 Methods for Model Evaluation

– The same considerations apply as for classification
  - Cross Validation: 10-fold (90% for training, 10% for testing in each iteration)
  - Holdout Validation: 80% random share for training, 20% for testing
– Estimating performance metrics in RapidMiner
  - Cross Validation Operator + Regression Performance Operator



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')
```

3.2 Metrics for Model Evaluation

- Mean Absolute Error (*MAE*) computes the average deviation between predicted value p_i and the actual value r_i

$$MAE = \frac{1}{n}\sum_{i=1}^{n} | p_i - r_i |$$

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

$$MSE = \frac{1}{n}\sum_{i=1}^{n} (p_i - r_i)^2$$

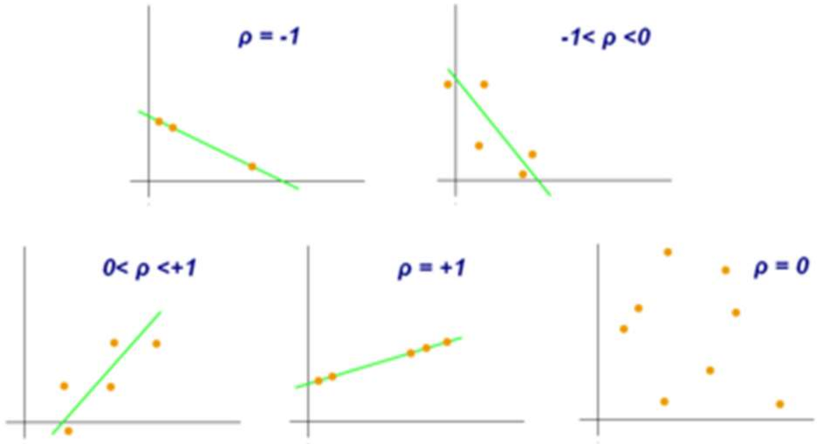
- Root Mean Squared Error (*RMSE*) has similar scale as *MAE* and places more emphasis on larger deviations

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (p_i - r_i)^2}$$

Metrics for Regression Model Evaluation

– Pearson's Correlation Coefficient (PCC)

- scores well if
  - high actual values get high predictions
  - low actual values get low predictions



$$PCC = \frac{\sum_{all\ examples} (pred - \overline{pred}) \times (act - \overline{act})}{\sqrt{\sum_{all\ examples} (pred - \overline{pred})^2} \times \sqrt{\sum_{all\ examples} (act - \overline{act})^2}}$$

– R Squared: Coefficient of Determination

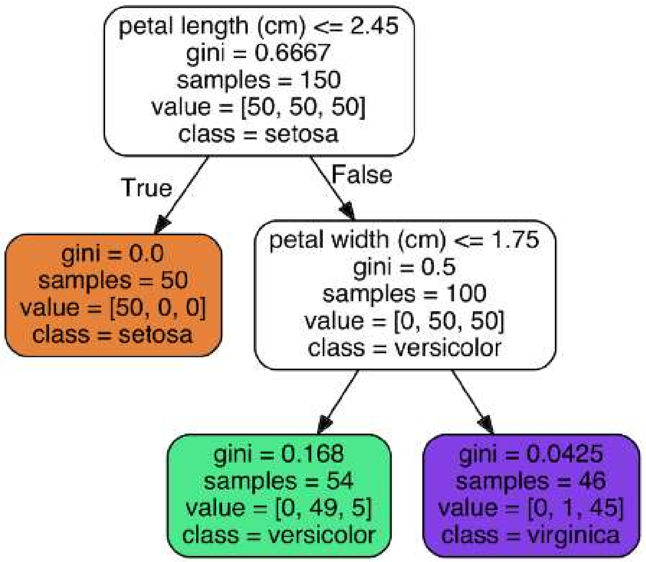
$$R^2 = \frac{\sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$$

- measures the part of the total variation in the dependent variable y that is predictable (explainable) from the explanatory variables X
- $R^2 = 1$: Perfect model as total variation of y can be completely explained from X
- R^2 is called 'squared correlation' in RapidMiner

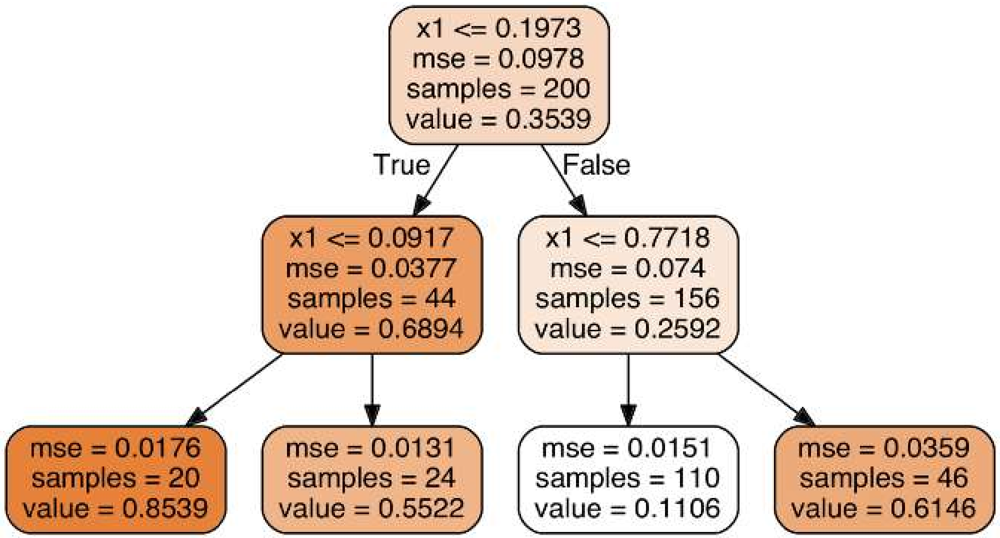
4. Regression Trees

- 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 or entropy)
  2. prediction is average value of the trainings examples in a specific leaf

Decision Tree



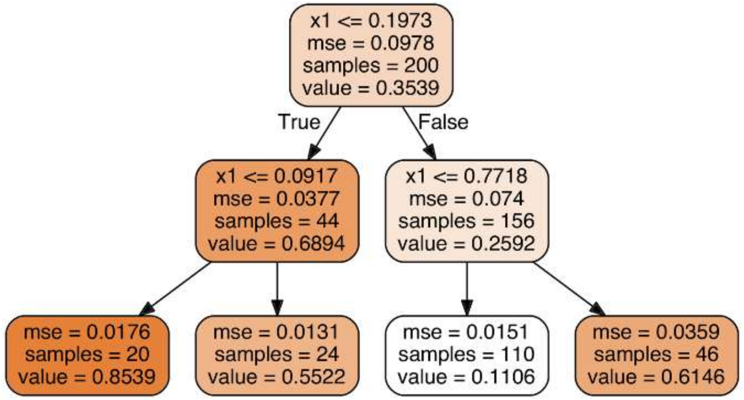
Regression Tree

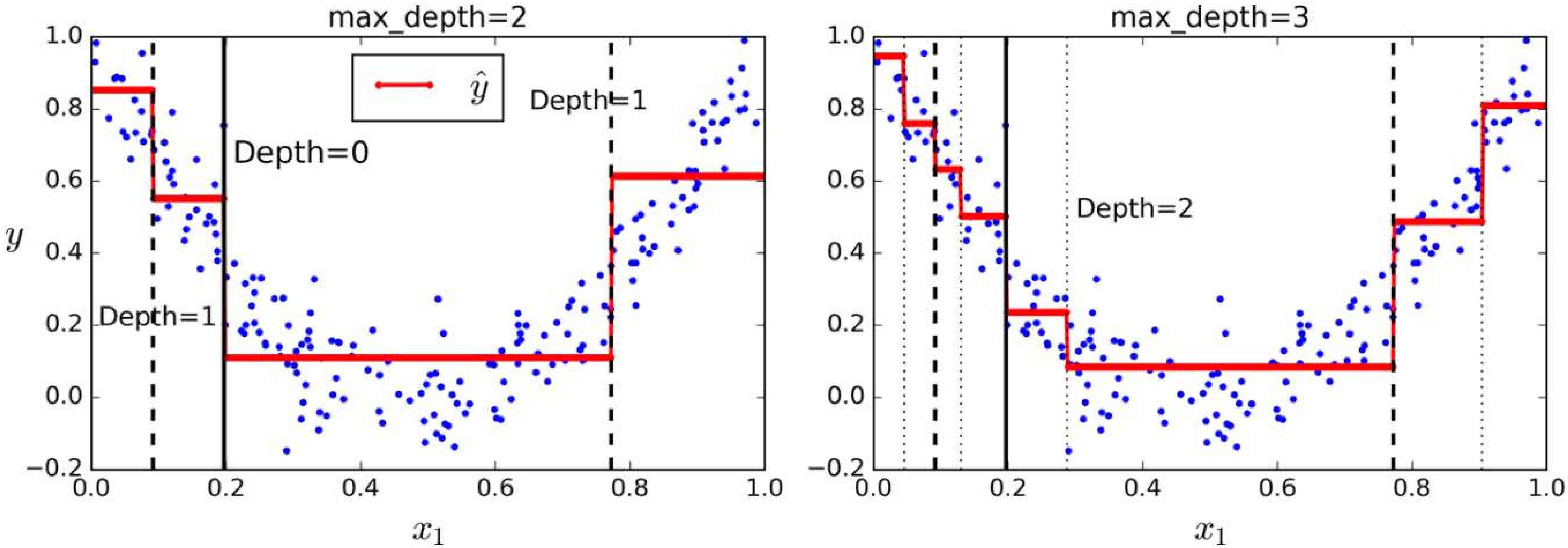


Regression Trees Fitting the Training Data

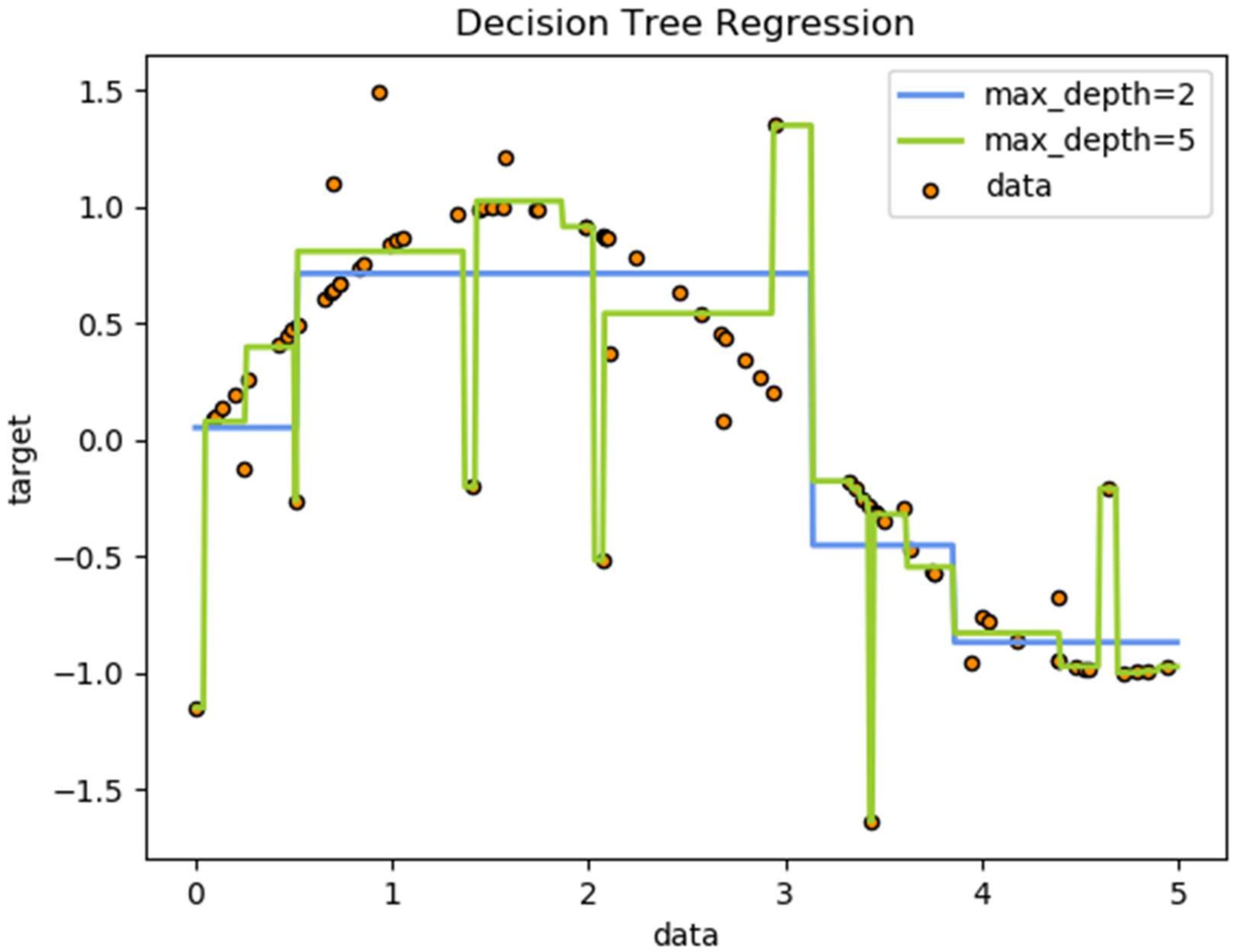
Pre-pruning parameters deterime how closely the tree fits the training data

- e.g. max_depth parameter





Overfitted Regression Tree

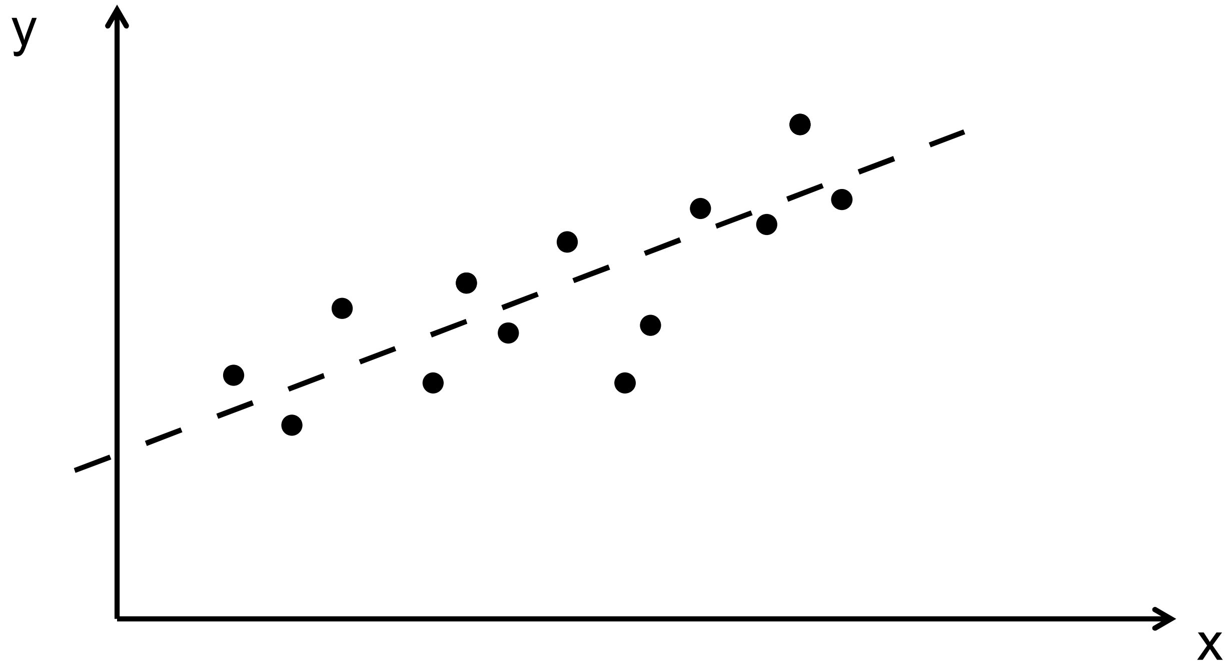


The learning algorithm uses available depth to cover strongest outliers

5. Linear Regression

Assumption of Linear Regression: The target variable y is (approximately) linearly dependent on explanatory variables X

- for visualization: we use one variable x (simple linear regression)
- in reality: vector X = $x_1 \ldots x_n$ (multiple linear regression)

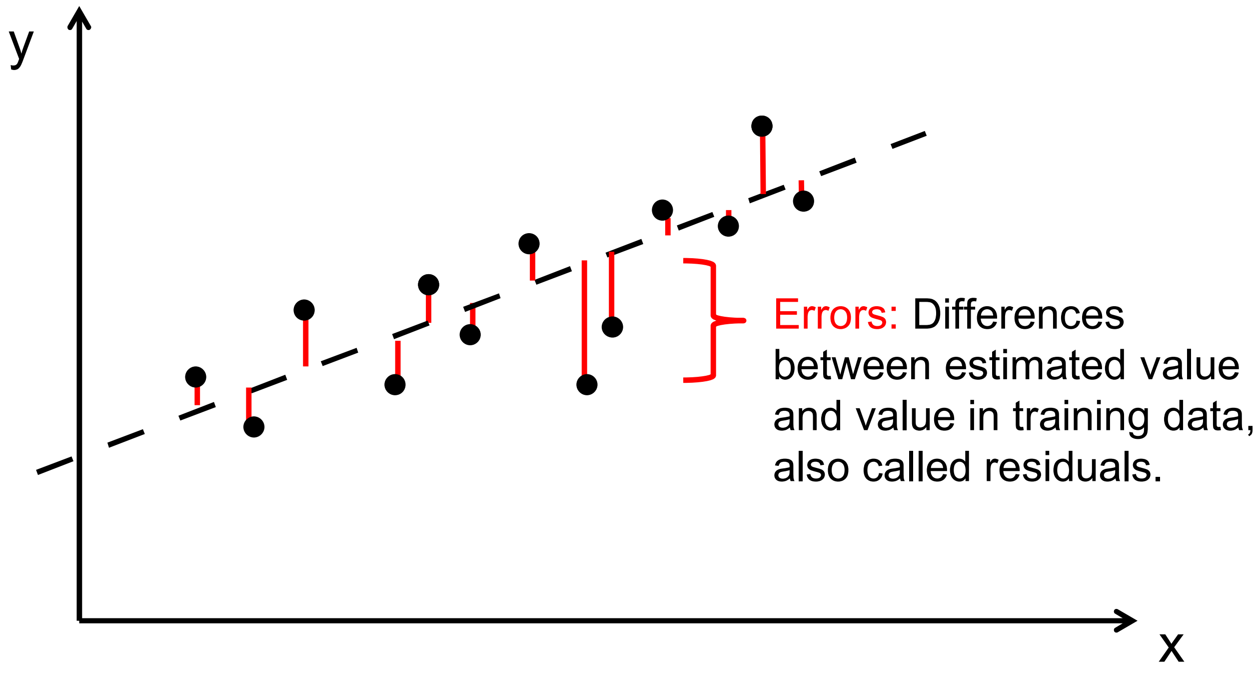


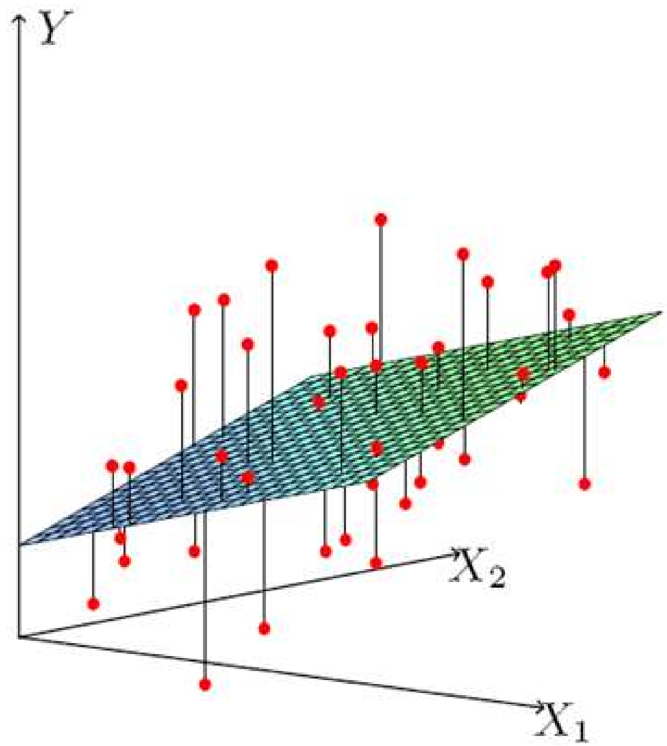
$$\hat{y}(X) = w_0 + w_1x_1 + w_2x_2 + \ldots + w_nx_n$$

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) for all training examples

$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}(X_i, W))^2$$



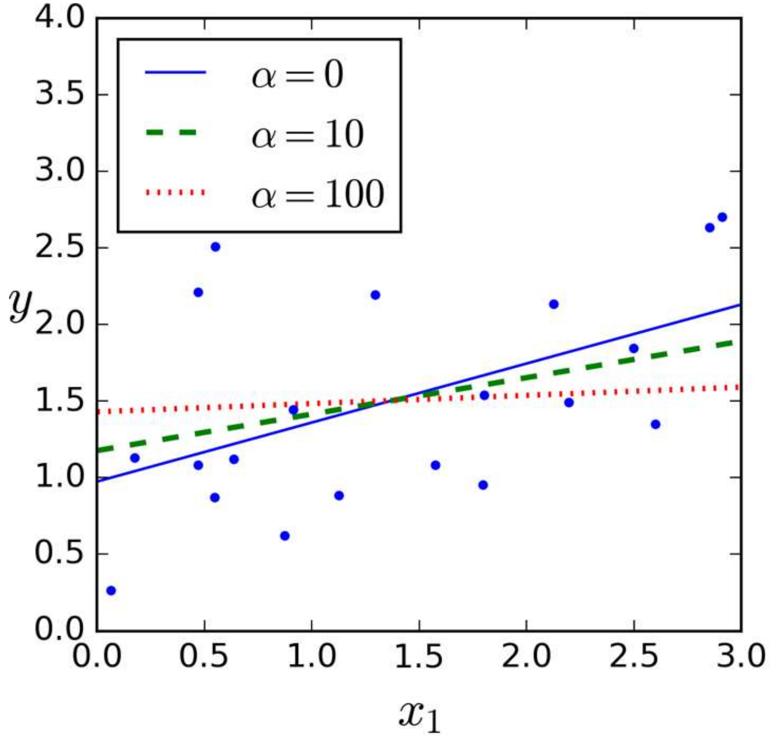


Ridge Regularization

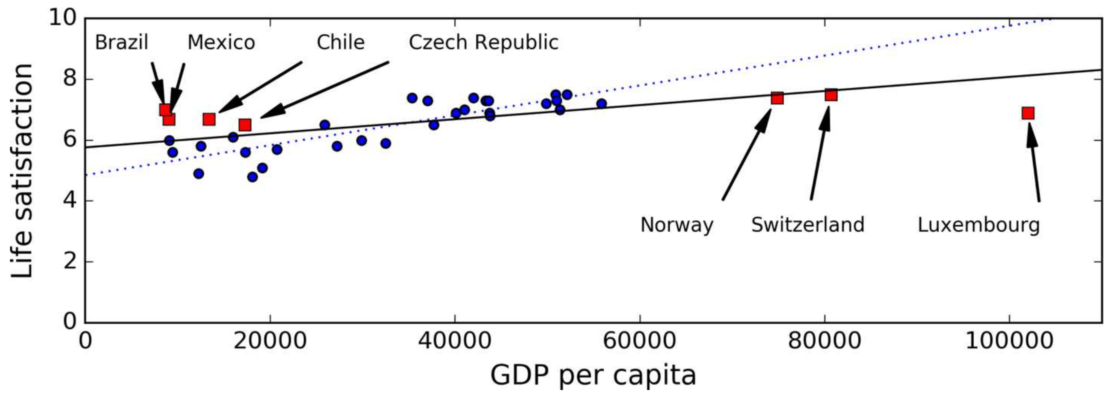
- Variation of least squares approach which tries to avoid overfitting by keeping the weights W small
- Ridge regression cost function to minimize

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

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



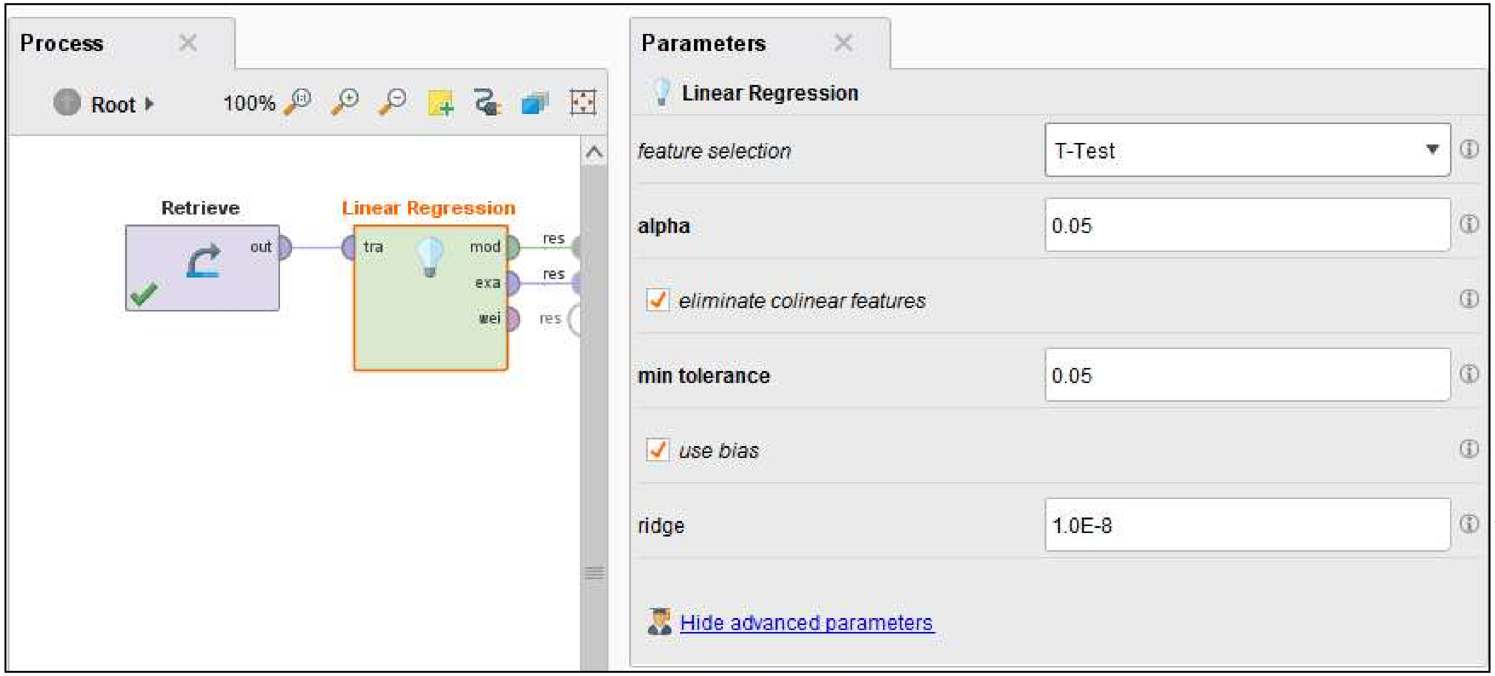
- Example of overfitting due to biased training data



Feature Selection

- 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

Linear Regression in RapidMiner



Choose feature selection method

Correlated features

Ridge (>0) or least squares (0) regression

Attribute	Coefficient	Std. Error	Std. Coeff...	Tolerance	t-Stat	p-Value	Code
a1	85.440	5.692	0.463	1.000	15.009	0	****
a2	127.001	5.701	0.689	0.998	22.276	0	****
a3	68.118	5.730	0.369	1.000	11.888	0	****
a4	10.302	5.728	0.056	1.000	1.799	0.074	*
a5	-12.452	5.723	-0.068	0.999	-2.176	0.031	**
(Intercept)	180.418	5.671	?	?	31.814	0	****

Feature quality code

p-Value

Linear Regression in Python

- Two different classes for linear and ridge regression
- Feature selection implemented as separate preprocessing step

Python

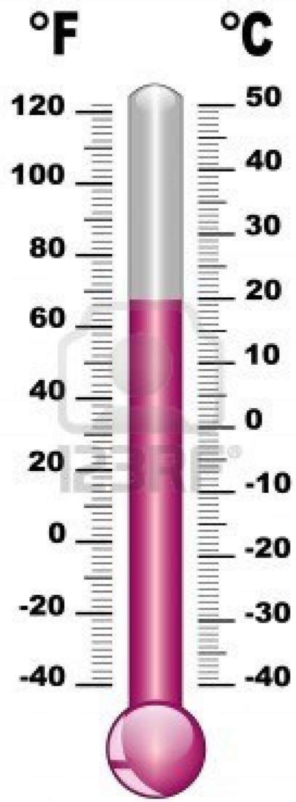
```
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import Ridge

from sklearn.feature_selection import SelectFwe
from sklearn.feature_selection import f_regression

selected_features = SelectFwe(f_regression, alpha=0.05).fit_transform(X, y)
estimator = LinearRegression()
estimator.fit(selected_features, y)
```

Interpolation vs. Extrapolation

- 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

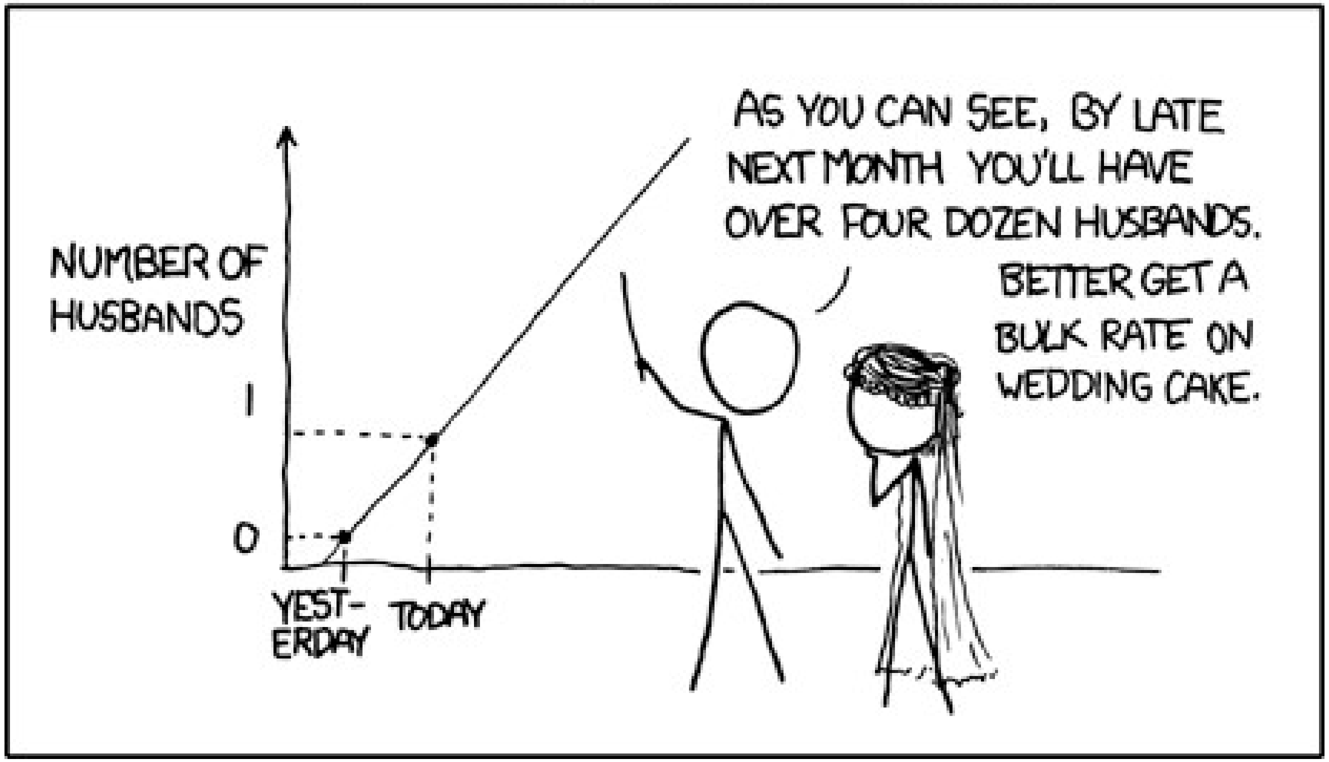


- Interpolating regression
  - only predicts values from the interval [-15°C,32°C]
- Extrapolating regression
  - may also predict values *outside* of this interval

Interpolation vs. Extrapolation

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

MY HOBBY: EXTRAPOLATING



http://xkcd.com/605/

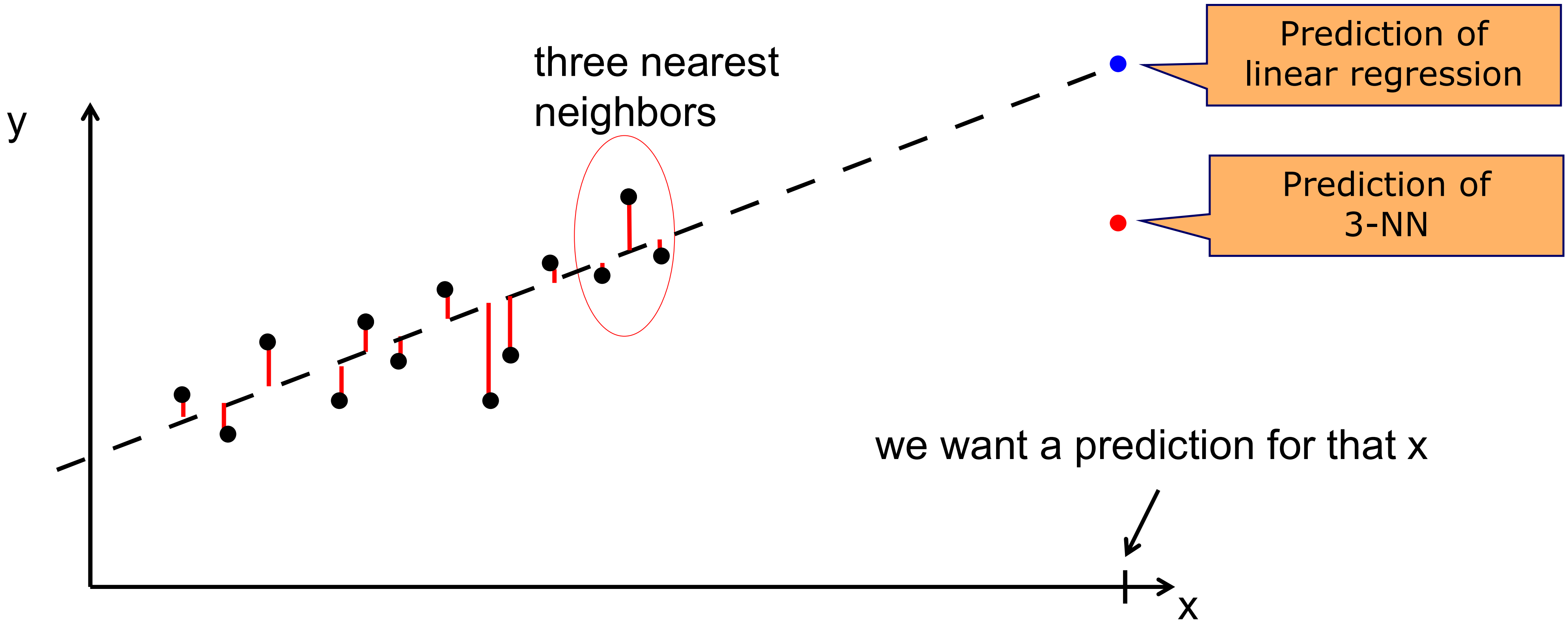
Interpolation vs. Extrapolation

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

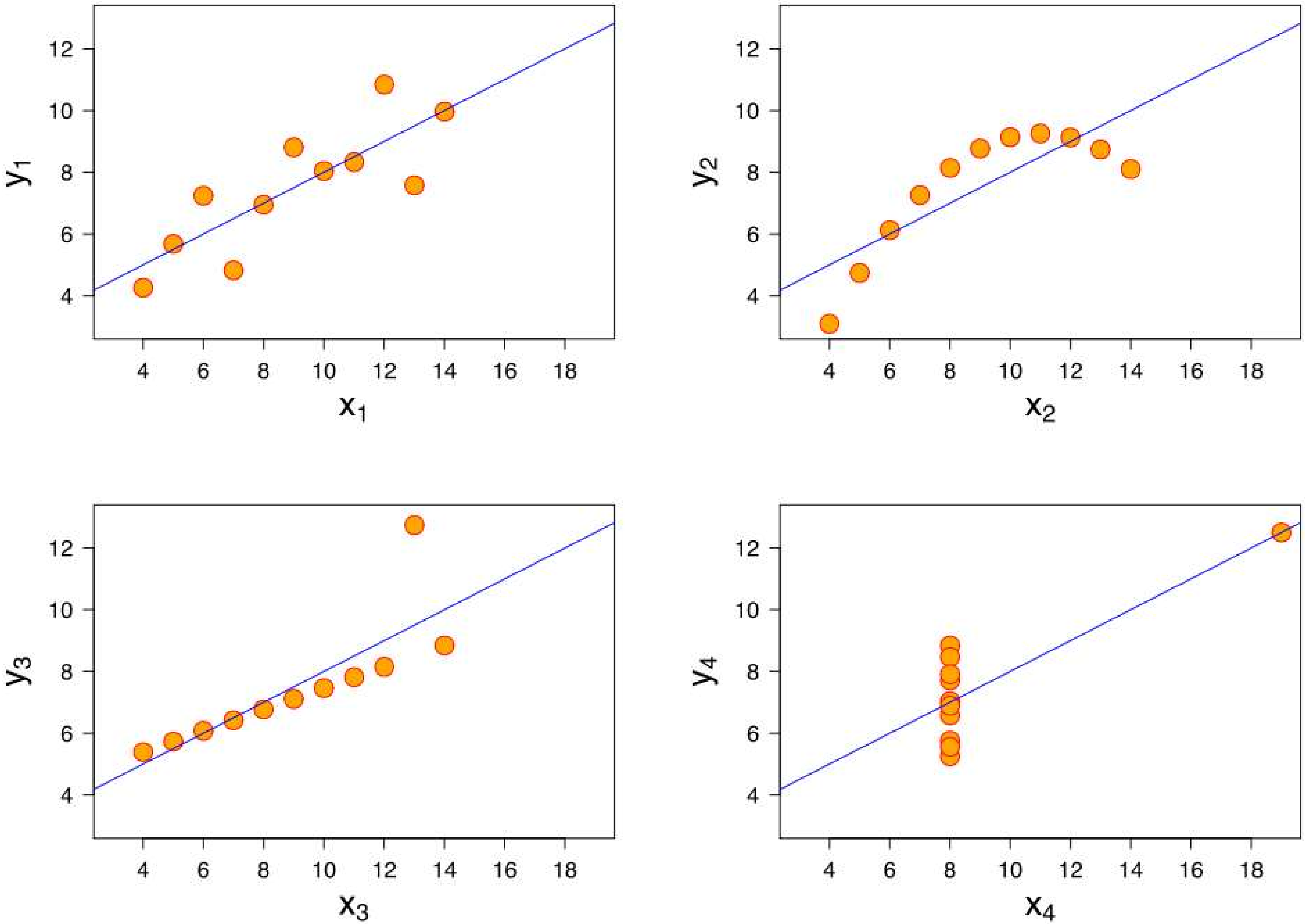
http://i1.ytimg.com/vi/FVfiujbGLfM/hqdefault.jpg

Linear Regression vs. K-NN Regression

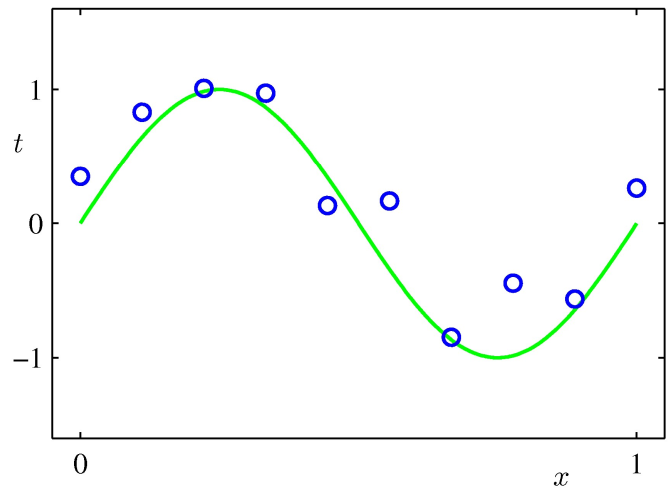
- Linear regression extrapolates
- K-NN and regression trees interpolate



Linear Regression Examples



… But What About Non-linear Problems?

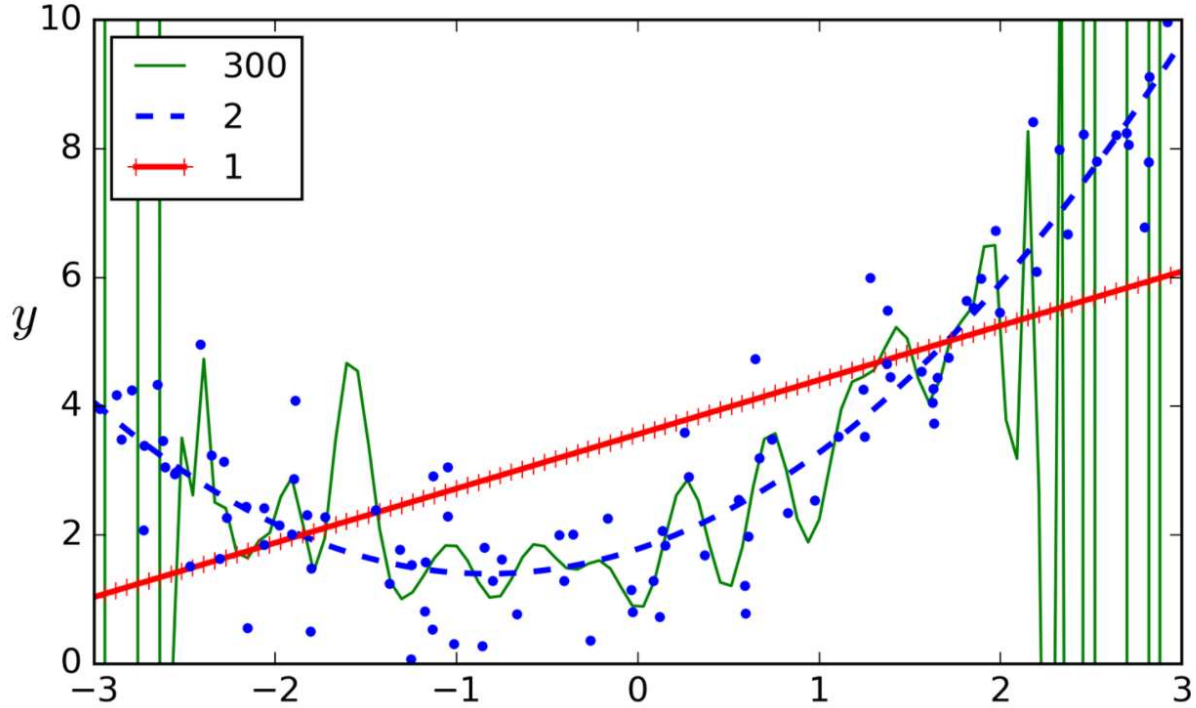


- One possibility is to apply transformations to the explanatory variables X within the regression function
  - e.g. log, exp, square root, square, etc.
    - example: : $\hat{y} = \omega_0 + \omega_1 \cdot x_1^2 + \omega_2 \cdot x_2^2$
  - polynomial transformation
    - example: $\hat{y} = \omega_0 + \omega_1 \cdot x + \omega_2 \cdot x^2 + \omega_3 \cdot x^3$
- This allows use of linear regression techniques to fit much more complicated non-linear datasets

6. Polynomial Regression

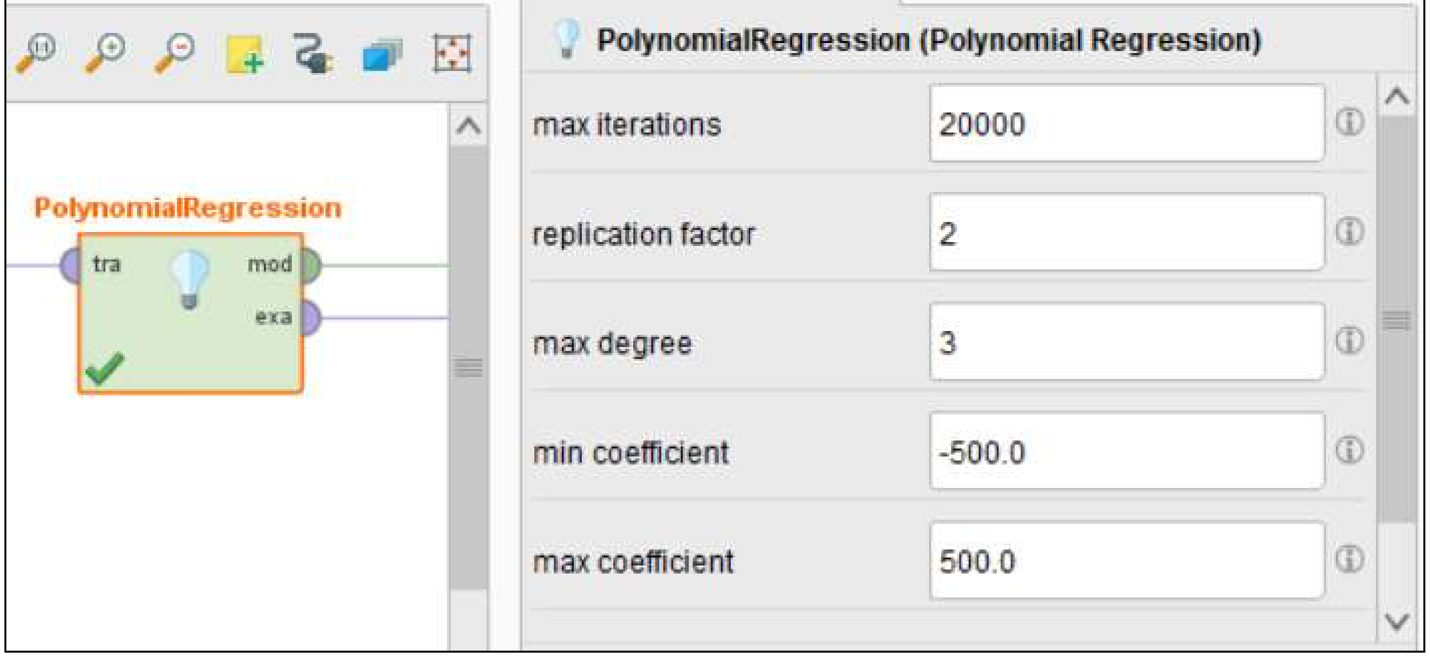
$$\hat{y}(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

- 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 M
- Workarounds:
  1. decrease M
  2. increase amount of training data



Polynomial Regression in RapidMiner and Python

RapidMiner



How often may each explanatory variable appear in the function.

Maximal degree to be used in the function

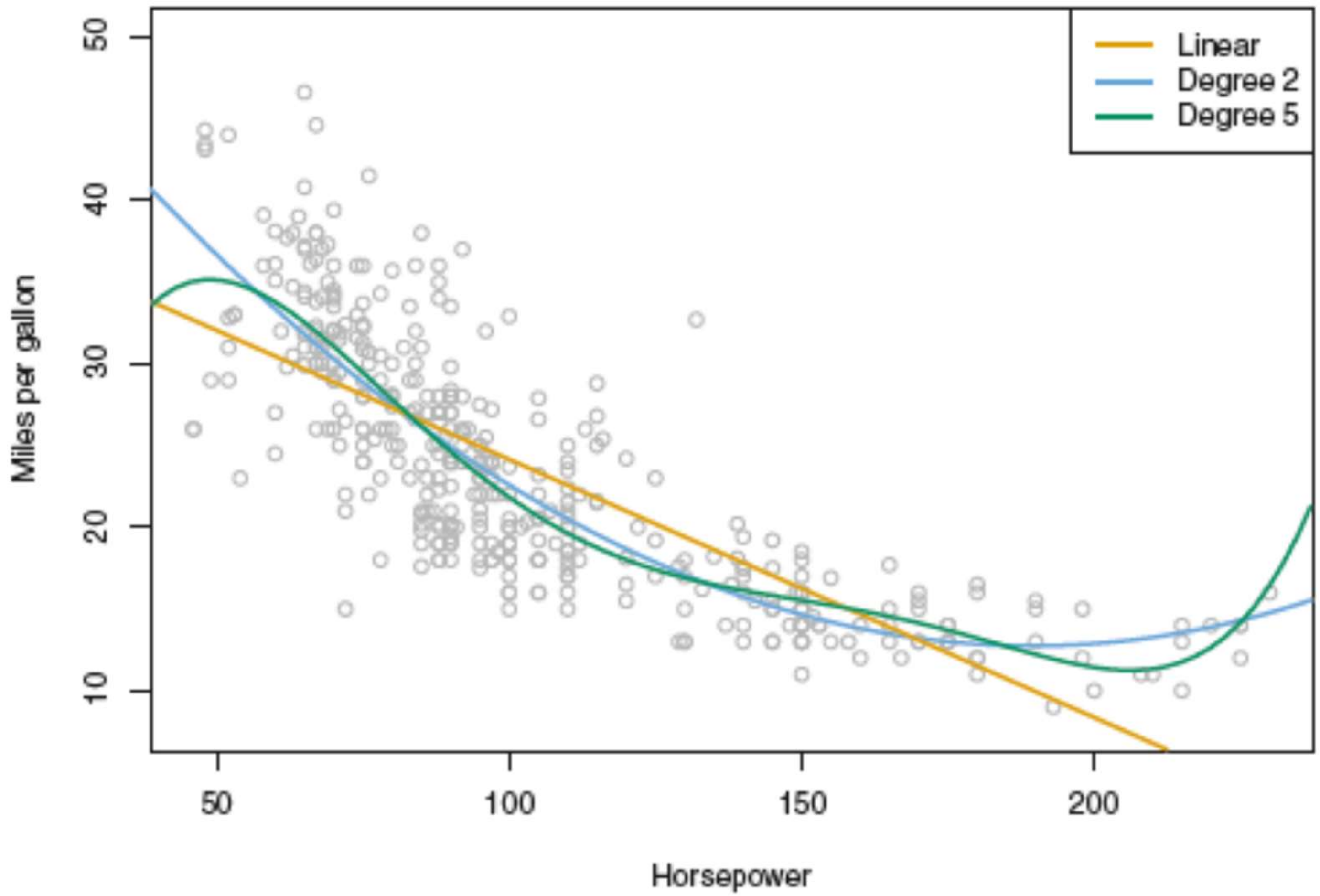
Boundaries for weights W

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

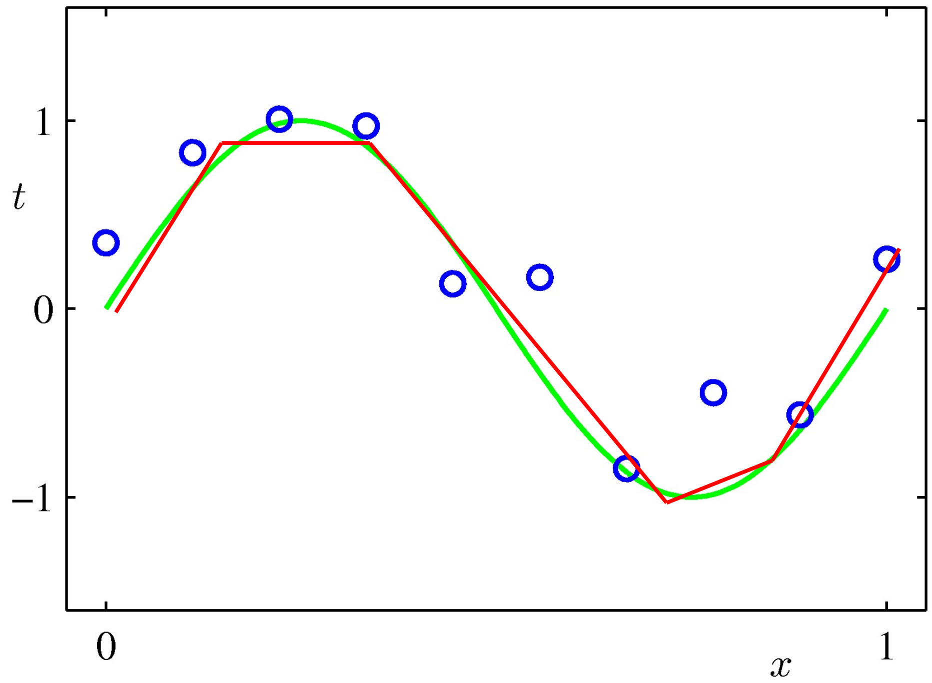


Overfitting often happens in sparse regions

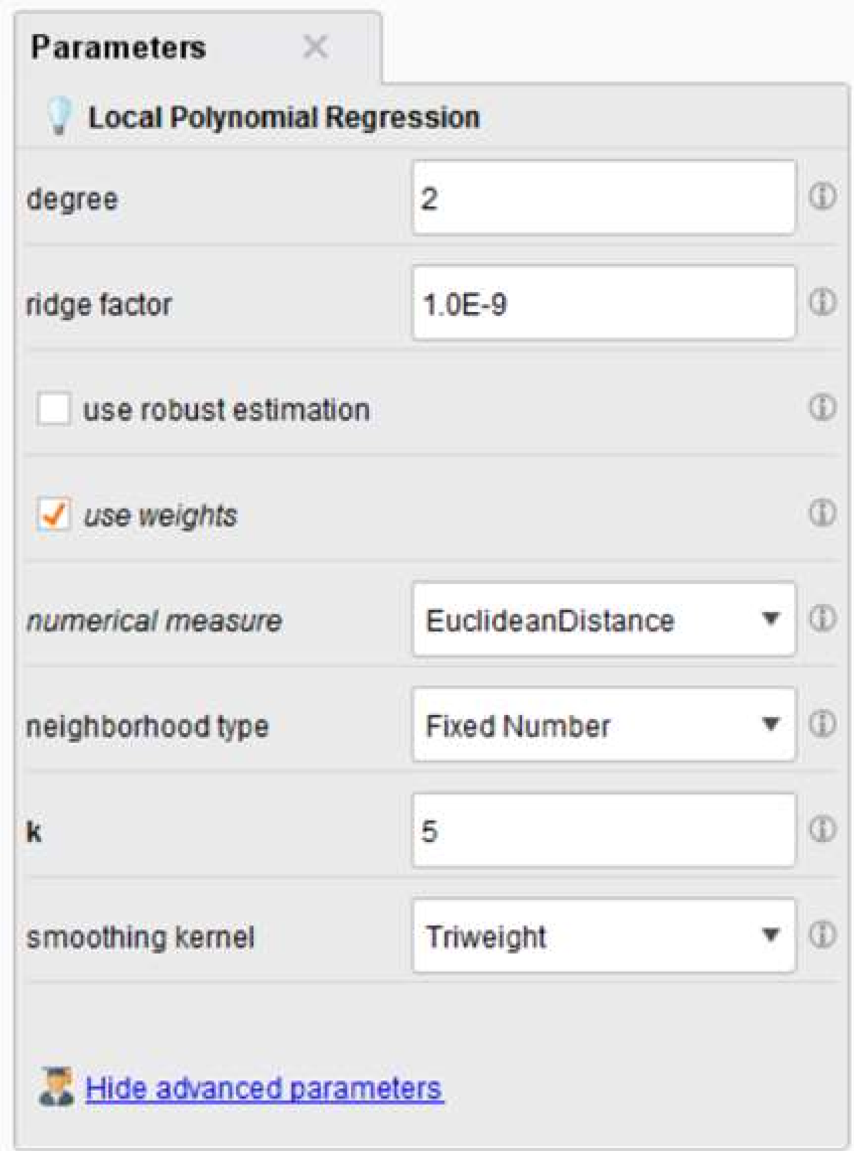
- left and right side of green line
- workaround: Local Regression

7. Local Regression

- Assumption: non-linear problems are approximately linear in local areas
- Idea: use linear regression locally for the data point at hand (lazy learning)
- A combination of
  - k nearest neighbors
  - linear regression
- Given a data point
  1. retrieve the k nearest neighbors
  2. learn a regression model using those neighbors
  3. use the learned model to predict y value



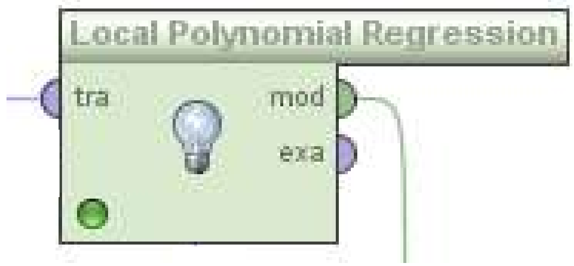
Local Regression in Rapidminer



Maximal degree to be used. Set to 1 for local linear regression

Distance function for determining neighborhood

Neighborhood size



Discussion of Local Regression

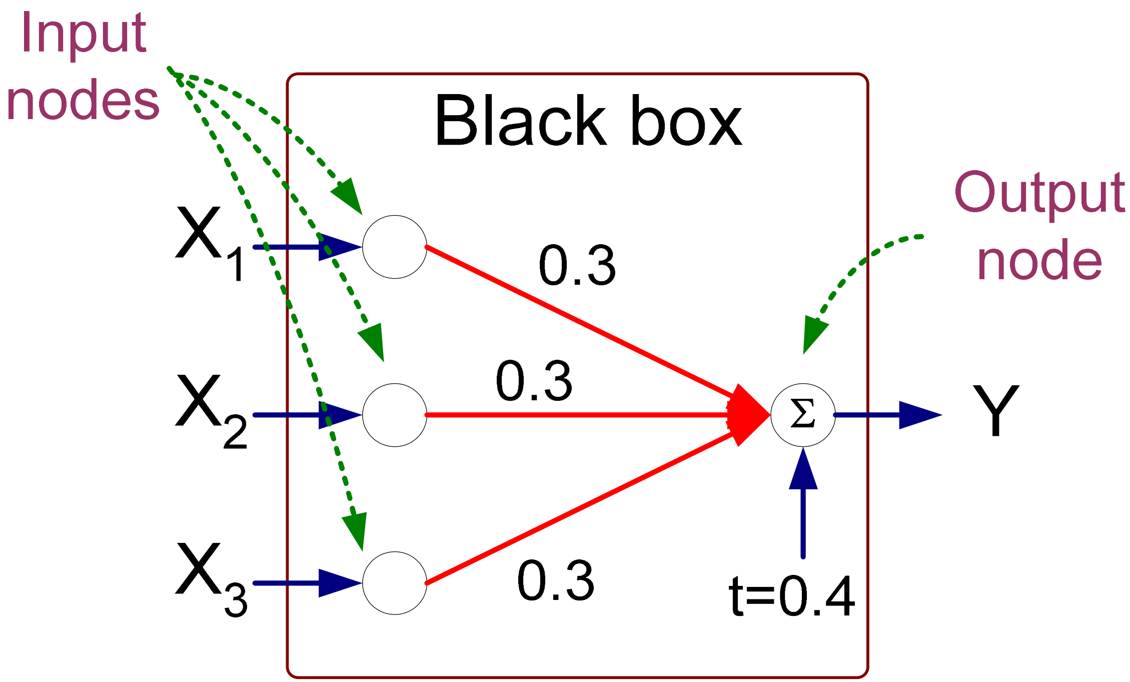
– Advantage: fits non-linear models well
  - good local approximation
  - often better than pure k-NN

– Disadvantage
  - slow at runtime
  - for each test example:
    - find k nearest neighbors
    - compute a local model

8. Artificial Neural Networks (ANNs) for Regression

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



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

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

Artificial Neural Networks for Regression

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

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

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

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

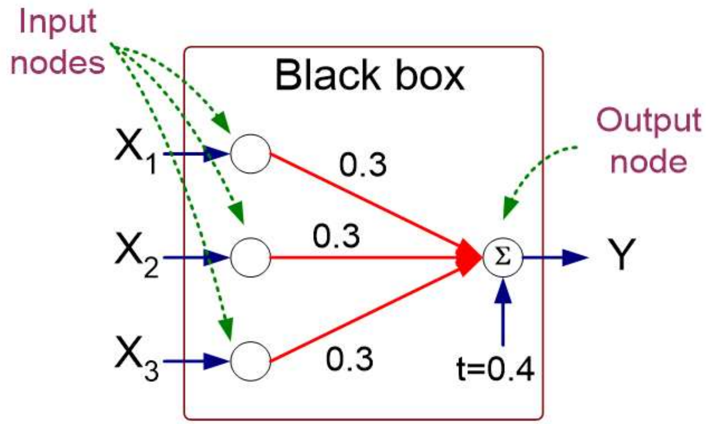
$$\hat{Y} = 0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4$$

– What has changed:
  - we do not use a cutoff for 0/1 predictions, but leave the numbers as they are

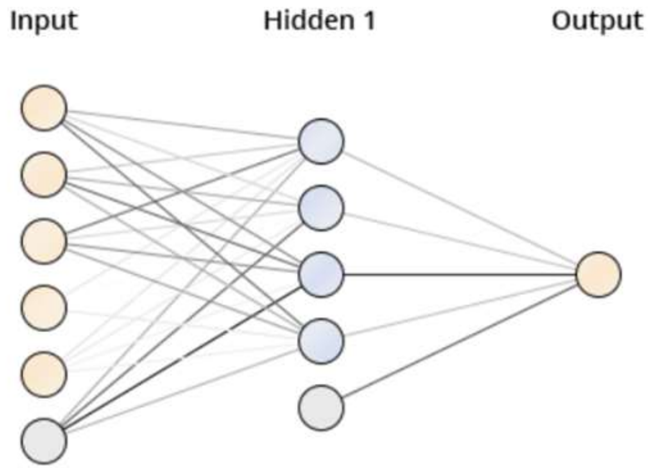
Artificial Neural Networks for Regression

– Given that our formula is of the form

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



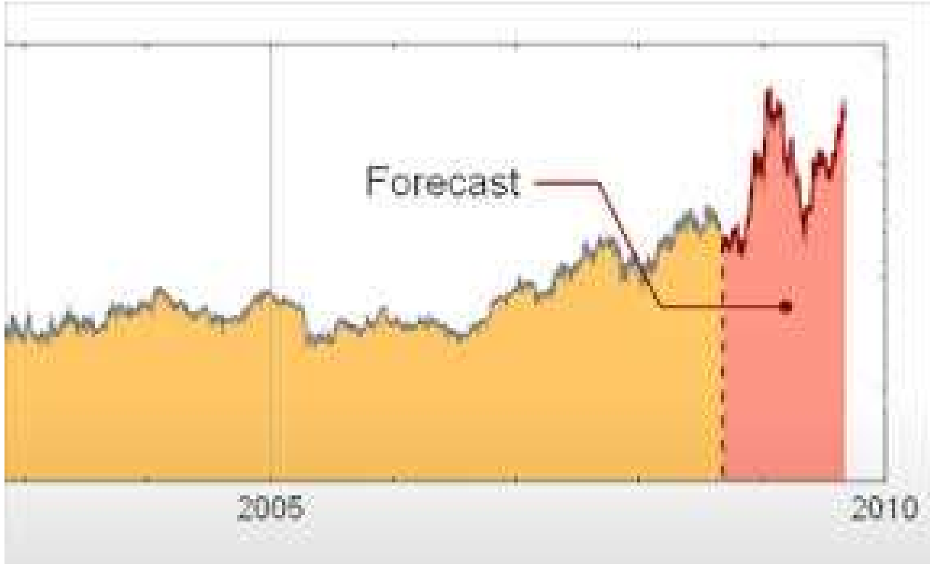
– we can learn only linear models
  - i.e., the target variable is a linear combination the input variables
– More complex regression problems can be approximated
  - by using multiple hidden layers
  - this allows for arbitrary functions



– Deep ANNs take this idea further by
  - employing millions of neurons
  - arranging them into specific network topologies
– If you use ANNs be cautions about overfitting!

9. Time Series Forecasting

– A **time series** is a series of data points indexed in time order
  - examples: Stock market prices, ocean tides, birth rates, temperature
– **Forecasting**: Given a time series, predict data points that continue the series into the future
  - explicitly deals with time, which is not explicitly considered by other regression techniques
  - aims to predict future values of the same variable
– Approaches:
  1. Data-driven: Smoothing
  2. Model-Driven:
     1. component models of time series
     2. other regression techniques



Smoothing

Simple Moving Average (SMA)

– average of the last n values, as more recent values might matter more

$$m_{\text{MA}}^{(n)}(t) = \frac{1}{n}\sum_{i=0}^{n-1} x(t-i)$$

Exponential Moving Average (EMA)

– exponentially decrease weight of older values

$$m_{\text{EMA}}^{(n)}(t) = \alpha \cdot x(t) + (1-\alpha) \cdot m_{\text{EMA}}^{(n)}(t-1)$$

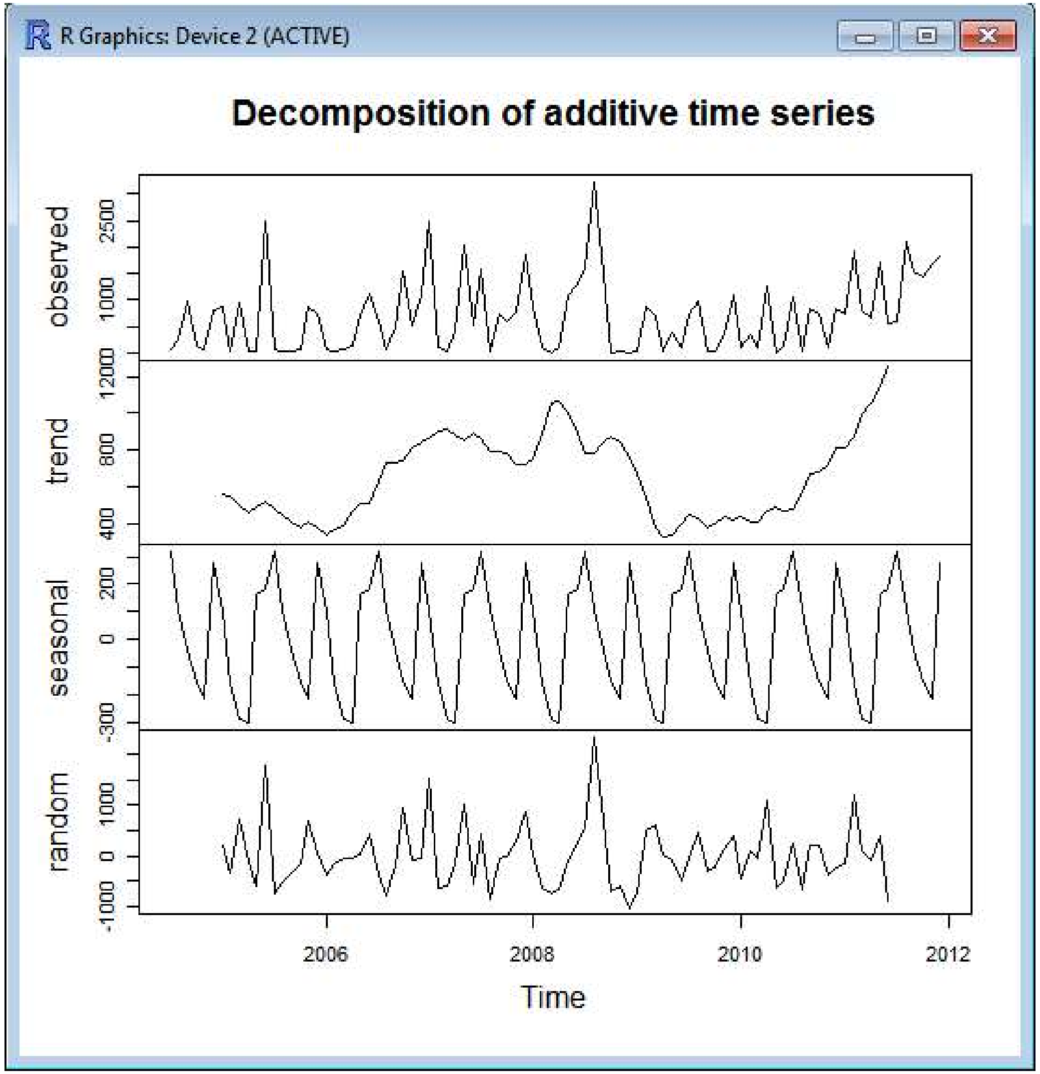
DAX: red = SMA(38 days), yellow = SMA(200 days)

Component Models of Time Series

Assume **time series** to consist of four components:

1. Long-term trend (T_t)
2. Cyclical effect (C_t)
3. Seasonal effect (S_t)
4. Random variation (R_t)

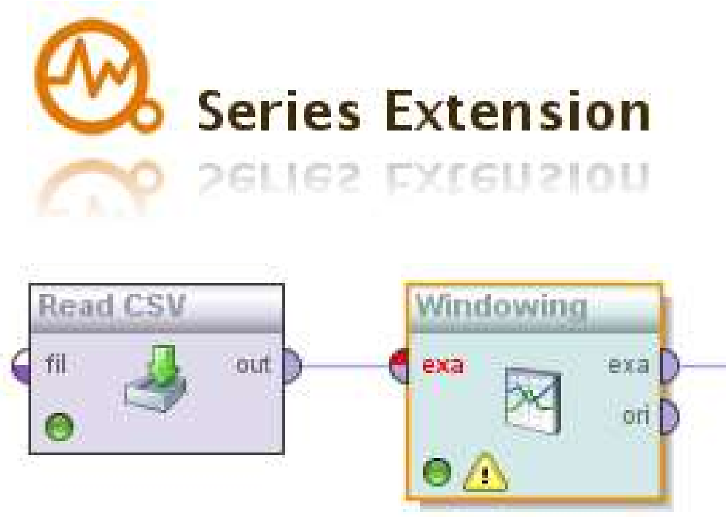
Series = $T_t + C_t + S_t + R_t$

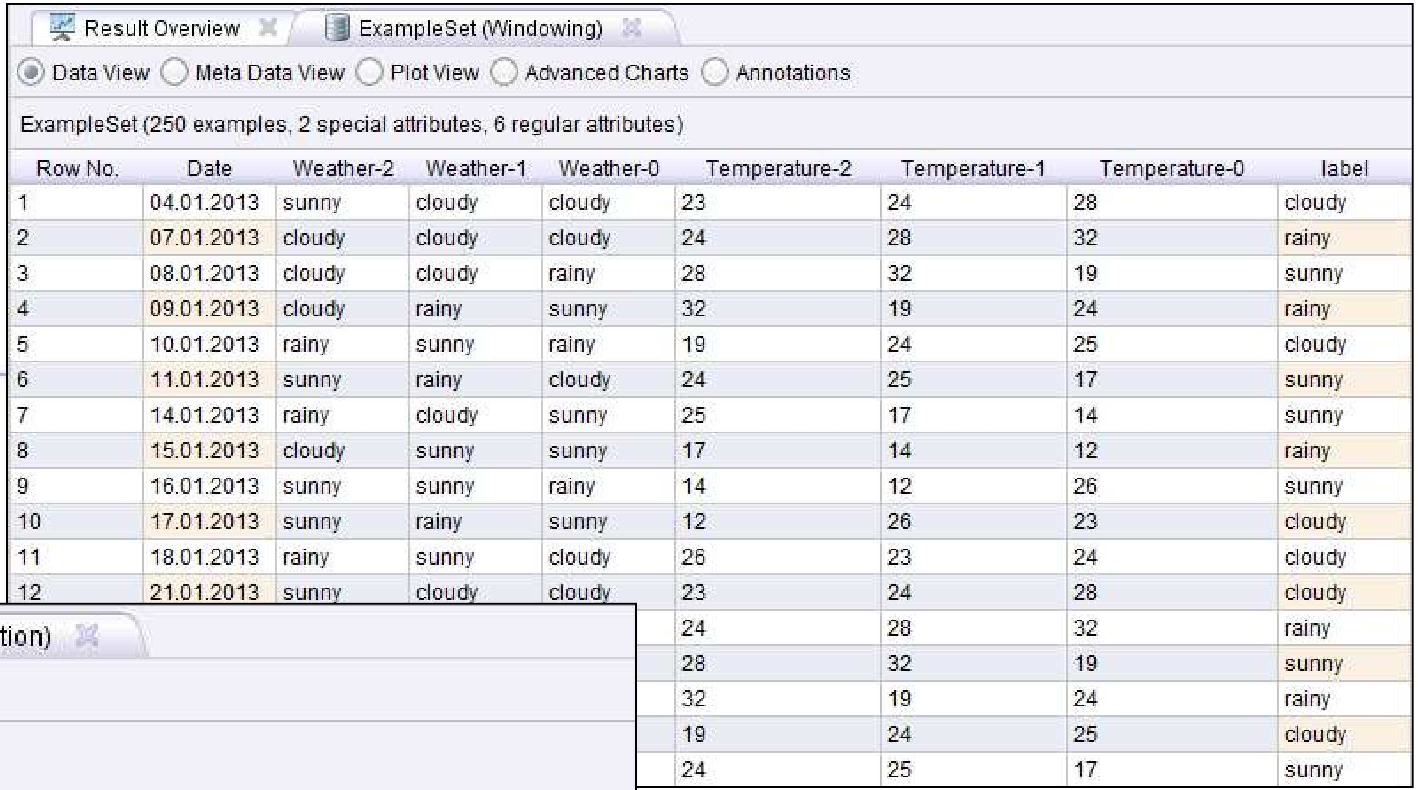


Windowing

- Idea: Transformation of forecasting problem into “classical” learning problem
  - either classification or regression
  - by only taking the last k time periods into account
- Example: Weather forecasting
  - using the weather from the three previous days
  - Possible model:
    - sunny, sunny, sunny → sunny
    - sunny, cloudy, rainy → rainy
    - sunny, cloudy, cloudy → rainy
- Assumption:
  - only the last k time periods matter for the forecast
  - the older past is irrelevant

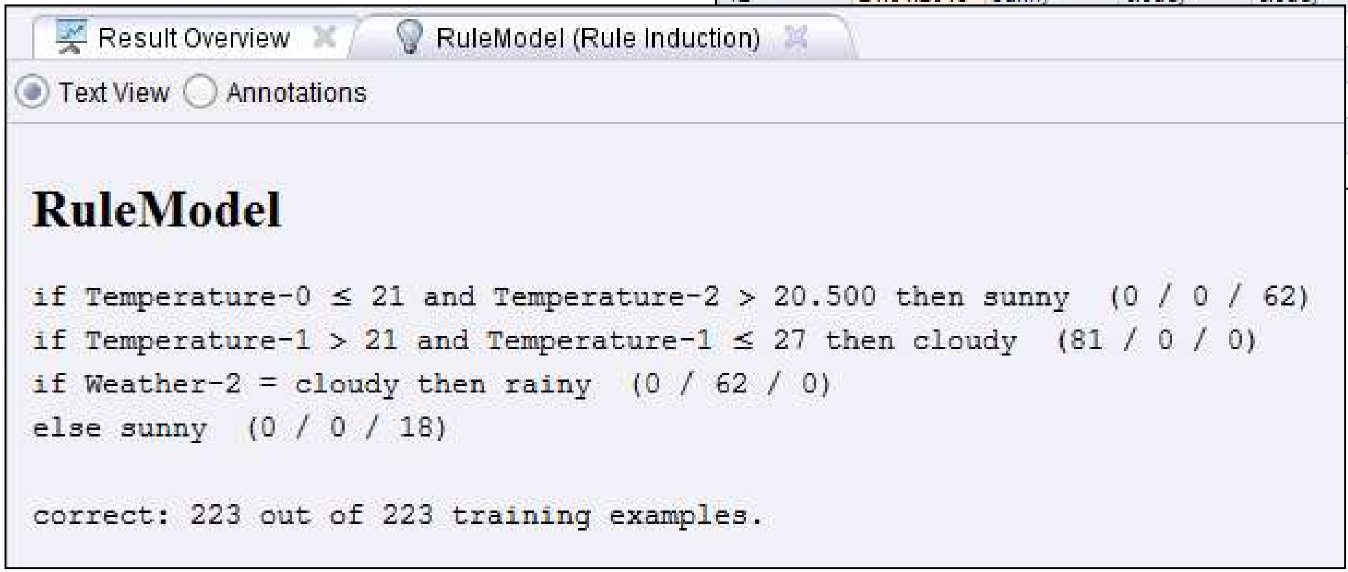
Windowing in RapidMiner and Python





ExampleSet (250 examples, 2 special attributes, 6 regular attributes)

Row No.	Date	Weather-2	Weather-1	Weather-0	Temperature-2	Temperature-1	Temperature-0	label
1	04.01.2013	sunny	cloudy	cloudy	23	24	28	cloudy
2	07.01.2013	cloudy	cloudy	cloudy	24	28	32	rainy
3	08.01.2013	cloudy	cloudy	rainy	28	32	19	sunny
4	09.01.2013	cloudy	rainy	sunny	32	19	24	rainy
5	10.01.2013	rainy	sunny	rainy	19	24	25	cloudy
6	11.01.2013	sunny	rainy	cloudy	24	25	17	sunny
7	14.01.2013	rainy	cloudy	sunny	25	17	14	sunny
8	15.01.2013	cloudy	sunny	sunny	17	14	12	rainy
9	16.01.2013	sunny	sunny	rainy	14	12	26	sunny
10	17.01.2013	sunny	rainy	sunny	12	26	23	cloudy
11	18.01.2013	rainy	sunny	cloudy	26	23	24	cloudy
12	21.01.2013	sunny	cloudy	cloudy	23	24	28	cloudy
					24	28	32	rainy
					28	32	19	sunny
					32	19	24	rainy
					19	24	25	cloudy
					24	25	17	sunny



RuleModel

```
if Temperature-0 ≤ 21 and Temperature-2 > 20.500 then sunny  (0 / 0 / 62)
if Temperature-1 > 21 and Temperature-1 ≤ 27 then cloudy  (81 / 0 / 0)
if Weather-2 = cloudy then rainy  (0 / 62 / 0)
else sunny  (0 / 0 / 18)

correct: 223 out of 223 training examples.
```

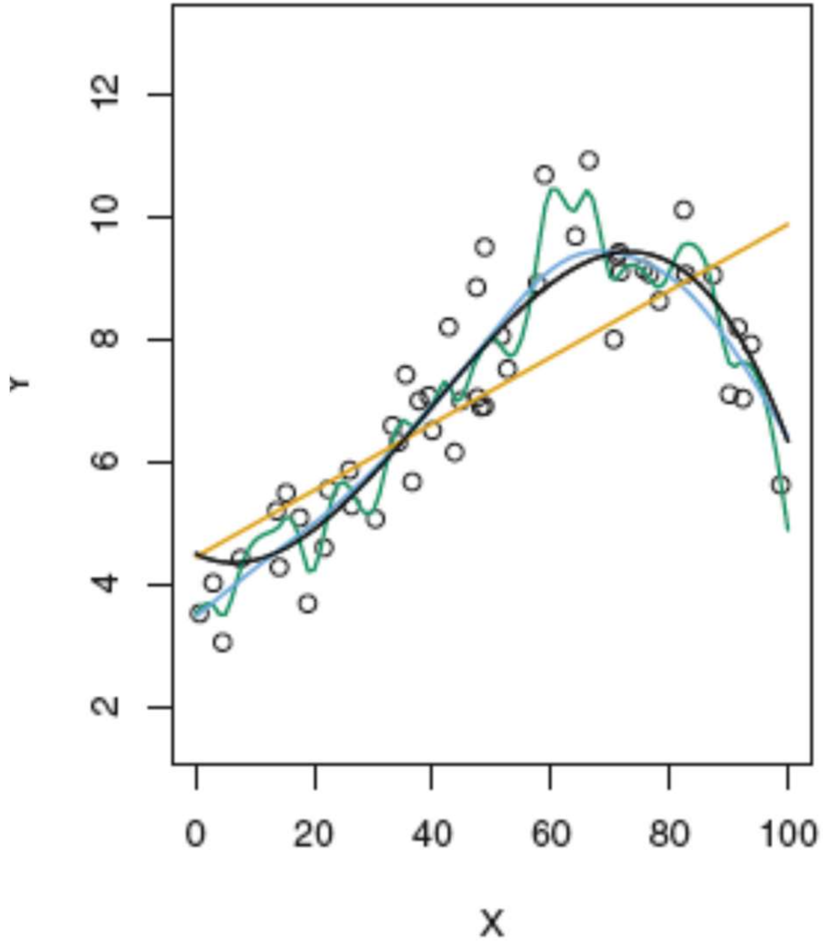
Python: Windowing is implemented using
pandas.DataFrame.shift()
pandas.DataFrame.rolling()

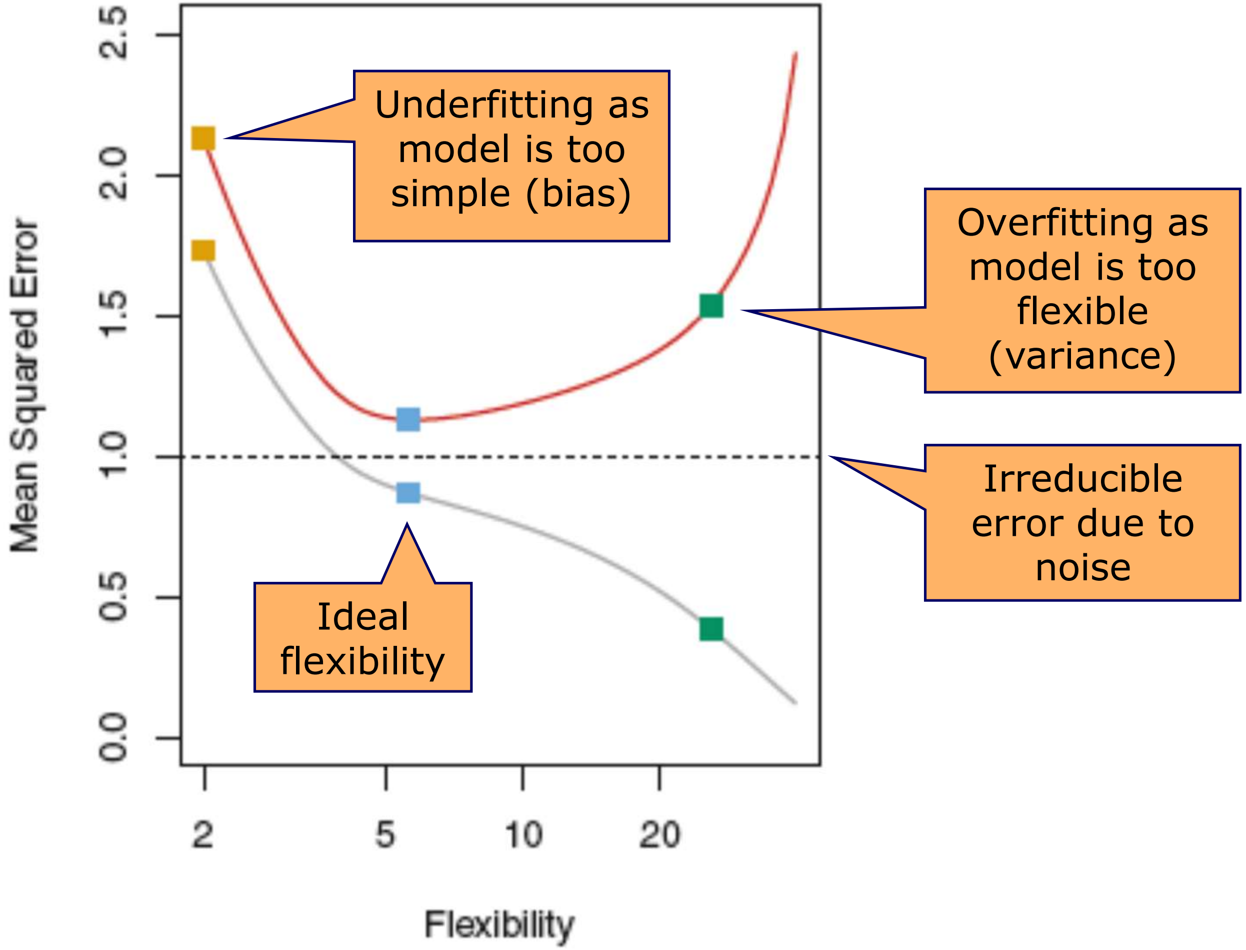
10. The Bias/Variance-Tradeoff

- 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:
  1. **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
  2. **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
  3. **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, fixing broken sensors)

The Bias/Variance-Tradeoff

- Left: Three models with different flexibility trying to fit a function
  - Orange: Linear regression. Green, blue: Polynomials of different degrees
- Right: Training error (gray) and test error (red) in relation to model flexibility

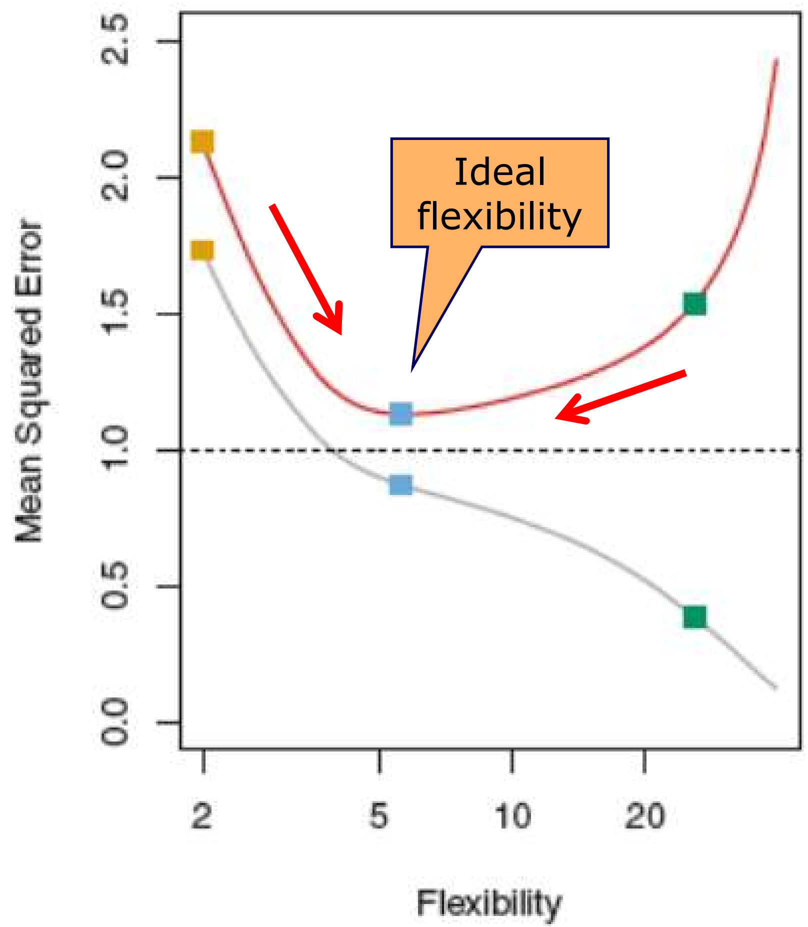




Learning Method and Hyperparameter Selection

We try to find the ideal flexibility (bias/variance-tradeoff) by

1. Testing different learning methods
   - Linear regression, polynomial regression, …
   - Decision Trees, ANNs, Naïve Bayes, …
2. Testing different hyperparameters
   - degree of polynomial, ridge
   - max depth of tree, min examples branch
   - number of hidden layers of ANN



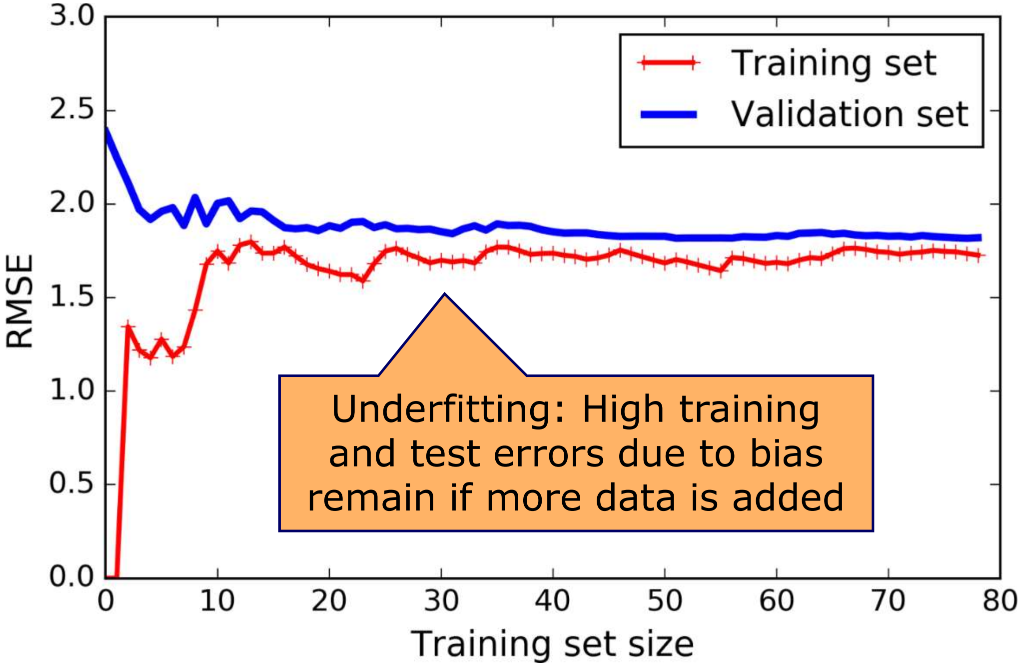
But we have three more options:

1. increase the amount of training data
2. increase the interestingness of the data by including more corner cases
3. cleanse the training data

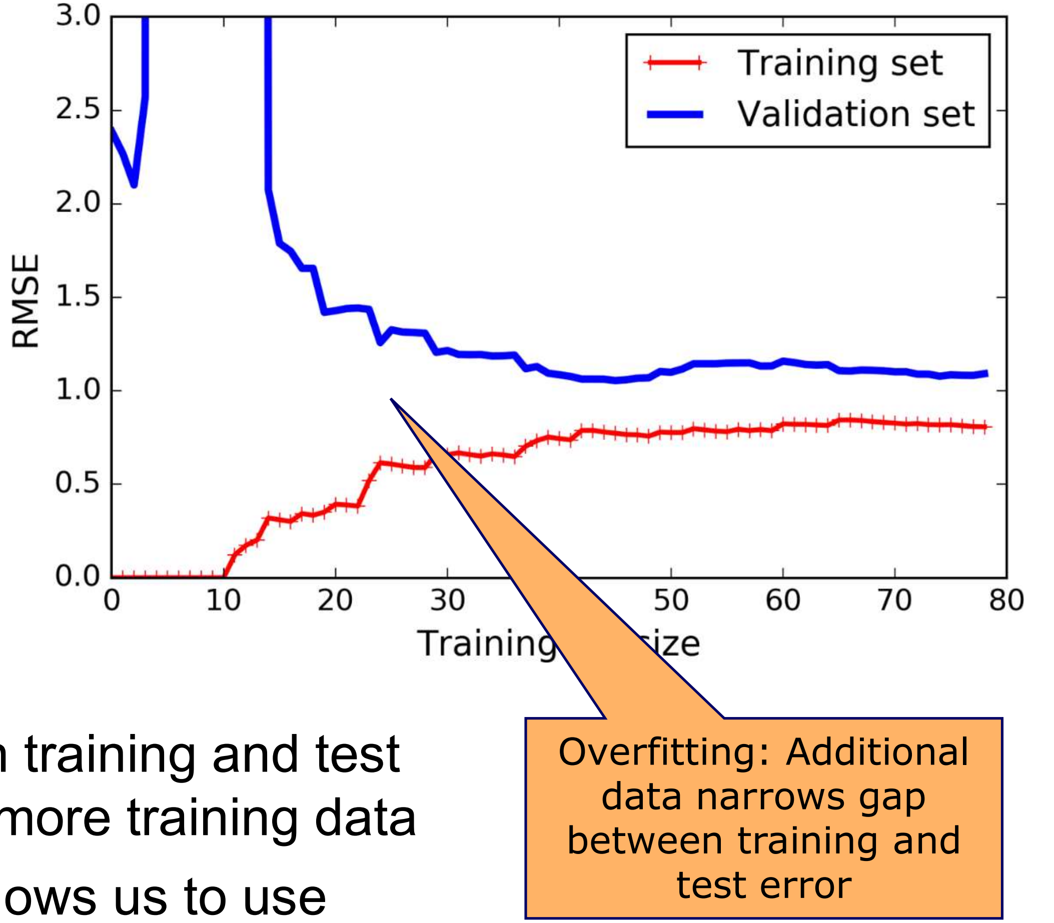
Learning Curves

– Visualize the training error and test error for different training set sizes

Low Flexibility Model (e.g. Linear regression)



High Flexibility Model (e.g. Polynomial regression)



– 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

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

Literature

– Solving practical regression tasks using:
  - RapidMiner: Kotu: Predictive Analytics - Chapter 5, 10
  - 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