

Data Mining

Regression

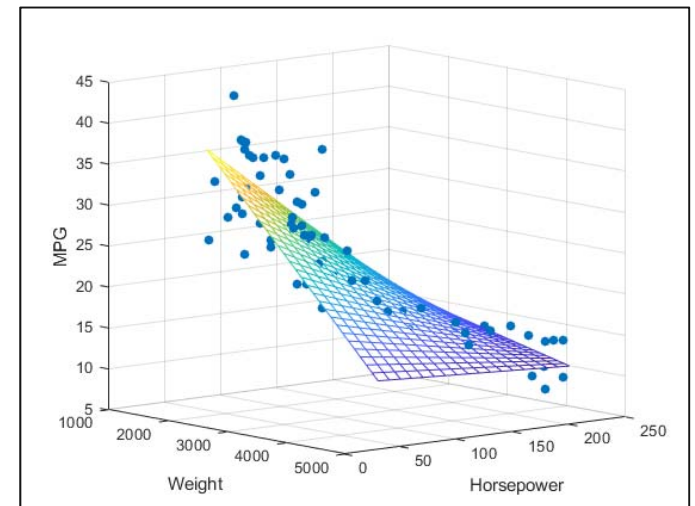
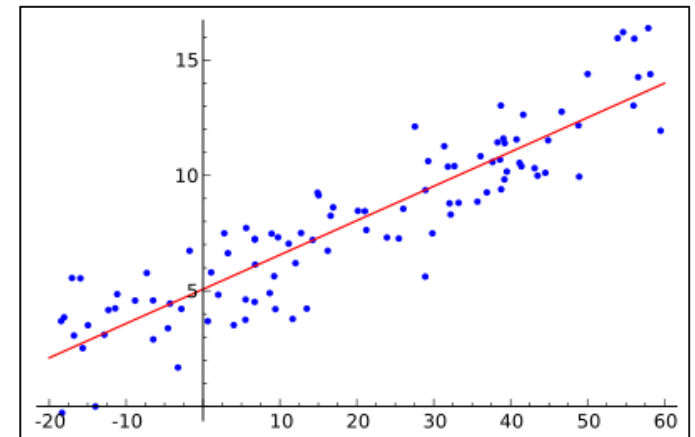


Outline

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

1. What is Regression?

- Goal: Predict the value of a **scalar 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 $X = x_1, x_2, \dots, x_n$
- Approach: Given training examples (X_i, y_i) learn a model f to predict \hat{y} from X .
- Difference to classification: The predicted attribute is continuous, while classification is used to predict nominal class attributes.



Regression Model Learning and Application

Explanatory variables

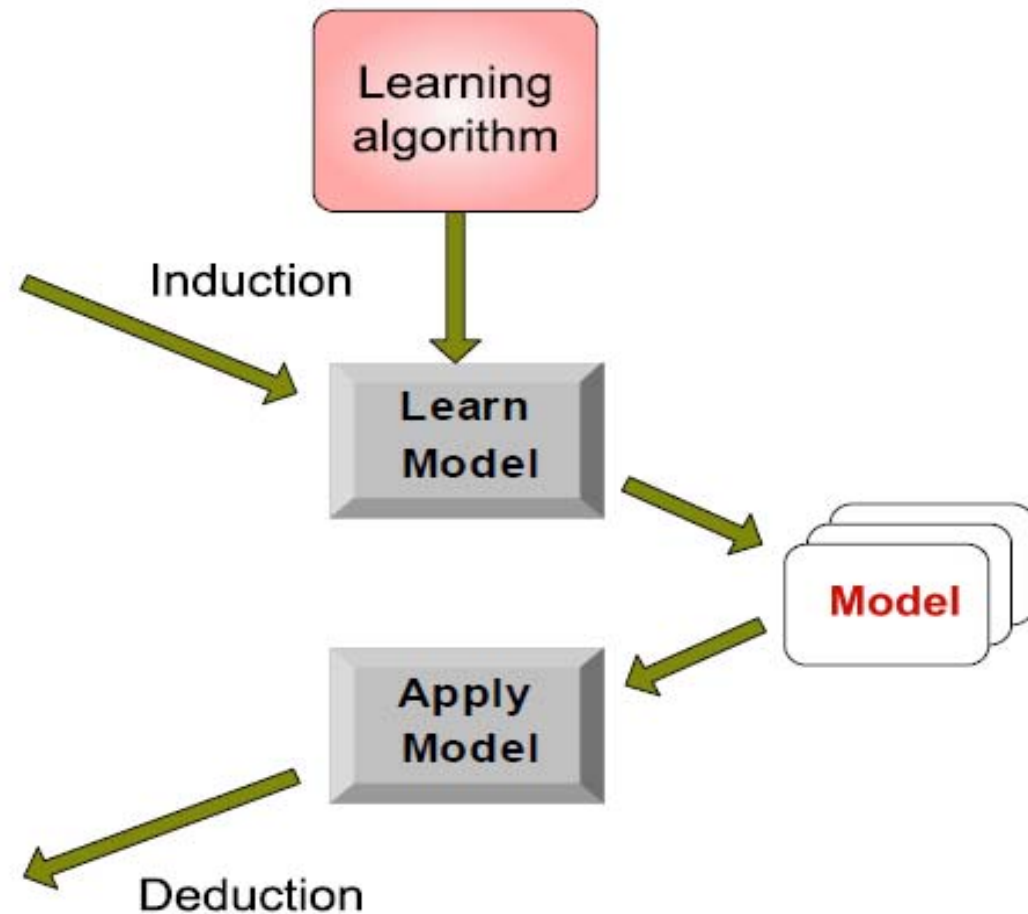
Dependent variable

Tid	Attrib1	Attrib2	Attrib3	y
1	Yes	Large	125K	12
2	No	Medium	100K	194
3	No	Small	70K	45
4	Yes	Medium	120K	78
5	No	Large	95K	2
6	No	Medium	60K	89
7	Yes	Large	220K	131
8	No	Small	85K	244
9	No	Medium	75K	669
10	No	Small	90K	4

Training Set

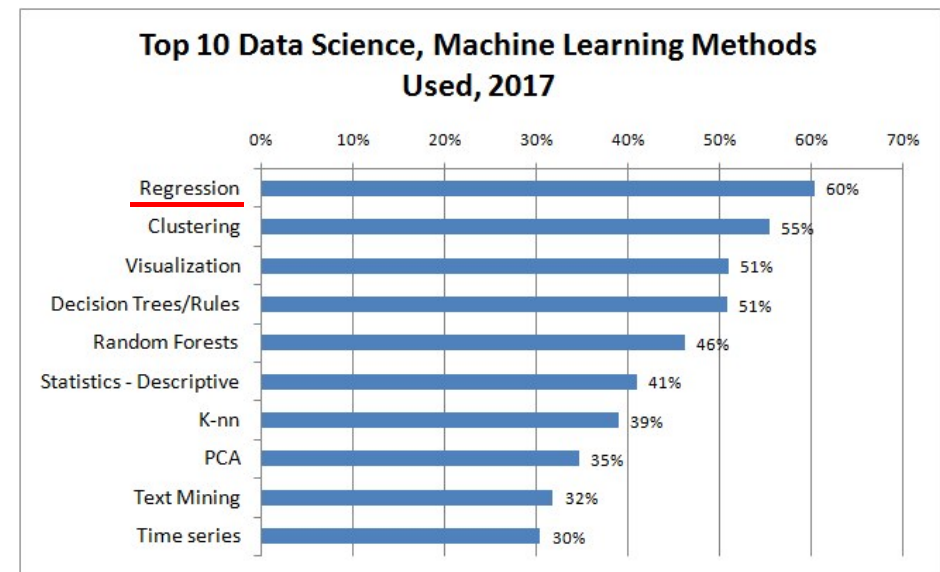
Tid	Attrib1	Attrib2	Attrib3	\hat{y}
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Unseen Records



Regression 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, weather forecast



Source: KDnuggets online poll, 732 votes

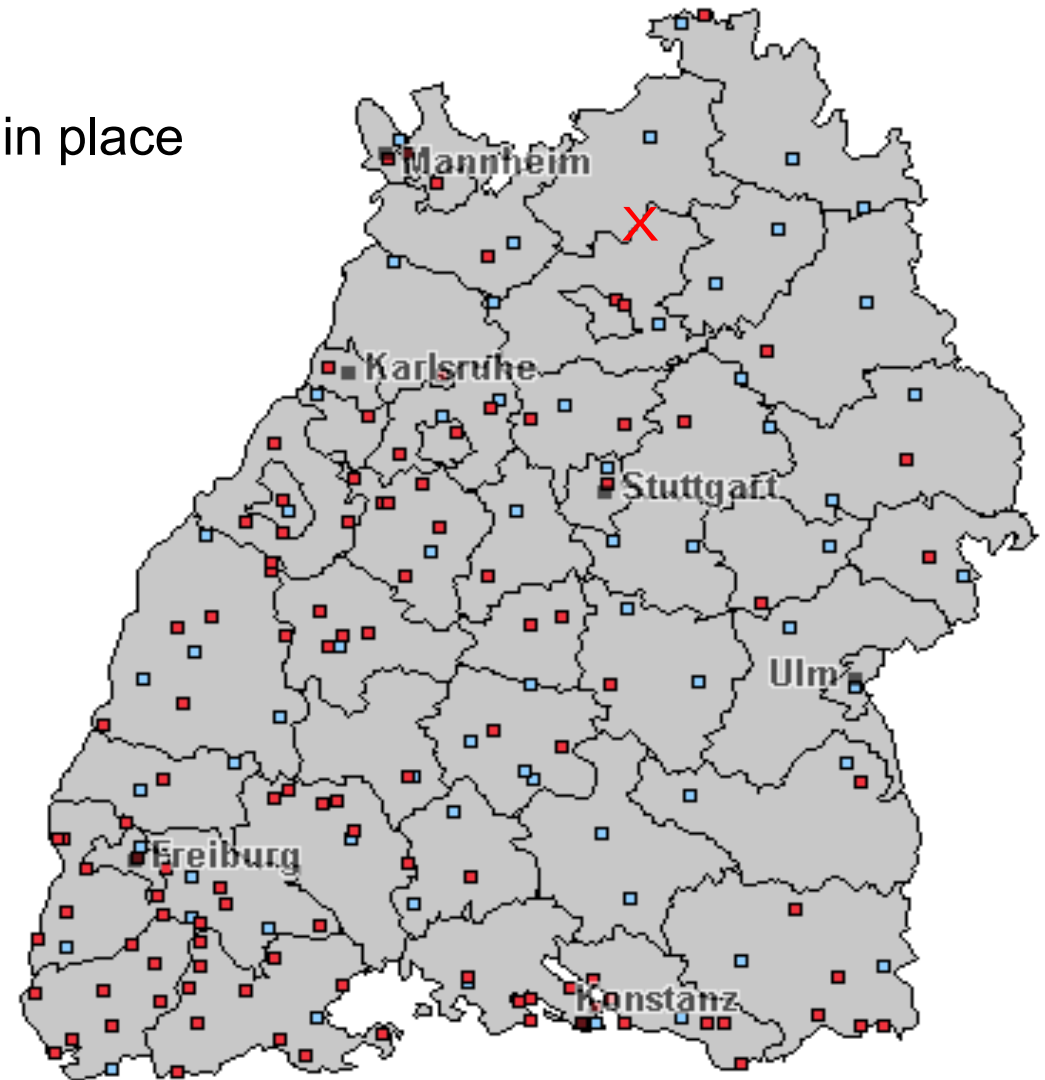
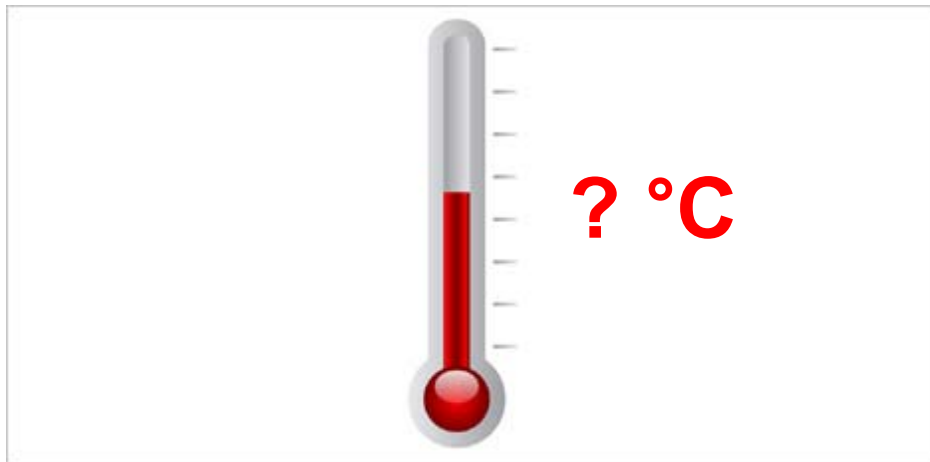
Regression Techniques

1. Linear Regression
2. Polynomial Regression
3. Local Regression
4. K-Nearest-Neighbors Regression
5. Regression Trees
6. Support Vector Machines
7. Artificial Neural Networks
8. Deep Neural Networks
9. Component Models of Time Series
10. Many others ...

2. K-Nearest-Neighbors Regression

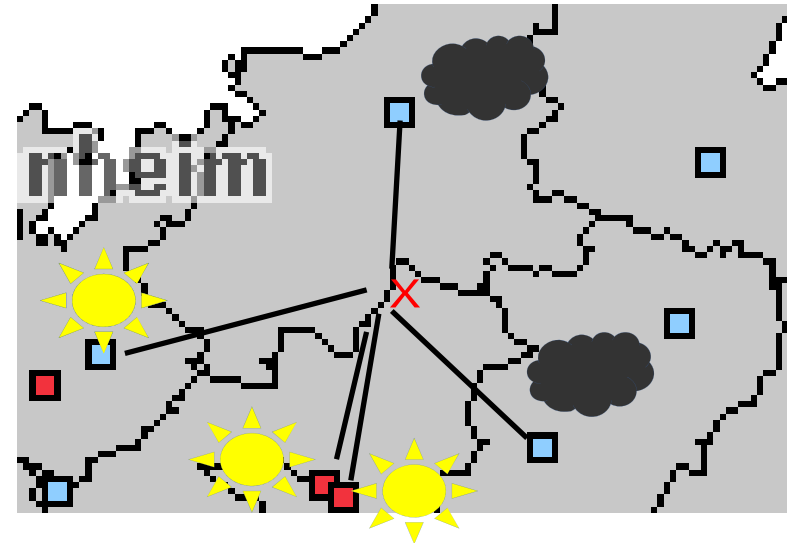
Problem

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



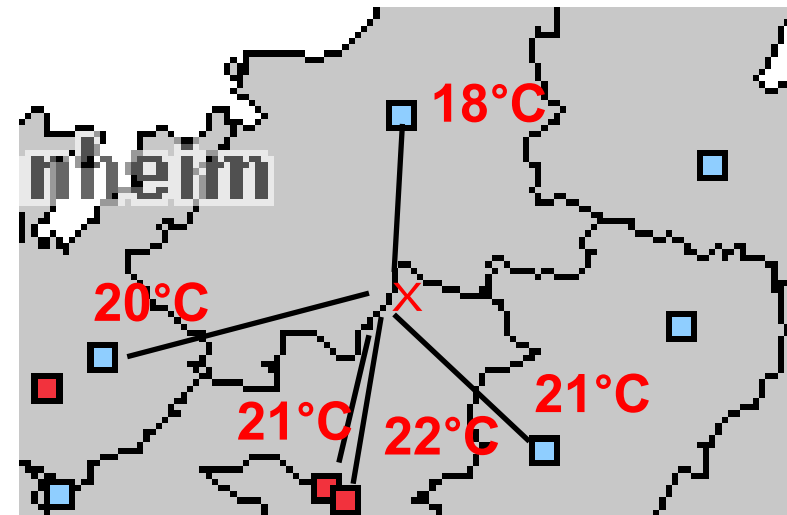
Recap: K-Nearest-Neighbors Classification

- Idea: use the average 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



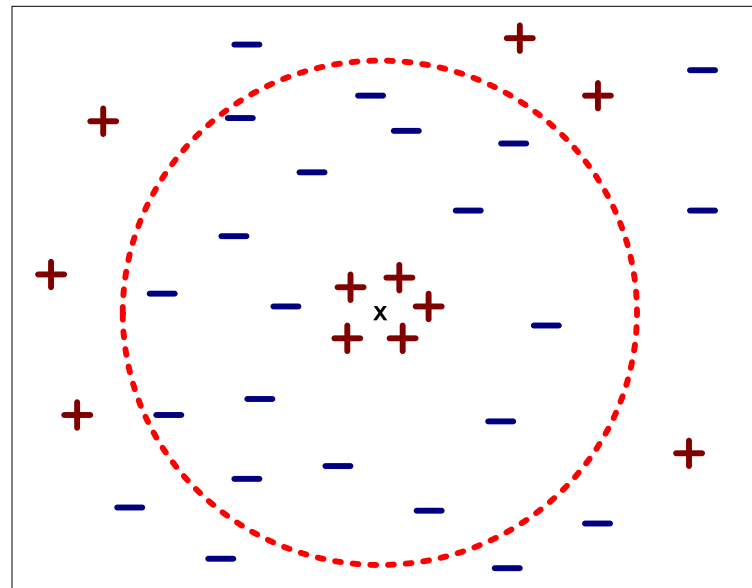
K-Nearest-Neighbors Regression

- 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: $\hat{y} = 20.4^\circ\text{C}$

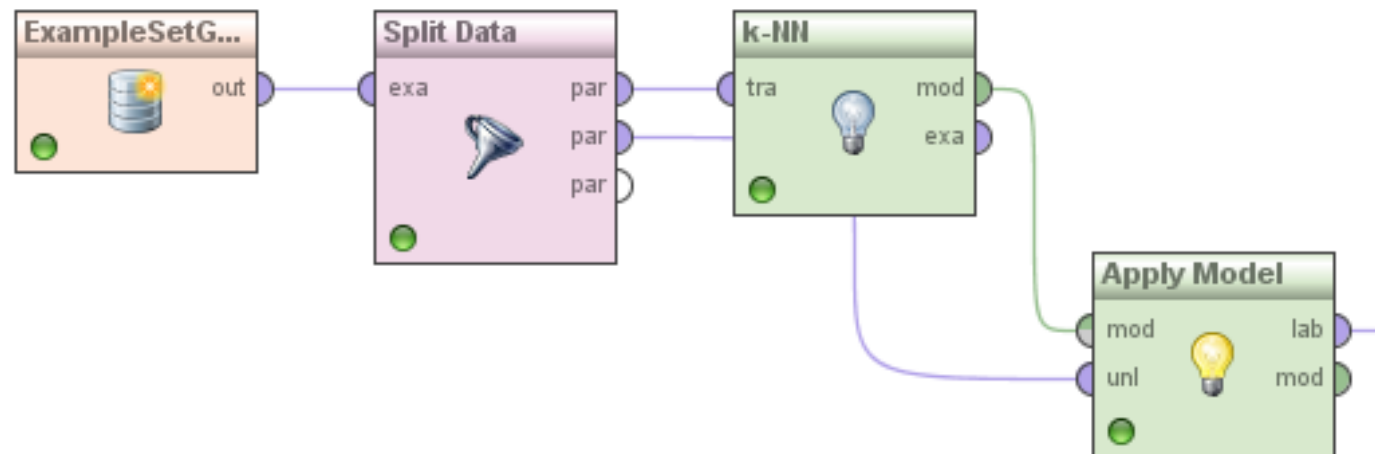


Choosing a Good Value for K

- 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, the neighborhood may include points from other classes
- Rule of thumb: Test k values between 1 and 10.



K-Nearest-Neighbor Regression in RapidMiner



☐ Data View
 ☒ Meta Data View
 ☐ Plot View
 ☐ Advanced Charts
 ☐ Annotations

ExampleSet (100 examples, 1 special attribute, 5 regular attributes)

Name	Role	Type	Statistics	Range	Missings
label	label	real	avg = 74.105 +/- 42	[-873.112 ; 968.407]	0
att1	regular	real	avg = 0.650 +/- 5.8%	[-9.645 ; 9.843]	0
att2	regular	real	avg = 0.460 +/- 6.3%	[-9.939 ; 9.798]	0
att3	regular	real	avg = 0.079 +/- 6.0%	[-9.661 ; 9.795]	0
att4	regular	real	avg = -1.355 +/- 5.2%	[-9.837 ; 9.612]	0
att5	regular	real	avg = -0.075 +/- 5.7%	[-9.968 ; 9.973]	0

Numeric Predictions are Added to the Dataset

Prediction

ExampleSet (Cross Validation)

ExampleSet (200 examples, 2 special attributes, 5 regular attributes) Filter (200 / 200 examples): all

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)

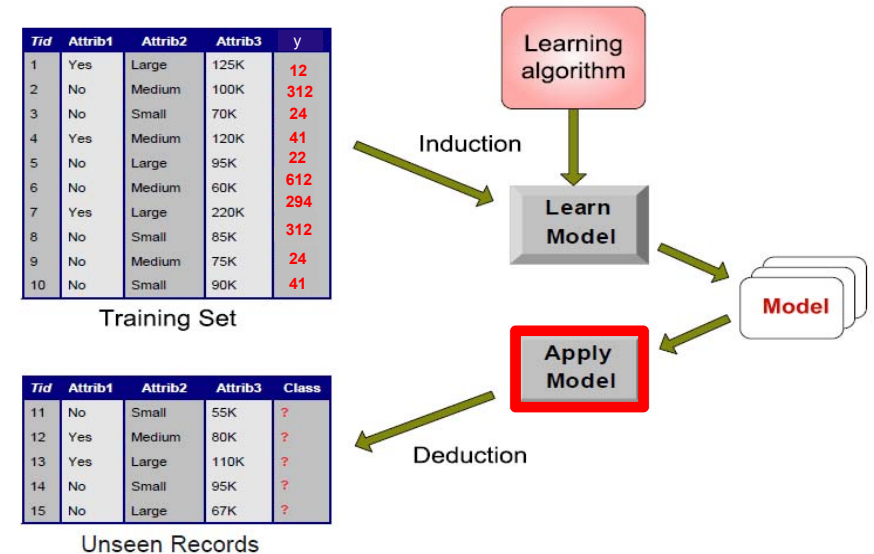
Name	Type	Missing	Statistics	Filter (7 / 7 attributes):
Label	Real	0	Min 0.143 Max 926.739 Average 180.418	Search for Attributes
Prediction	Real	0	Min -32.614 Max 898.428 Average 177.064	
a1	Real	0	Min 0.081 Max 9.940 Average 5.000	
a2	Real	0	Min 0.009 Max 9.986 Average 4.812	

Prediction

3. Model Evaluation

Central Question:

How good is a model at predicting the dependent variable?



3.1 Methods for Model Evaluation

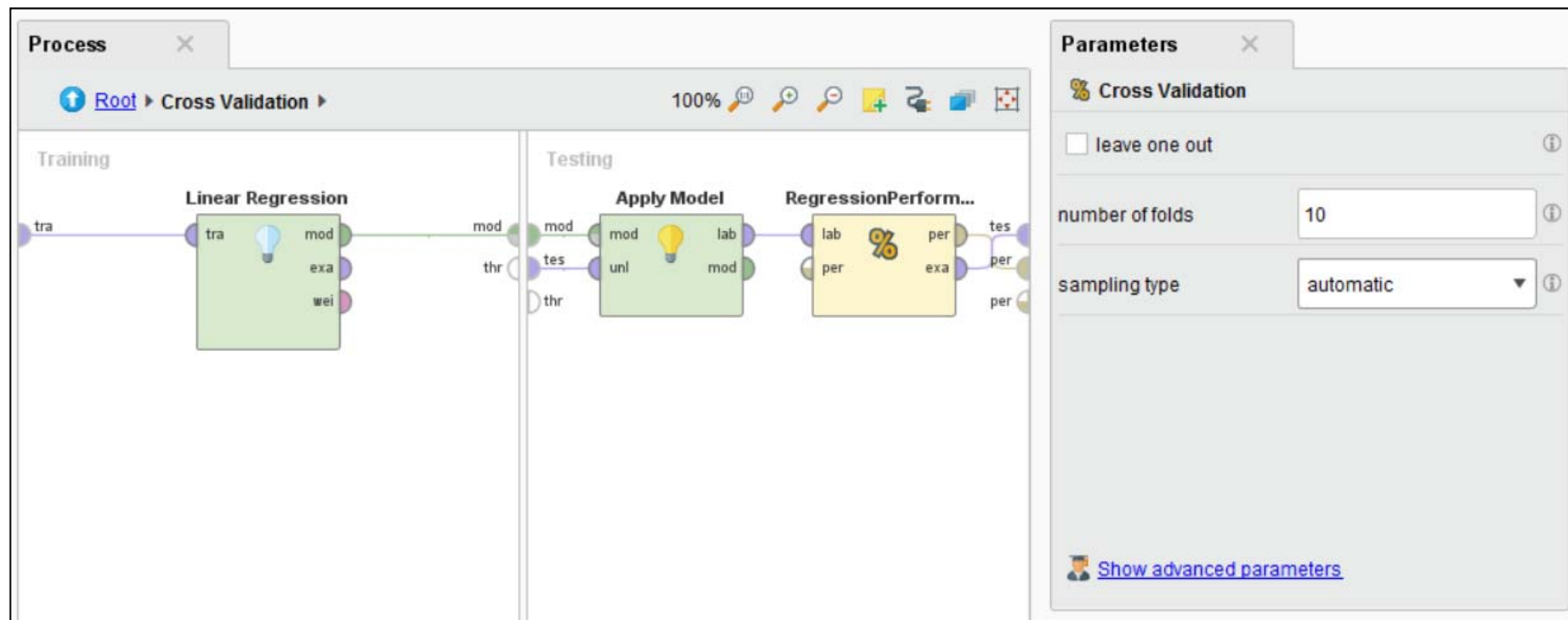
- How to obtain reliable estimates?

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
 - X-Validation: 10-fold (90% for training, 10% for testing in each iteration)
 - Split Validation: 80% random share for training, 20% for testing
- Estimating performance metrics in RapidMiner
 - X-Validation Operator + Regression Performance Operator



3.2 Metrics for Model Evaluation

Recap: Which metrics did we use for classification?

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN} = \frac{\text{Correct predictions}}{\text{All predictions}}$$

	PREDICTED CLASS		
		Class= Yes	Class= No
	Class= Yes	TP 25	FN 4
ACTUAL CLASS	Class= No	FP 6	TN 15

$$\text{Acc} = \frac{25 + 15}{25 + 15 + 6 + 4} = 0.80$$

Metrics for Regression 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 Square Error (MSE)** is similar to MAE , but places more emphasis on larger deviation

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

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

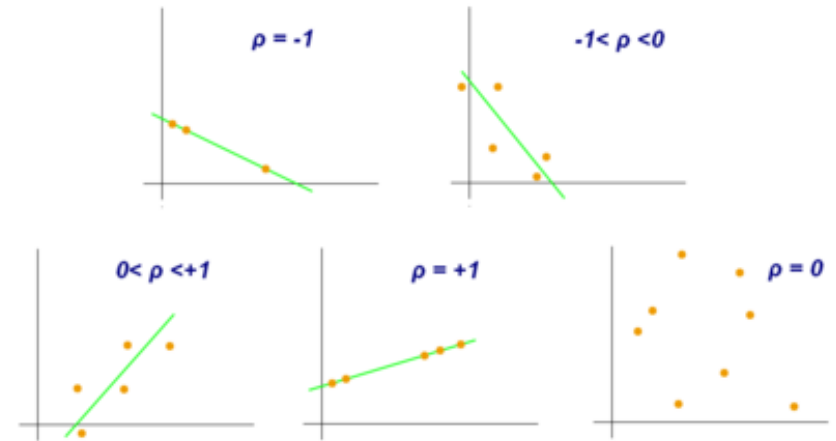
$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (p_i - r_i)^2}$$

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

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



– R Squared: Coefficient of Determination

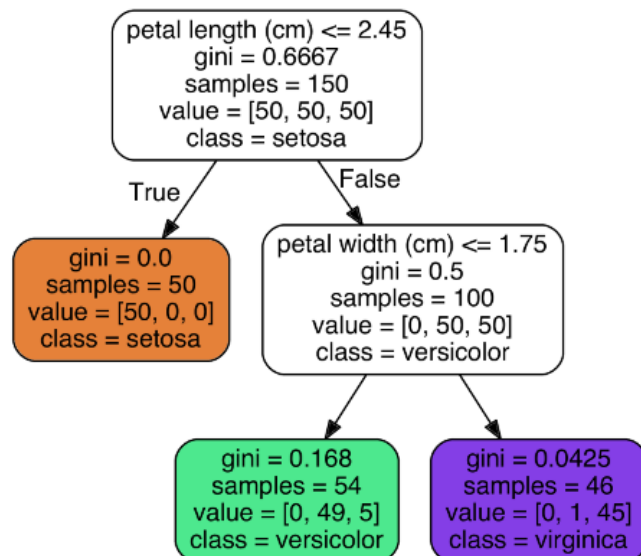
- measures the part of the variation in the dependent variable y that is predictable from the explanatory variables X .
- $R^2 = 1$: Perfect model as y can be completely explained from X .
- called Squared Correlation in RapidMiner

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

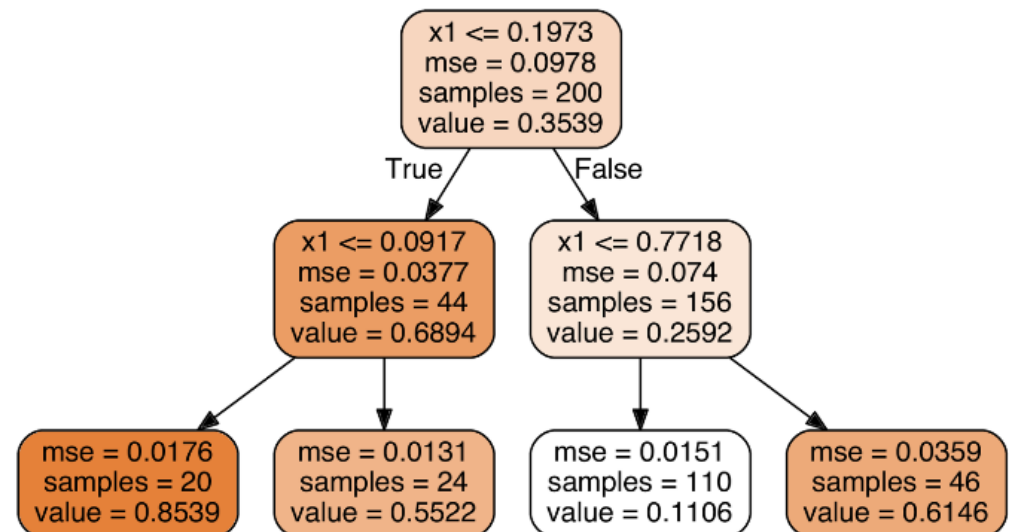
4. Regression Trees

- 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 InfoGain)
 2. Predict the average value of the trainings examples in a specific leaf.

Decision Tree



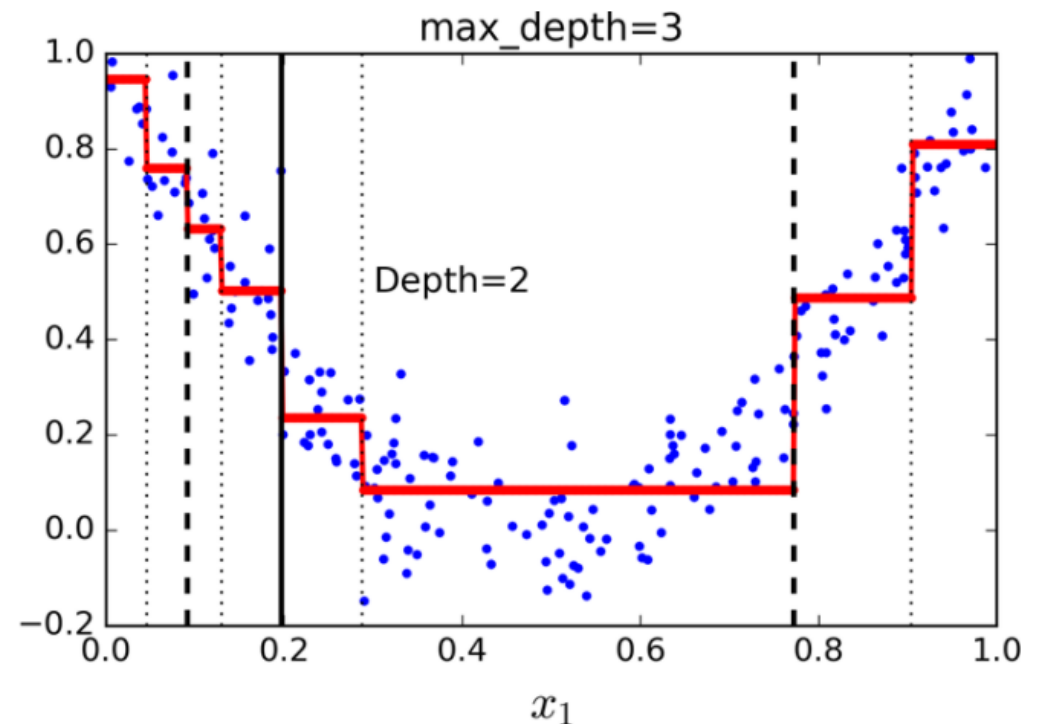
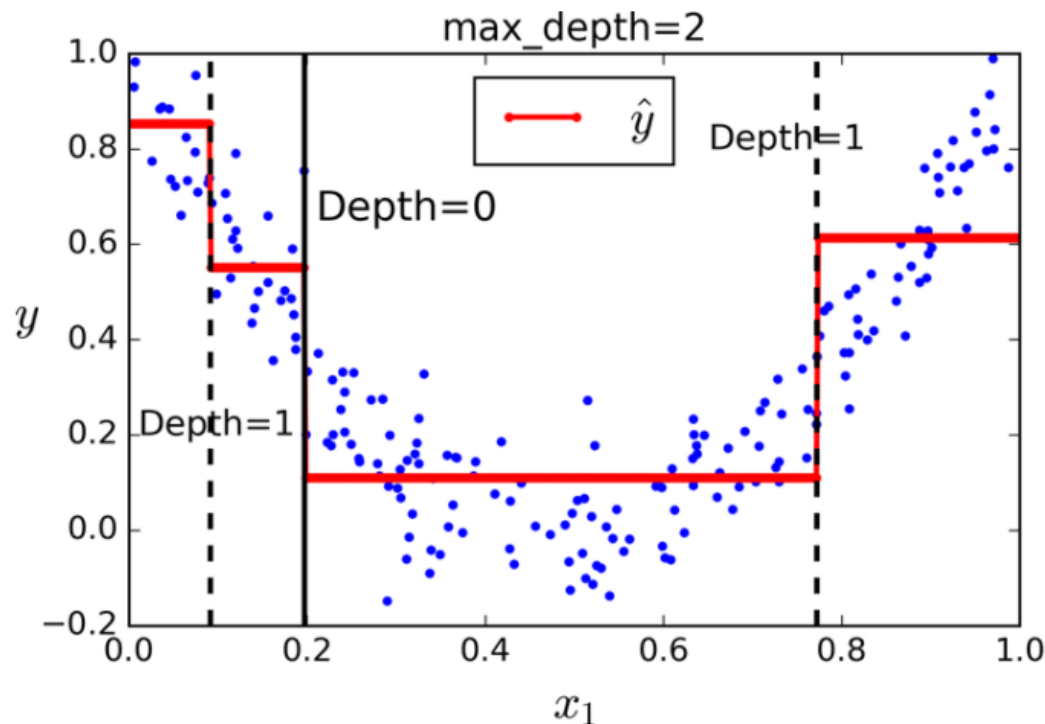
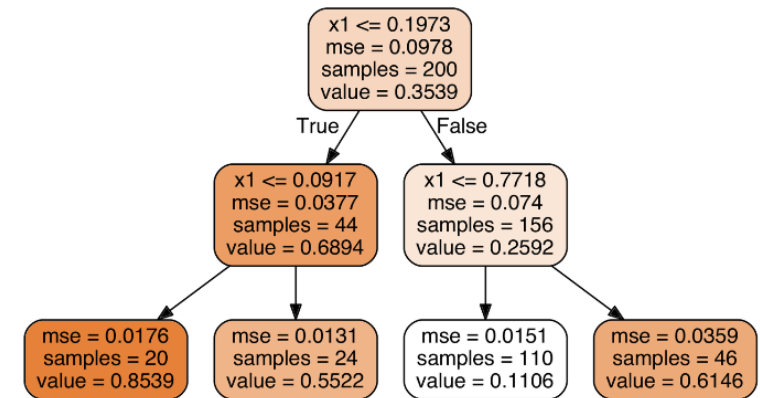
Regression Tree



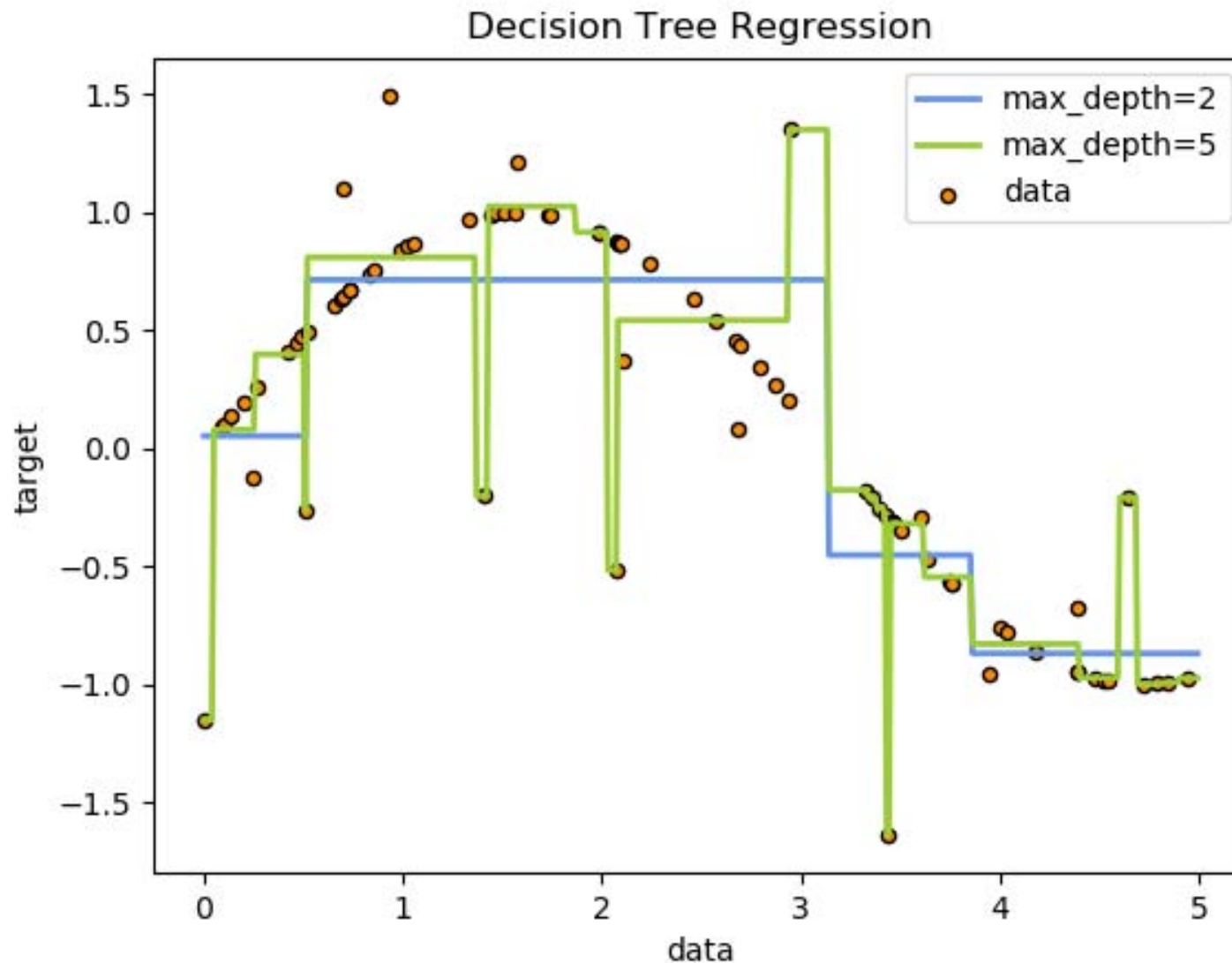
Regression Trees Fitting the Training Data

Pre-pruning parameters determine how closely the tree fits the training data.

- e.g. `max_depth` parameter



Overfitted Regression Tree

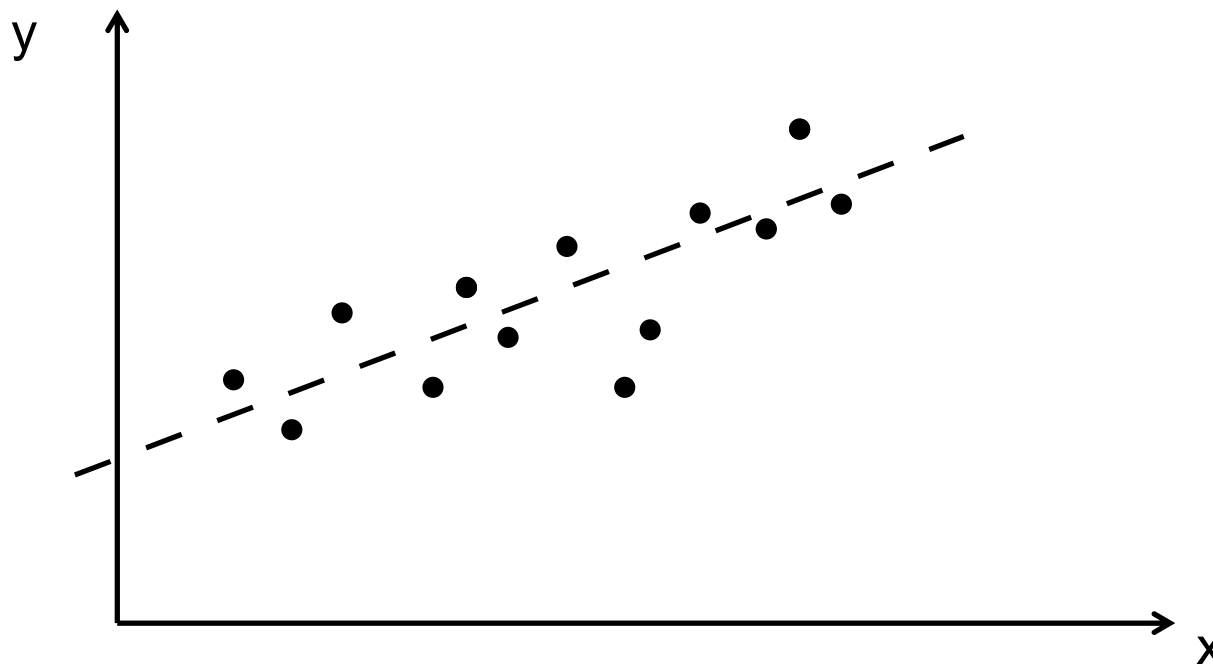


The learning algorithm uses available depth to cover strongest outliers.

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 $X = x_1 \dots x_n$ (multiple linear regression)

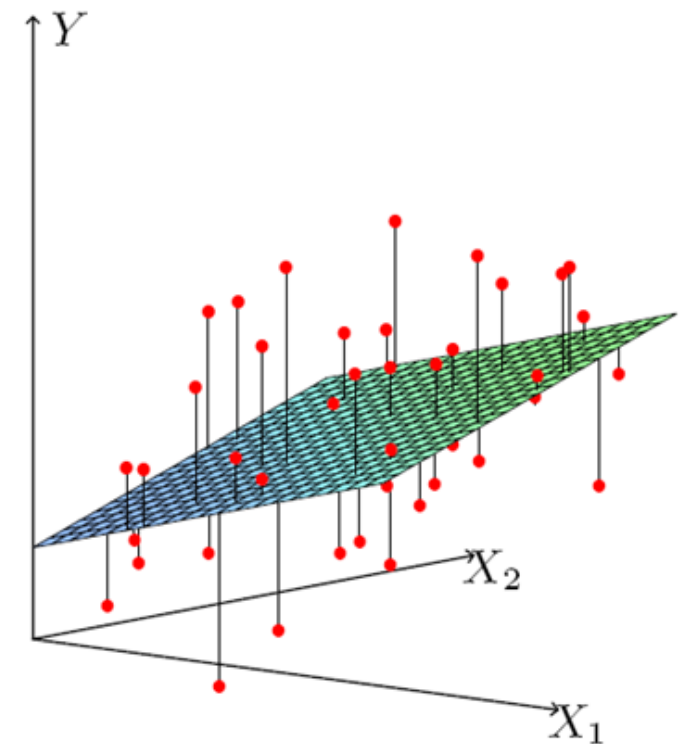
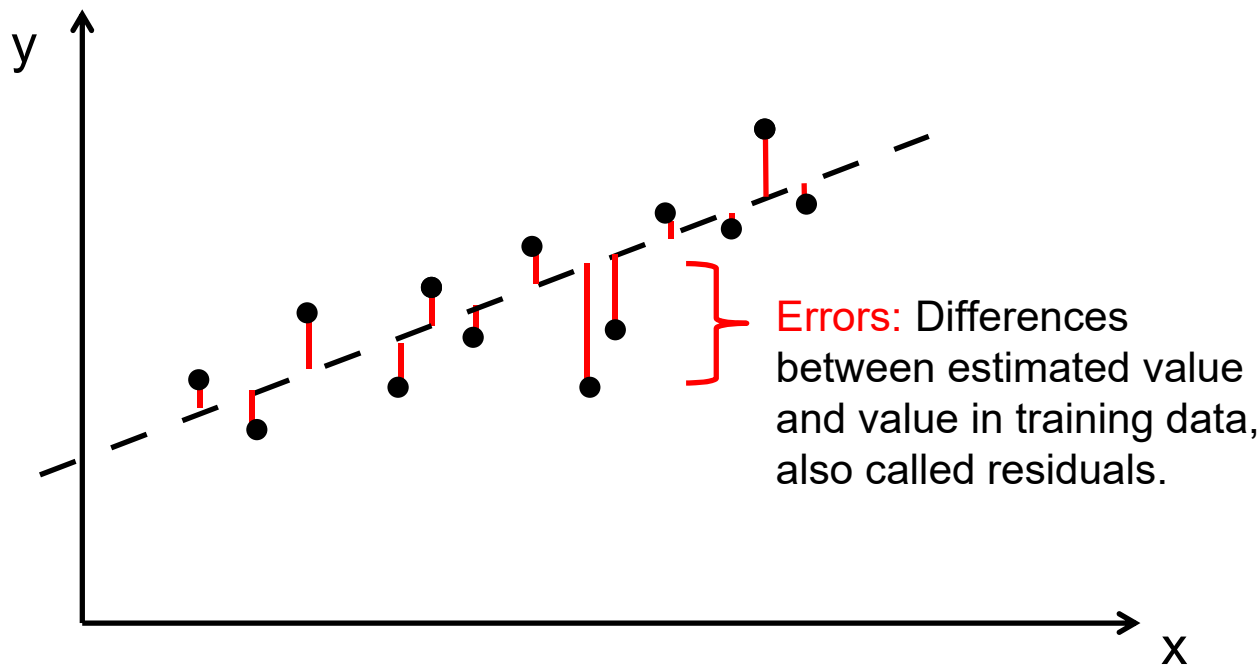


$$\hat{y}(X) = w_0 + w_1 x_1 + w_2 x_2 + \dots + w_n x_n$$

Fitting a Regression Function

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

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

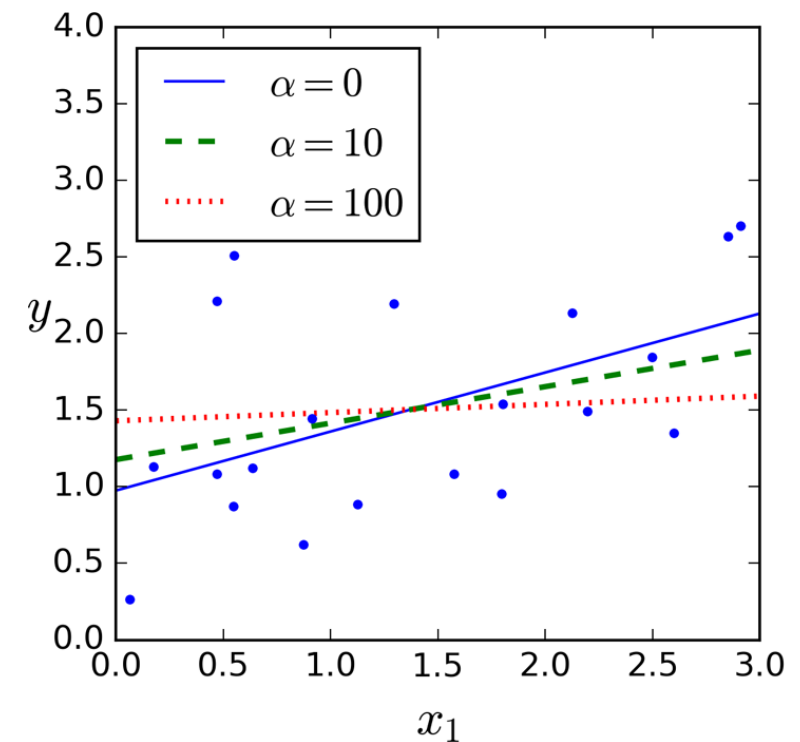
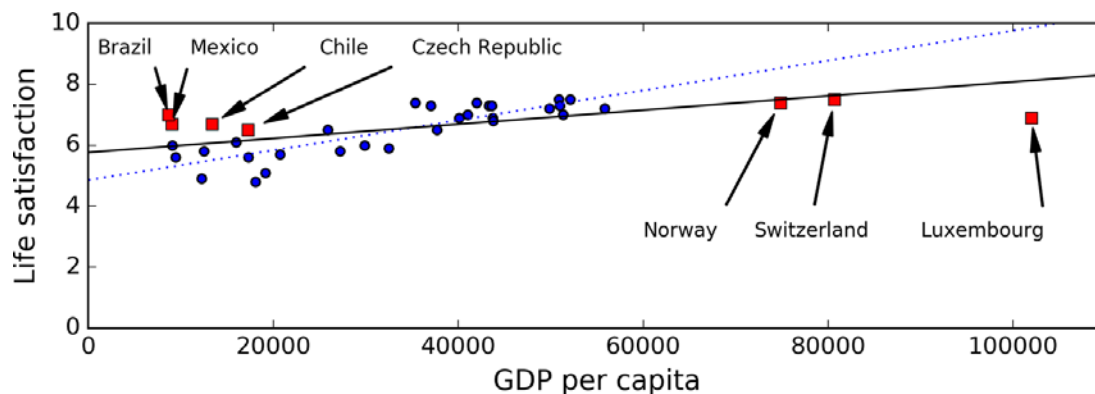


Ridge Regularization

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

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

- $\alpha = 0$: Normal least squares regression
 - $\alpha = 100$: 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 null-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

Process ×

Root ▶ 100%

Linear Regression

Retrieve → Linear Regression

Parameters ×

Linear Regression

feature selection: T-Test

alpha: 0.05

☒ eliminate colinear features

min tolerance: 0.05

☒ use bias

ridge: 1.0E-8

[Hide advanced parameters](#)

Choose feature selection method

Correlated features

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

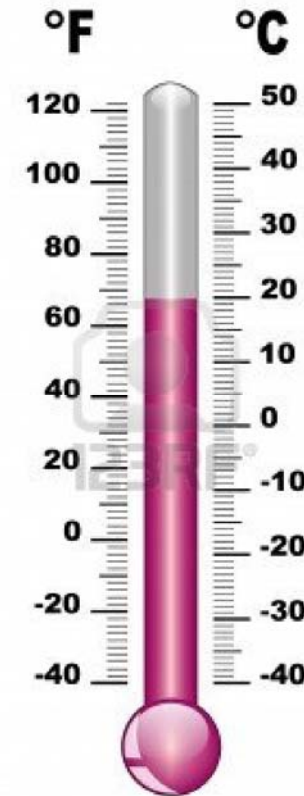
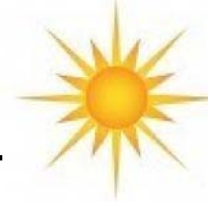
Attribute	Coefficient	Std. Error	Std. Coeff...	Tolerance	t-Stat	p-Value	Code
a1	85.440	5.692	0.463	1.000	15.009	0	****
a2	127.001	5.701	0.689	0.998	22.276	0	****
a3	68.118	5.730	0.369	1.000	11.888	0	****
a4	10.302	5.728	0.056	1.000	1.799	0.074	*
a5	-12.452	5.723	-0.068	0.999	-2.176	0.031	**
(Intercept)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

Feature quality code

p-Value

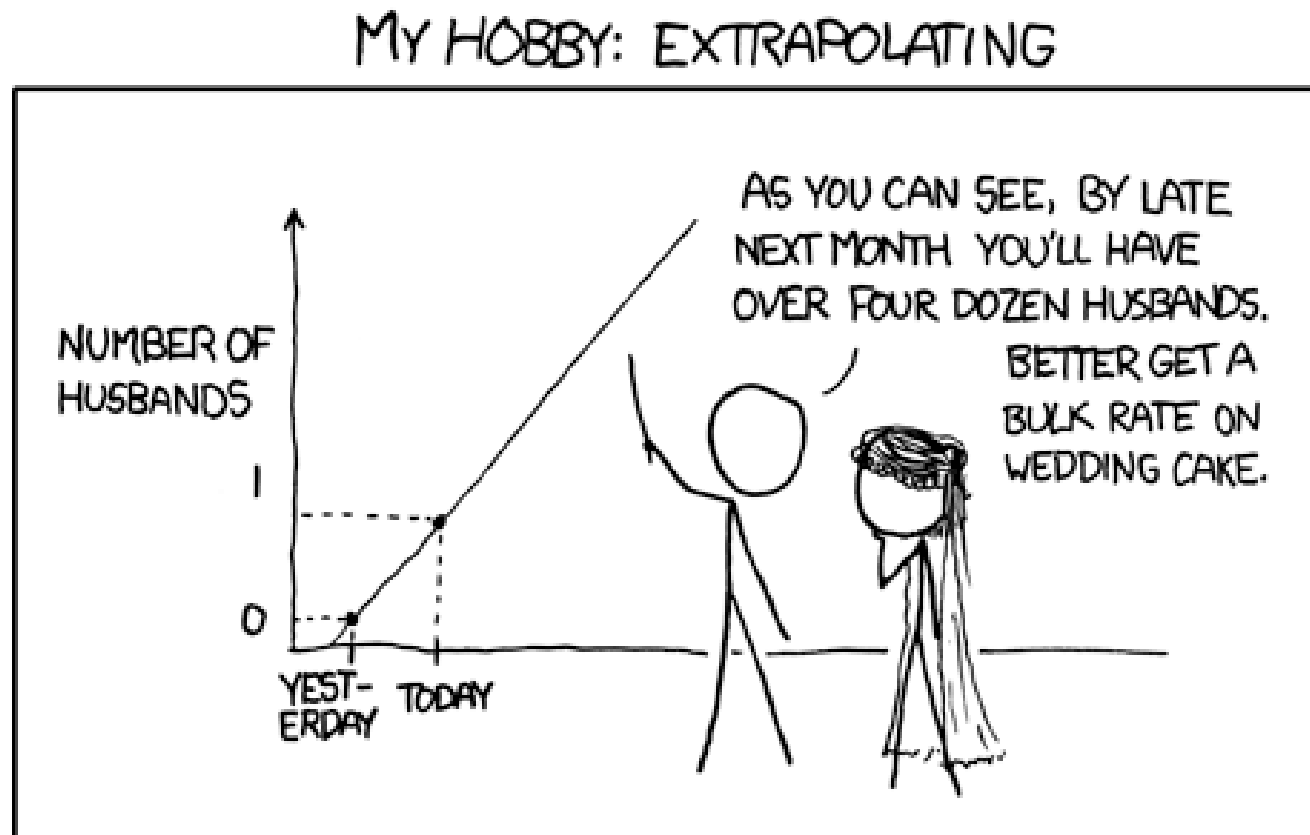
Interpolation vs. Extrapolation

- 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 $[-15^{\circ}\text{C}, 32^{\circ}\text{C}]$
- 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



<http://xkcd.com/605/>

Interpolation vs. Extrapolation

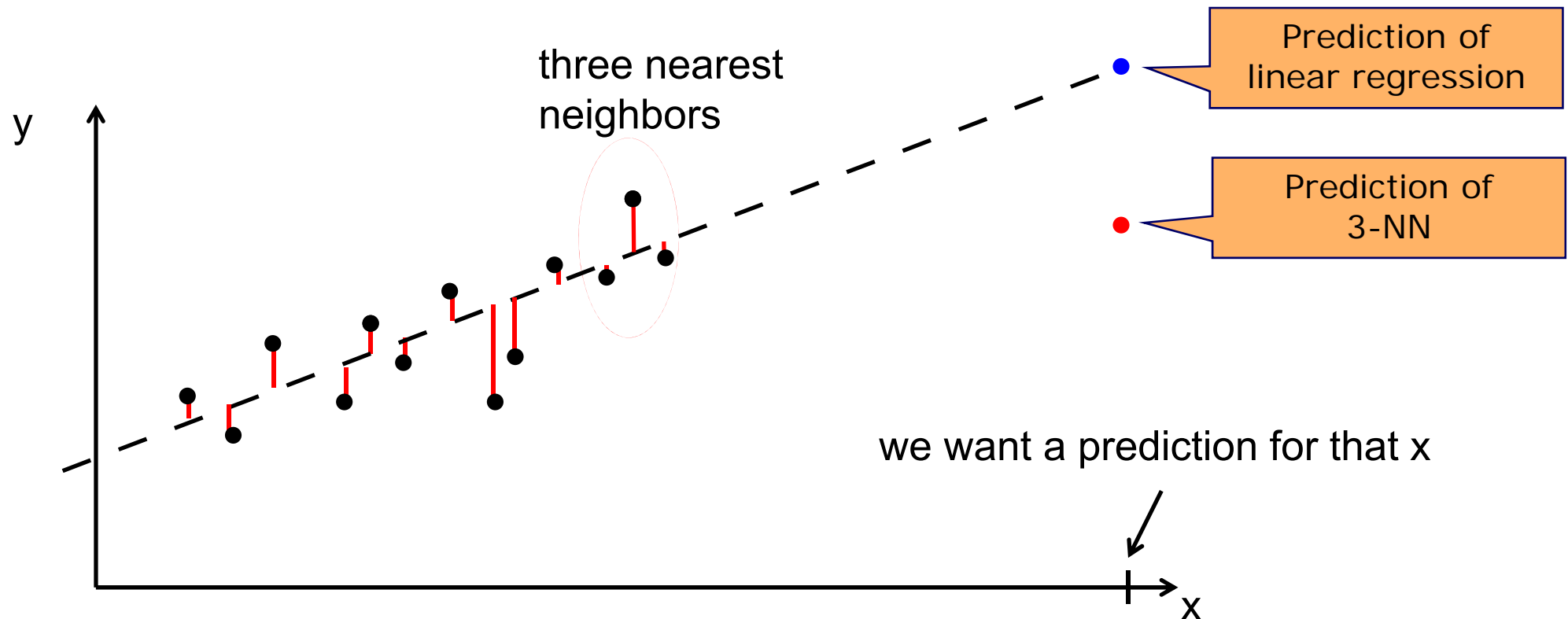
- Sometimes, however, only extrapolation is interesting
 - how far will the sea level have risen by 2050?
 - how much will the temperature rise in my nuclear power plant?



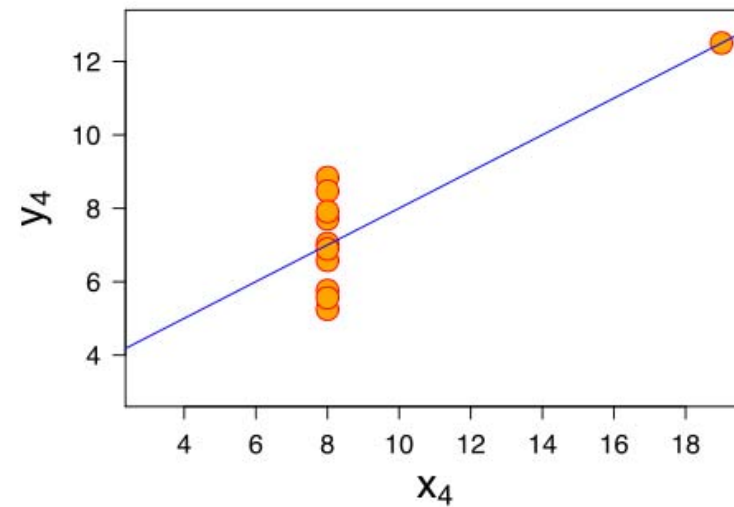
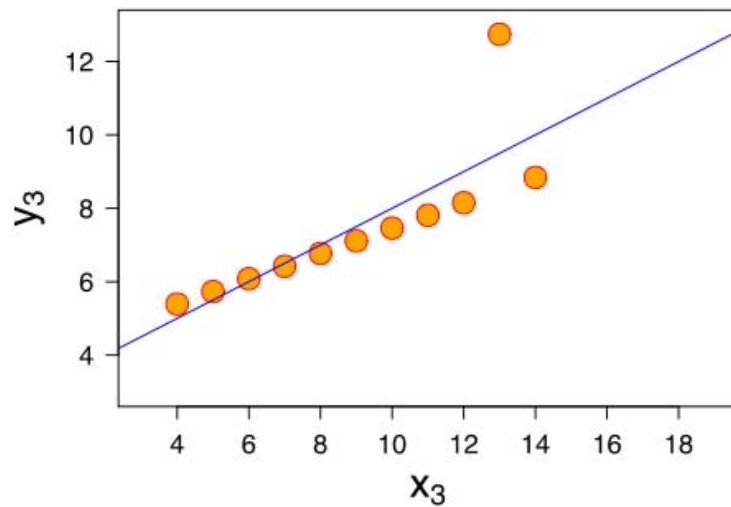
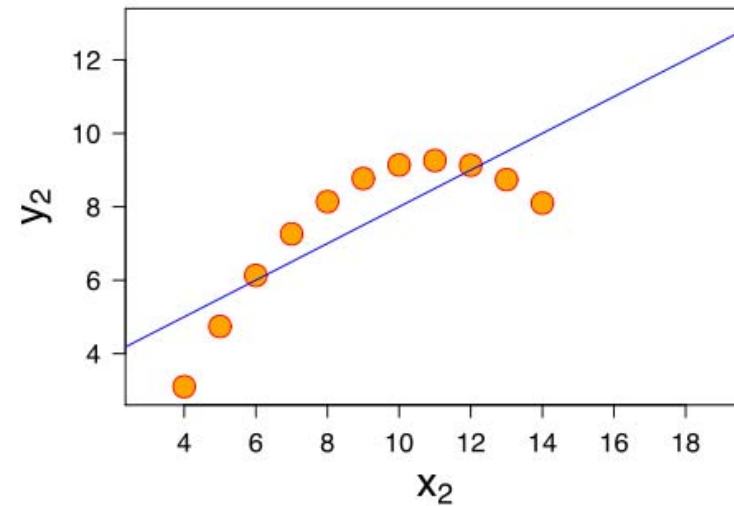
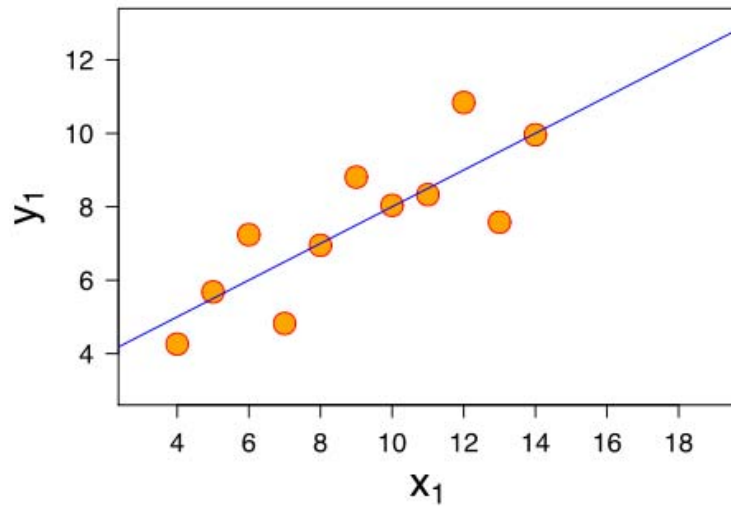
<http://i1.ytimg.com/vi/FVfiujbGLfM/hqdefault.jpg>

Linear Regression vs. K-NN Regression

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

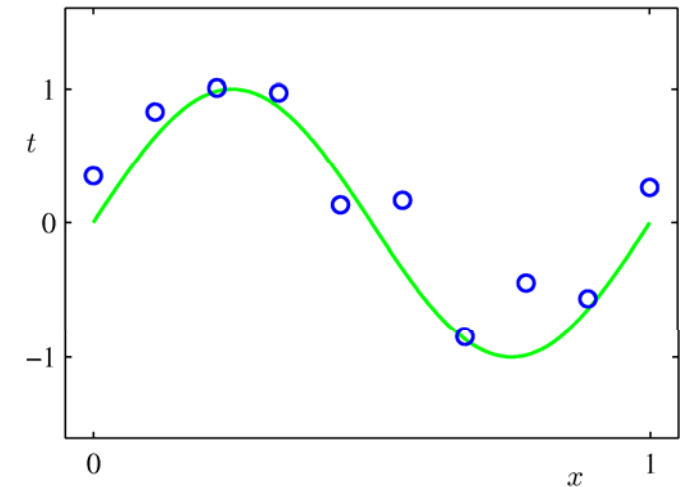


Linear Regression Examples



...but what about non-linear Problems?

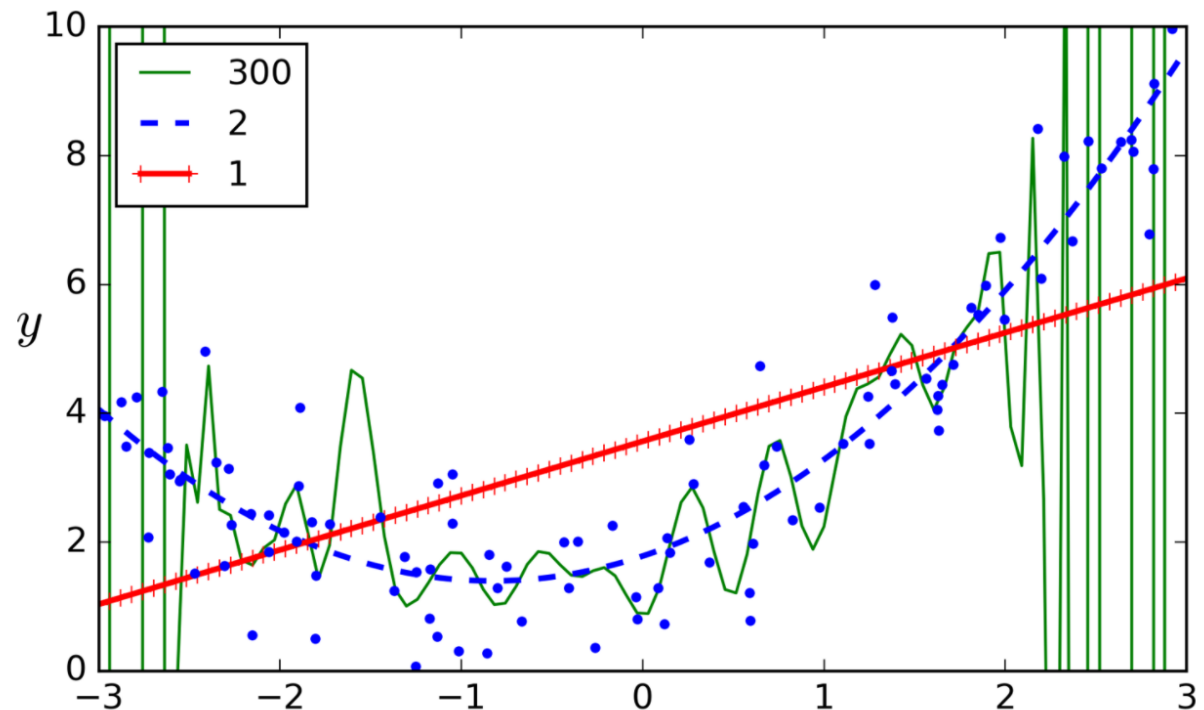
- One possibility is to apply transformations to the explanatory variables X within the regression function.
 - e.g. log, exp, square root, square, etc.
 - example: : $\hat{y} = \omega_0 + \omega_1 \cdot x_1^2 + \omega_2 \cdot x_2^2$
 - polynomial transformation
 - example: $\hat{y} = \omega_0 + \omega_1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



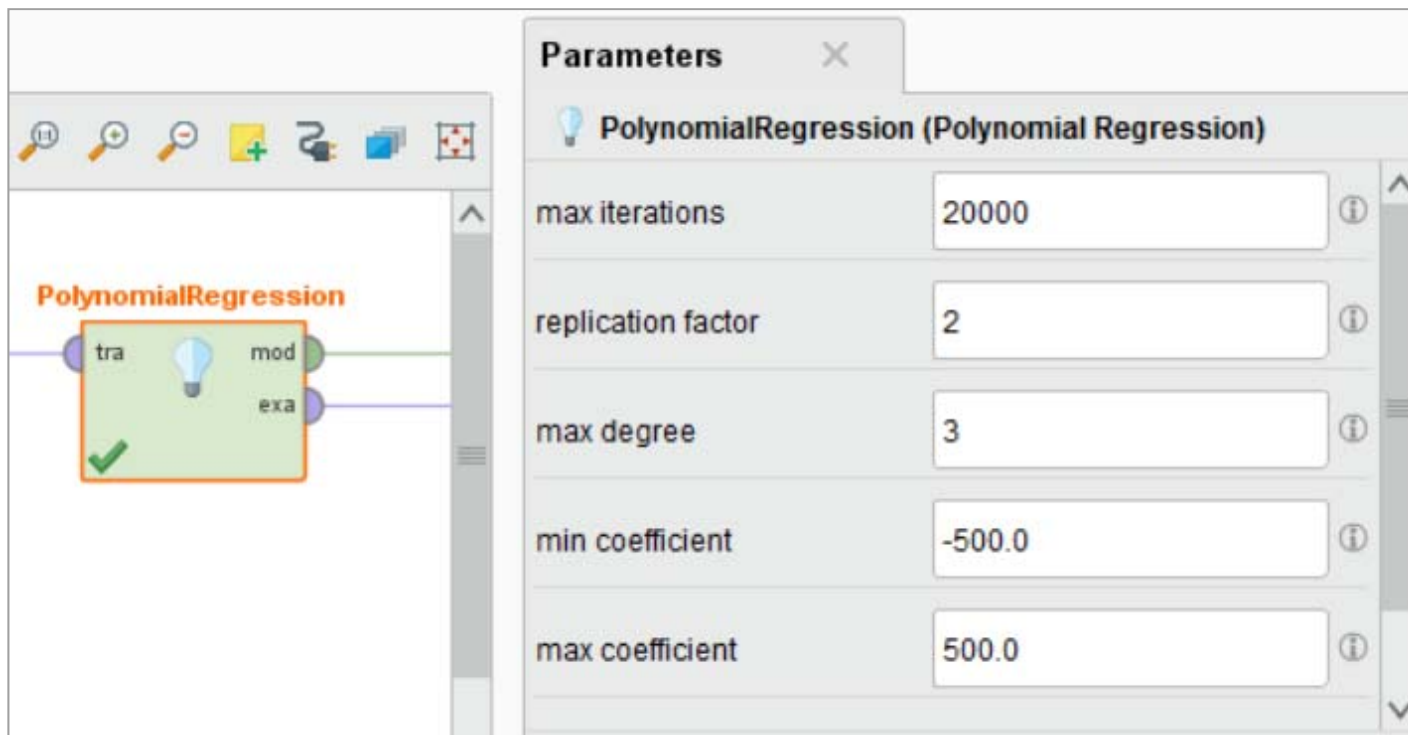
6. Polynomial Regression

$$\hat{y}(x, \mathbf{w}) = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M = \sum_{j=0}^M w_jx^j$$

- 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



How often may each explanatory variable appear in the function.

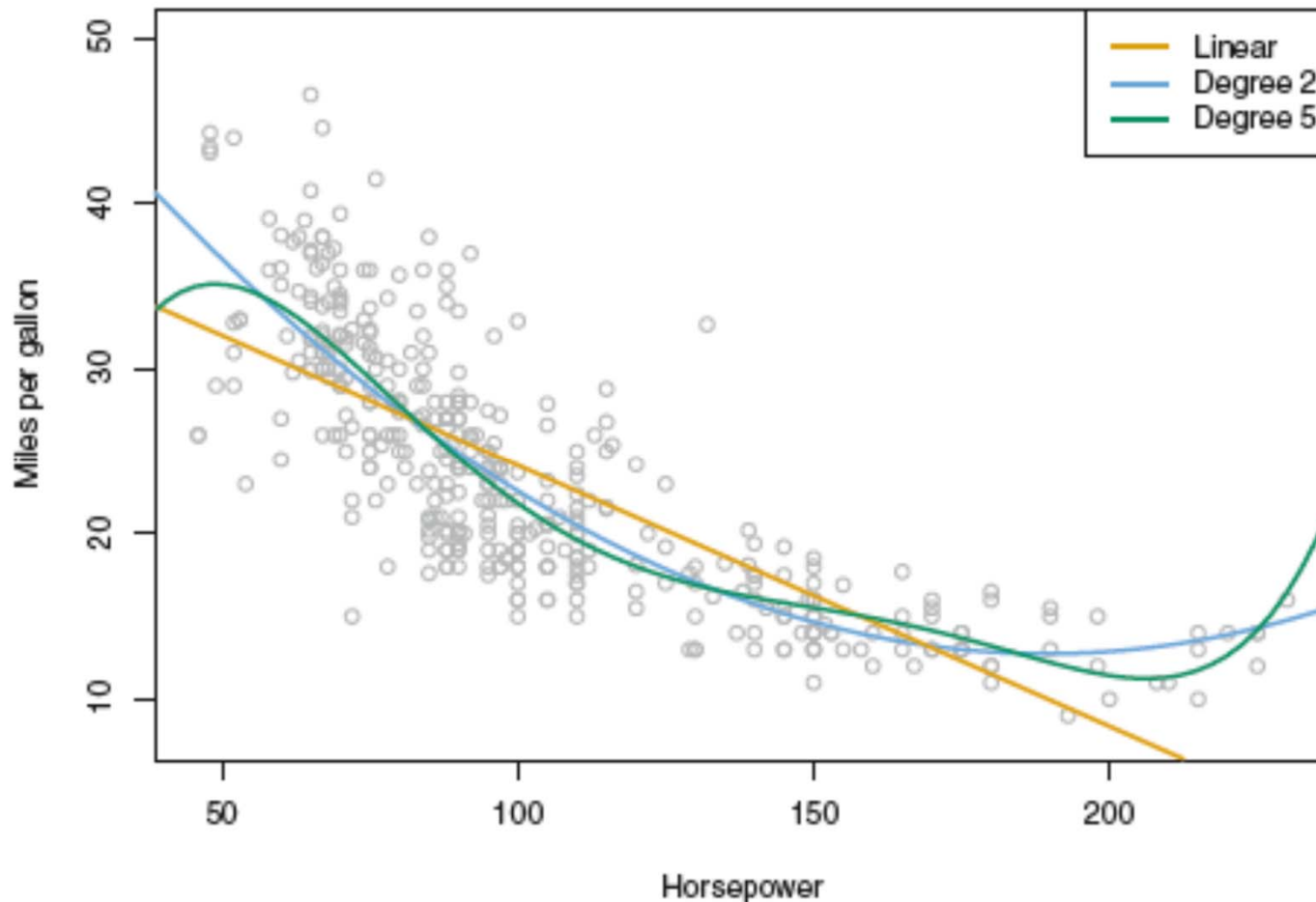
Maximal degree to be used in the function

Boundaries for weights W

$$\begin{aligned} Y = & 100.000 * att1 ^ 3.000 - 16.644 * att1 ^ 2.000 \\ & - 31.516 * att2 ^ 2.000 + 58.019 * att2 ^ 1.000 \\ & + 18.014 * att3 ^ 1.000 - 9.555 * att3 ^ 2.000 \\ & - 7.056 \end{aligned}$$

Example of a function learned using the parameters shown above.

Polynomial Regression Overfitting Training Data

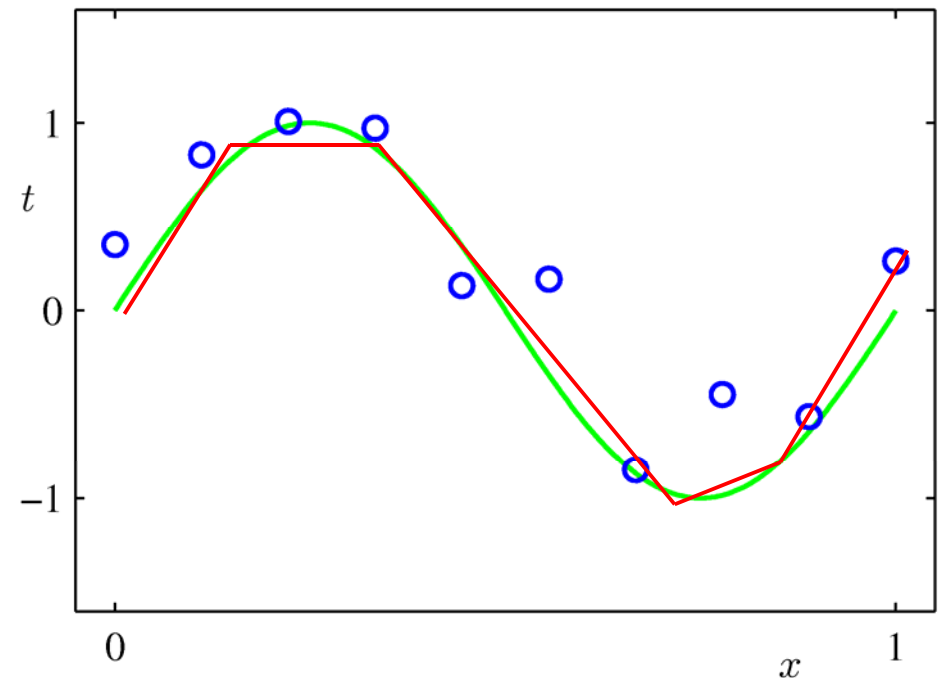


Overfitting often happens in sparse regions.

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

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

The screenshot shows the 'Parameters' window for 'Local Polynomial Regression'. It includes a lightbulb icon and the title 'Local Polynomial Regression'. The parameters are as follows:

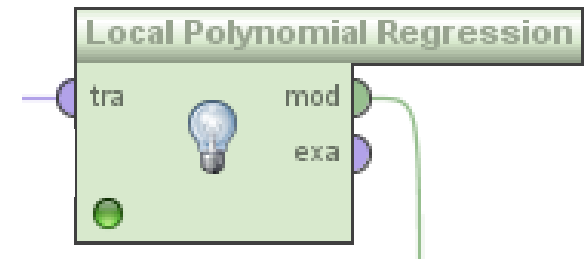
Parameter	Value
degree	2
ridge factor	1.0E-9
use robust estimation	<input type="checkbox"/>
use weights	<input checked="" type="checkbox"/>
numerical measure	EuclideanDistance
neighborhood type	Fixed Number
k	5
smoothing kernel	Triweight

At the bottom, there is a link: [Hide advanced parameters](#)

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

Distance function for determining neighborhood

Neighborhood size

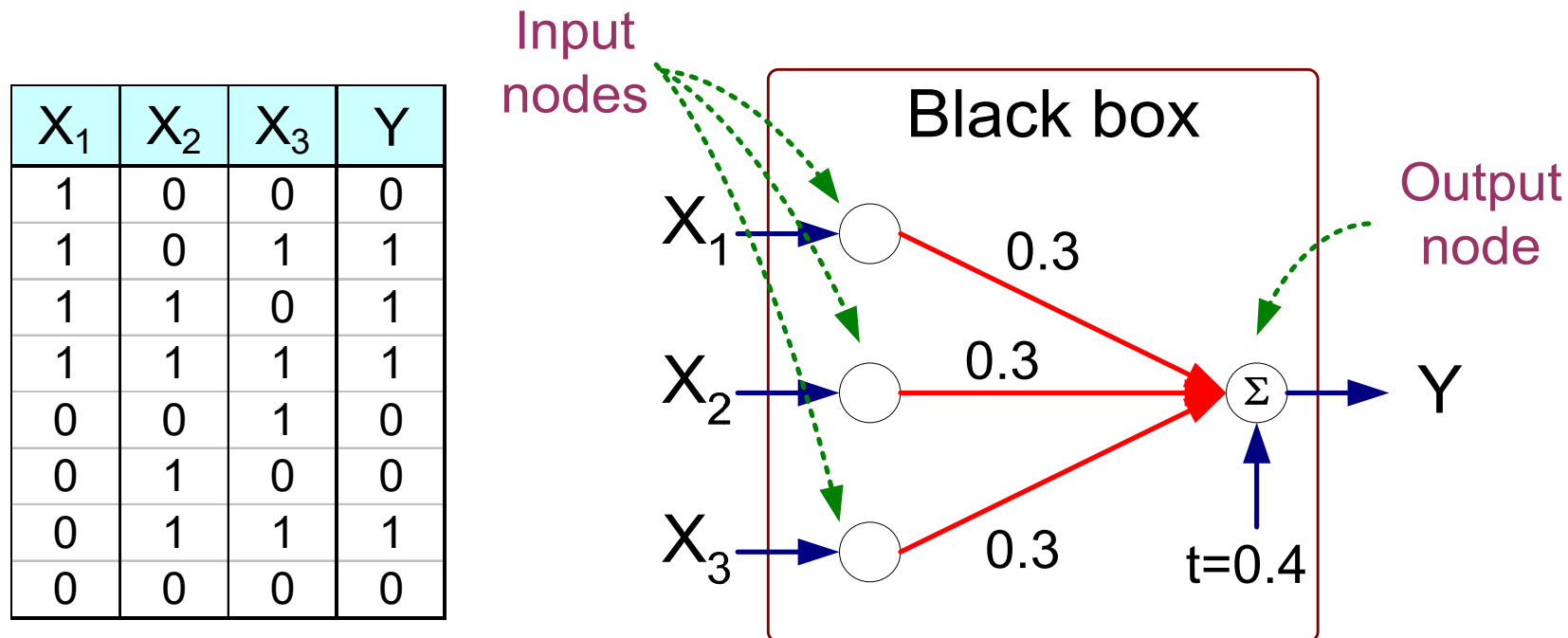


Discussion of Local Regression

- 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

7. Artificial Neural Networks (ANNs) for Regression

Recap: How did we use ANNs for classification?



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

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

ANNs for Regression

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

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

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

- 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
- Training examples:
 - pairs (y_i, X_i) , \hat{y}_i = scalar dependent variable, X_i = vector of explanatory variables

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.

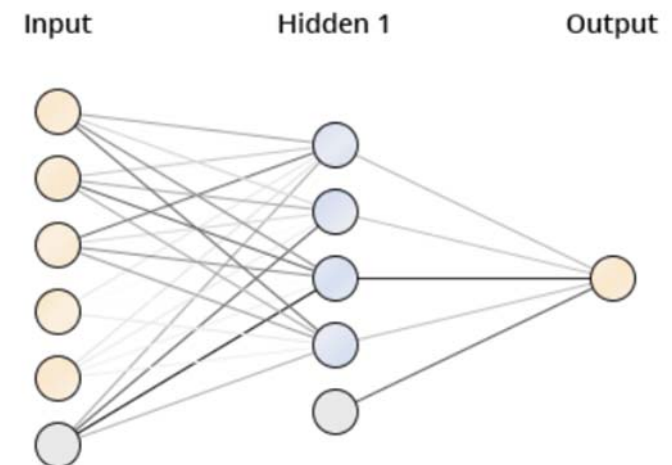
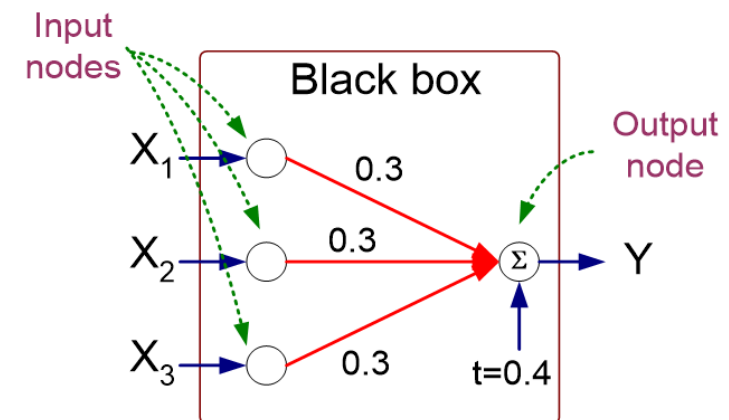
- More complex regression problems can be approximated

- by using multiple hidden layers
 - this allows for arbitrary functions

- Deep ANNs take this idea further by

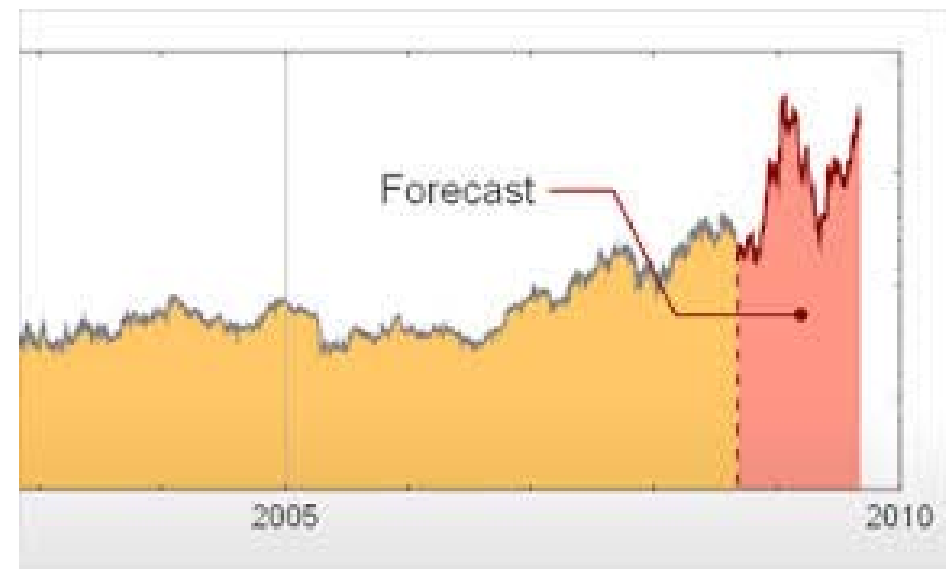
- employing millions of neurons
 - arranging them into specific network topologies
 - more on Deep Learning in Data Mining II

- With all ANNs be cautious 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)

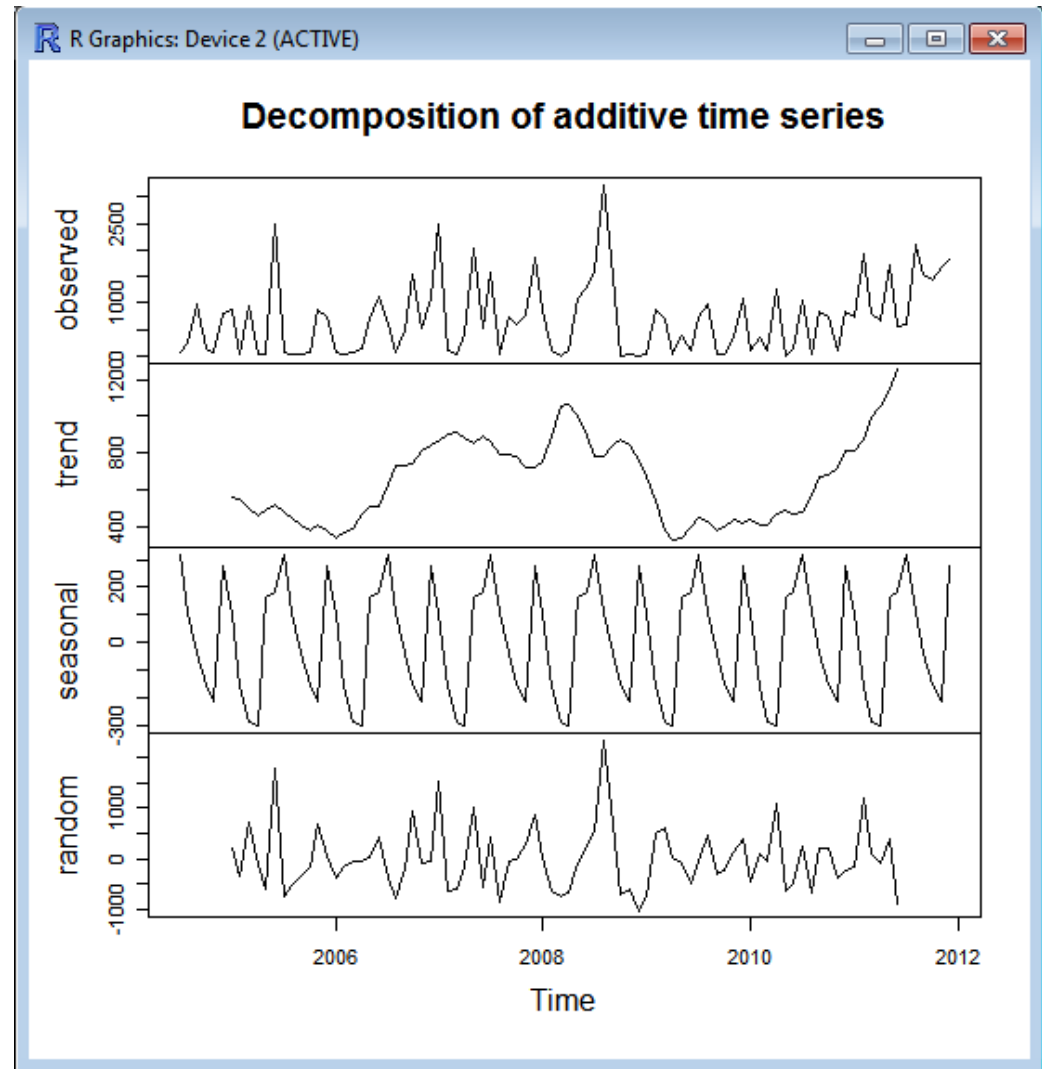
Component Models of Time Series

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)

$$\text{Series} = T_t + C_t + S_t + R_t$$

**Details in
Data Mining II**

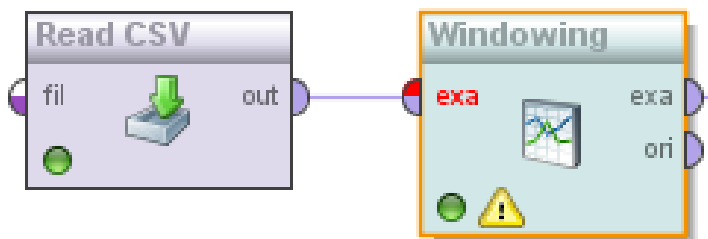


Windowing

- Idea: Transformation of forecasting problem into “classical” learning problem.
 - either classification or regression
 - by only taking the last k days 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 days matter for the forecast
 - the older past is irrelevant

**Details in
Data Mining II**

Windowing in RapidMiner



The diagram shows a 'Read CSV' operator with inputs 'fil' and 'out' connected to a 'Windowing' operator. The 'Windowing' operator has an 'exa' output and an 'ori' output.

Result Overview
ExampleSet (Windowing)

☒ Data View
 ☐ Meta Data View
 ☐ Plot View
 ☐ Advanced Charts
 ☐ Annotations

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

Result Overview
RuleModel (Rule Induction)


☒ Text View
 ☐ Annotations

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.
            
```



Series Extension

26162 EXAMPLES

Summary

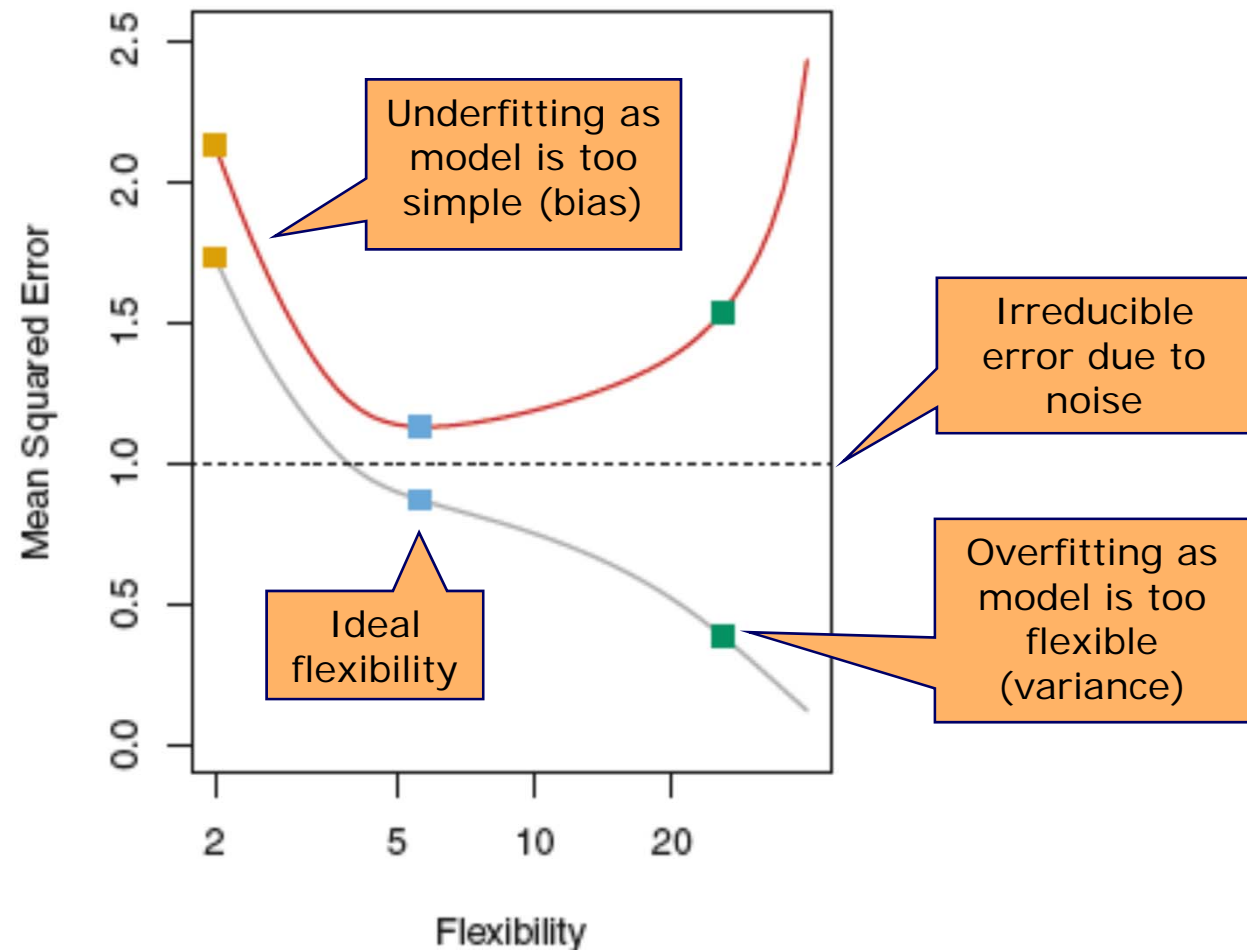
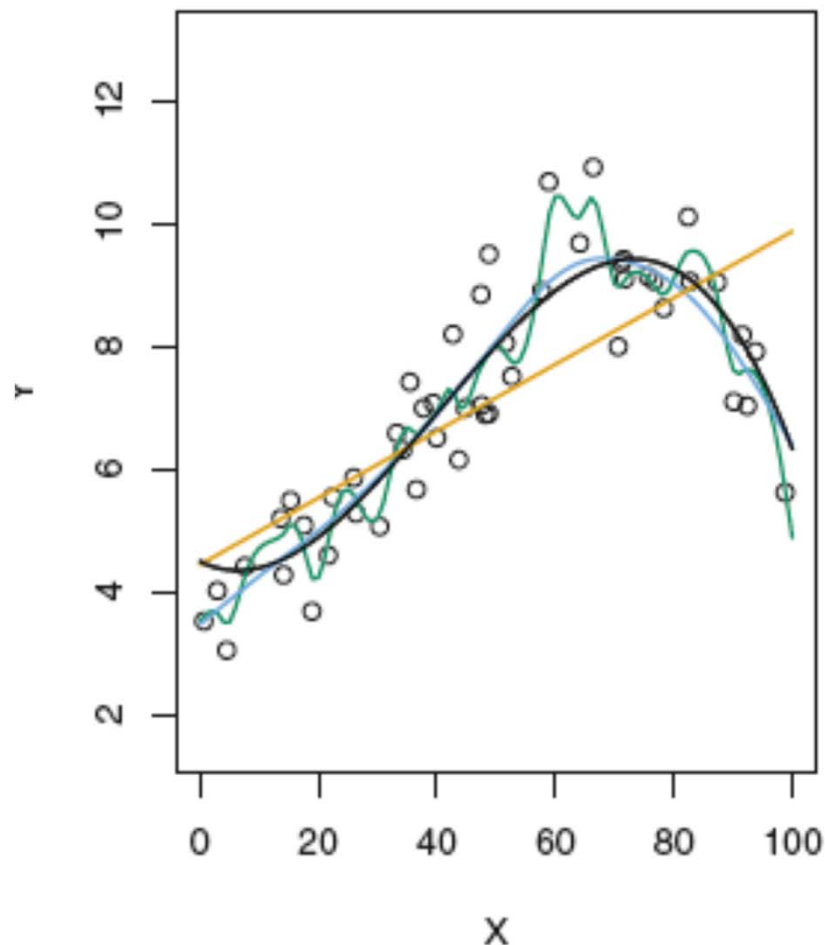
- Regression
 - predict numerical values instead of classes
- Performance measuring
 - absolute or squared error, Pearson correlation, R squared, ...
- Methods
 - k Nearest Neighbors
 - Regression trees
 - Artificial neural networks
 - Linear regression
 - Polynomial regression
 - Local regression
 - Time Series Prediction
 - ...

Final Remarks: Learning Classification and Regression Models

- 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.



Method Selection and Parameter Tuning

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

1. Testing different methods

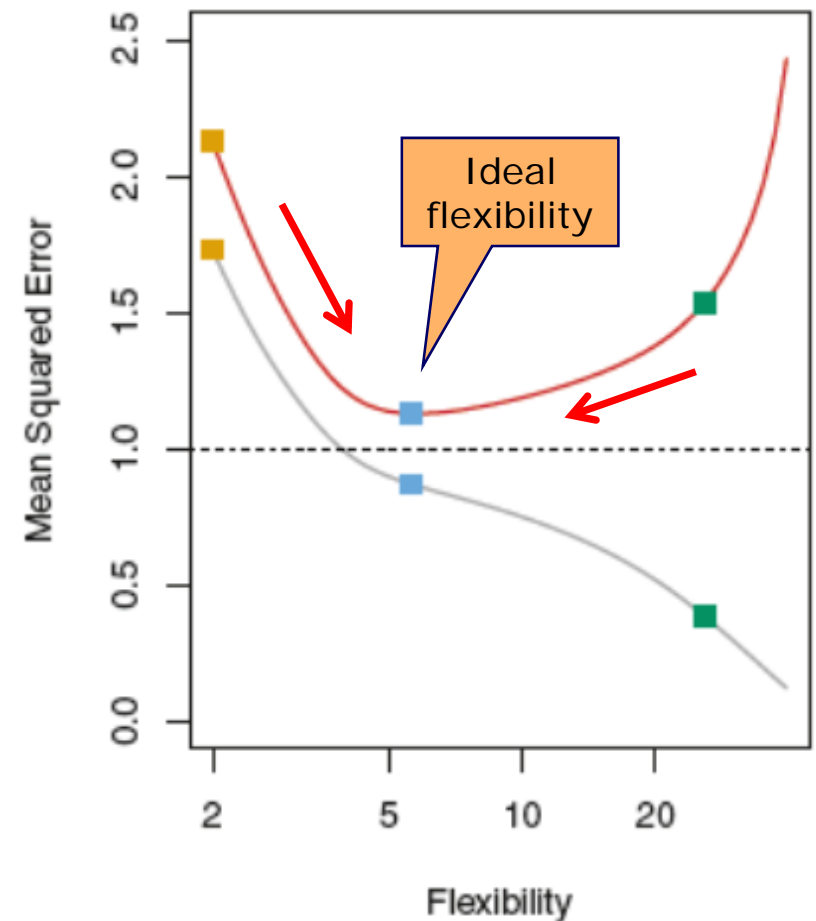
- Linear regression, polynomial regression, ...
- Decision Trees, ANNs, Naïve Bayes, ...

2. Testing different hyperparameters

- degree of polynomial, ridge
- depth of tree, min examples branch
- number of hidden layers

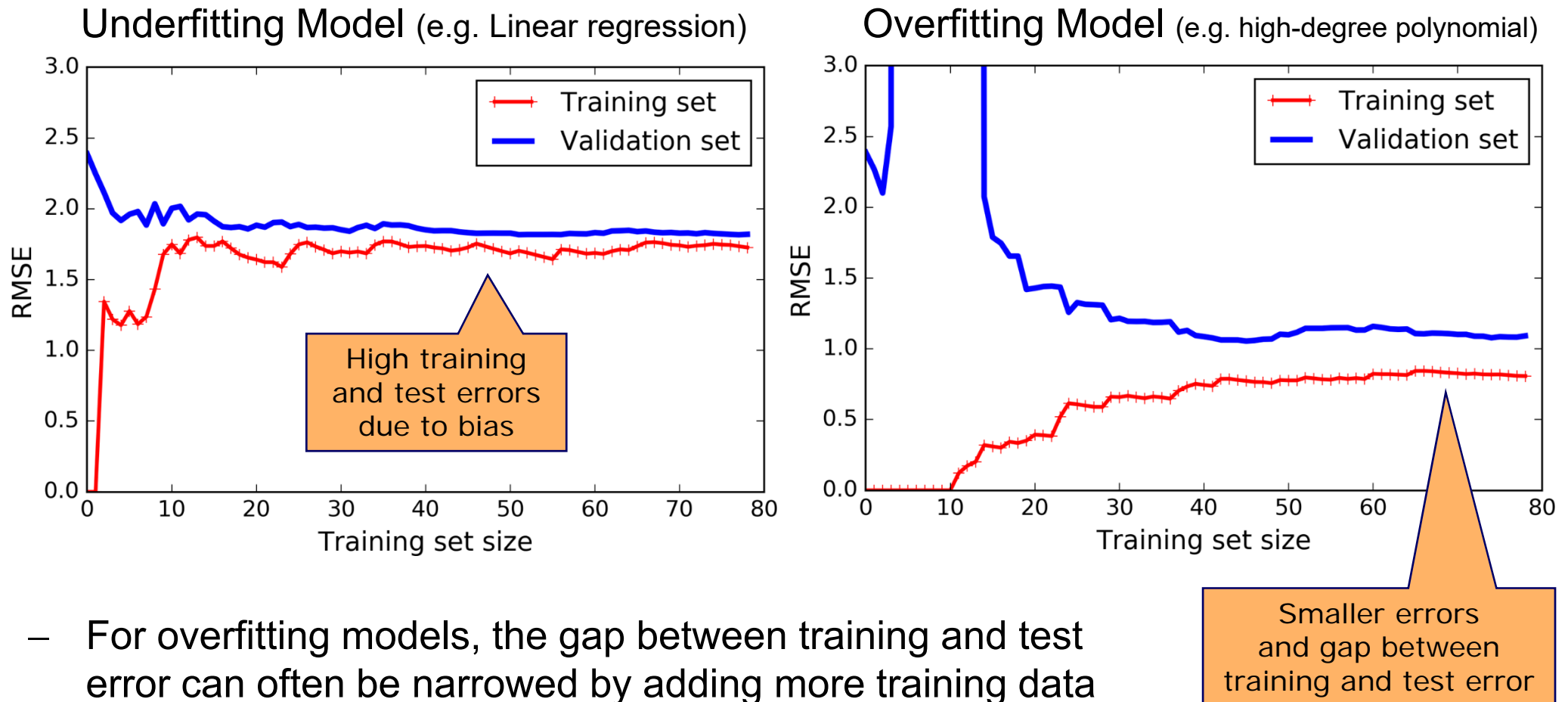
But we have two more options:

1. Increase the amount of training data
2. Cleanse the training data



Learning Curves

- 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 more flexible models, e.g. Deep Learning (Details in Data Mining II)

Literature

- Solving practical regression tasks using:
 - RapidMiner: Kotu: Predictive Analytics - Chapter 5, 10
 - Python: Geron: Hands-on Machine Learning - Chapter 4
- Deeper coverage including theoretical background
 - James, Witten, et al.: An Introduction to Statistical Learning Chapters 3, 7, 8

