UNIVERSITÄT MANNHEIM

Data Mining
Regression

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Regression

- Classification
  - covered in the previous lectures
  - predict a label from a finite collection
  - e.g., true/false, low/medium/high, ...

- Regression
  - predict a *numerical* value
  - from a possibly infinite set of possible values
- Examples
  - temperature
  - sales figures
  - stock market prices
  - ...

Contents

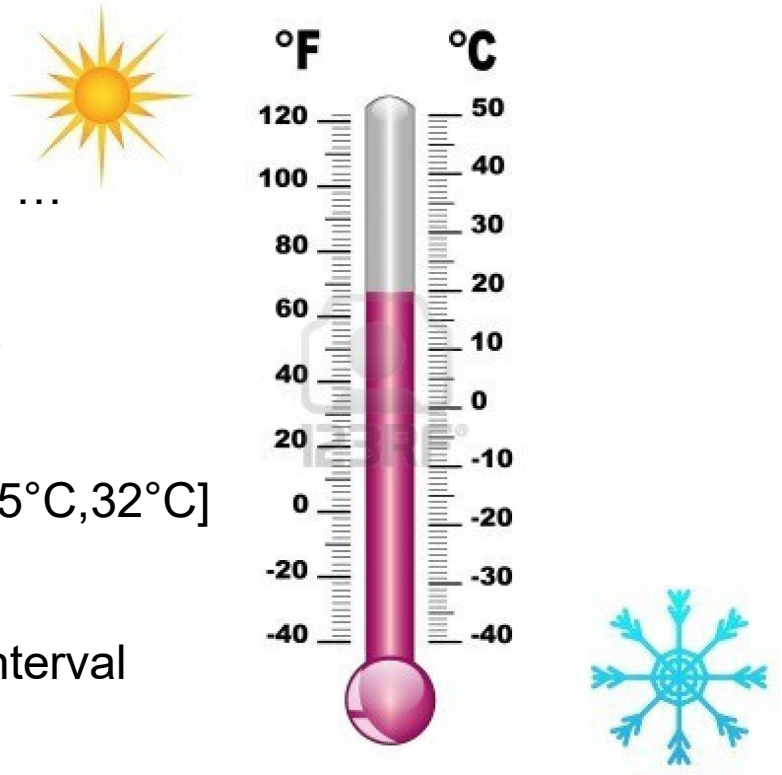
- A closer look at the problem
  - e.g., interpolation vs. extrapolation
  - measuring regression performance
- Revisiting classifiers we already know
  - which can also be used for regression
- Adoption of classifiers for regression
  - model trees
  - support vector machines
  - artificial neural networks
- Other methods of regression
  - linear regression and its regularized variants
  - isotonic regression
  - local regression

The Regression Problem

- 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

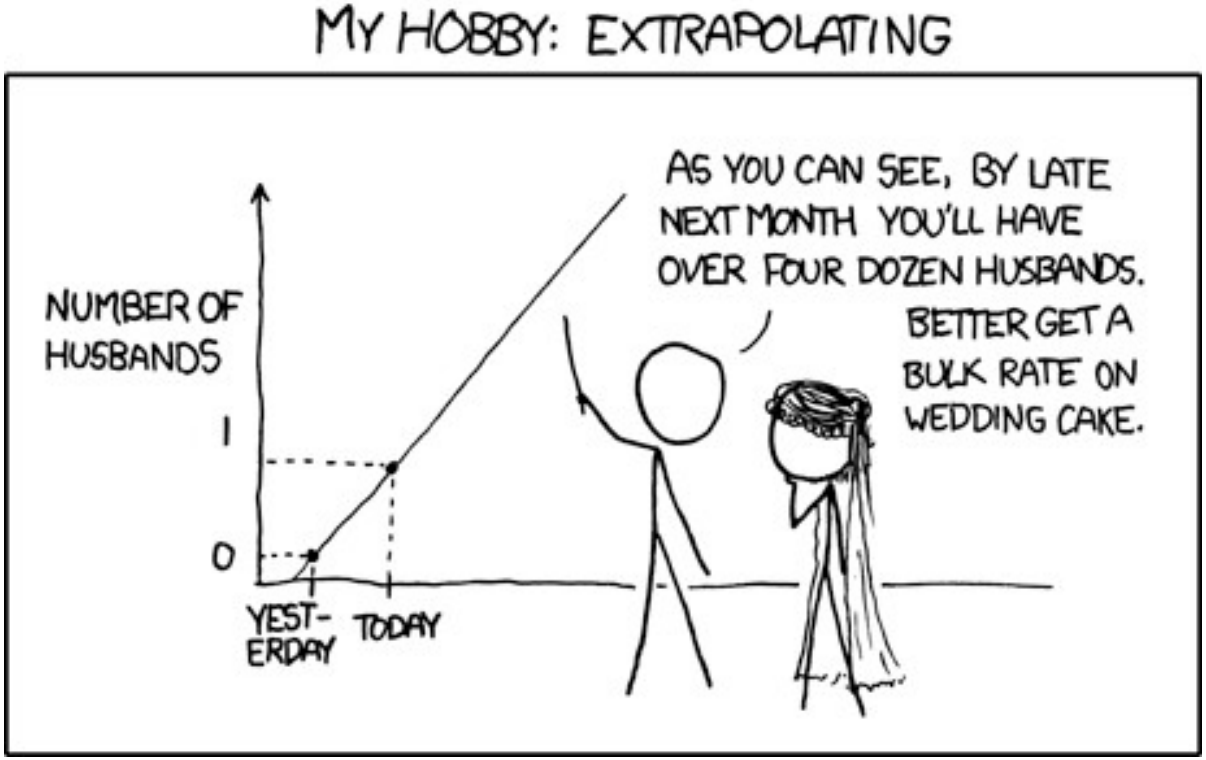
Interpolation vs. Extrapolation

- 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



http://xkcd.com/605/

Interpolation vs. Extrapolation

- Sometimes, however, only extrapolation is interesting
  - how far will the sea level have risen by 2050?
  - will there be a nuclear meltdown in my power plant?

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

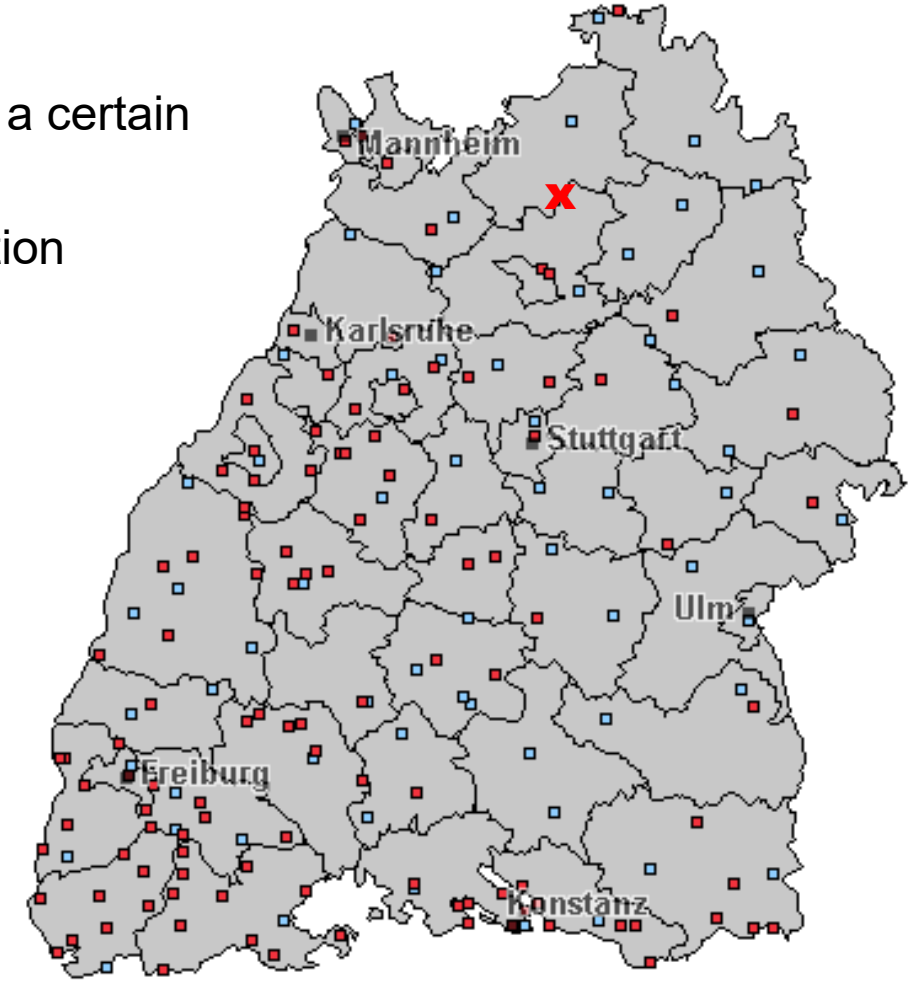
Baseline Prediction

- For classification: predict most frequent label
- For regression:
  - predict average value
  - or median
  - or mode
  - in any case: only interpolating regression
- often a strong baseline

http://xkcd.com/937/

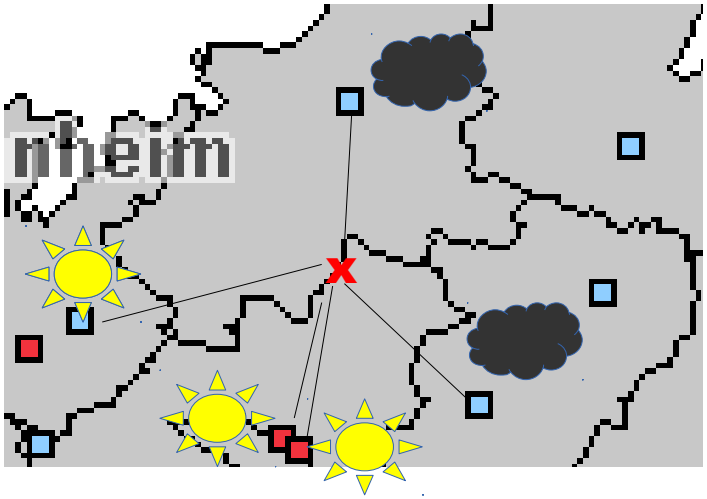
k Nearest Neighbors Revisited

- Problem
  - find out what the weather is in a certain place
  - where there is no weather station
  - how could you do that?



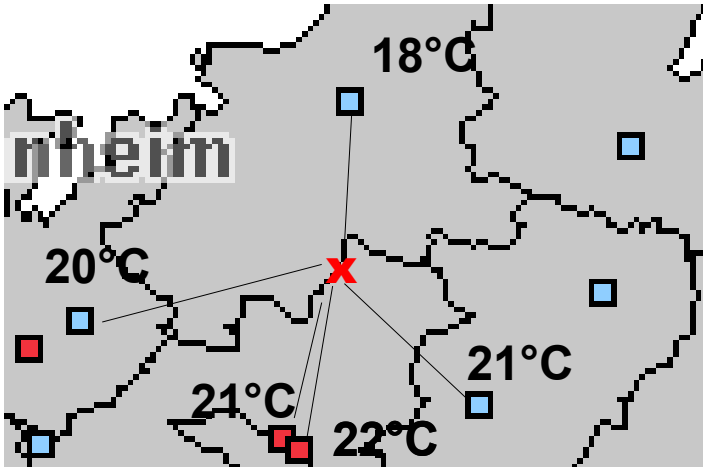
k Nearest Neighbors Revisited

- 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



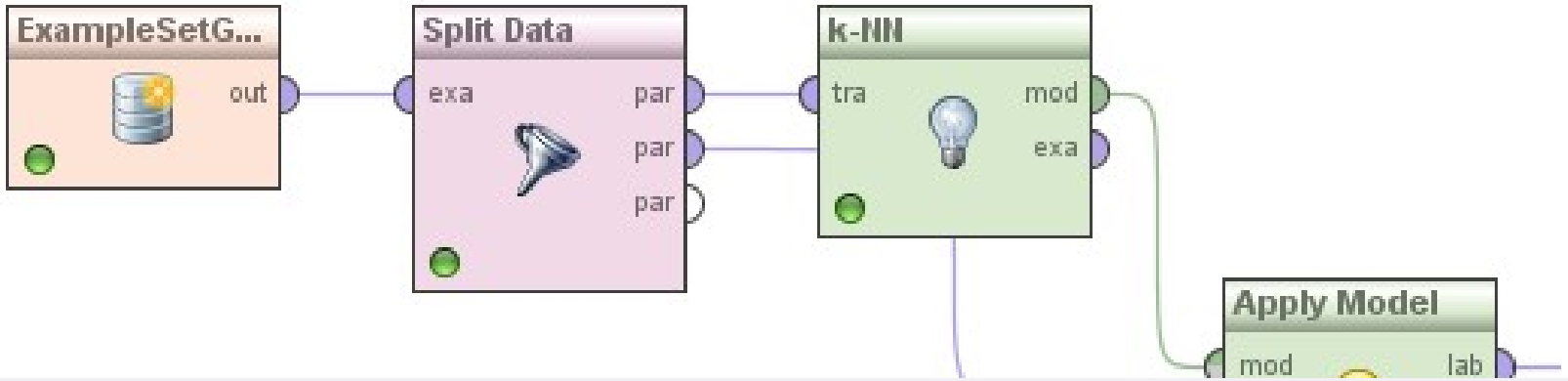
k Nearest Neighbors for Regression

- 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
  - (18+20+21+22+21)/5
  - prediction: 20.4°C



- Only interpolating regression!

k Nearest Neighbor Regression in RapidMiner



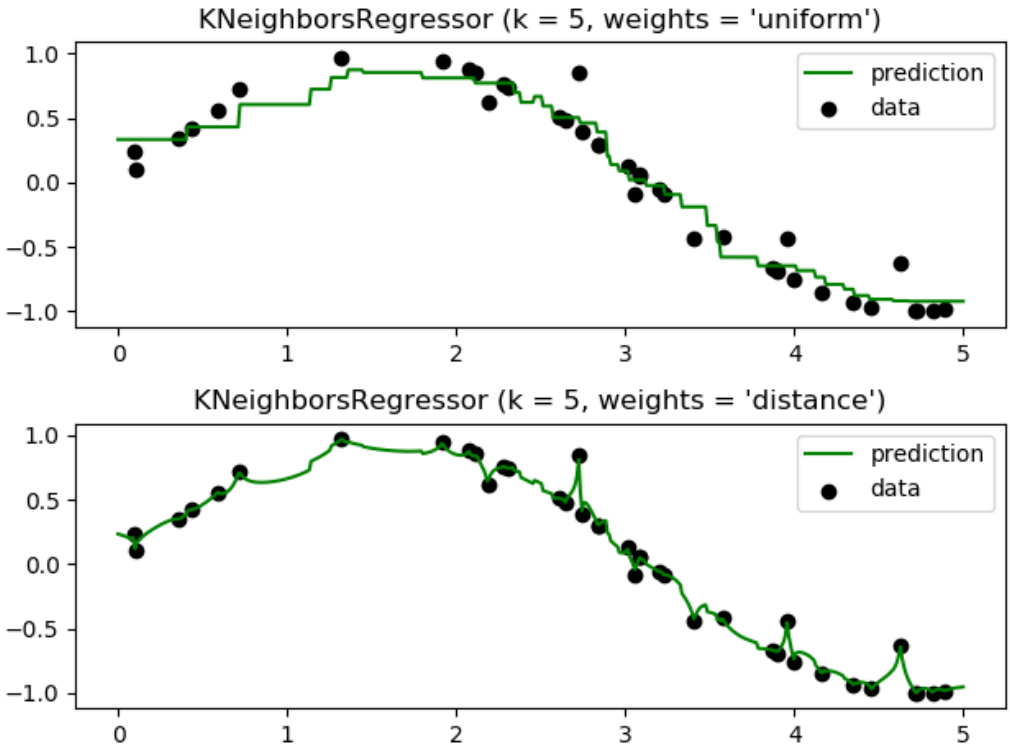
Data View | Meta Data View | Plot View | Advanced Charts | Annotations

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

k Nearest Neighbor Regression in Python

```
model = KNeighborsRegressor(k=number,
          weights='uniform'/'distance')
model.fit(X,Y)
```



Performance Measures

- Recap: measuring performance for classification:

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

- If we use the numbers 0 and 1 for class labels, we can reformulate this as

$$\text{Accuracy} = 1 - \frac{\sum_{\text{all examples}} |predicted - actual|}{N}$$

Why?

- the nominator is the sum of all correctly classified examples
  - i.e., the difference of the prediction and the actual label is 0
- the denominator is the total number of examples

Mean Absolute Error

- We have

$$\text{Accuracy} = 1 - \frac{\sum_{\text{all examples}} |predicted - actual|}{N}$$

- For an arbitrary numerical target, we can define

$$\text{MAE} = \frac{\sum_{\text{all examples}} |predicted - actual|}{N}$$

- Mean Absolute Error
  - intuition: how much does the prediction differ from the actual value on average?

(Root) Mean Squared Error

- Mean Squared Error:

$$\mathrm{MSE} = \frac{\sum_{all\ examples} |predicted - actual|^2}{N}$$

- Root Mean Squared Error:

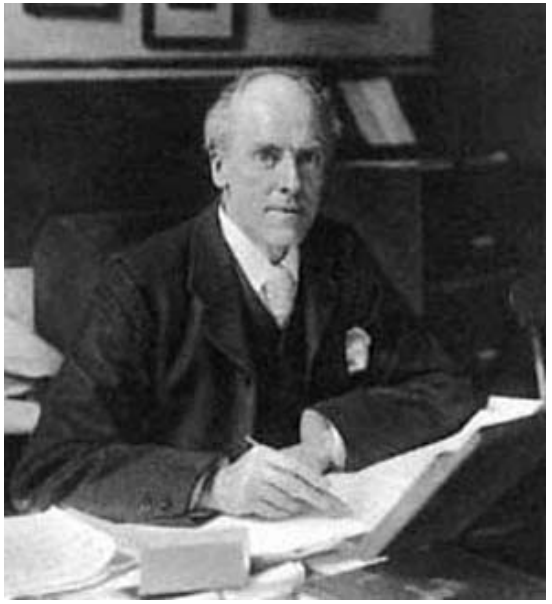
$$\mathrm{RMSE} = \sqrt{\frac{\sum_{all\ examples} |predicted - actual|^2}{N}}$$

- More severe errors are weighted higher by MSE and RMSE

Correlation

- Pearson's correlation coefficient
- Scores well if
  - high actual values get high predictions
  - low actual values get low predictions
- Caution: PCC is scale-invariant!
  - actual income: \$1, \$2, \$3
  - predicted income: \$1,000, \$2,000, \$3,000

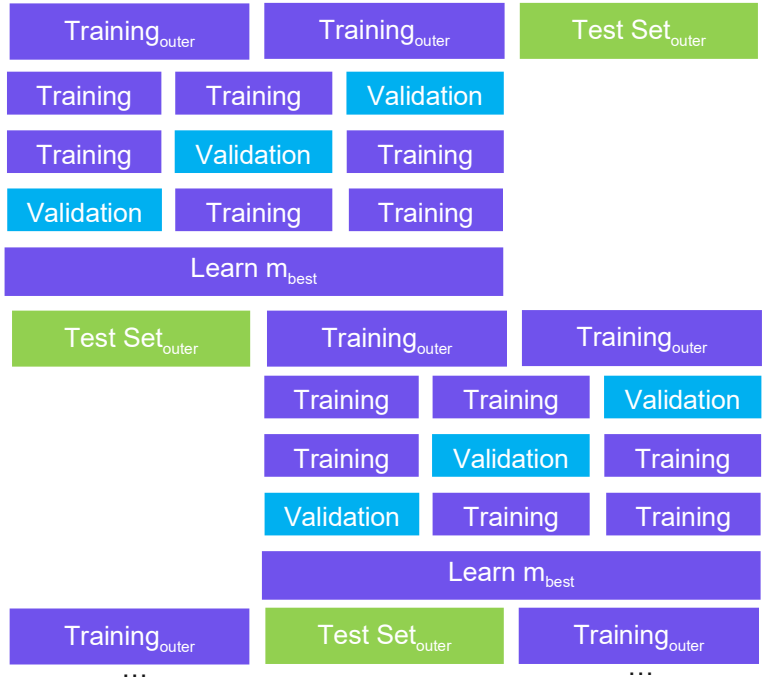
  → PCC = 1



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

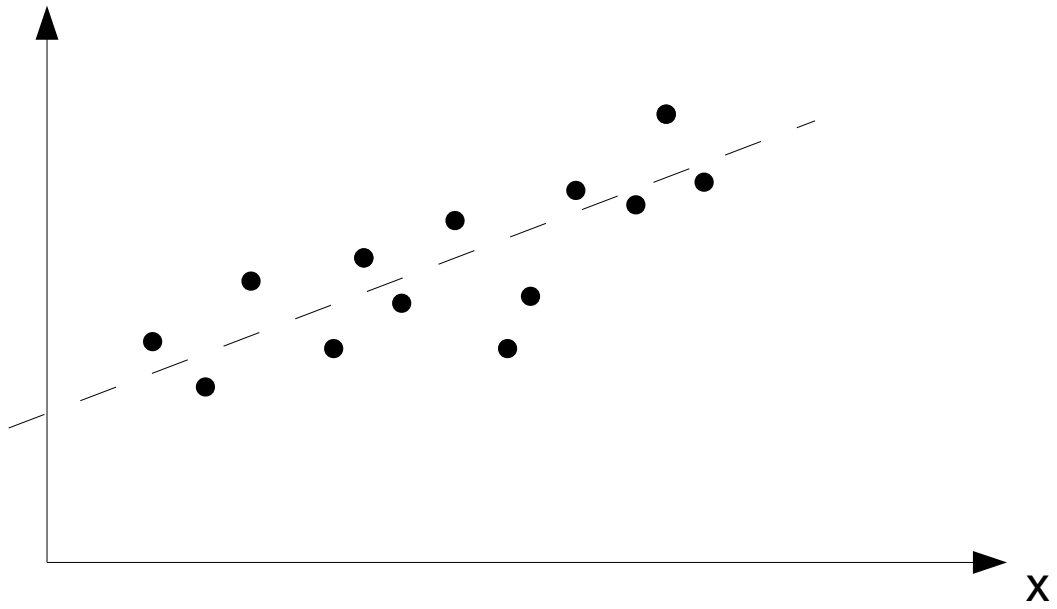
Evaluation Protocols

- Just as for classification
  - we are interested in performance on *unseen* data
  - we want to avoid *overfitting*
- Recap
  - split/cross validation
  - hyperparameter tuning in nested cross validation



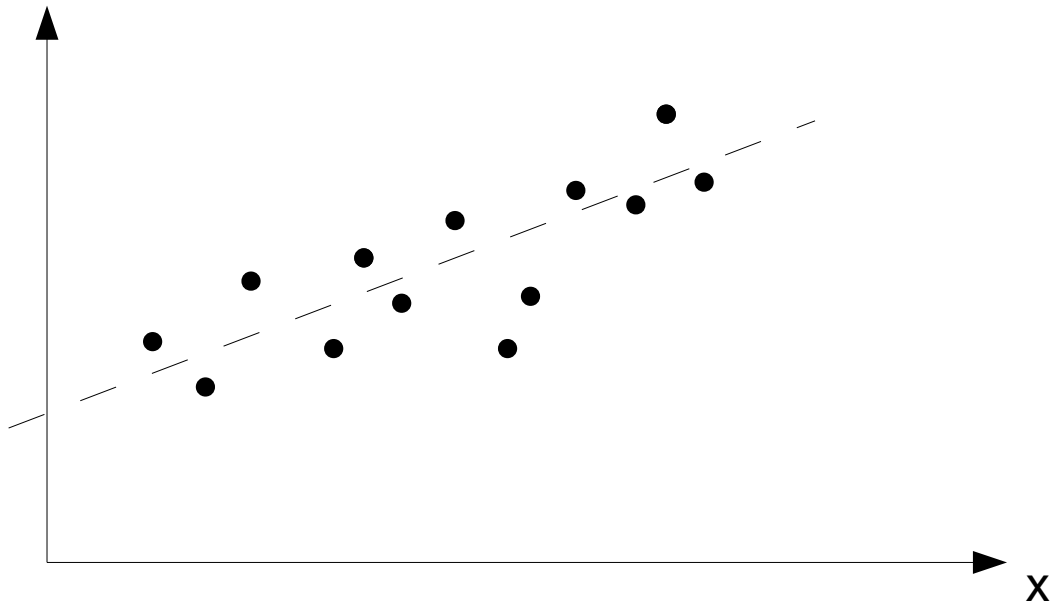
Linear Regression

- Assumption: target variable y is (approximately) linearly dependent on attributes
  - for visualization: one attribute x
  - in reality: $x_1 ... x_n$



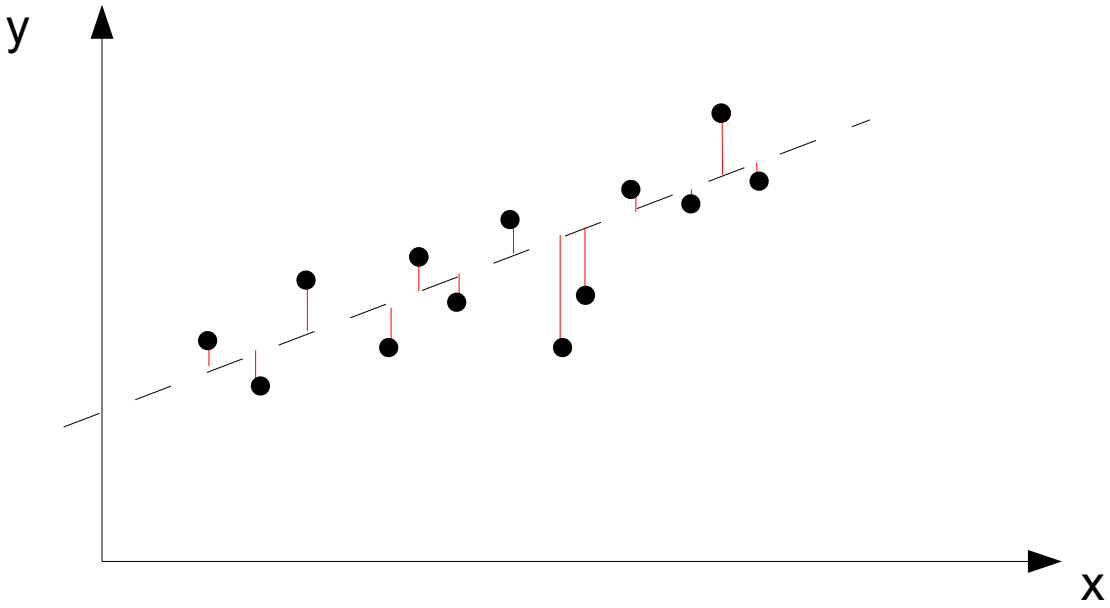
Linear Regression

- Target: find a linear function f: $f(x)=w_0 + w_1x_1 + w_2x_2 + \ldots + w_nx_n$
  - so that the error is minimized
  - i.e., for all examples $(x_1,...x_n,y)$, f(x) should be a *correct* prediction for y
  - given a performance measure



Linear Regression

- Typical performance measure used: Mean Squared Error
- Task: find w_0....w_n so that $\sum_{\textit{all examples}} \left(w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_n \cdot x_n - y\right)^2$ is minimized
- note: we omit the denominator N



Linear Regression: Multi Dimensional Example

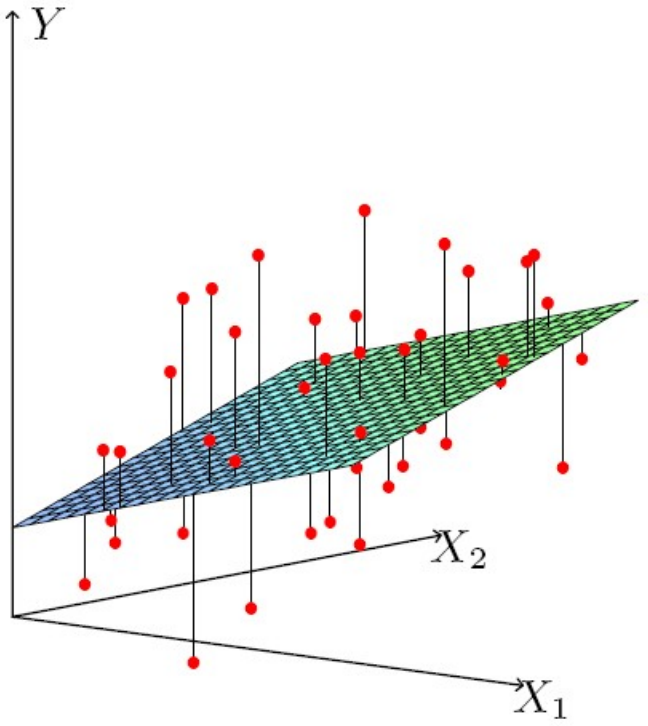
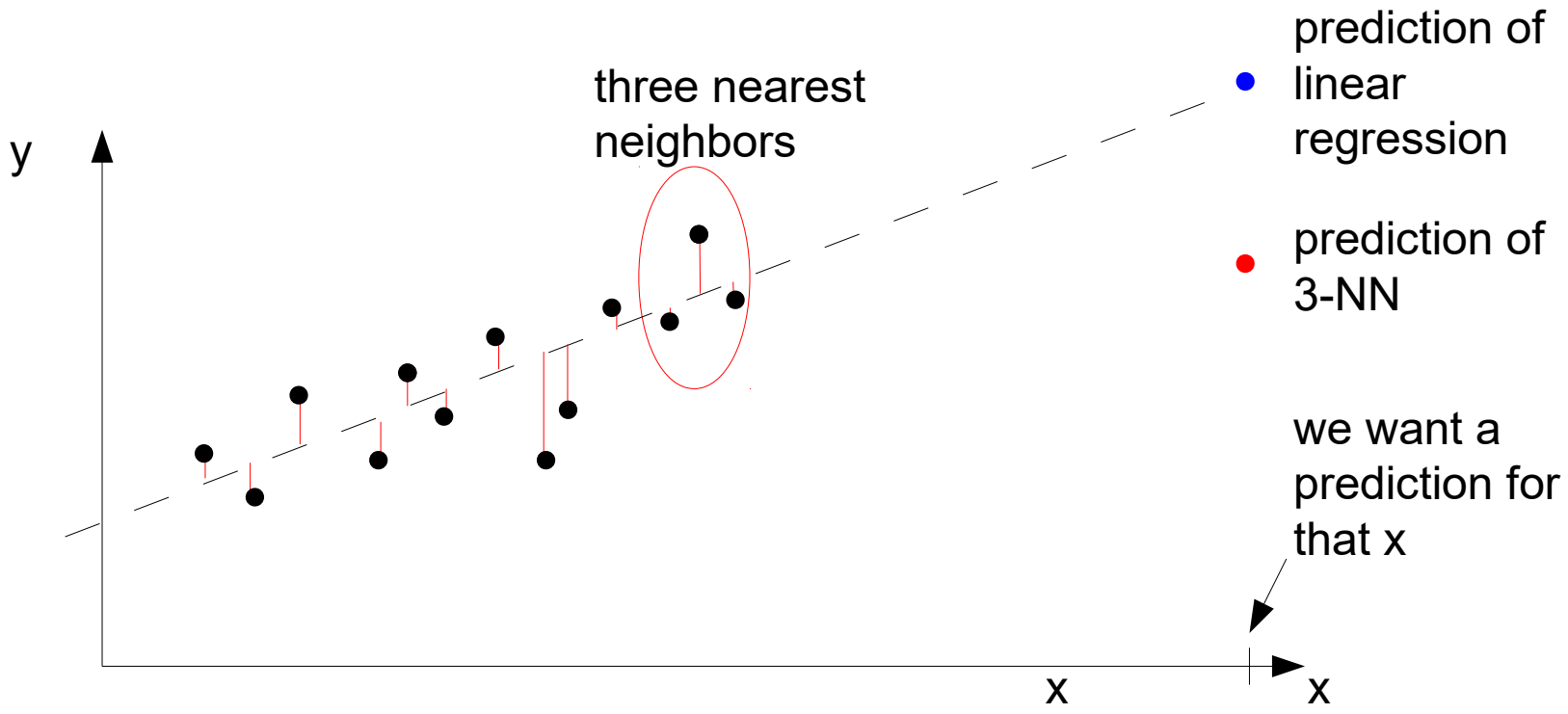


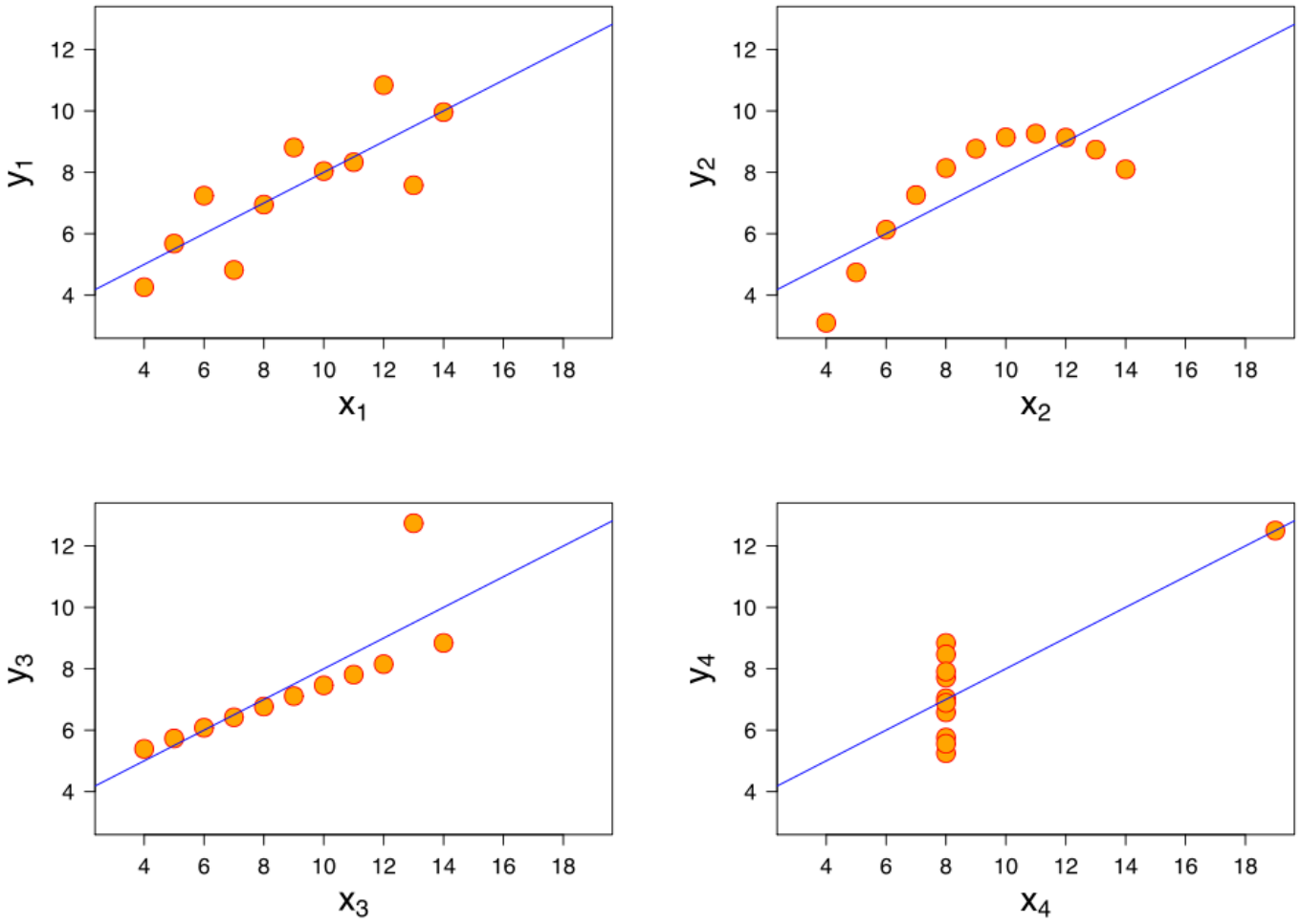
FIGURE 3.1. *Linear least squares fitting with* $X \in \mathbb{R}^2$. *We seek the linear function of* X *that minimizes the sum of squared residuals from* Y.

Linear Regression vs. k-NN Regression

- Recap: Linear regression extrapolates, k-NN interpolates



Linear Regression Examples



Linear Regression and Overfitting

- Given two regression models
  - One using five variables to explain a phenomenon
  - Another one using 100 variables
- Which one do you prefer?
- Recap: Occam's Razor
  - out of two theories explaining the same phenomenon, prefer the smaller one

Ridge Regression

- Linear regression only minimizes the errors on the training data
  - i.e., $\sum_{all\ examples} \left(w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_n \cdot x_n - y \right)^2$
- With *many* variables, we can have a large set of very small w_i
  - this might be a sign of overfitting!
- Ridge Regression:
  - introduces *regularization*
  - create a simpler model by favoring larger factors, minimize

$$\sum_{all\ examples} \left(w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_n \cdot x_n - y \right)^2 + \lambda \sum_{all\ variables} w_i^2$$

Ridge & Lasso Regression

- Ridge Regression optimizes

$$\sum_{\text{all examples}} \left(w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_n \cdot x_n - y\right)^2 + \lambda \sum_{\text{all variables}} w_i^2$$

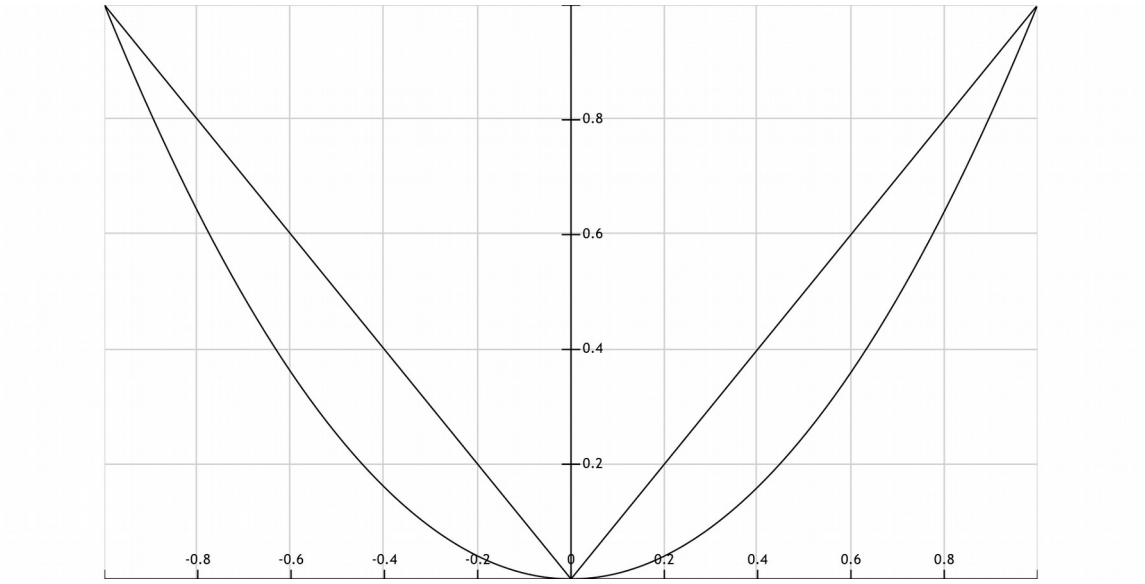
- Lasso Regression optimizes

$$\sum_{\text{all examples}} \left(w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_n \cdot x_n - y\right)^2 + \lambda \sum_{\text{all variables}} |w_i|$$

- Observations
  - Ridge Regression yields small, but non-zero coefficients
  - Lasso Regression tends to yield zero coefficients
  - $\lambda=0$: no normalization (i.e., ordinary linear regression) $\rightarrow$ overfitting
  - $\lambda \rightarrow \infty$: all weights will ultimately vanish $\rightarrow$ underfitting

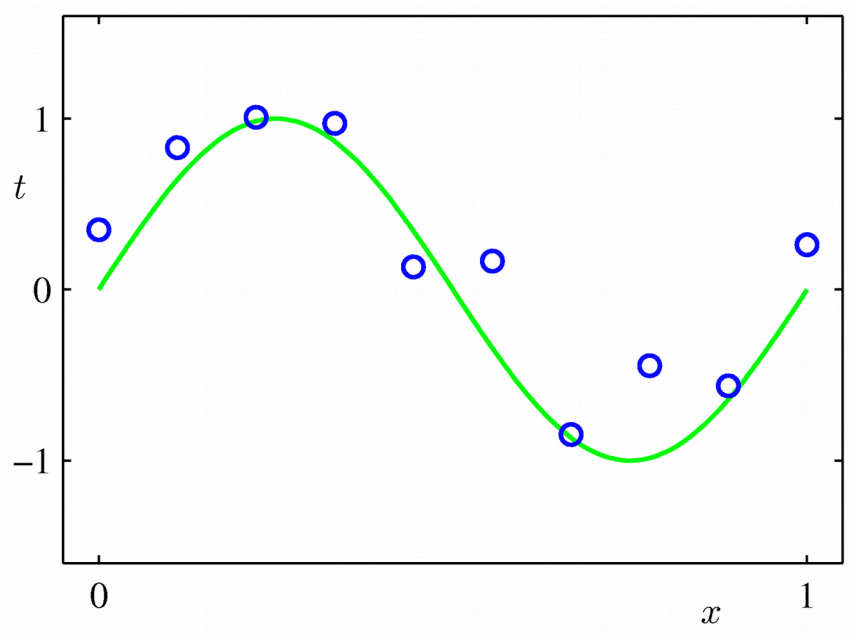
Lasso vs. Ridge Regression

- For w_i<close to 0, the contribution to the squared error is often smaller than the contribution to the regularization
  - Hence, minimization pushes small weights down to 0



$$\sum_{\text{all examples}} \left(w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_n \cdot x_n - y\right)^2 + \lambda \sum_{\text{all variables}} |w_i|$$

…but what about Non-linear Problems?



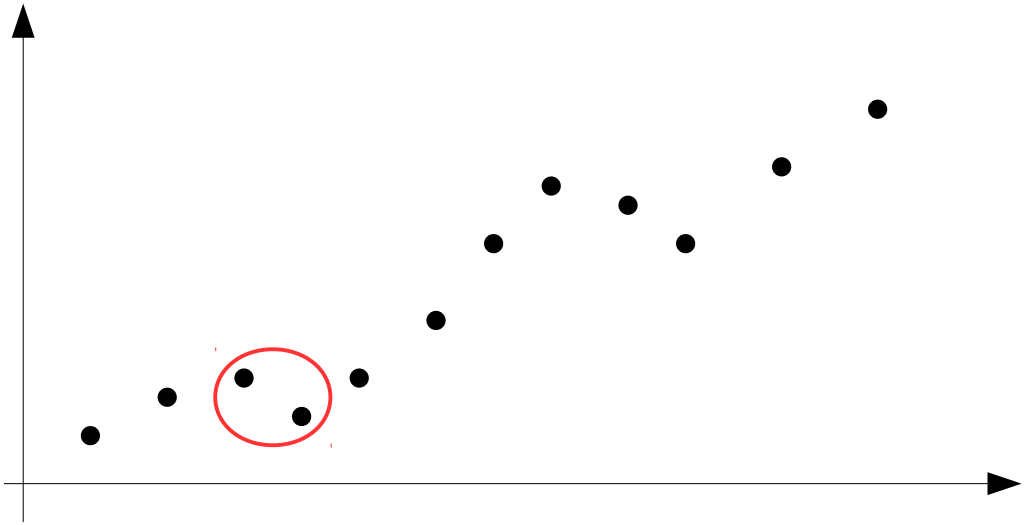
Isotonic Regression

- Special case:
  - Target function is *monotonous*
    - i.e., $f(x_1) \leq f(x_2)$ for $x_1 < x_2$
  - For that class of problem, efficient algorithms exist

- Simplest: Pool Adjacent Violators Algorithm (PAVA)

Isotonic Regression

- Identify adjacent violators, i.e., $f(x_i)>(x_{i+1})$
- Replace them with new values $f'(x_i)=f'(x_{i+1})$
  so that sum of squared errors is minimized
  - ...and *pool* them, i.e., they are going to be handled as one point
- Repeat until no more adjacent violators are left



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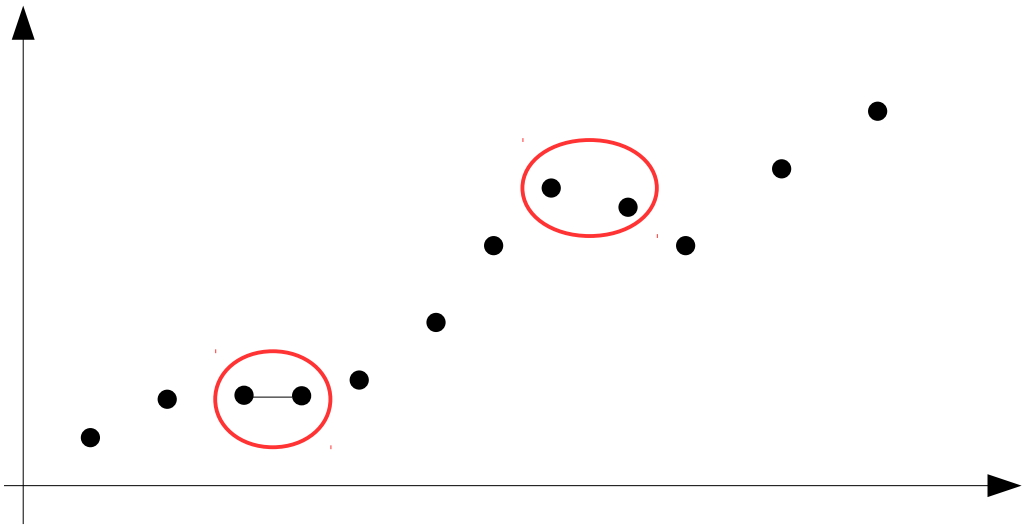

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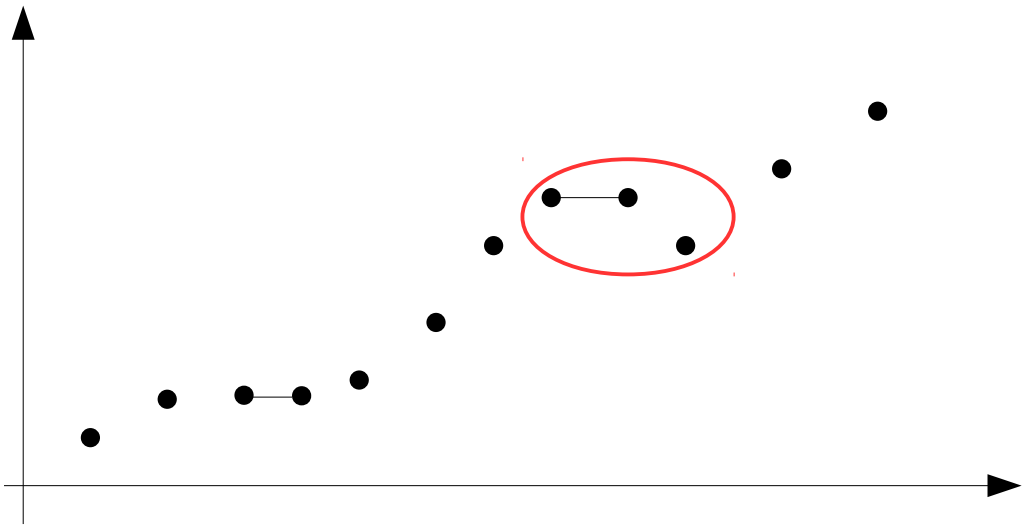

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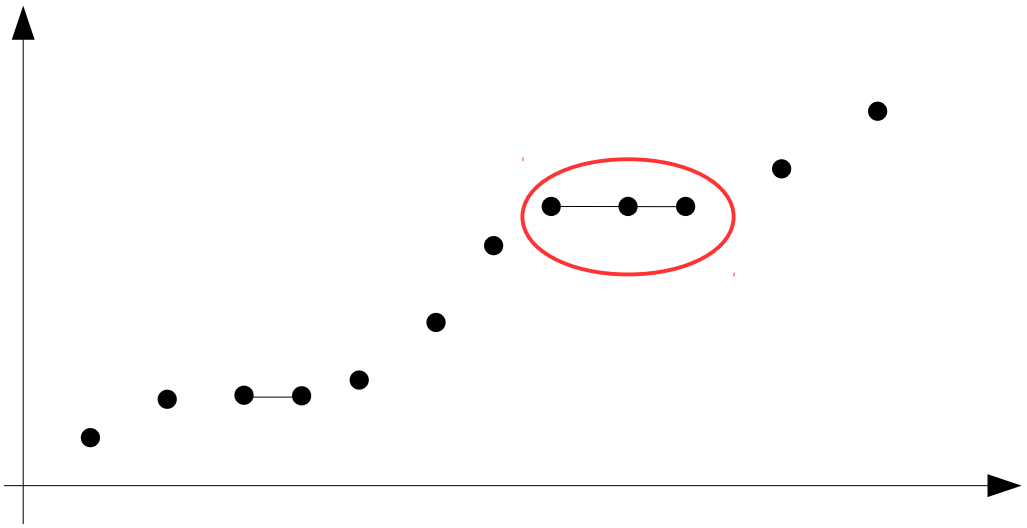
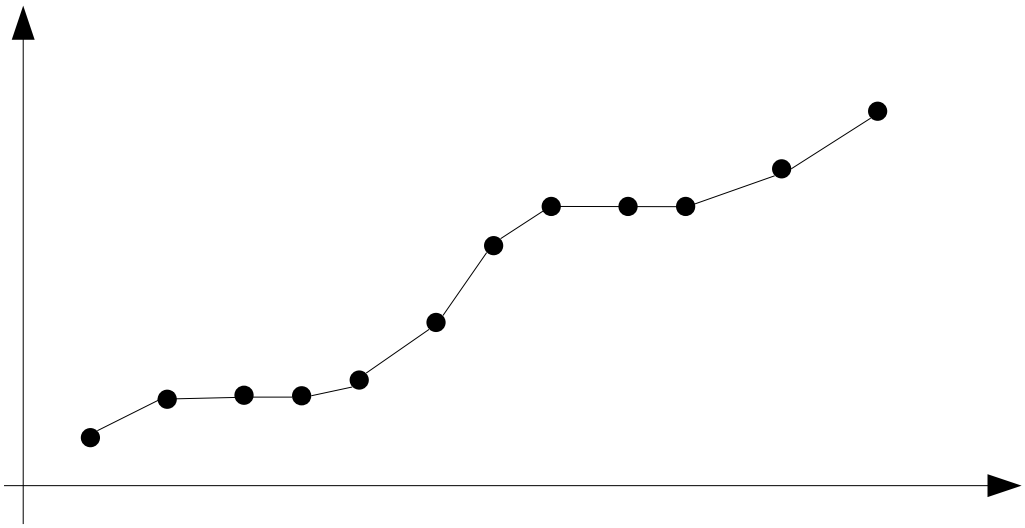


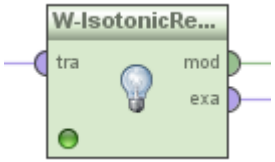
Isotonic Regression

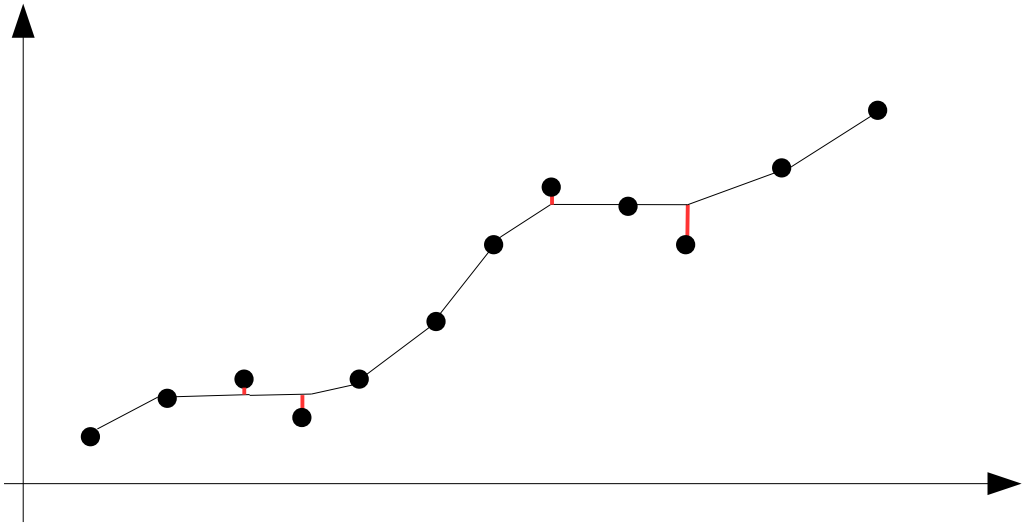
- After all points are reordered so that $f'(x_i)=f'(x_{i+1})$ holds for every i
  - Connect the points with a piecewise linear function



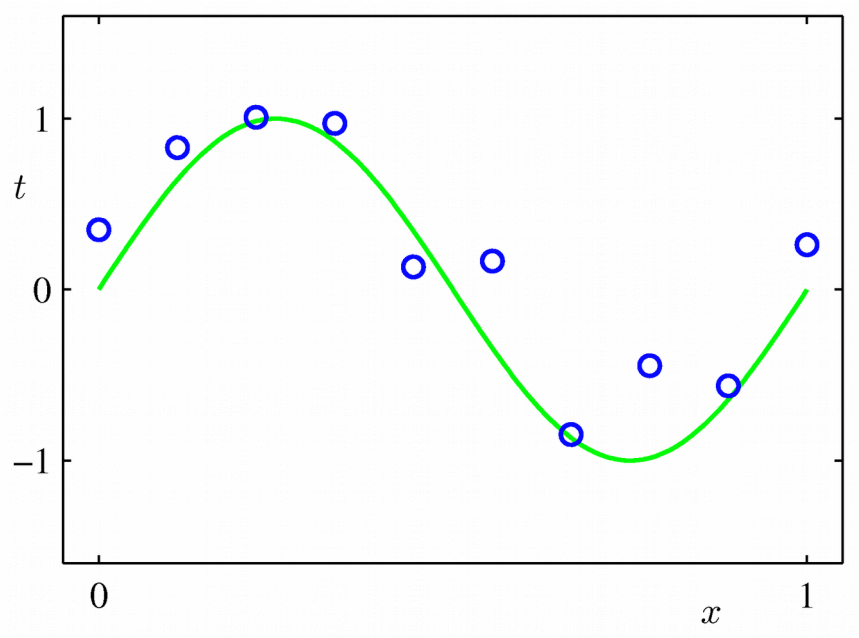
Isotonic Regression

- Comparison to the original points
  - Plateaus exist where the points are not monotonous
  - Overall, the mean squared error is minimized
- Operator in RapidMiner: from the Weka Extension
- Python: `IsotonicRegression` (caution: only increasing case)





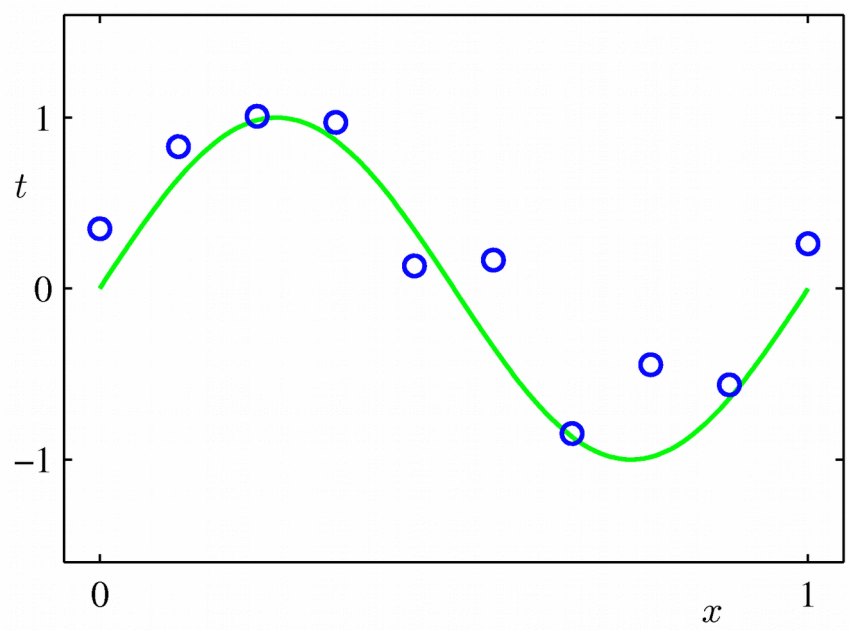
…but what about non-linear, *non-monotonous* Problems?

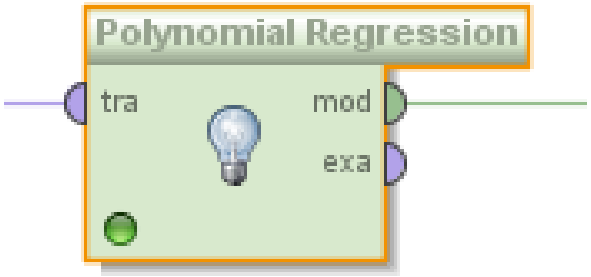


Possible Option: new Attributes

- The attributes **X** for linear regression can be:
  - Original attributes **X**
  - Transformation of original attributes,
    e.g. log, exp, square root, square, etc.
  - Polynomial transformation
    - example: $y = \beta_0 + \beta_1 \cdot x + \beta_2 \cdot x^2 + \beta_3 \cdot x^3$
  - Basis expansions
  - Interactions between variables
    - example: $x_3 = x_1 \cdot x_2$
- This allows use of linear regression techniques to fit much more complicated non-linear datasets

Example with Polynomially Transformed Attributes





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

```
Xp = PolynomialFeatures(degree=M).fit_transform(X)
```

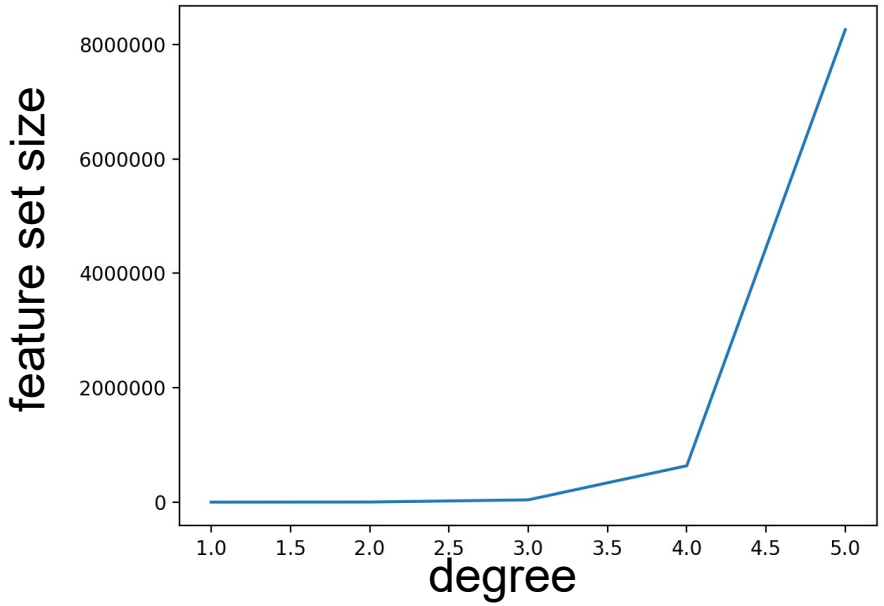
Polynomial Regression & Overfitting

- Creating polynomial features of degree d for a dataset with f features: $O(f^d)$ features
- Consider: three features x,y,z, d=3
  - 6 new features d=2: x^2, y^2, z^2, xy, xz, yz
  - 10 new features d=3: x^3, y^3, z^3, x^2y, x^2z, y^2x, y^2z, z^2x, z^2y, xyz

- With higher values for f and d,
  we are likely to generate a very large number of additional features

Polynomial Regression & Overfitting

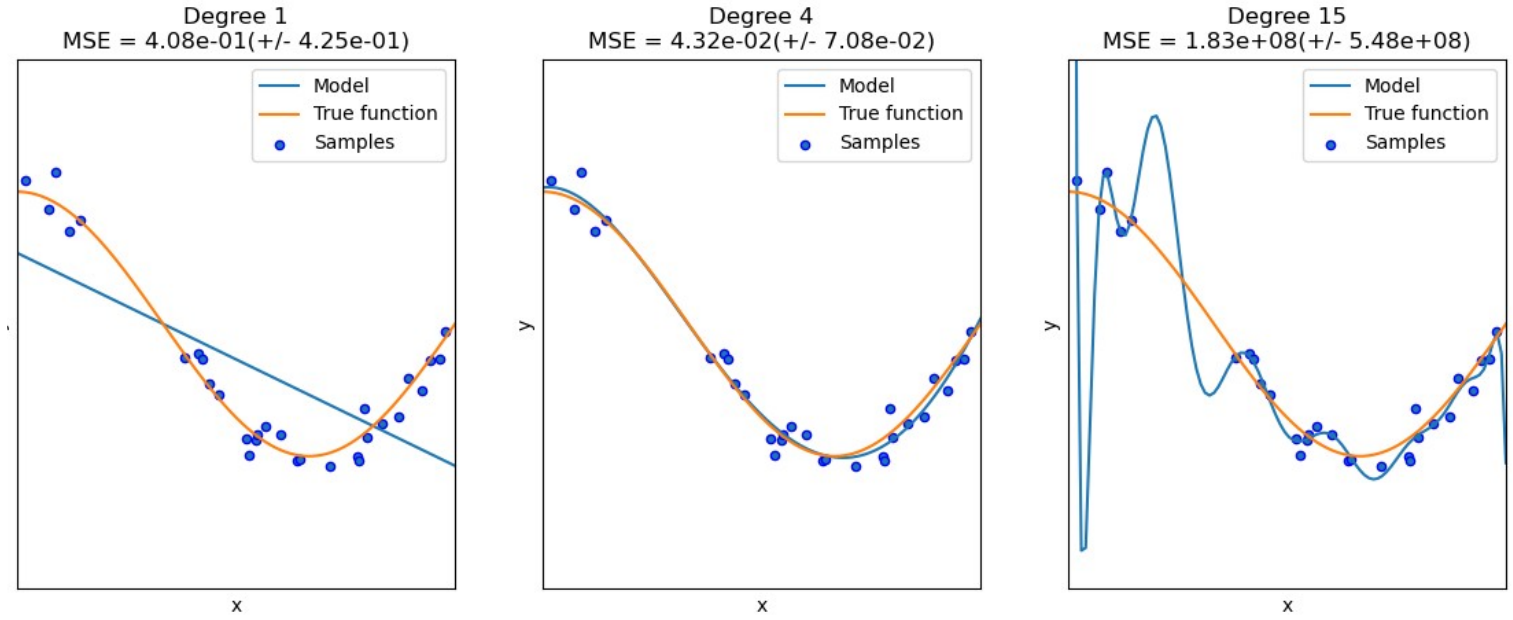
- Creating polynomial features of degree d for a dataset with f features: $O(f^d)$ features
- Example: Sonar dataset (60 features)



https://machinelearningmastery.com/polynomial-features-transforms-for-machine-learning/

Polynomial Regression & Overfitting

- Larger feature sets lead to higher degrees of overfitting

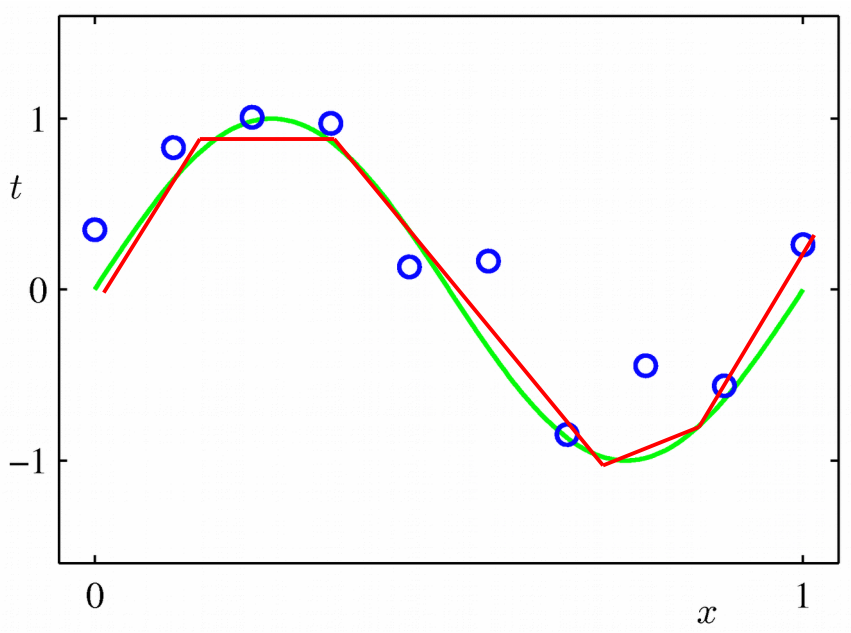


Polynomial Regression & Overfitting

- Why are larger feature sets dangerous?
  - Think of overfitting as “memorizing”
- With 1k variables and 1k examples
  - we can probably identify each example by a unique feature combination
  - but with 2 variables for 1k examples, the model is forced to abstract
- Rule of thumb
  - Datasets should never be wider than long!

Local Regression

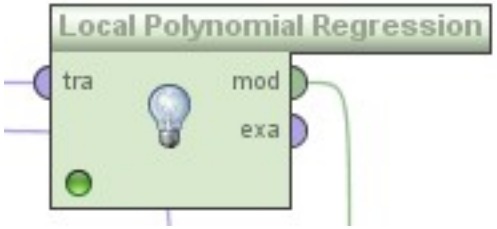
- Assumption: non-linear problems are approximately linear in local areas
  - idea: use linear regression locally
  - only for the data point at hand (lazy learning)



Local Regression

- A combination of
  - k nearest neighbors
  - local regression

- Given a data point
  - retrieve the k nearest neighbors
  - compute a regression model using those neighbors
  - locally weighted regression:
    uses distance as weight for error computation



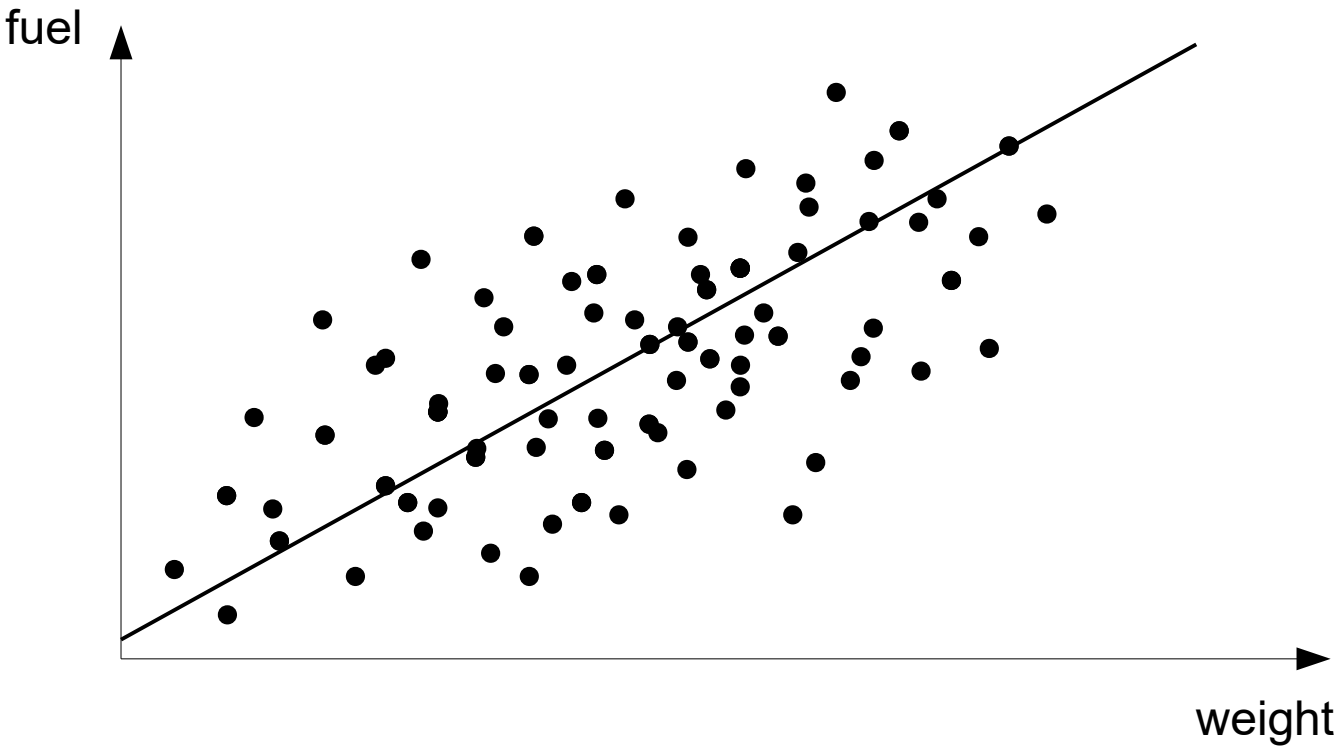
Local Regression

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

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

Combining Decision Trees and Regression

- Idea: split data first so that it becomes “more linear”
- example: fuel consumption by car weight



Combining Decision Trees and Regression

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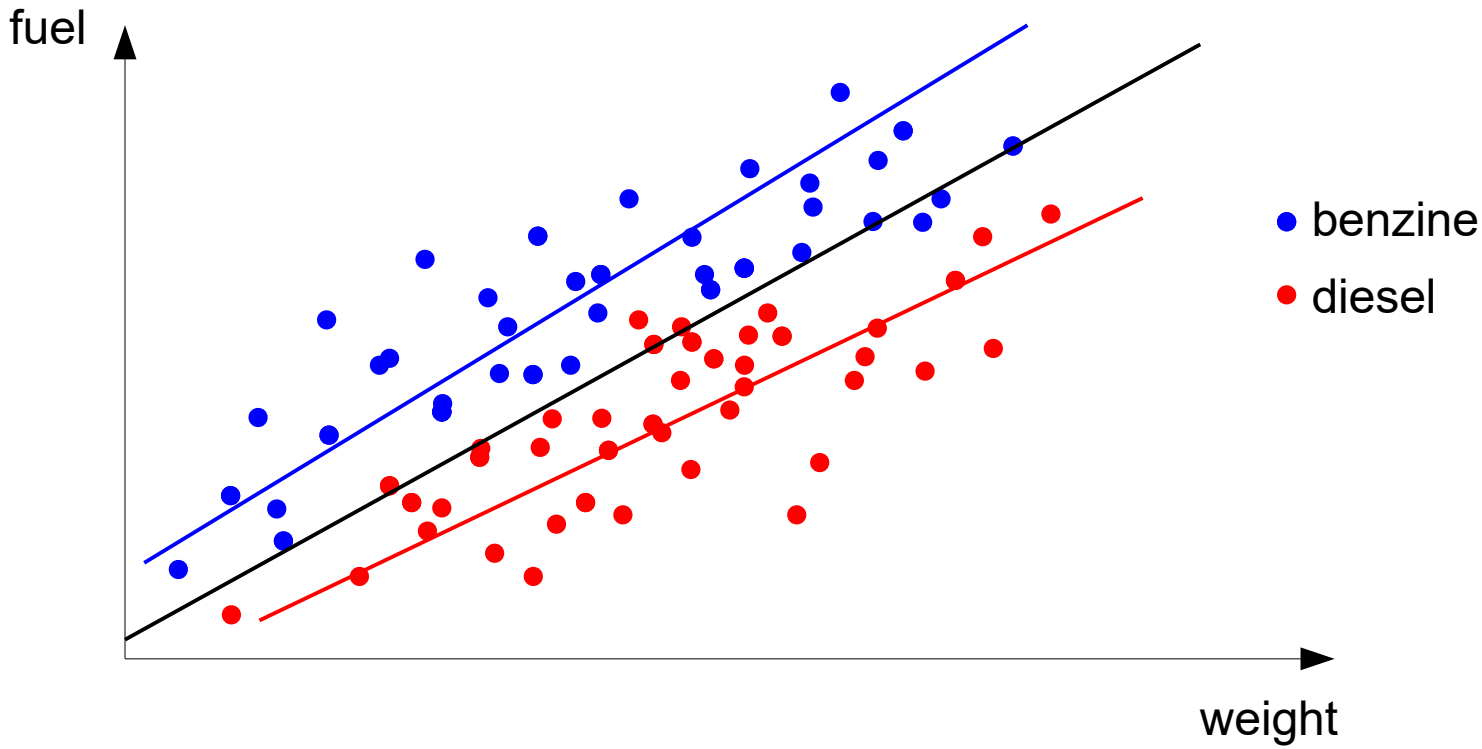
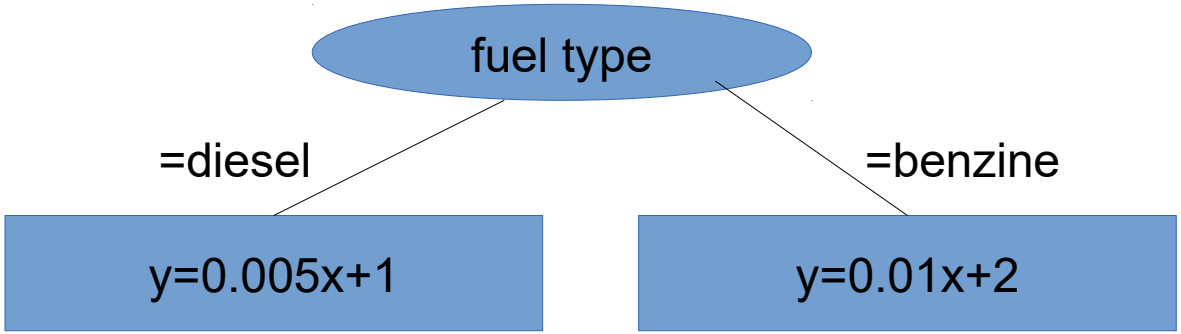


Combining Decision Trees and Regression

- Observation:
  - by cleverly splitting the data, we get more accurate linear models
- Regression trees:
  - decision tree for splitting data
  - constants as leaves
- Model trees:
  - more advanced
  - linear functions as leaves



Regression Trees

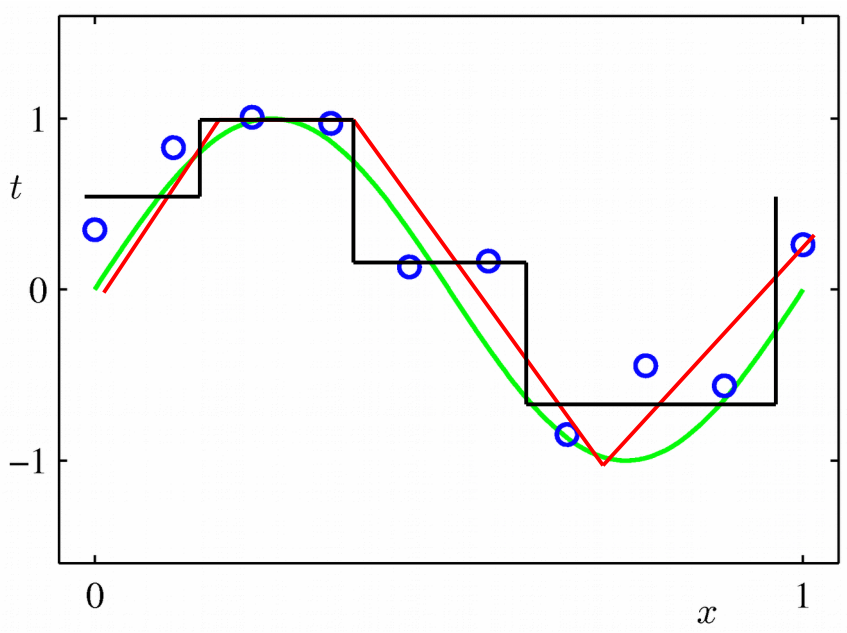
- Differences to classification decision trees:
  - Splitting criterion: minimize intra-subset variation
  - Termination criterion: standard deviation becomes small
  - Pruning criterion: based on numeric error measure
  - Prediction: Leaf predicts average class values of instances
- Easy to interpret
- Resulting model: piecewise *constant* function

Model Trees

- Build a regression tree
  - For each leaf $\Rightarrow$ learn linear regression function
- Need linear regression function at each *node*
- Prediction: go down tree, then apply function
- Resulting model: piecewise *linear* function

Local Regression and Regression/Model Trees

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



piecewise linear (model tree)

piecewise constant (regression tree)

Building the Tree

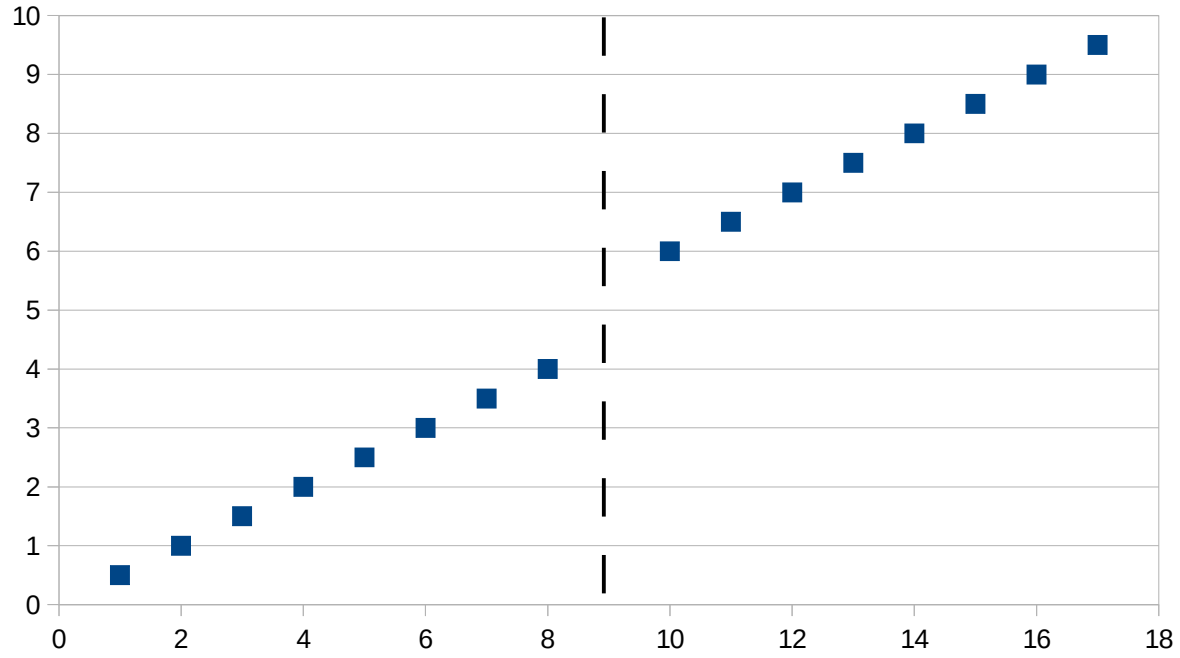
- Splitting: standard deviation reduction

$$SDR = sd(T) - \sum_i \left|\frac{T_i}{T}\right| \times sd(T_i)$$

- Termination:
  - Standard deviation < 5% of its value on full training set
  - Too few instances remain (e.g. < 4)
- Pruning:
  - Proceed bottom up:
    - Compute LR model at internal node
    - Compare LR model error to error of subtree
    - Prune if the subtree's error is not significantly smaller
  - Heavy pruning: single model may replace whole subtree

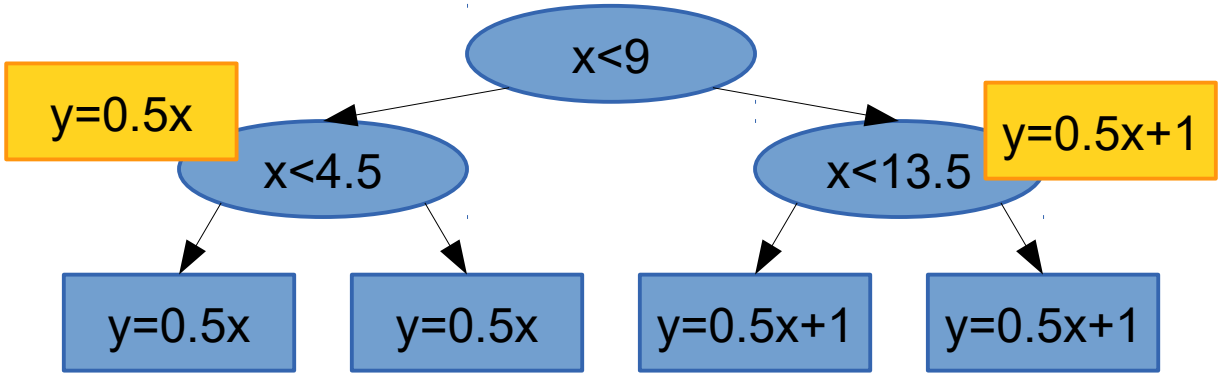
Model Tree Learning Illustrated

- Standard deviation of complete value set: 3.08
- Standard deviation of two subsets after split x>9: 1.22
  - Standard deviation reduction: 1.86
  - This is the best split

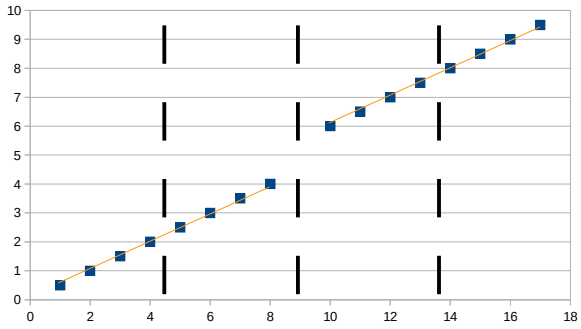


Model Tree Learning Illustrated

- Assume that we have split further (min. 4 instances per leaf)
  - Standard deviation reduction for the new splits is still 0.57
- Resulting model tree:

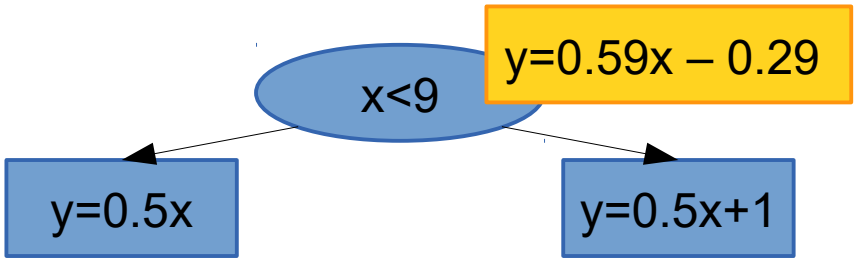


- The error of the inner nodes is the same as for the root nodes → prune

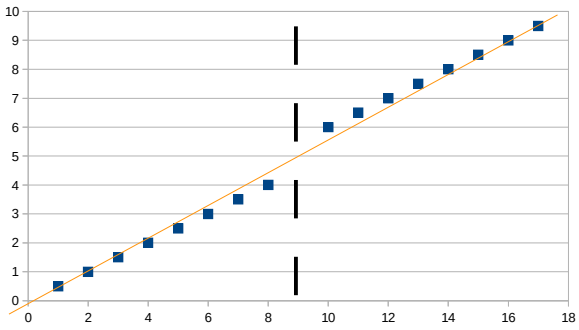


Model Tree Learning Illustrated

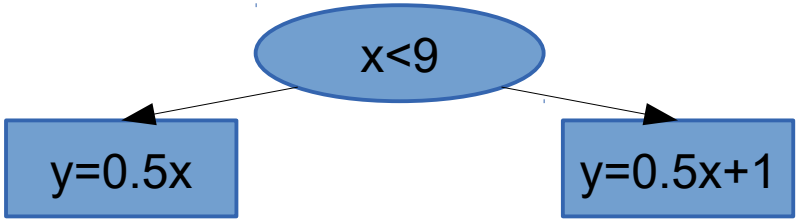
- Assume that we have split further (min. 4 instances per leaf)
  - Standard deviation reduction for the new splits is still 0.57
- Resulting model tree:

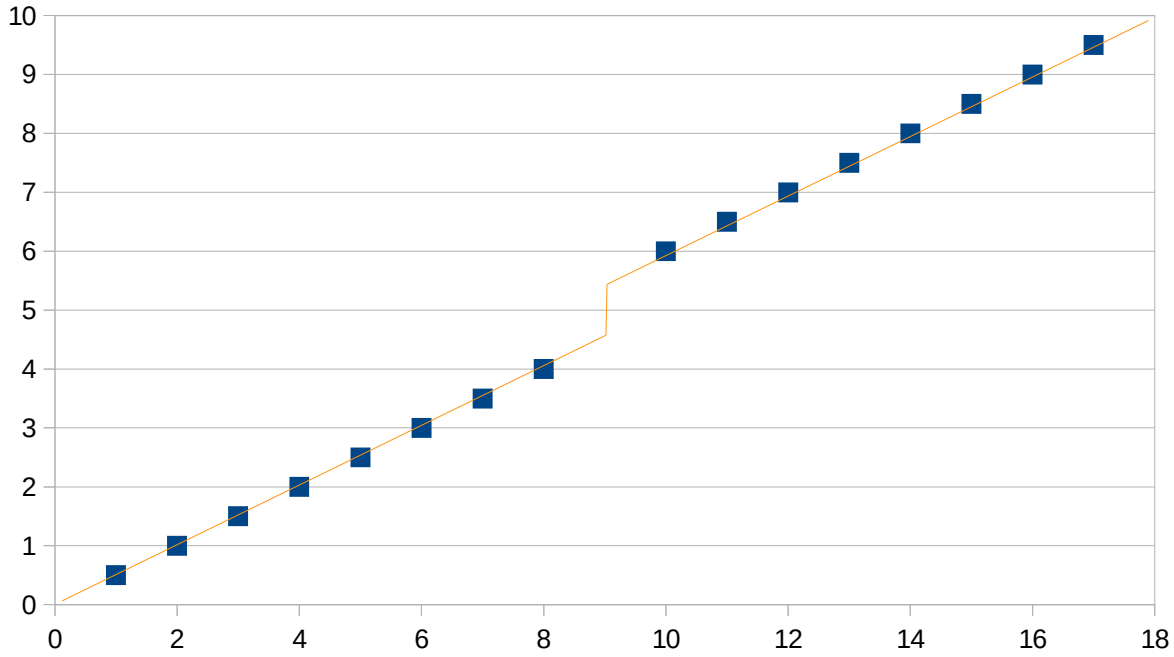


- The error of the root node is larger than that of the leaf nodes → keep leaf nodes

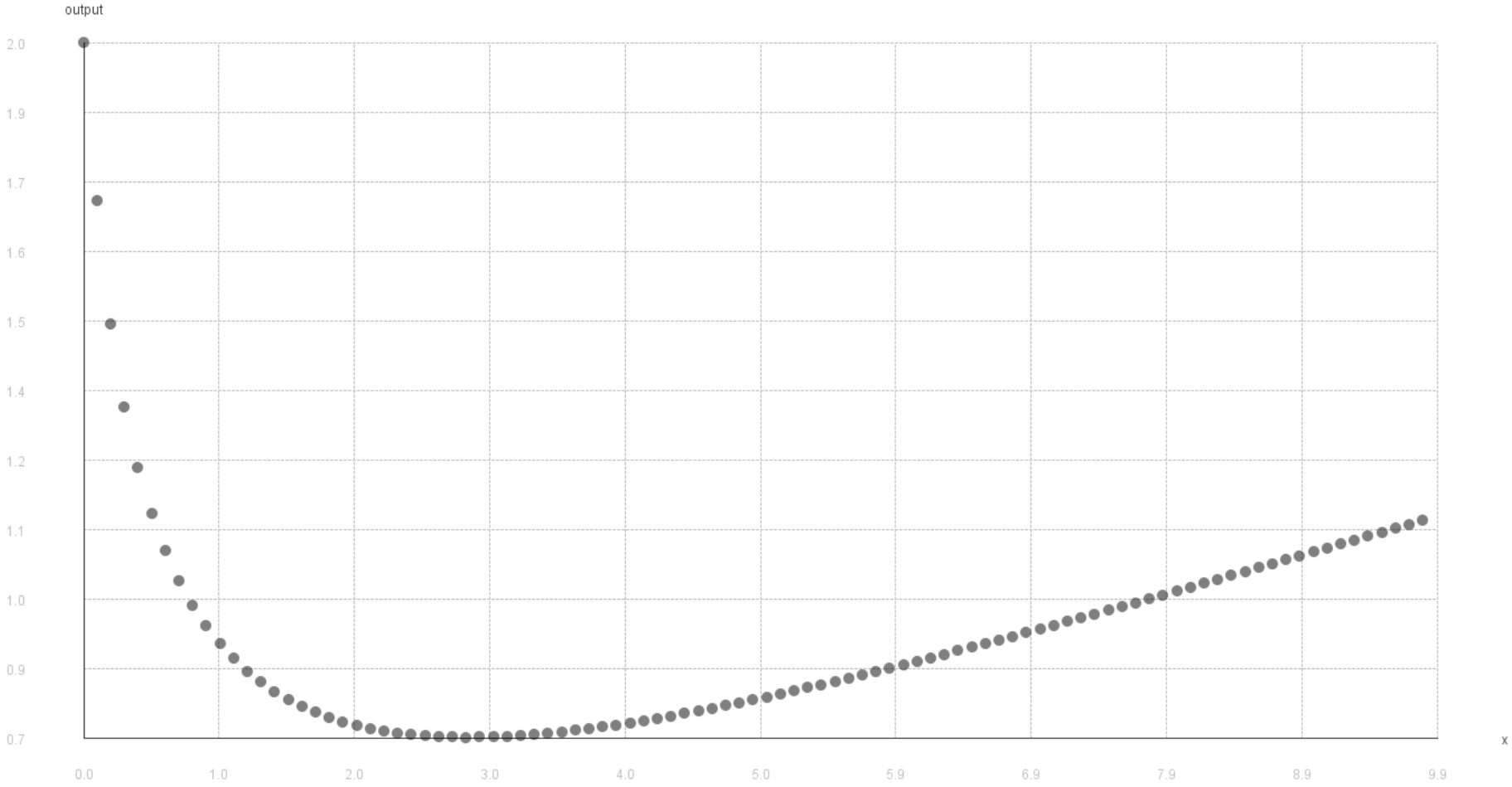


Model Tree Learning Illustrated

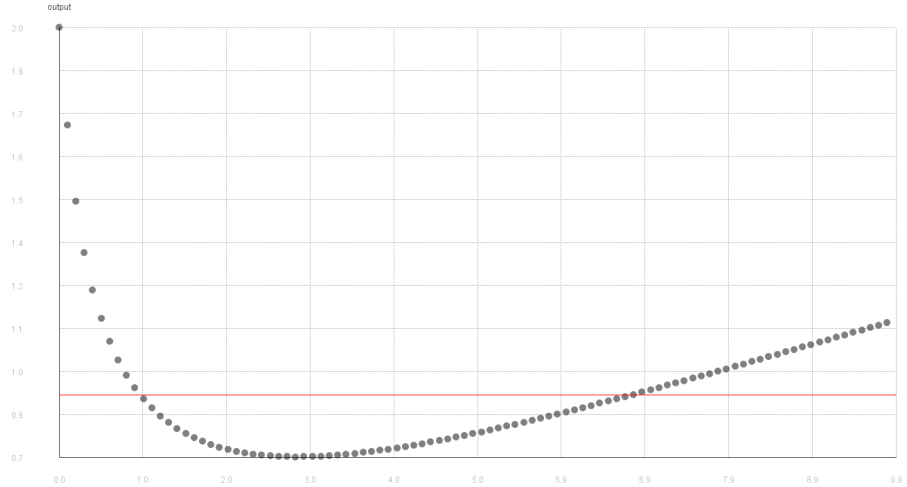


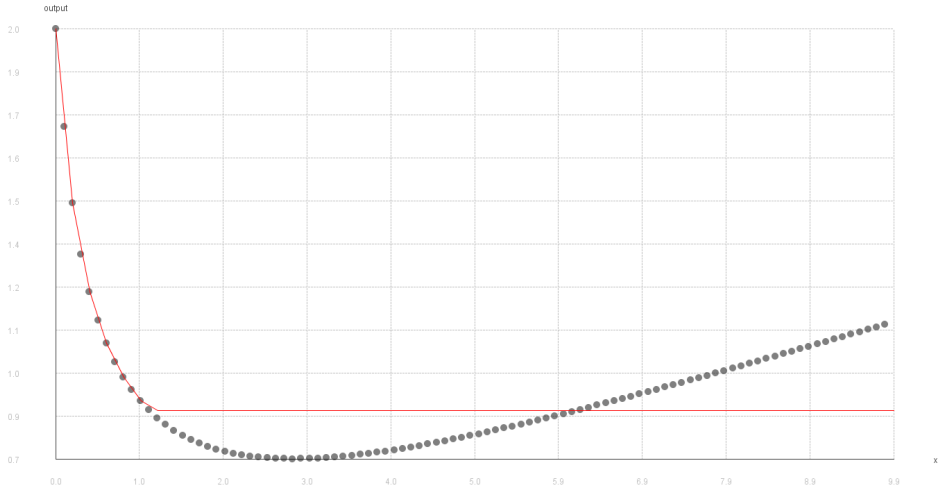


Comparison

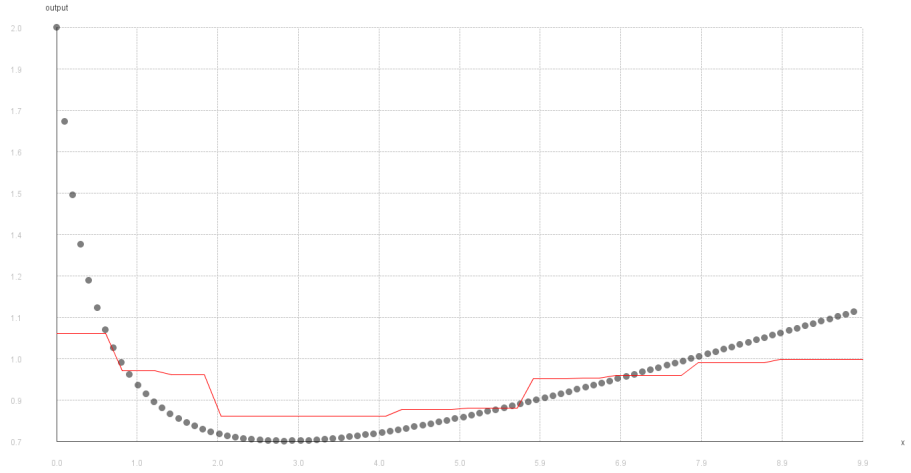

output
2.0
1.9
1.7
1.6
1.5
1.4
1.2
1.1
1.0
0.9
0.7
0.0
1.0
2.0
3.0
4.0
5.0
5.9
6.9
7.9
8.9
9.9
x

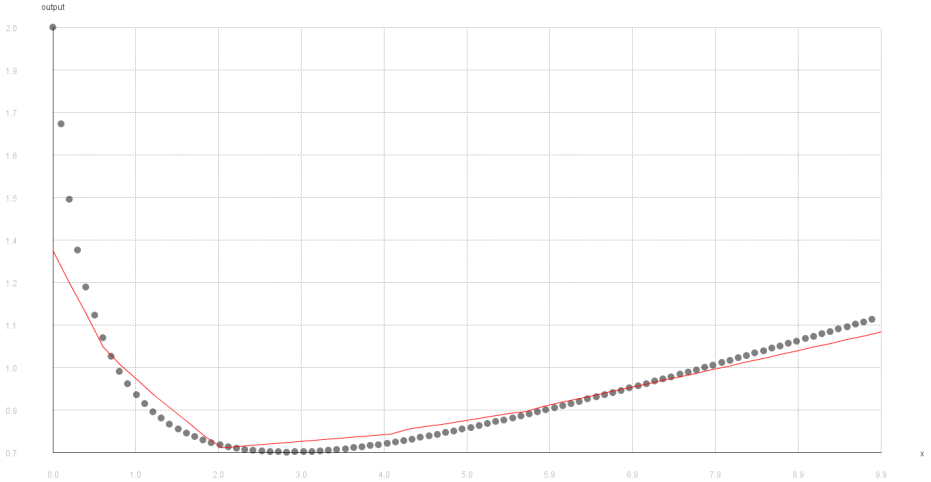
Comparison – Linear and Isotonic Regression



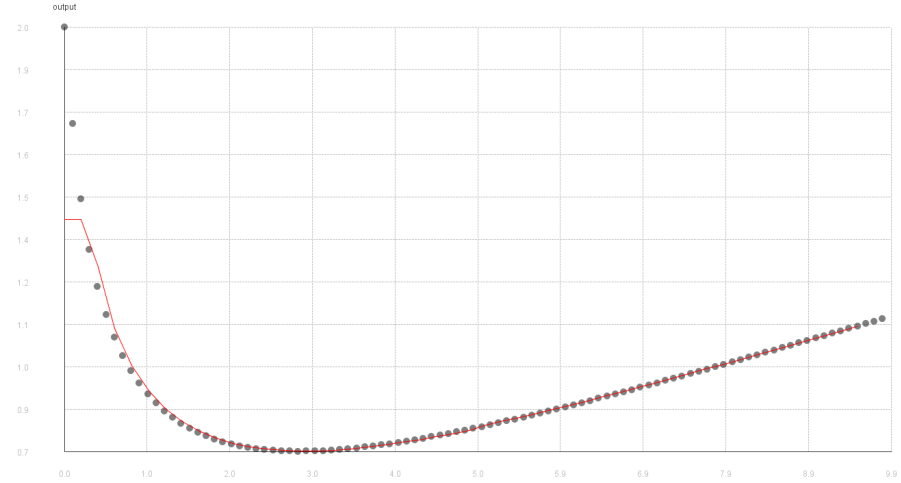


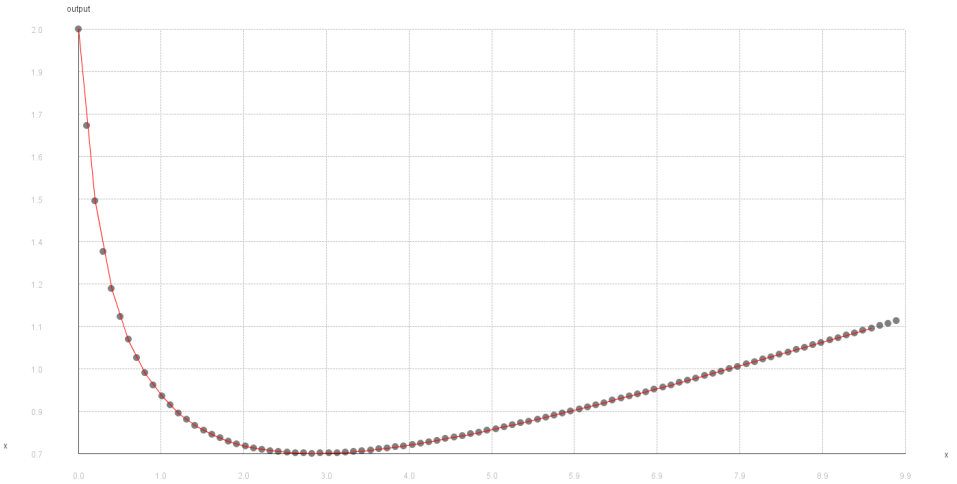
Comparison – M5' Regression and Model Tree





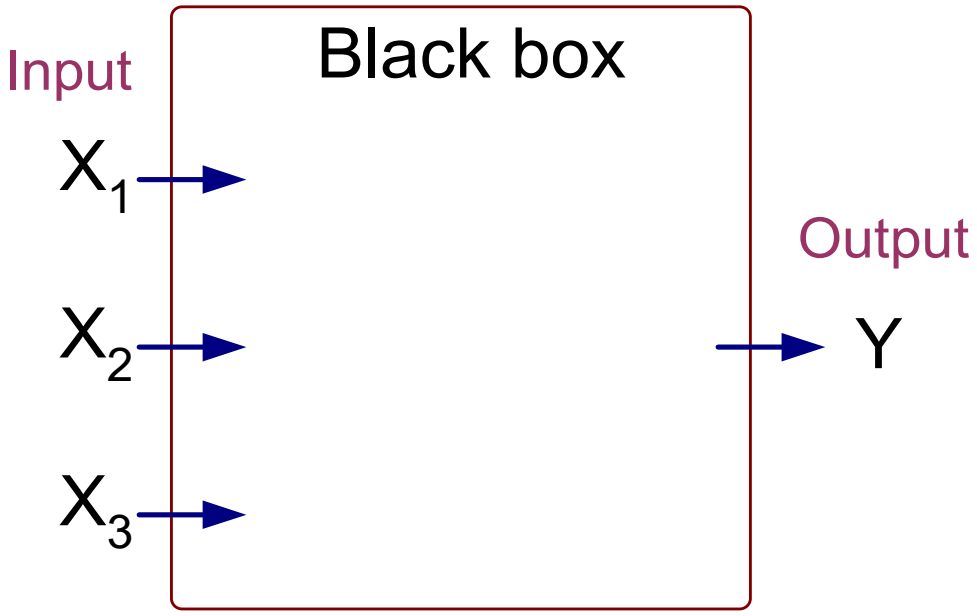
k-NN and Local Polynomial Regression (k=7)





Artificial Neural Networks Revisited

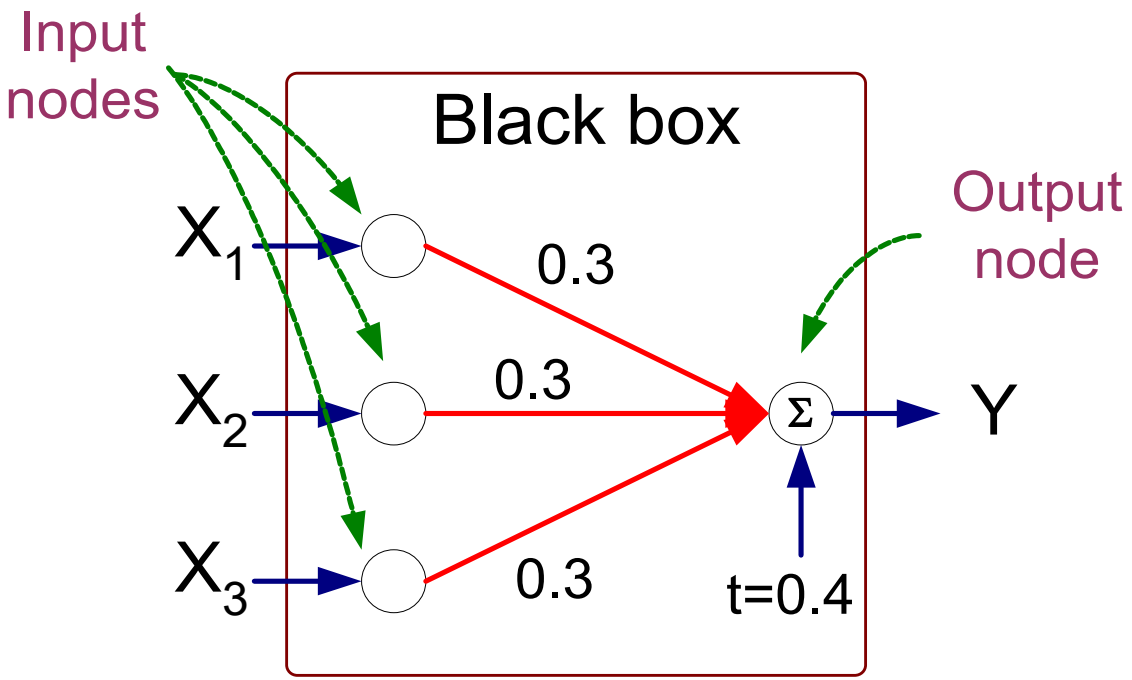
X_1	X_2	X_3	Y
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	0
0	1	0	0
0	1	1	1
0	0	0	0



Output Y is 1 if at least two of the three inputs are equal to 1.

Artificial Neural Networks Revisited

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 Revisited

- This final function was used to separate two classes:

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

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

- However, we may simply use it to predict a numerical value (between 0 and 1) by changing it to:

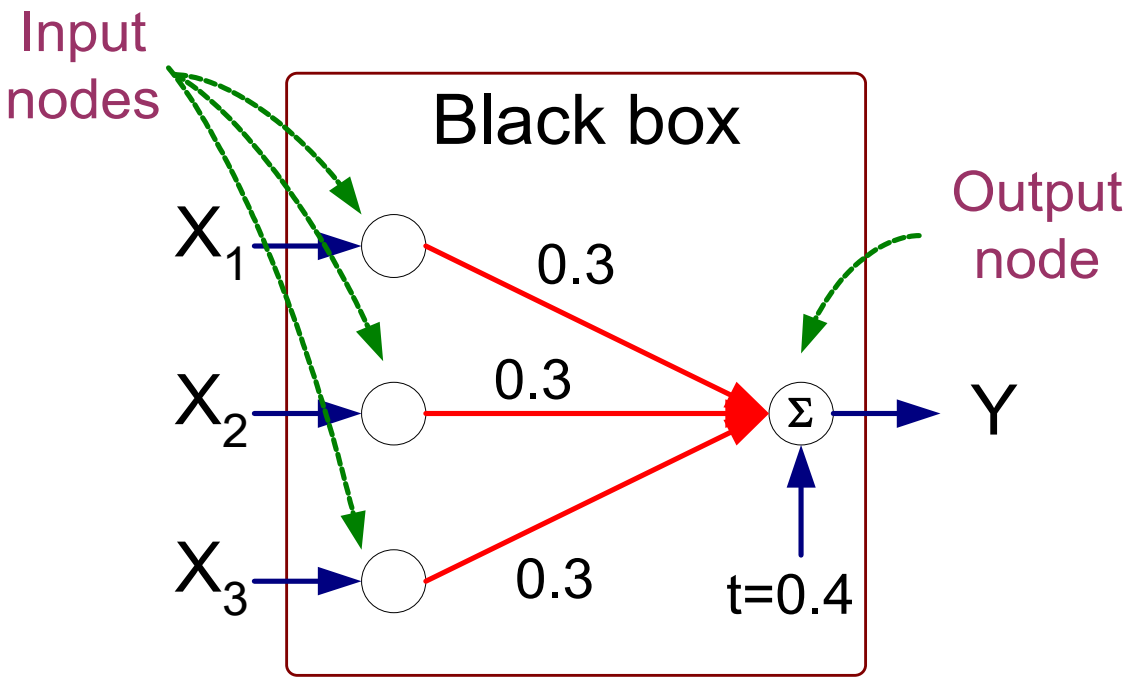
$$Y = 0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4$$

Artificial Neural Networks for Regression

- What has changed:
  - we do not use a cutoff for 0/1 predictions
  - but leave the numbers as they are
- Training examples:
  - attribute vectors – not with a class label, but numerical target
- Error measure:
  - Not classification error, but mean squared error

Artificial Neural Networks for Regression

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



$$Y = 0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4$$

Artificial Neural Networks for Regression

- Given that our target formula is of the form

$$Y = 0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4$$

- we can learn only linear problems
  - i.e., the target variable is a linear combination the input variables

- More complex regression problems can be approximated
  - by combining several perceptrons
    - in neural networks: hidden layers
    - with non-linear activation functions!
  - this allows for arbitrary functions
- Hear more about ANNs in Data Mining 2!

From Classification to Regression and Back

- We have got to known classification first
  - and asked: how can we get from classification to regression?

- Turning the question upside down:
  - can we use regression algorithms for classification?

- Transformation:
  - for binary classification: encode true as 1.0 and false as 0.0
    - learn regression model
    - predict true for (-∞,0.5] and false for (0.5,∞)
  - similarly for ordinal (e.g., good, medium, bad)
  - non-ordinal multi-class problems are trickier

Summary

- Regression
  - predict numerical values instead of classes
- Performance measuring
  - absolute or relative error, correlation, …
- Methods
  - k nearest neighbors
  - linear regression and regularized variants
  - polynomial regression
  - isotonic regression
  - model trees
  - artificial neural networks
  - ...

Questions?