UNIVERSITÄT MANNHEIM

Data Mining
Regression

Heiko Paulheim

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

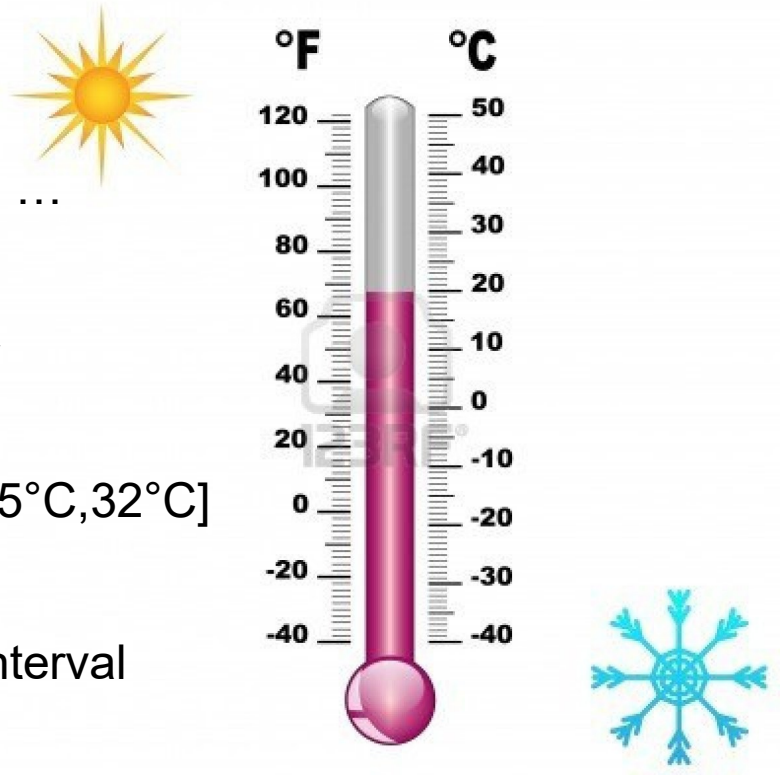
- A closer look at the problem
  - e.g., interpolation vs. extrapolation
  - measuring regression performance
- Revisiting classifiers we already know
  - which can also be used for regression
- Adoption of classifiers for regression
  - model trees
  - support vector machines
  - artificial neural networks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

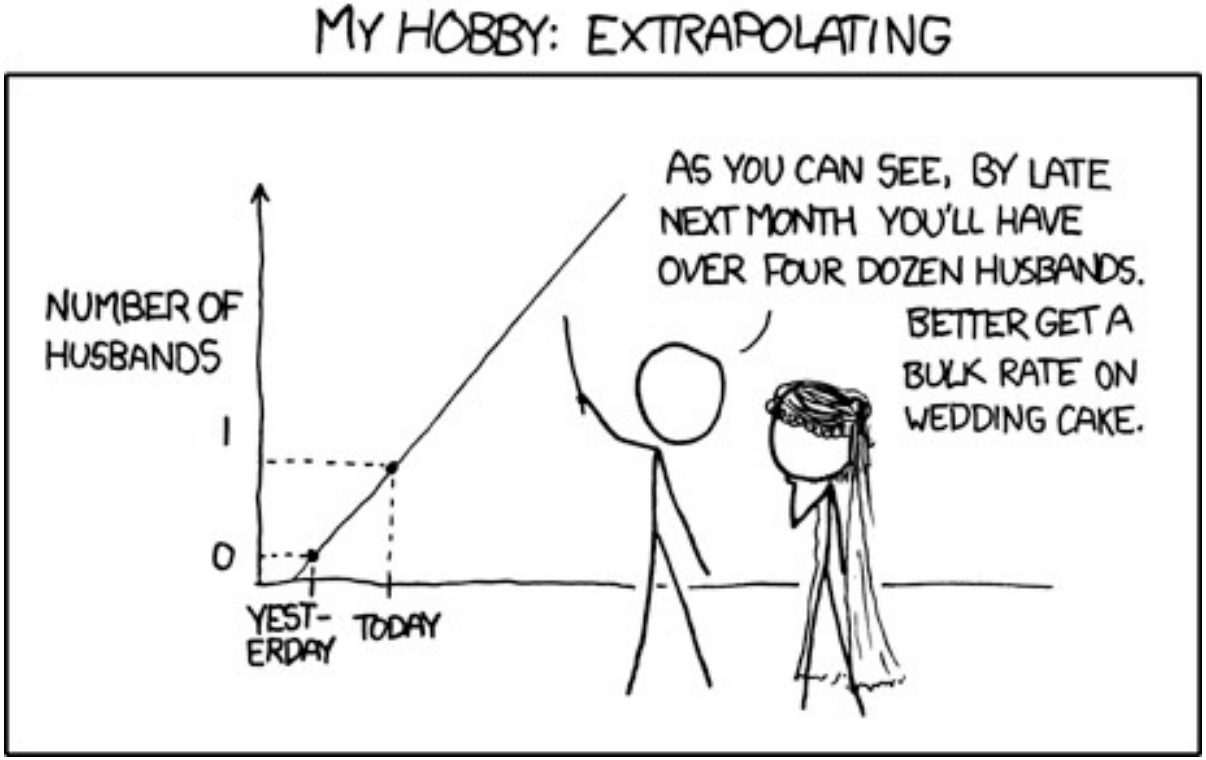
Interpolation vs. Extrapolation

- 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

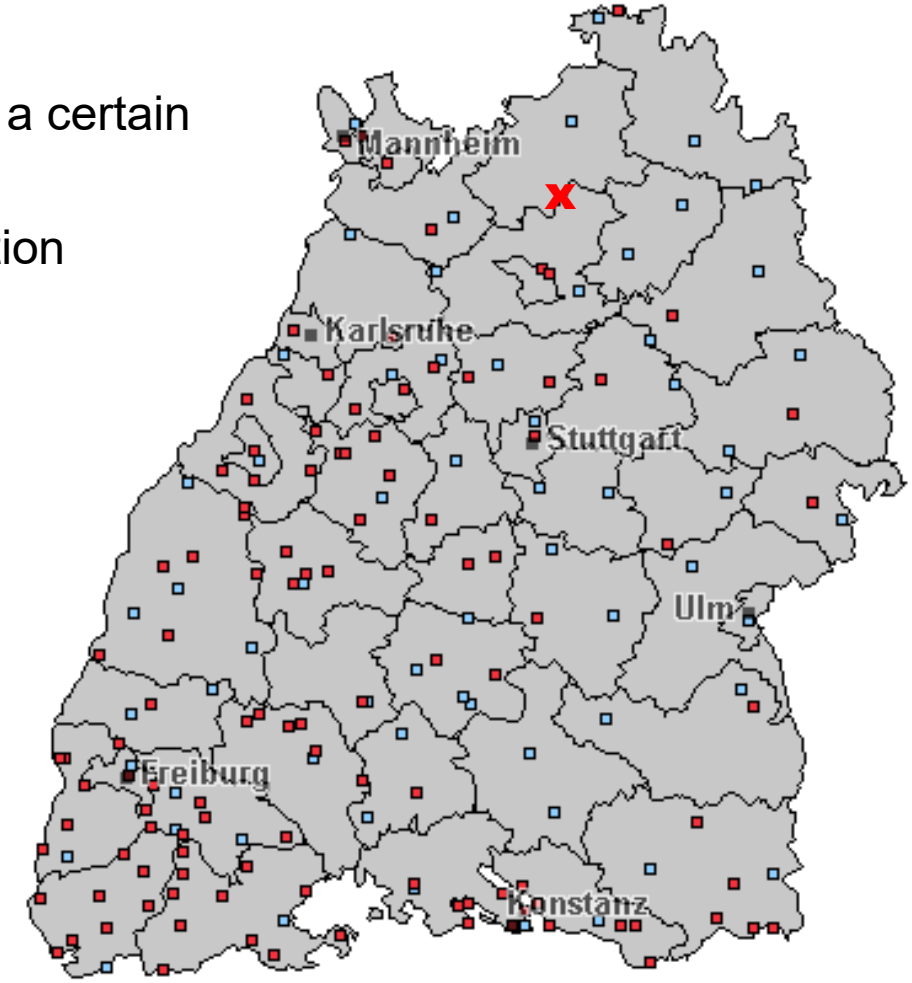
Baseline Prediction

- 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/

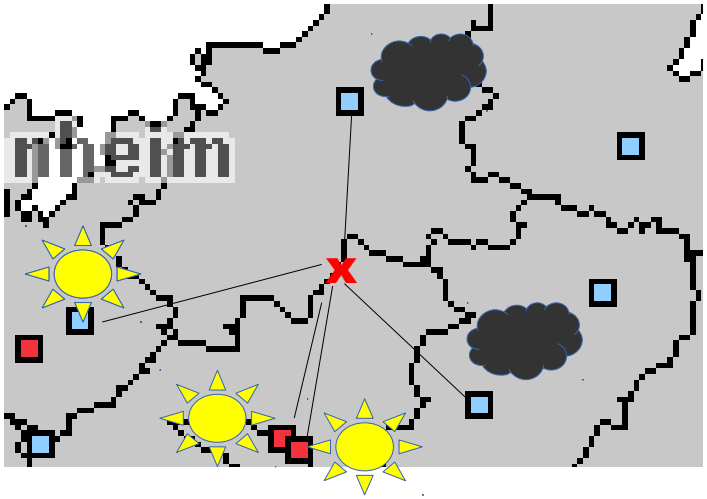
k Nearest Neighbors Revisited

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



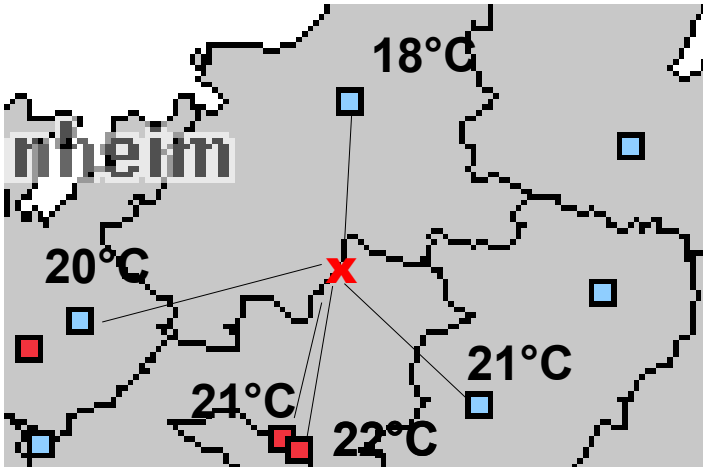
k Nearest Neighbors Revisited

- 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



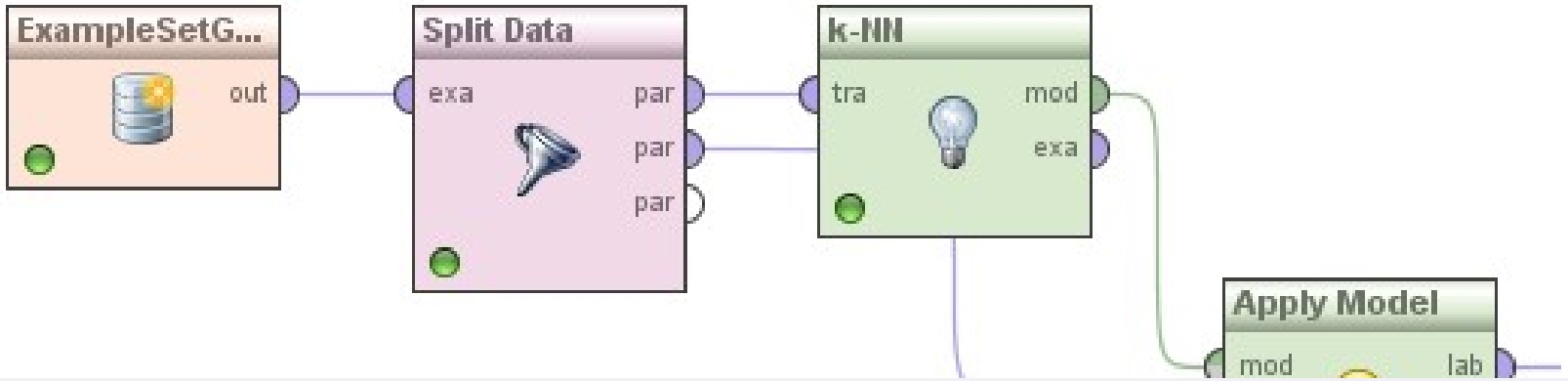
k Nearest Neighbors for Regression

- 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



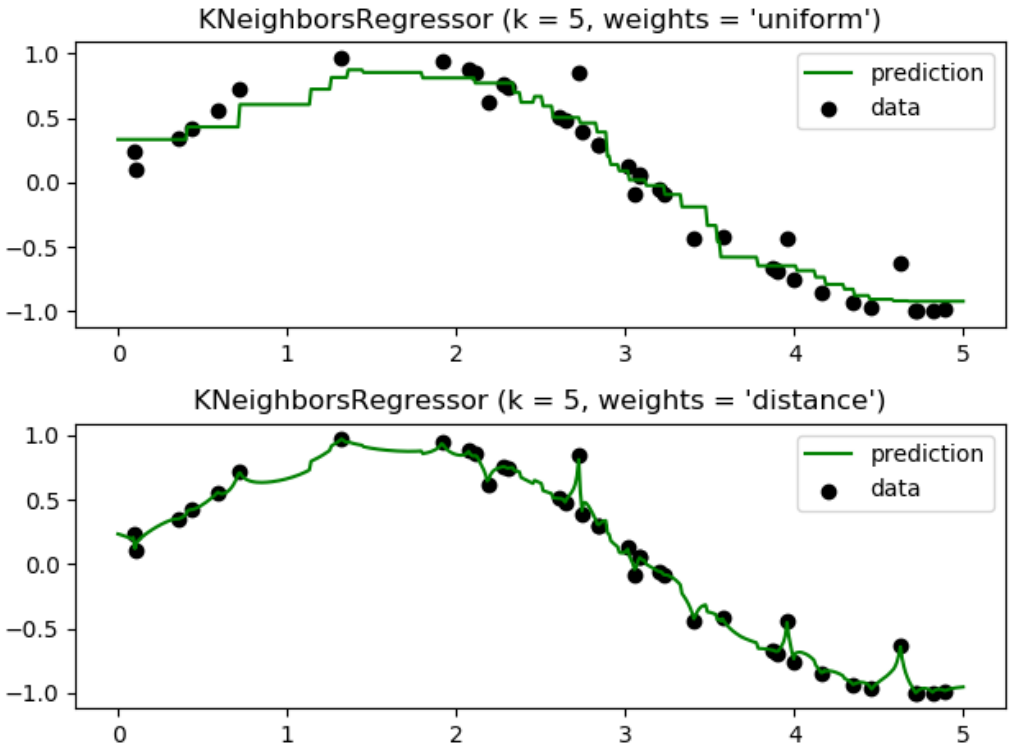
Data View | Meta Data View | Plot View | Advanced Charts | Annotations

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:

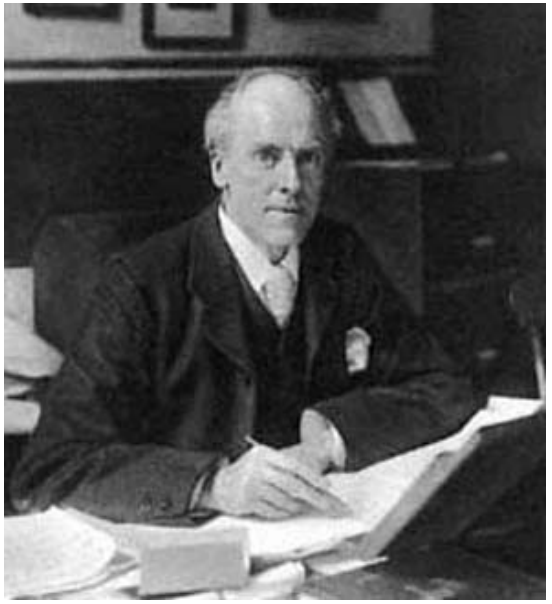
$$\mathrm{RMSE} = \sqrt{\frac{\sum_{all\ examples} |predicted - actual|^2}{N}}$$

- 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

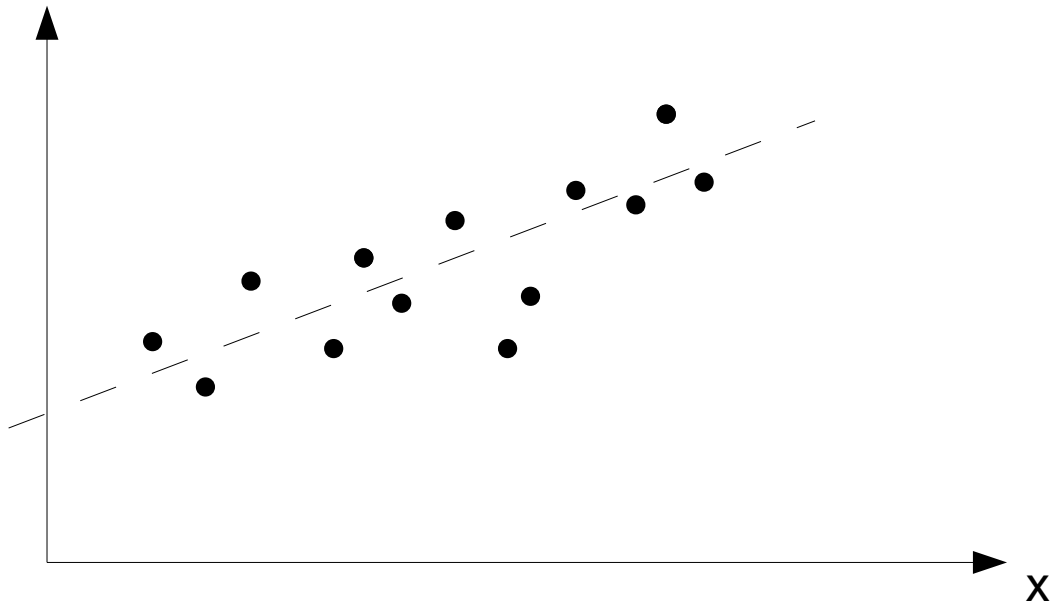
  → PCC = 1



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

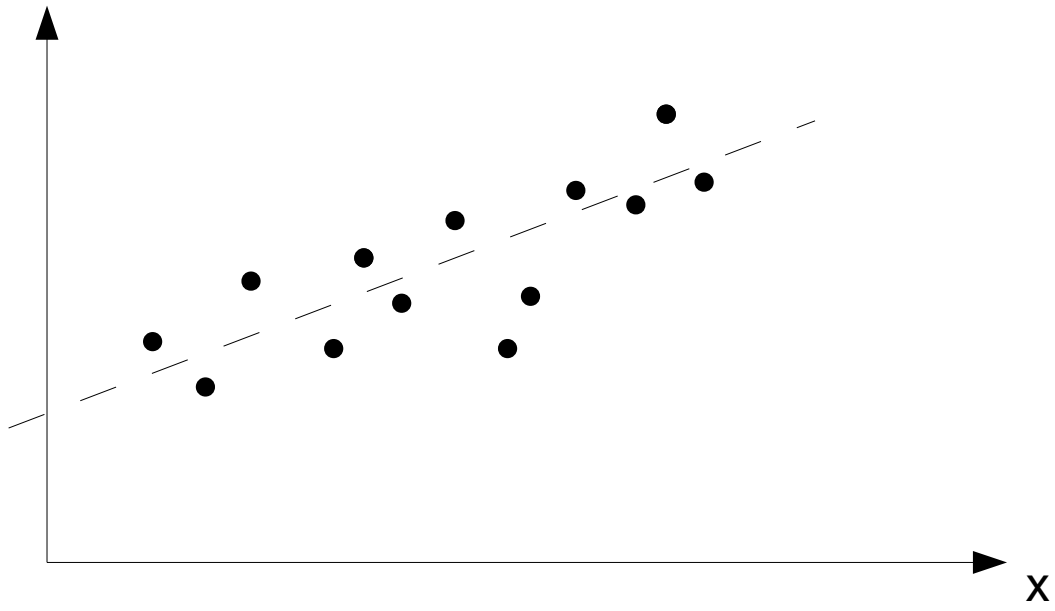
Linear Regression

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



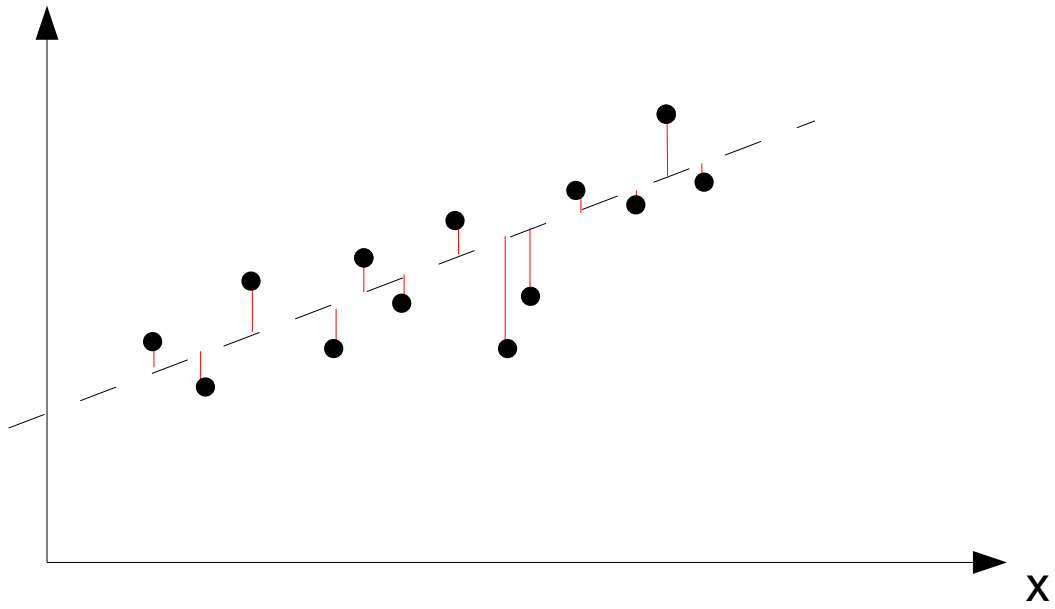
Linear Regression

- 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 $\sum_{\text{all examples}} \left(w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_n \cdot x_n - y\right)^2$ is minimized
- note: we omit the denominator N



Linear Regression: Multi Dimensional Example

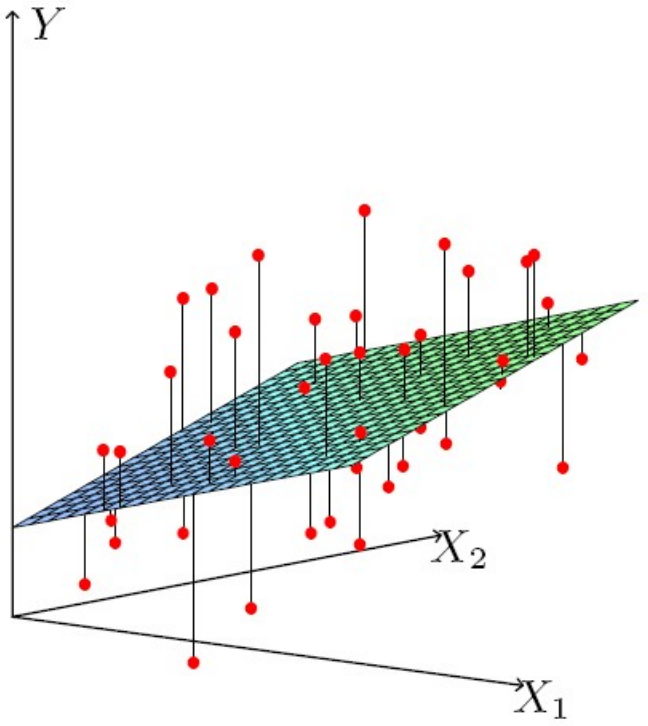
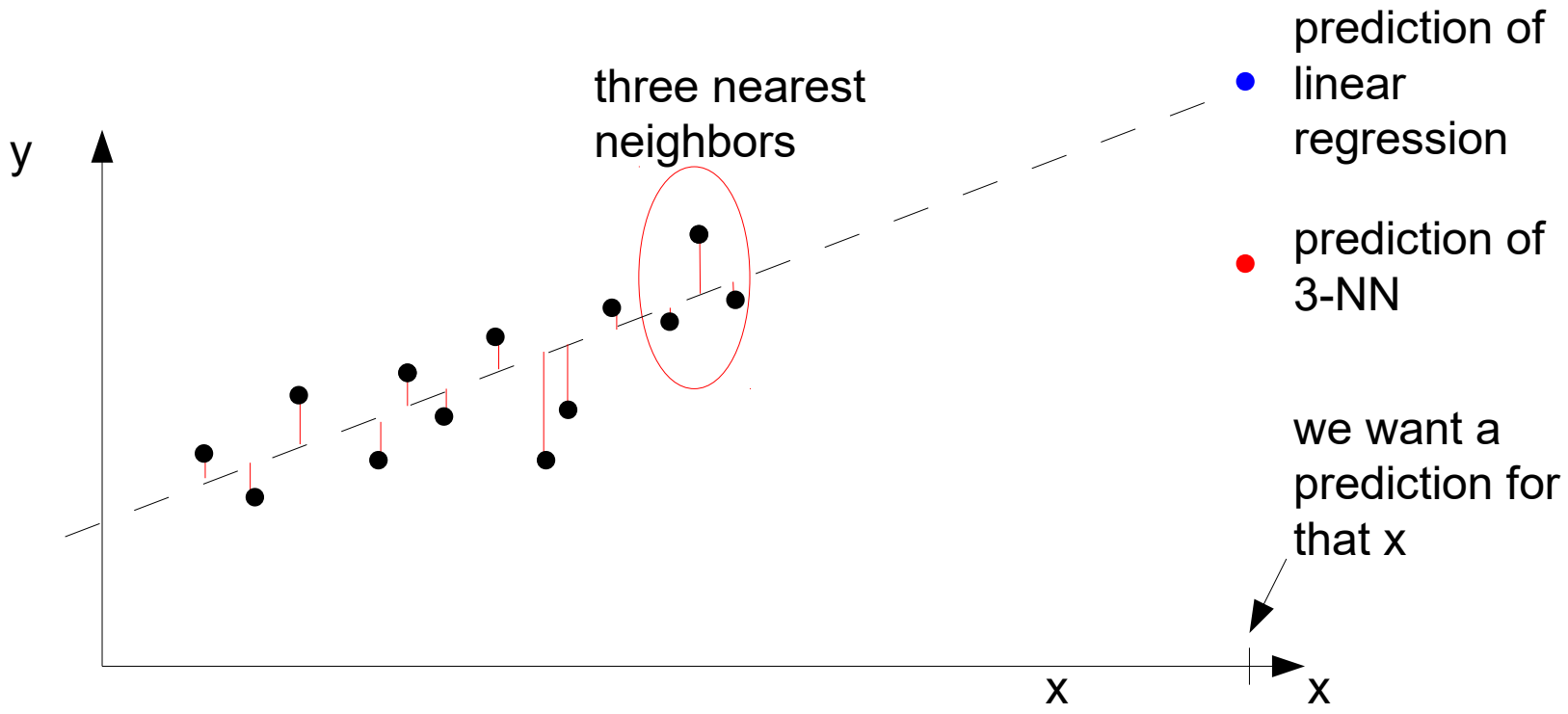


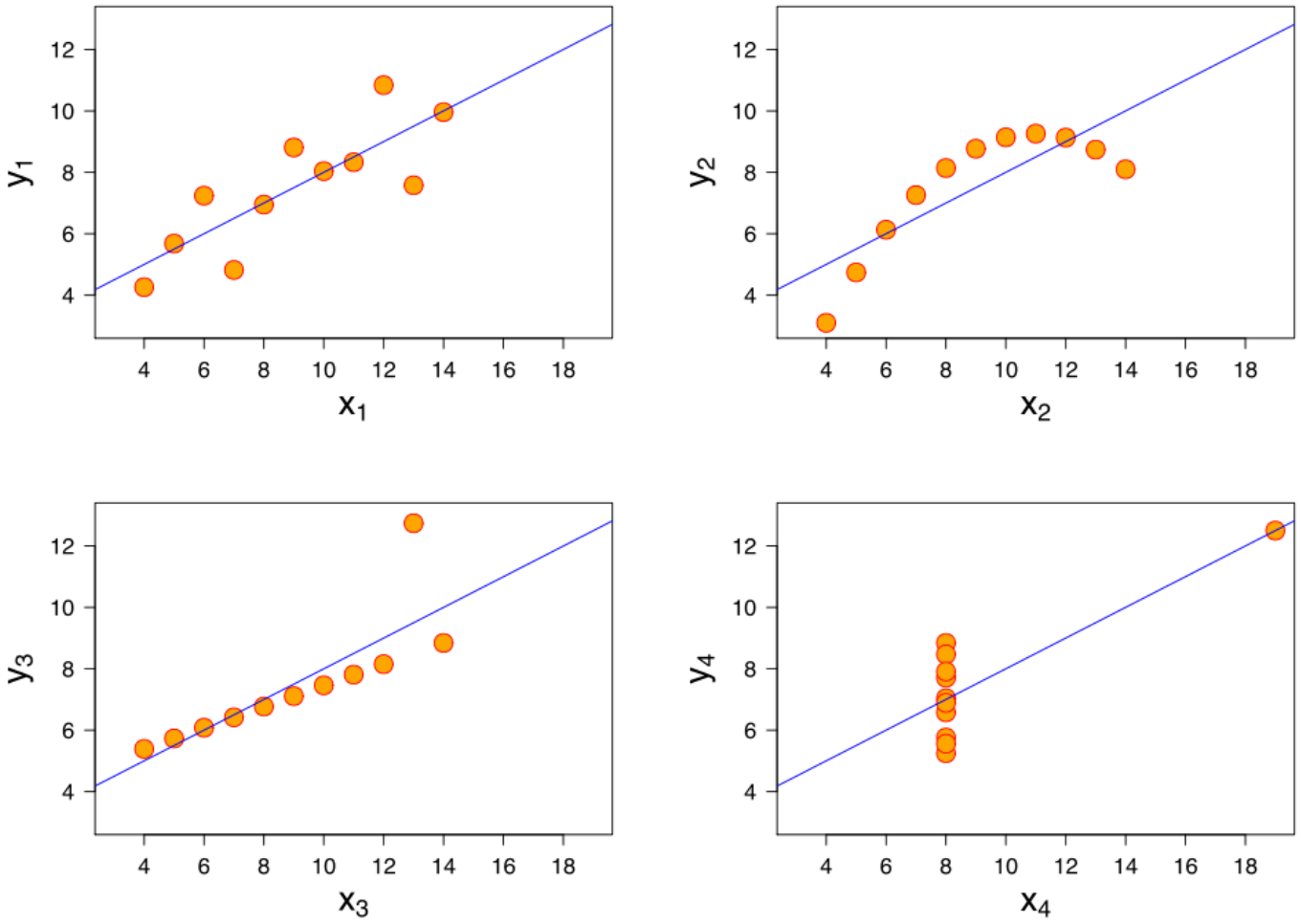
FIGURE 3.1. *Linear least squares fitting with* $X \in \mathbb{R}^2$. *We seek the linear function of* X *that minimizes the sum of squared residuals from* Y.

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

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

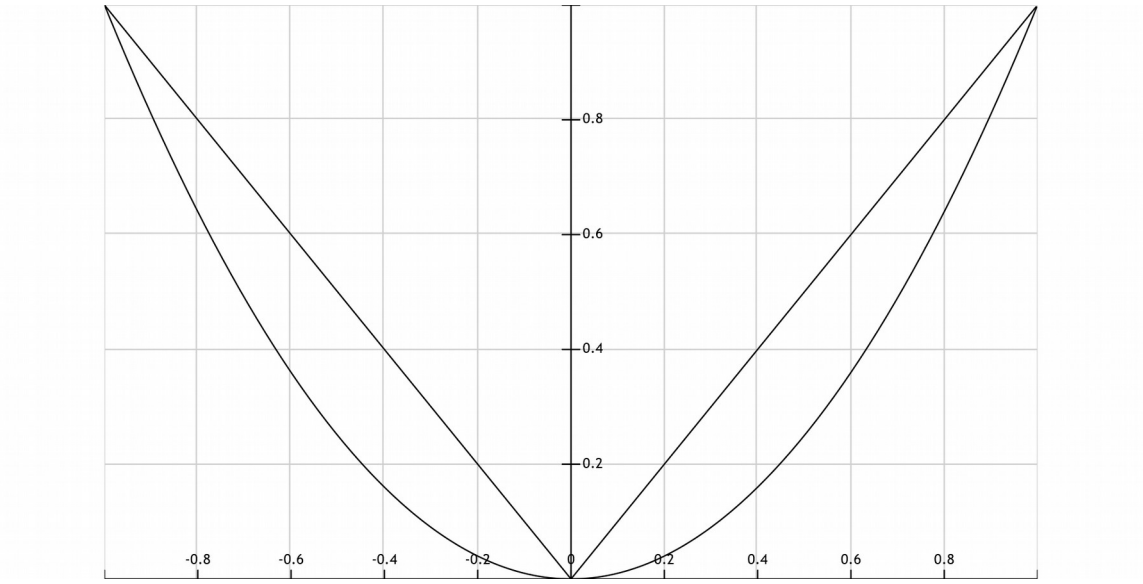
- Lasso Regression optimizes

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

- 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

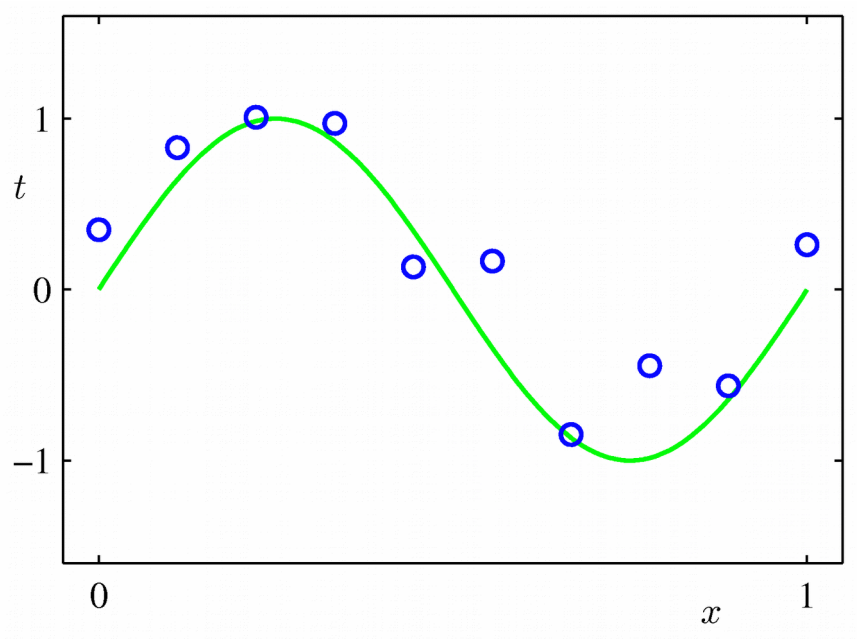
Lasso vs. Ridge Regression

- 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?



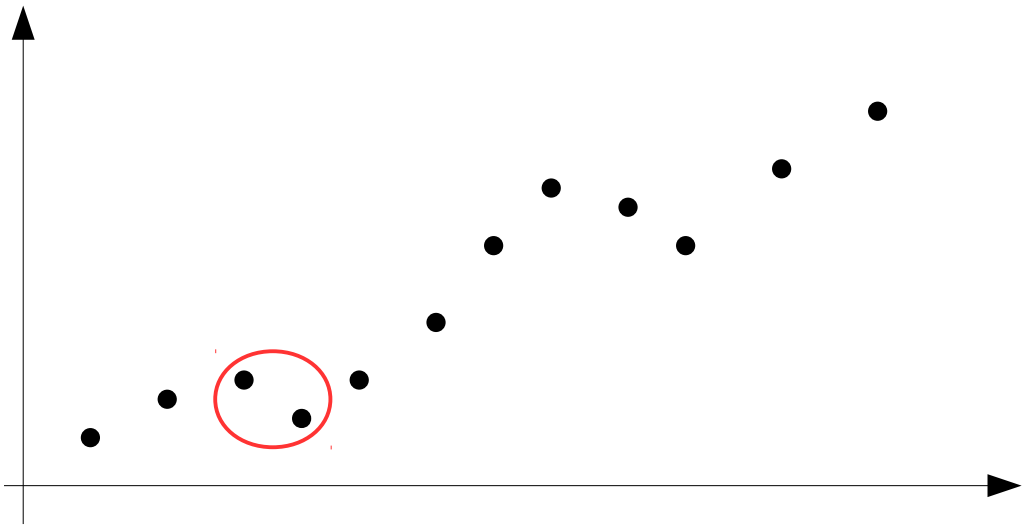
Isotonic Regression

- 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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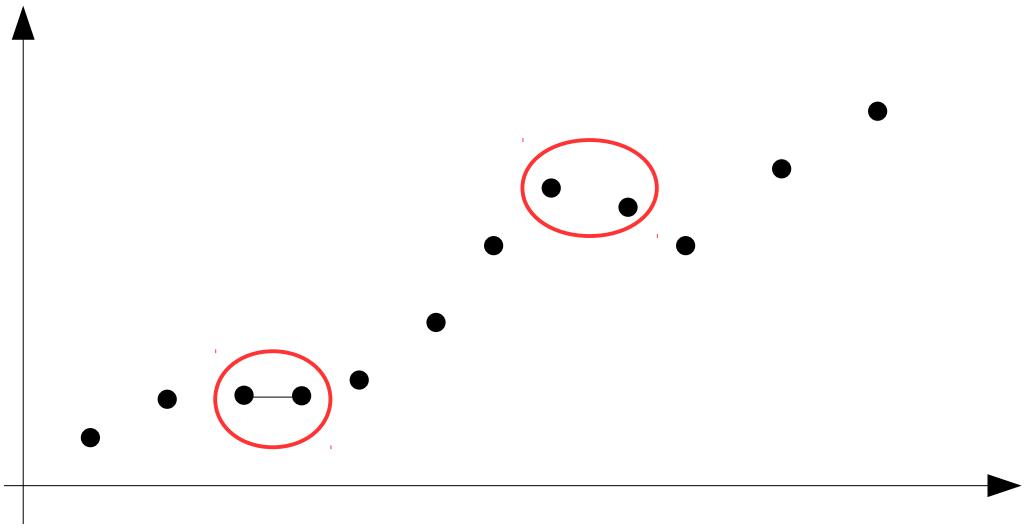

Isotonic Regression

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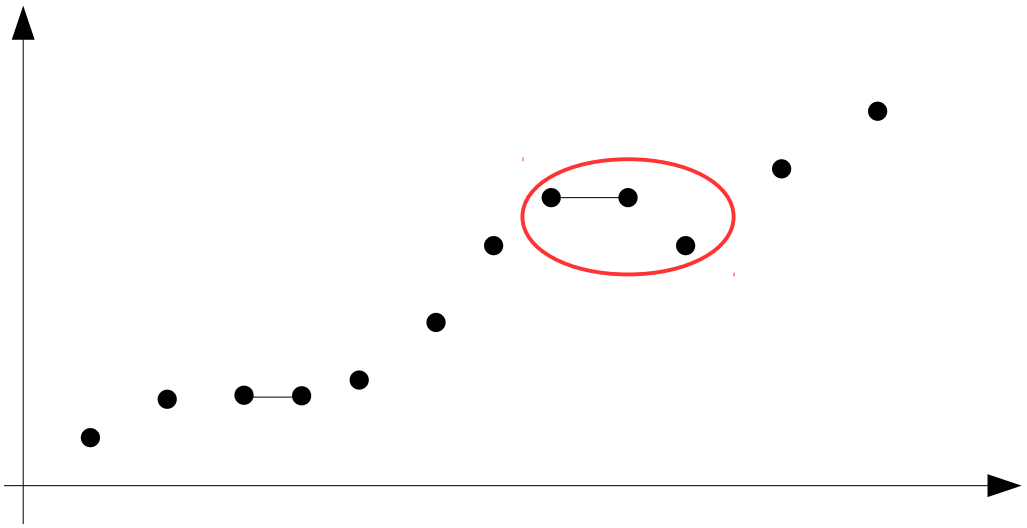

Isotonic Regression

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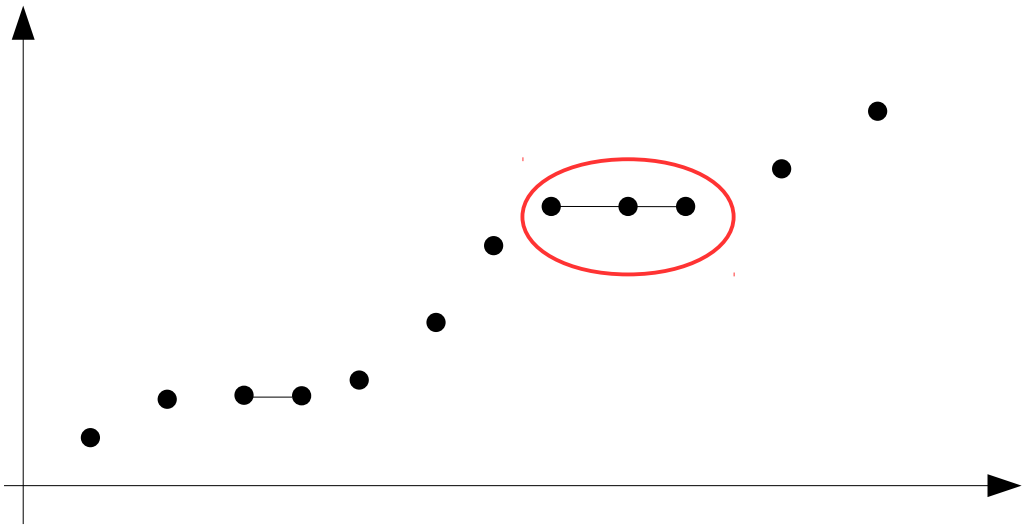
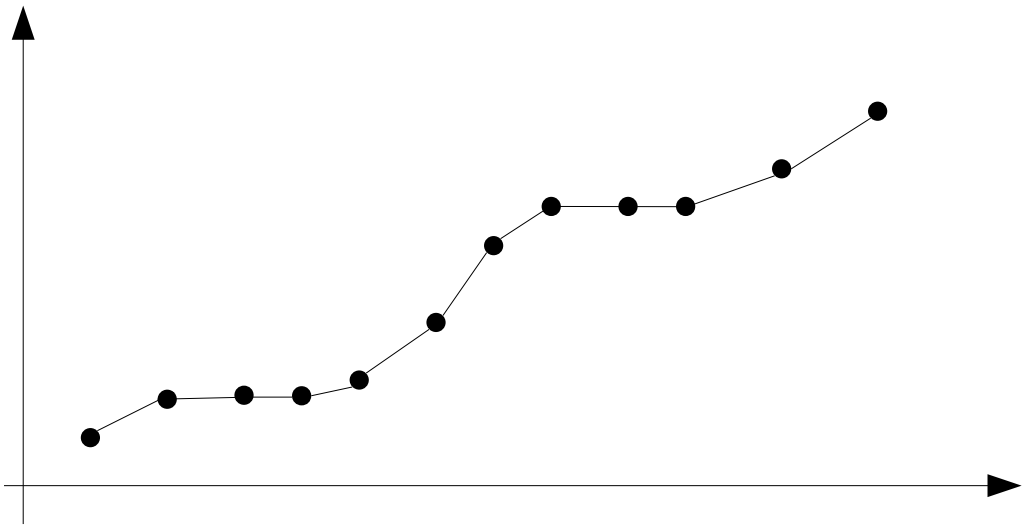


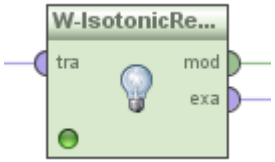
Isotonic Regression

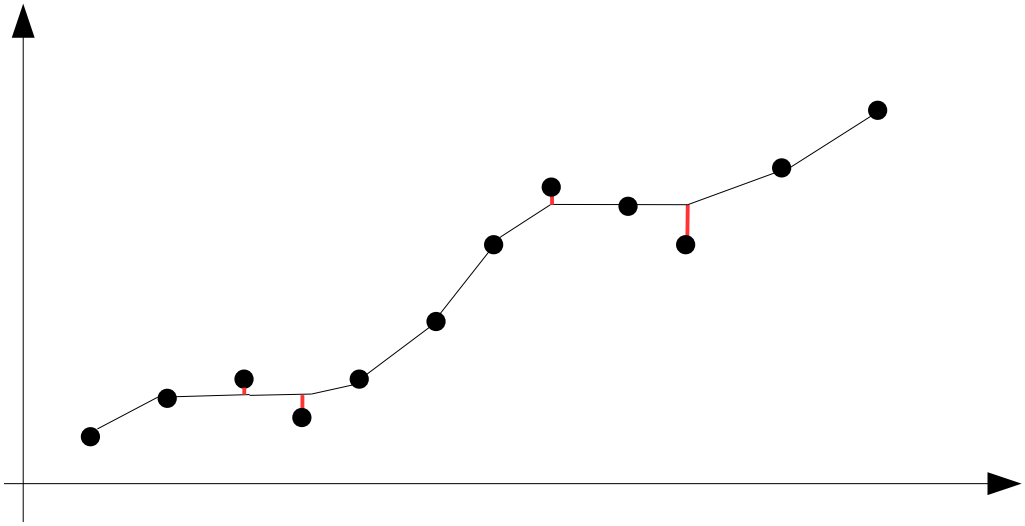
- After all points are reordered so that $f'(x_i)=f'(x_{i+1})$ holds for every i
  - Connect the points with a piecewise linear function



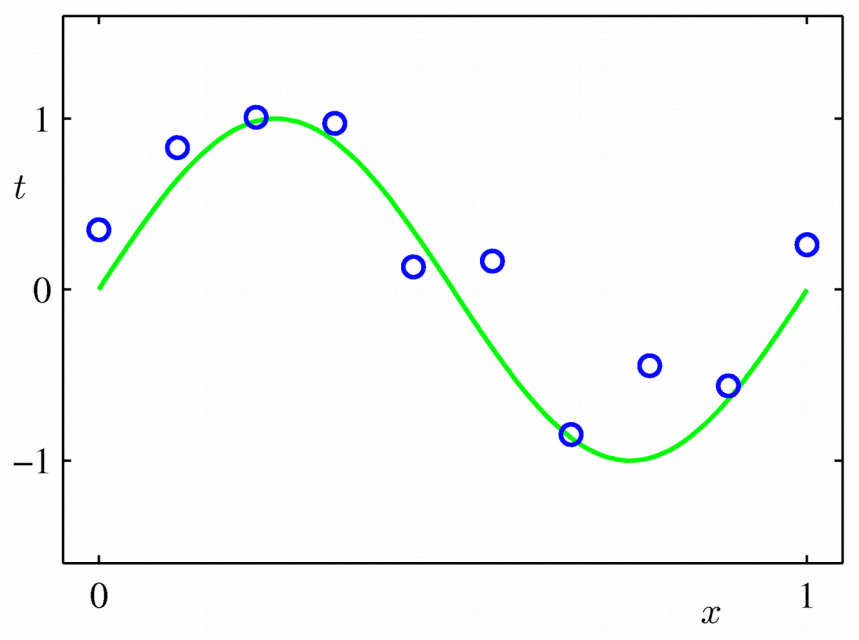
Isotonic Regression

- 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)





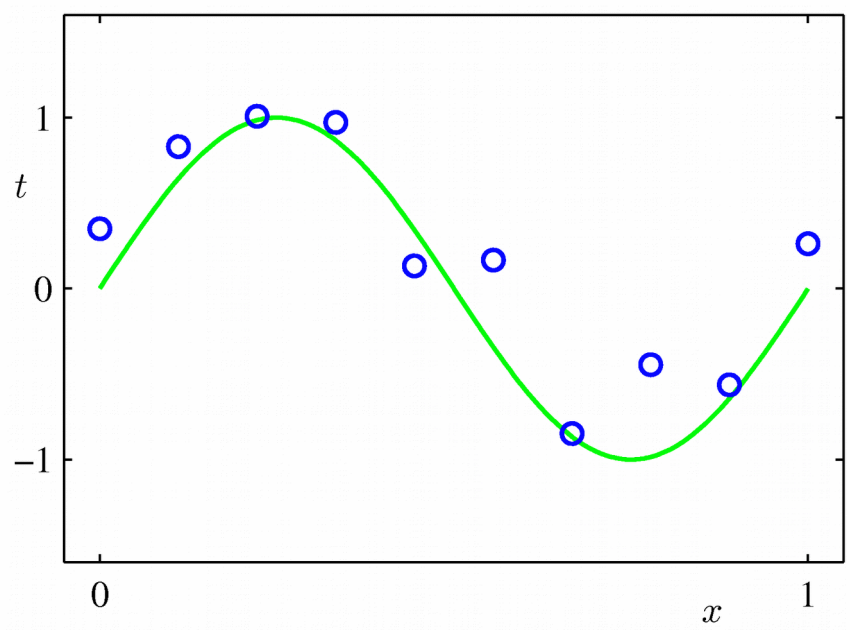
…but what about non-linear, *non-monotonous* Problems?

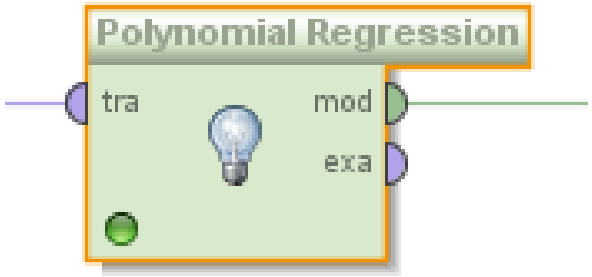


Possible Option: new Attributes

- 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

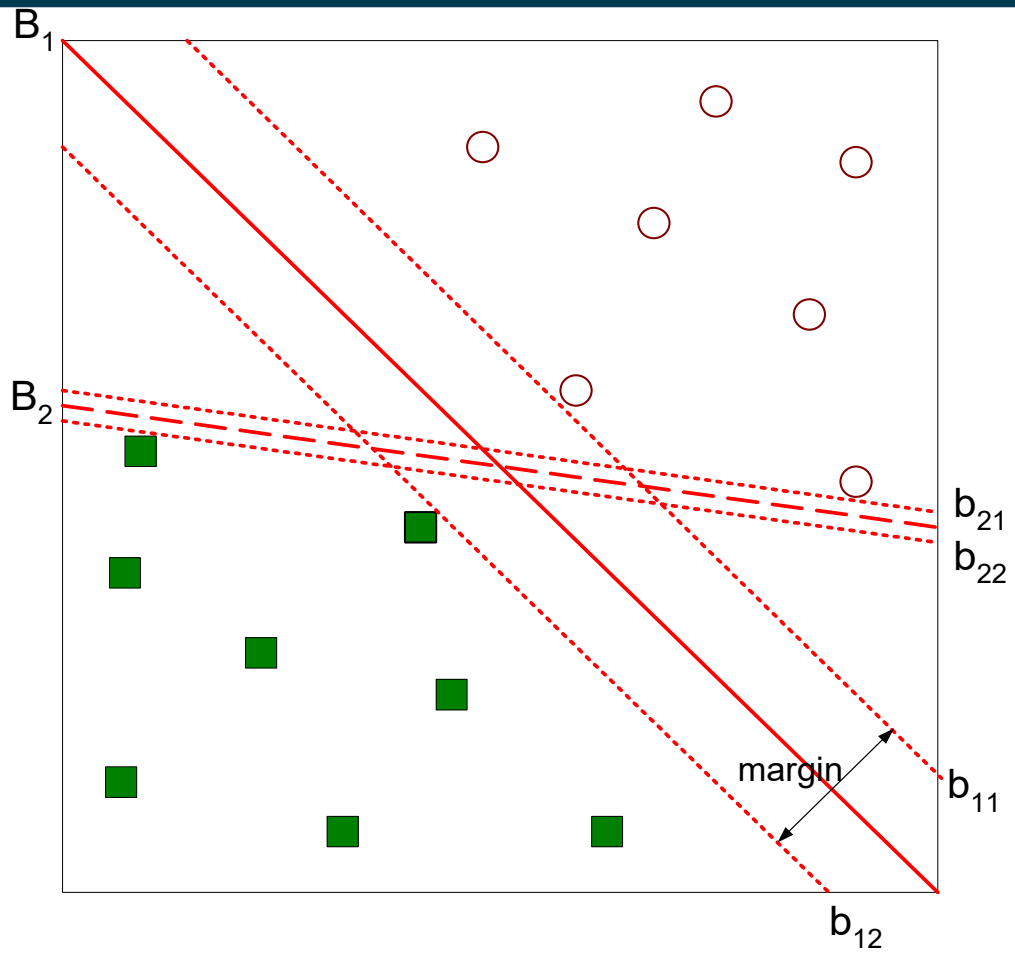




$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

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

Support Vector Machines Revisited



- Find hyperplane maximizes the margin => B1 is better than B2

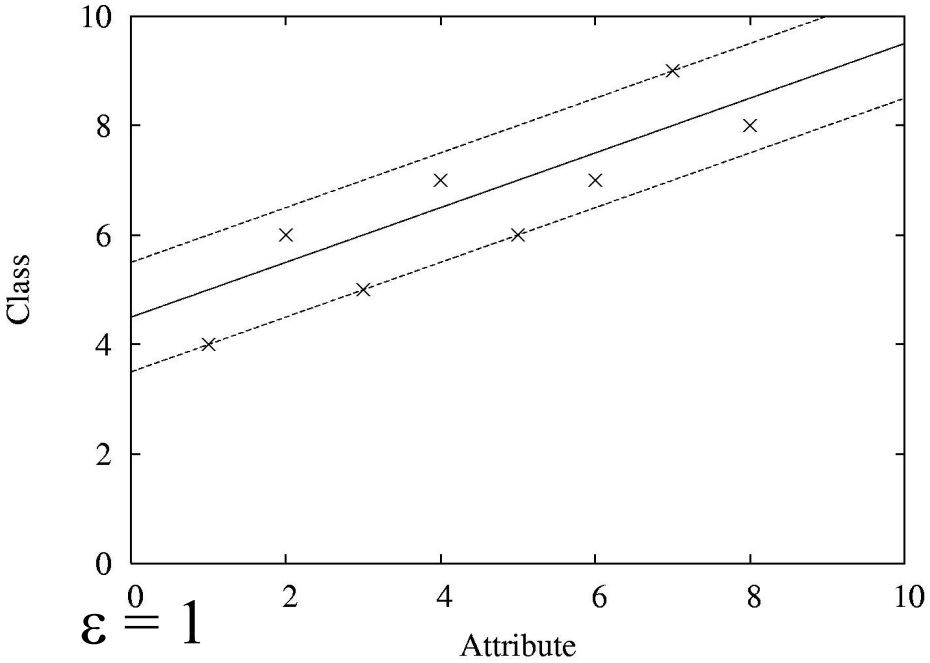
Linear Regression and SVM

- Linear Regression
  - find a linear function that *minimizes* the distance to data points w.r.t. the attribute to predict
- Support Vector Machine
  - find a linear function that *maximizes* the distance to data points (from different classes)
- Both problems are similar
  - hence, many SVMs also support regression

Support Vector Regression

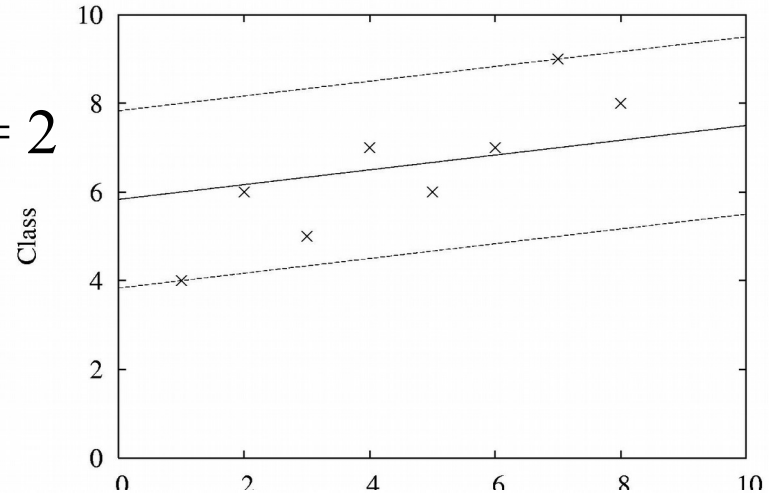
- Maximum margin hyperplane only applies to classification
- However, idea of support vectors and kernel functions can be used for regression
- Basic method same as in linear regression: want to minimize error
  - Difference A: ignore errors smaller than ε and use absolute error instead of squared error
  - Difference B: simultaneously aim to maximize flatness of function
- User-specified parameter ε defines “tube”

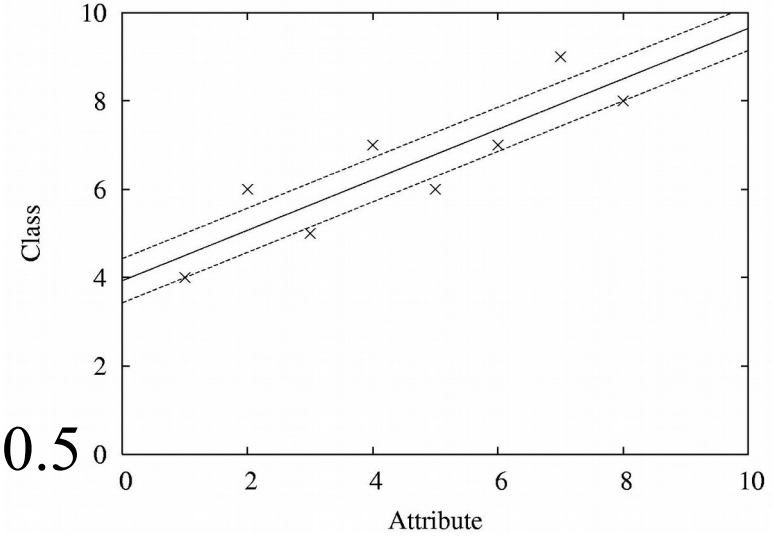
Examples



$\varepsilon = 1$

$\varepsilon = 2$





$\varepsilon = 0.5$

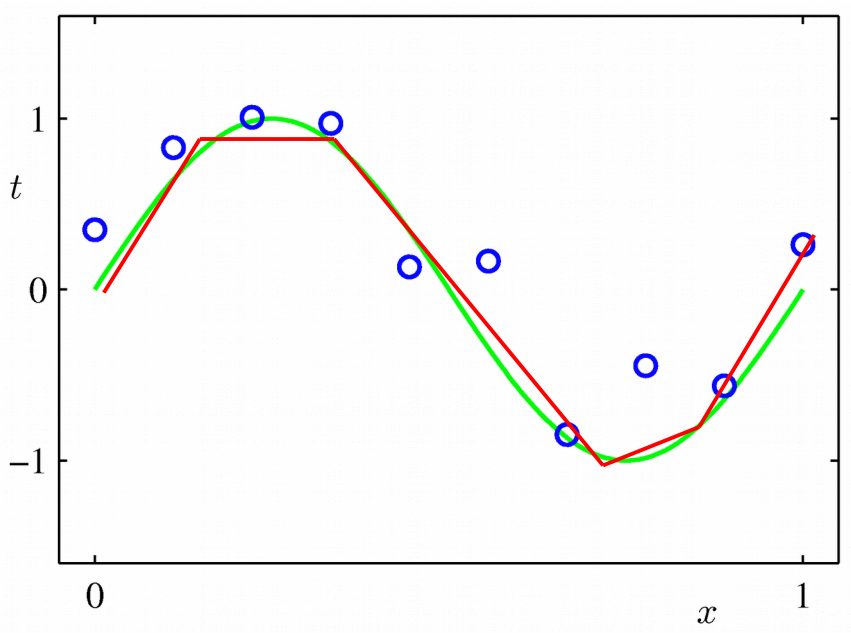
SVMs vs. Polynomial Regression

- Polynomial regression:
  - Create polynomial recombinations as additional features
  - Perform linear regression

- Support vector machine
  - Transform vector space with kernel function (e.g., polynomial kernel)
  - Find linear hyperplane

Local Regression

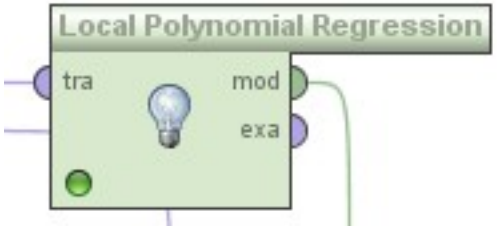
- Assumption: non-linear problems are approximately linear in local areas
  - idea: use linear regression locally
  - only for the data point at hand (lazy learning)



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



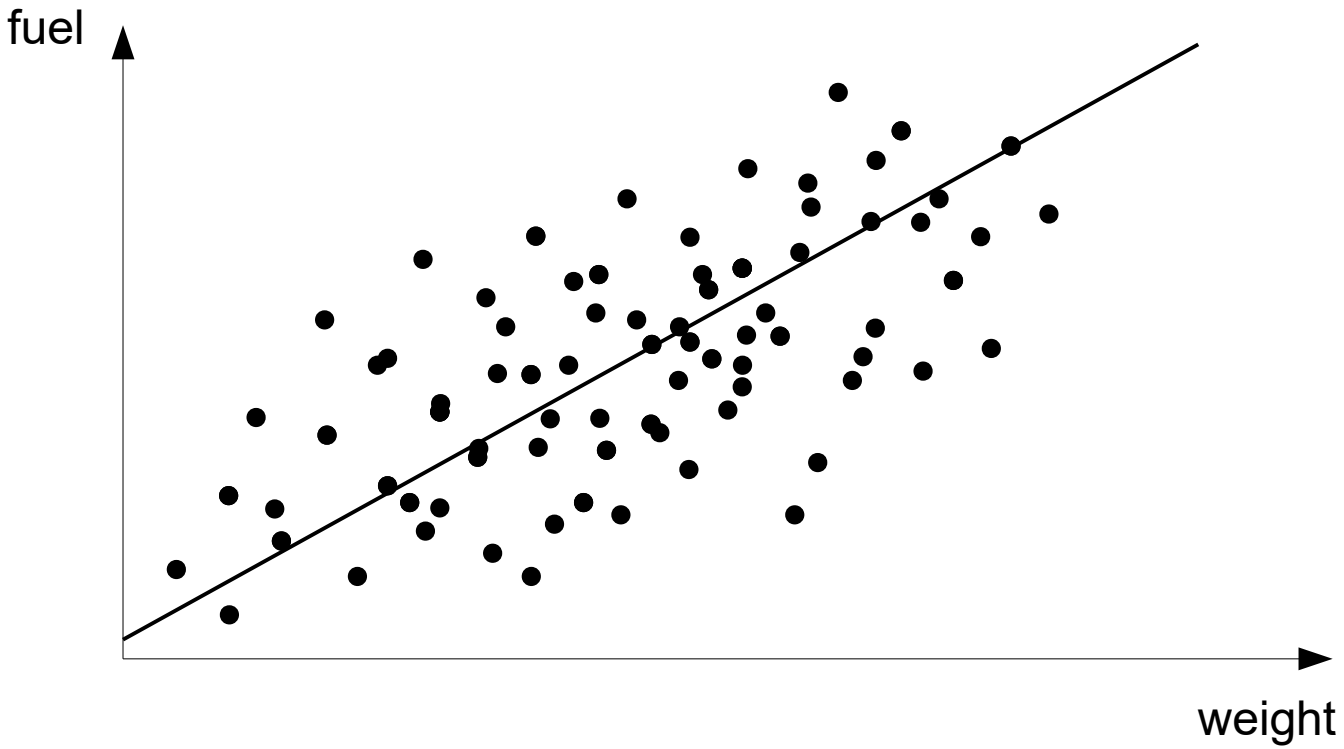
Local Regression

- 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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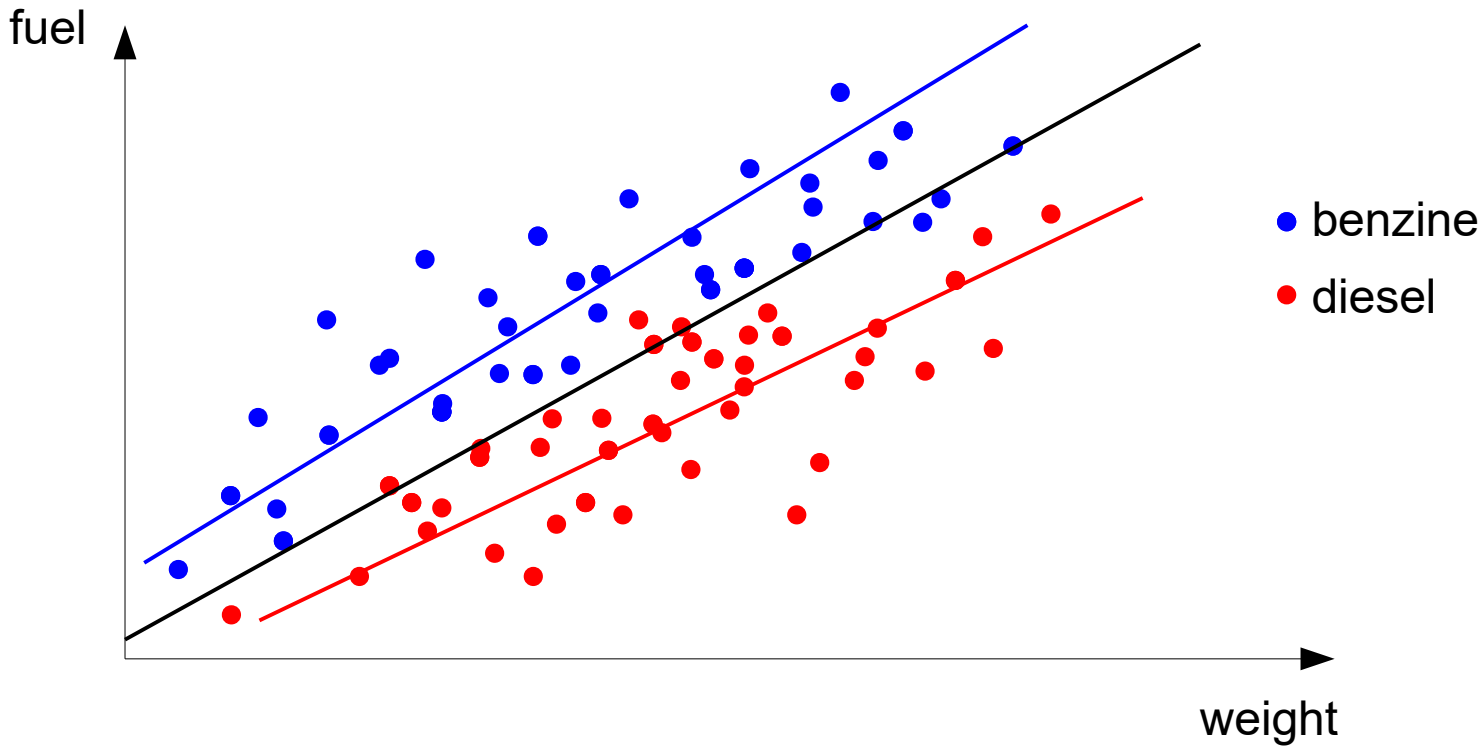
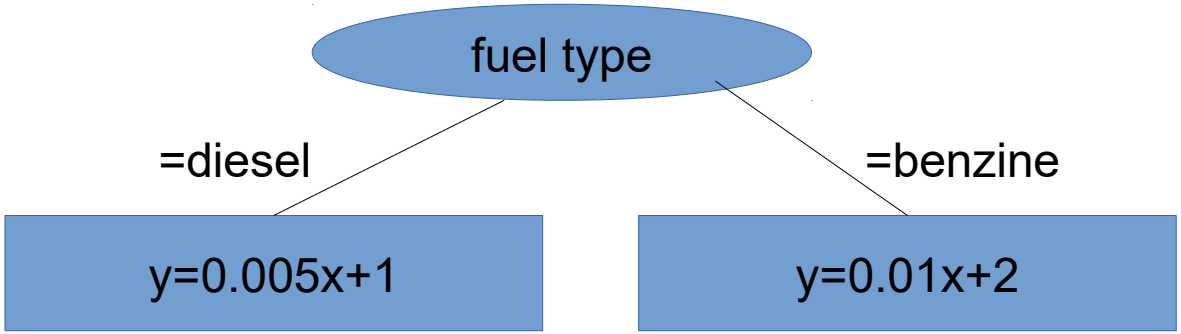


Combining Decision Trees and Regression

- 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

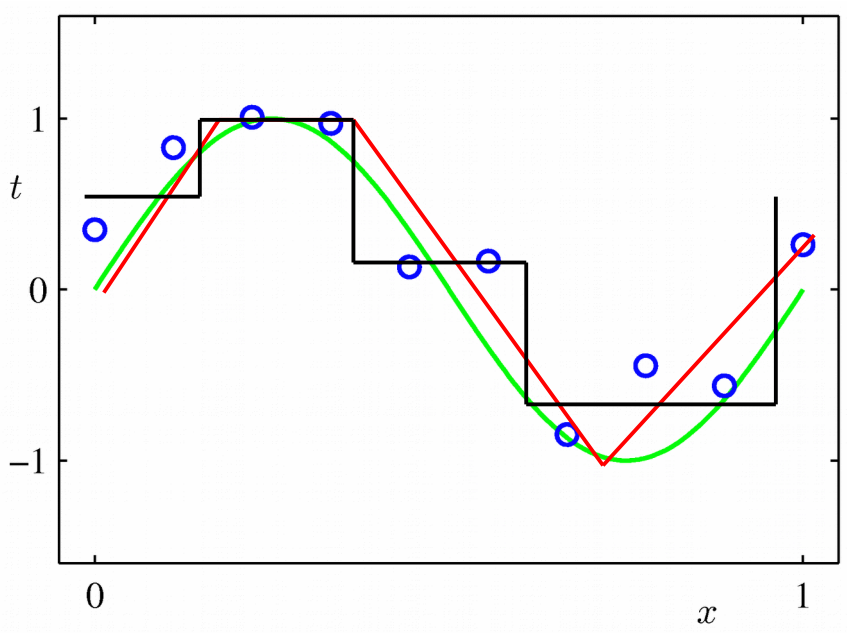
- Differences to classification decision trees:
  - Splitting criterion: minimize intra-subset variation
  - Termination criterion: standard deviation becomes small
  - Pruning criterion: based on numeric error measure
  - Prediction: Leaf predicts average class values of instances
- Easy to interpret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

Model Trees

- Build a regression tree
  - For each leaf ⇒ 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

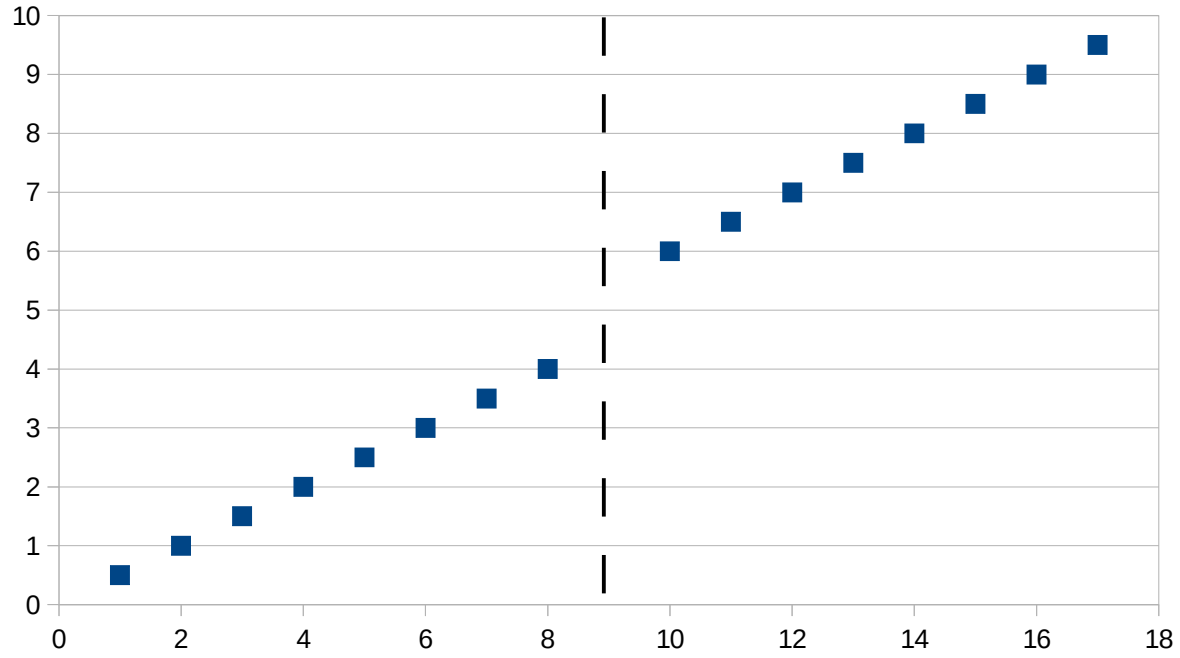
- Splitting: standard deviation reduction

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

- 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

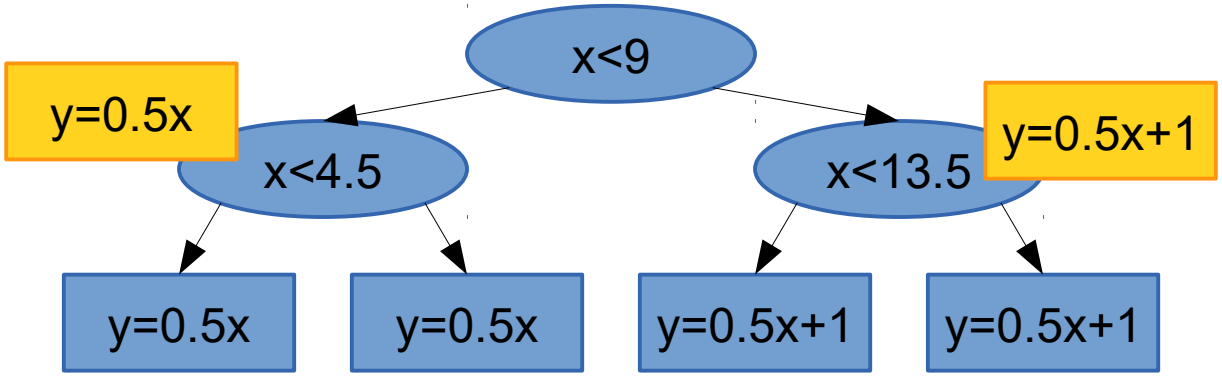
Model Tree Learning Illustrated

- 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

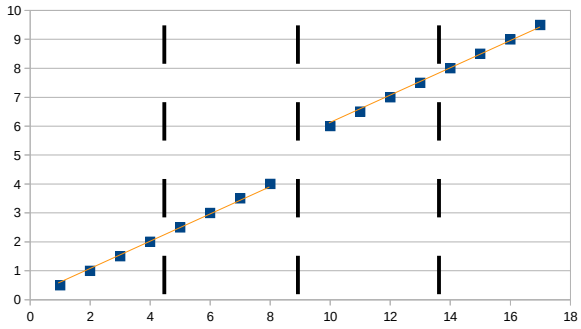


Model Tree Learning Illustrated

- 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

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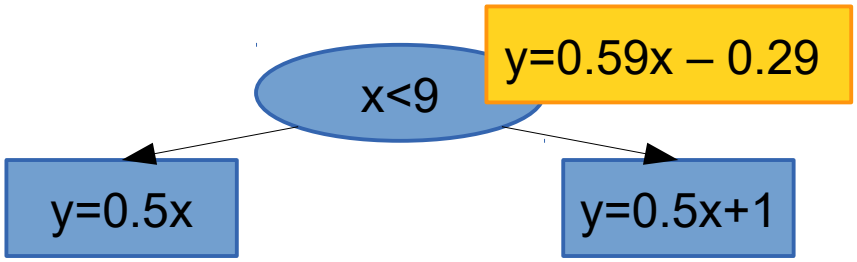
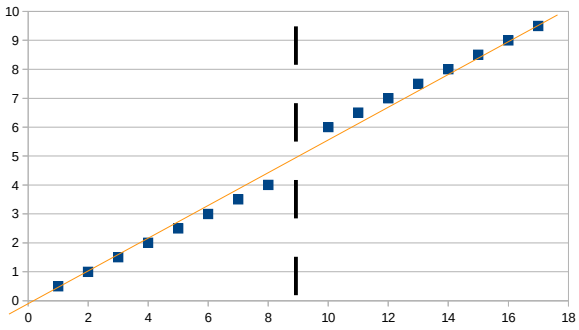
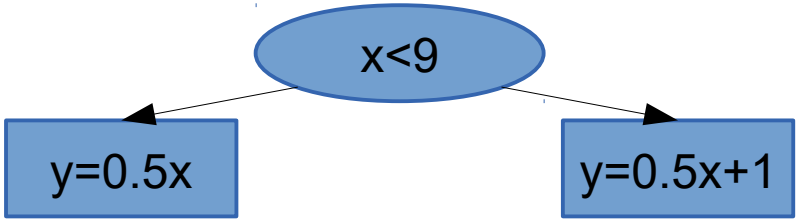
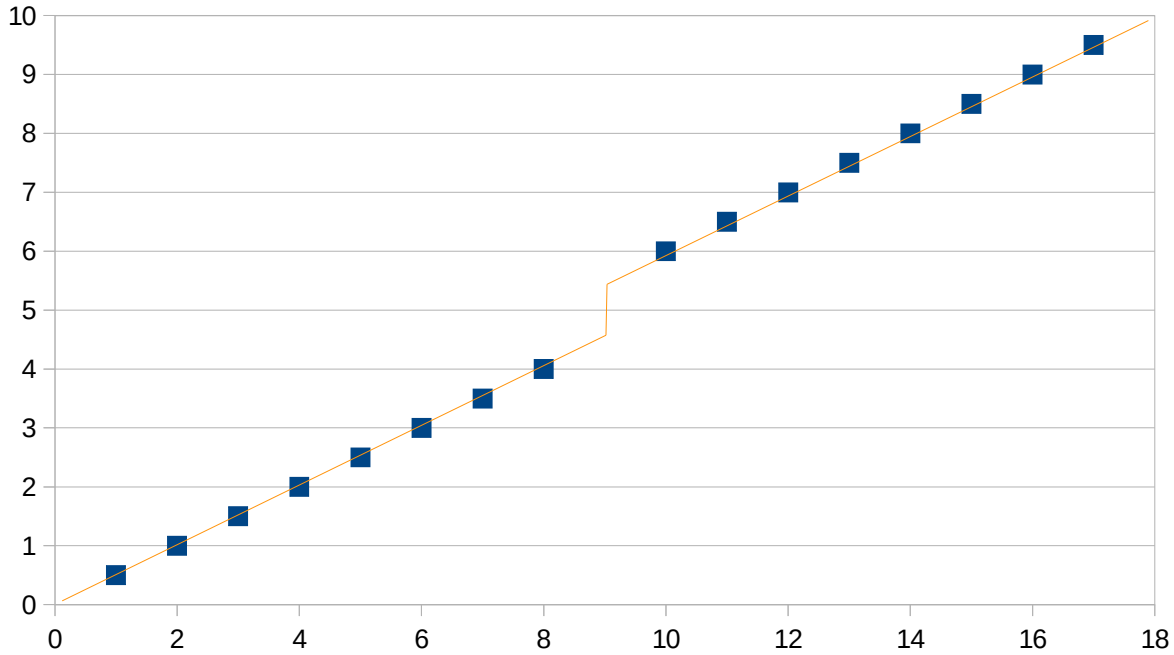


- The error of the root node is larger than that of the leaf nodes → keep leaf nodes



Model Tree Learning Illustrated

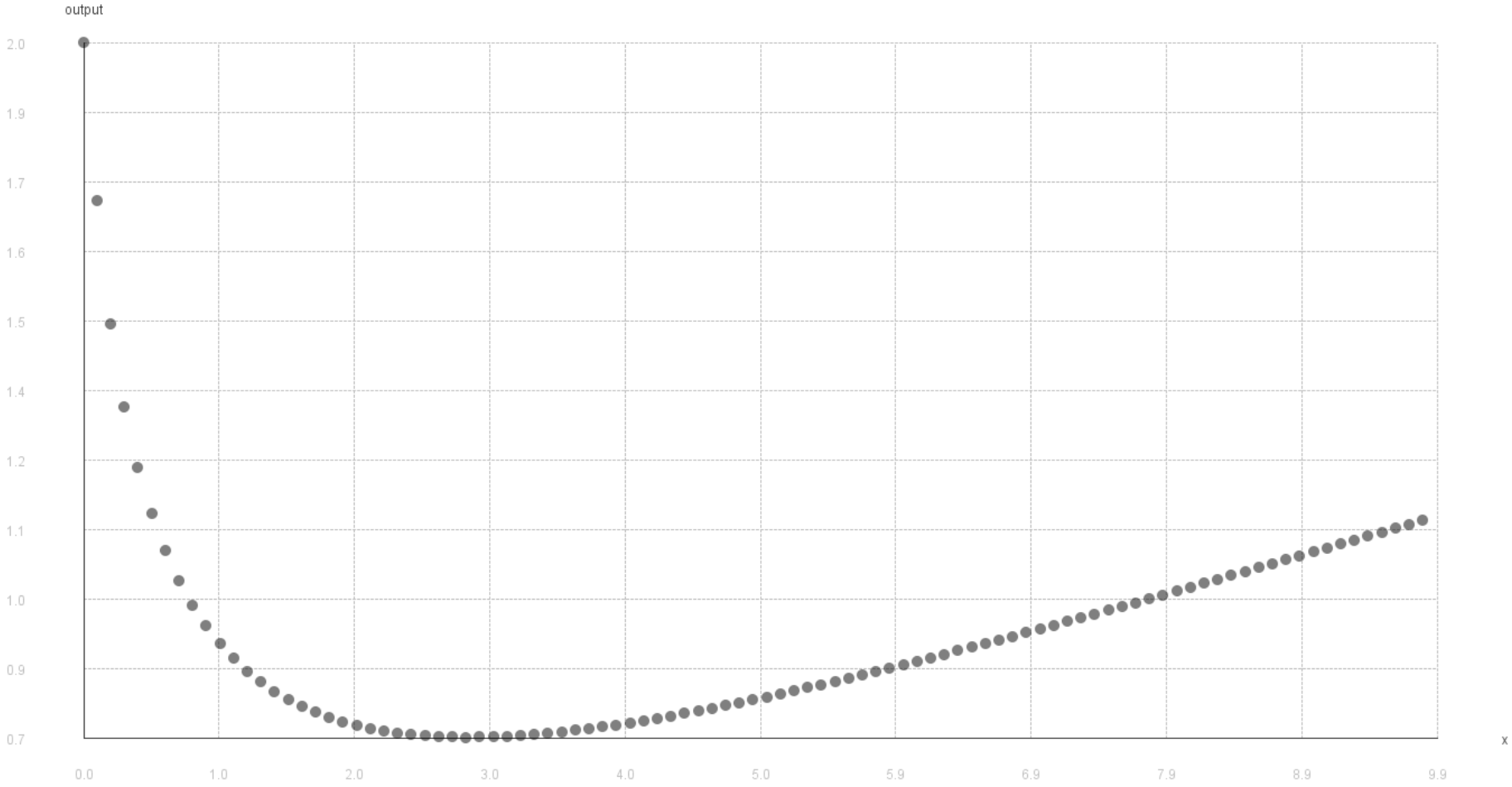




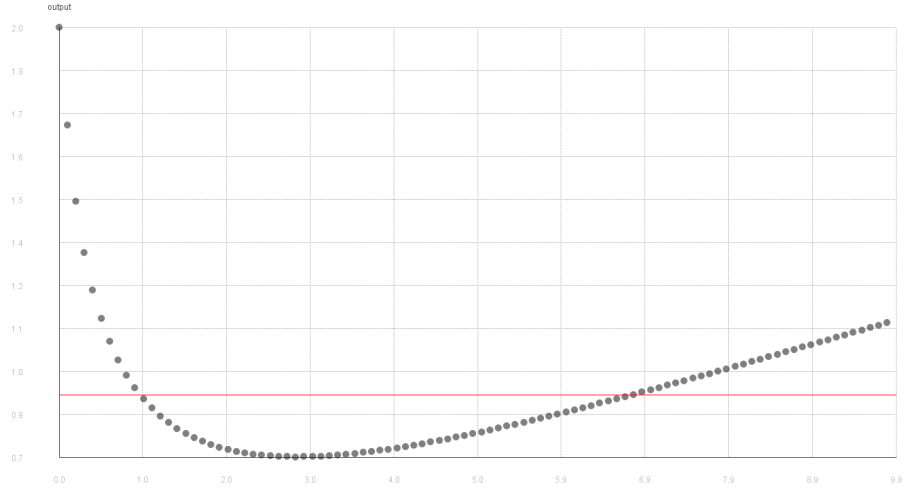
Rules from Model Trees

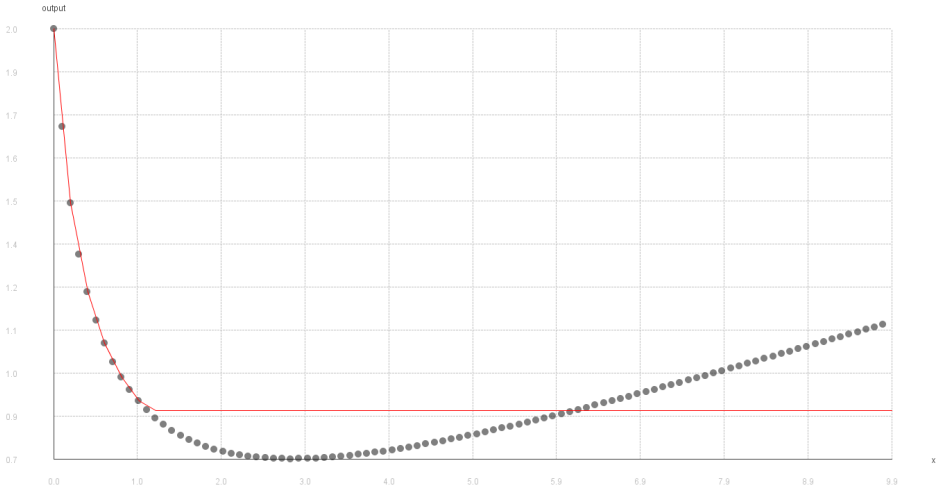
- Recap: PART algorithm generates classification rules by building partial decision trees
- M5Rules uses the same method to build rule sets for regression
  - Use model trees instead of decision trees
  - Use variance instead of entropy to choose node to expand when building partial tree
- Rules will have linear models on right-hand side

Comparison

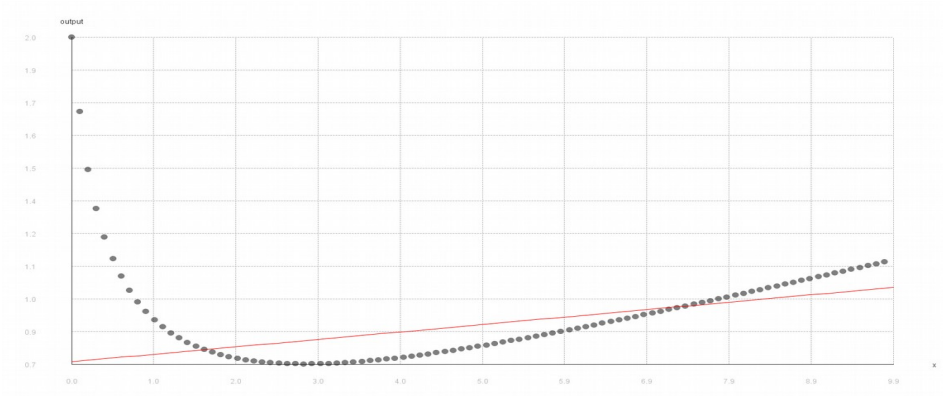

output
2.0
1.9
1.7
1.6
1.5
1.4
1.2
1.1
1.0
0.9
0.7
0.0
1.0
2.0
3.0
4.0
5.0
5.9
6.9
7.9
8.9
9.9
x

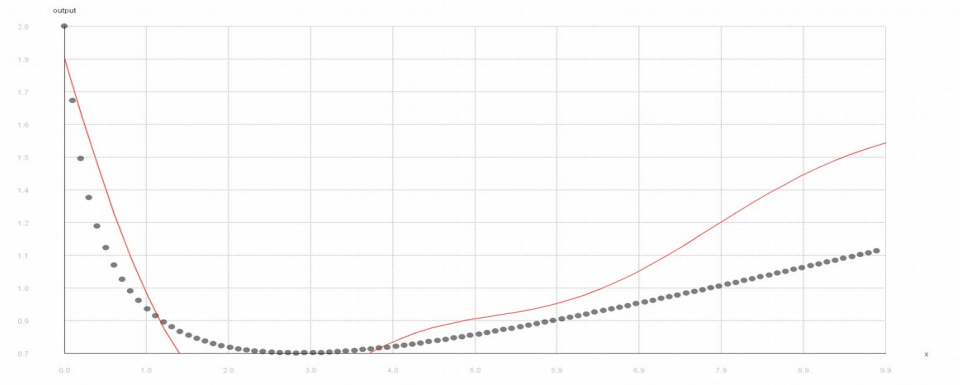
Comparison – Linear and Isotonic Regression



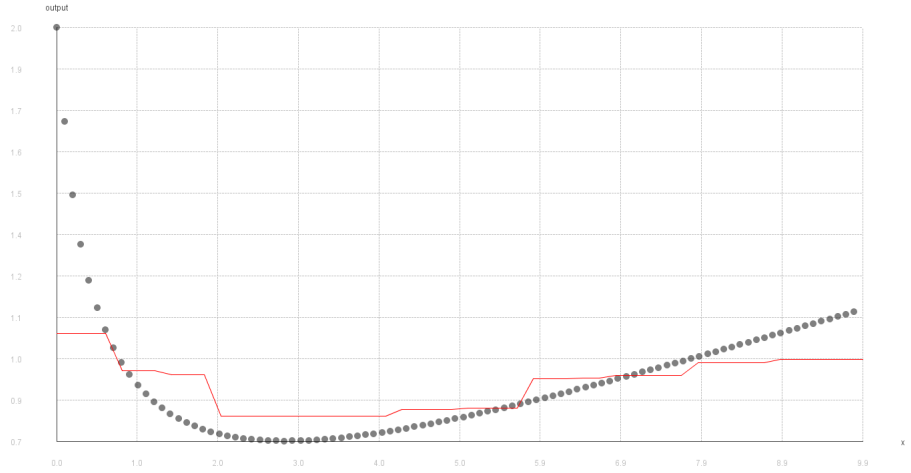


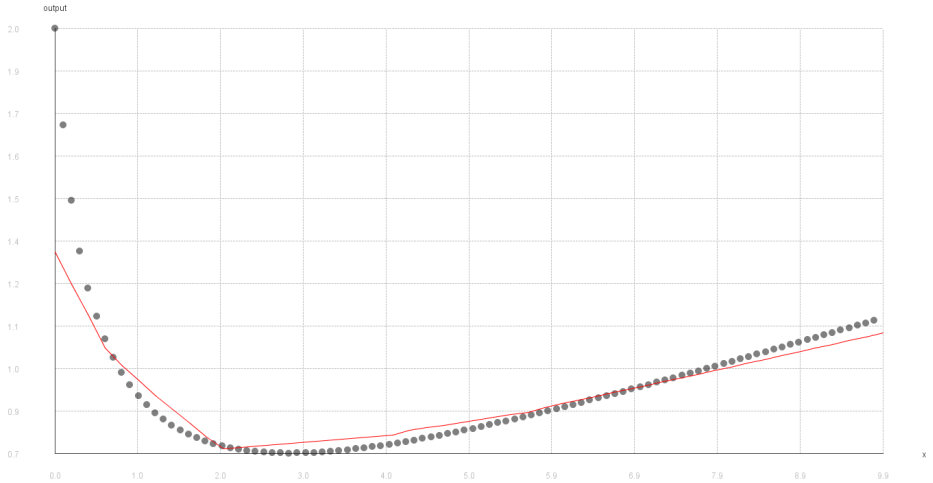
Comparison – SVM with Linear and RBF Kernel



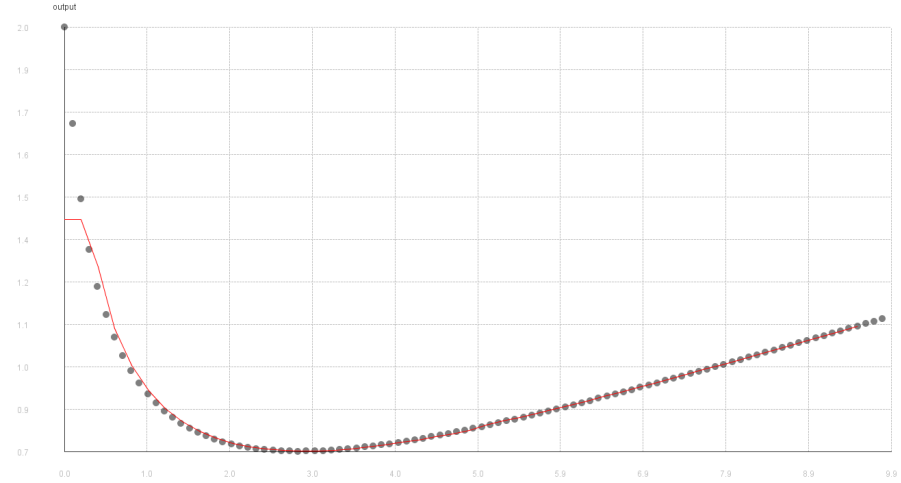


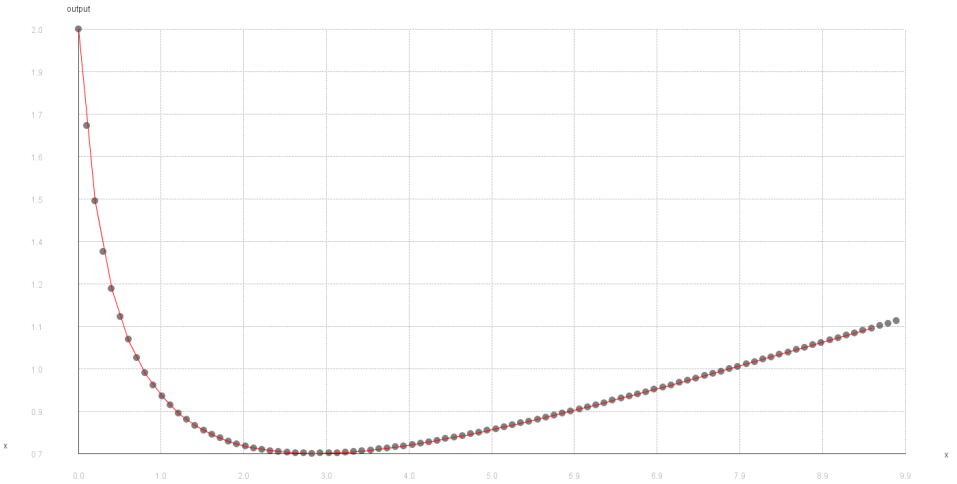
Comparison – M5' Regression and Model Tree





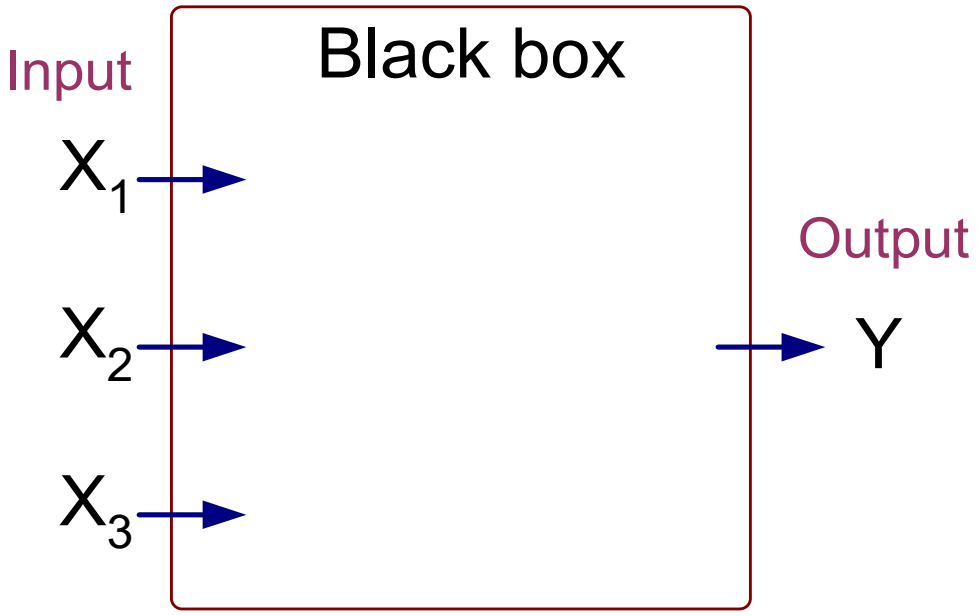
k-NN and Local Polynomial Regression (k=7)





Artificial Neural Networks Revisited

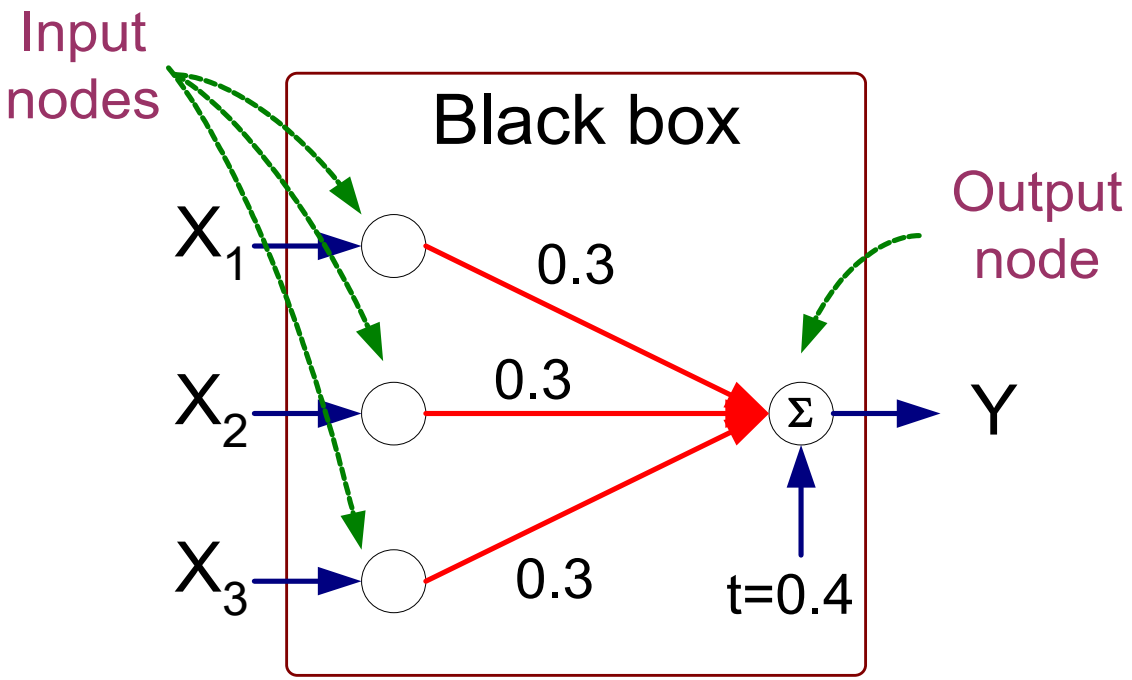
X_1	X_2	X_3	Y
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	0
0	1	0	0
0	1	1	1
0	0	0	0



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:

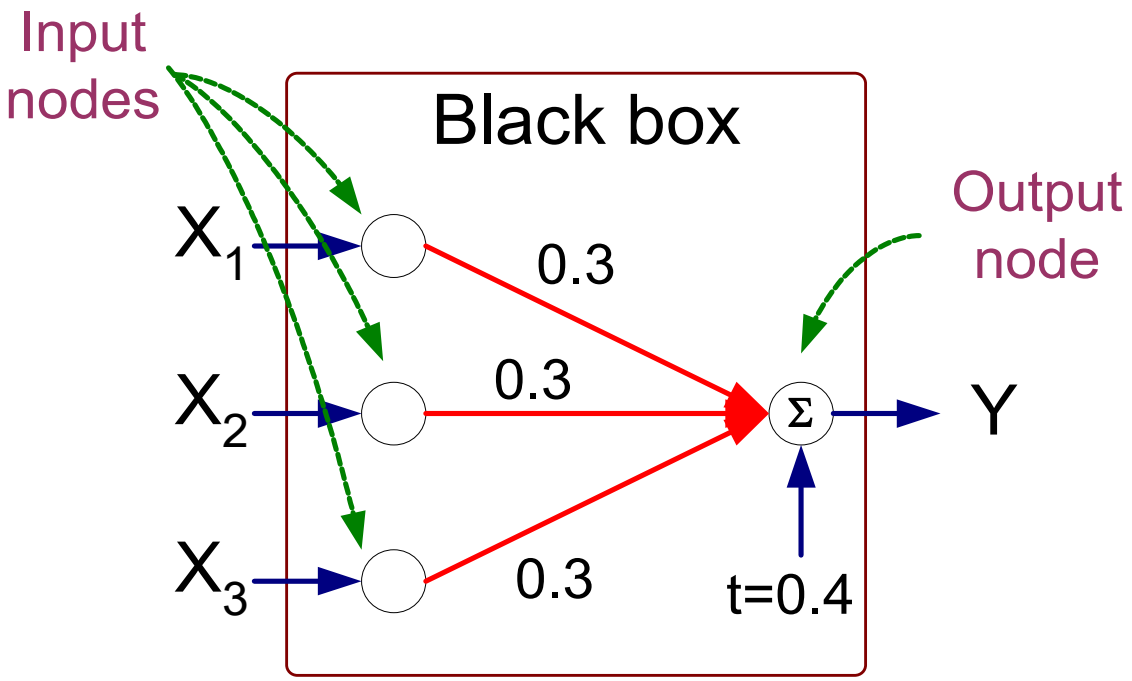
$$Y = 0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4$$

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!

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
  - SVMs
  - model trees
  - artificial neural networks

Questions?