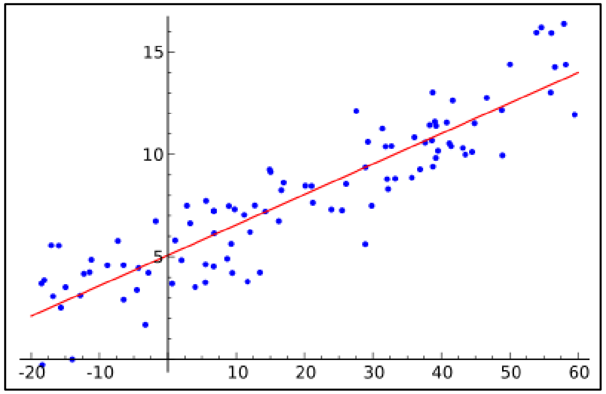
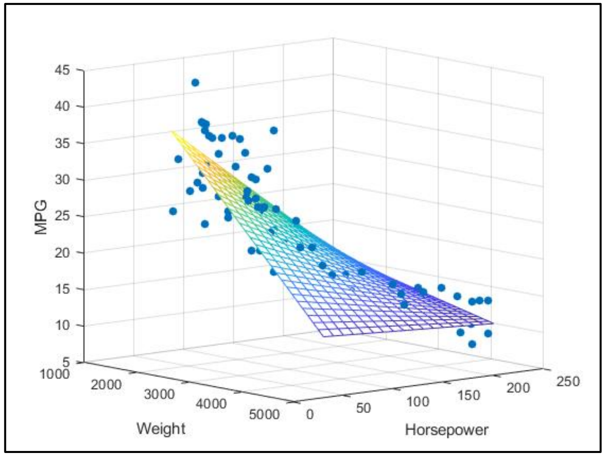
Regression

IE500 Data Mining

What is Regression?

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





The Regression Problem

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

Switching from Classification to Regression

- Many classification approaches
  can also be used for regression (with modifications)

- In the following slides each approach will be discussed
  - K-Nearest-Neighbors -> K-Nearest-Neighbors Regression
  - Decision Trees -> Regression Tree, Model Tree
  - Artificial Neural Networks (ANNs) -> ANNs for Regression

Outline

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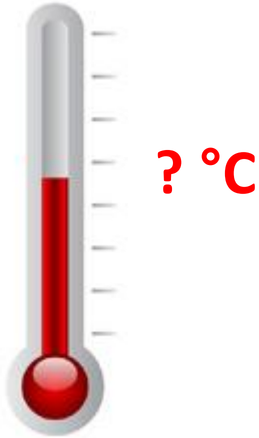
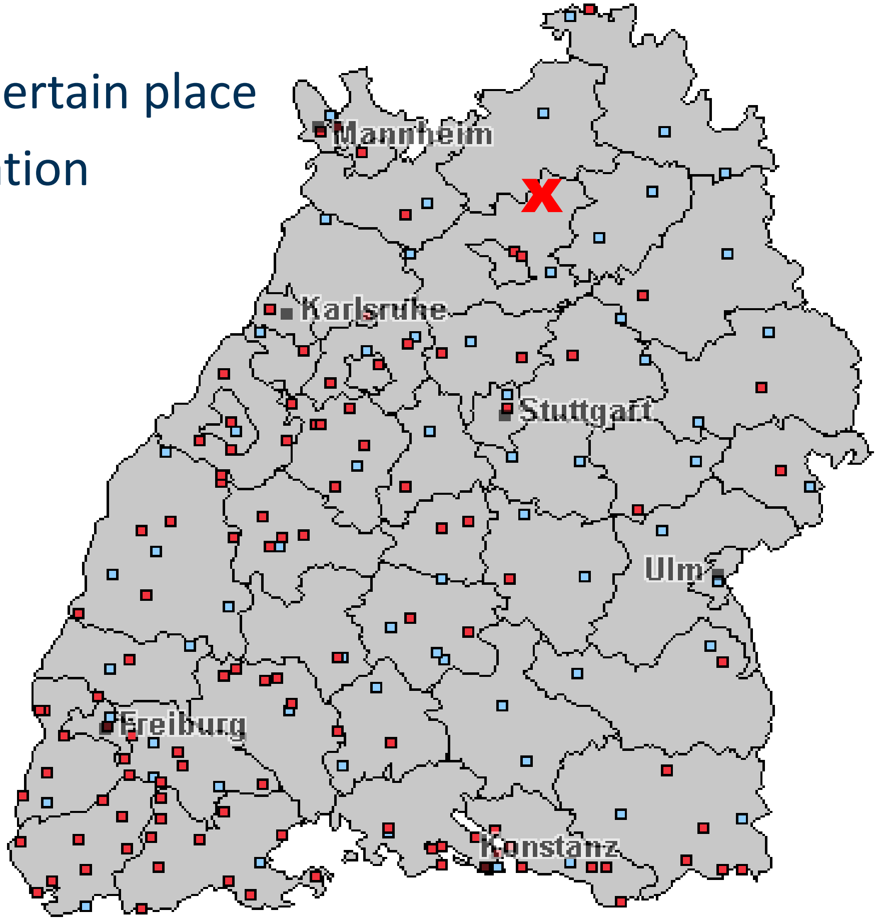
- KNN for Regression
- Evaluation Metrics
- Regression Trees, Model Trees
- Linear Regression, Ridge / Lasso Regression
- Isotonic Regression
- Polynominal Regression
- Local Regression
- ANNs for Regression
- The Bias/Variance-Tradeoff

K-Nearest-Neighbors Regression

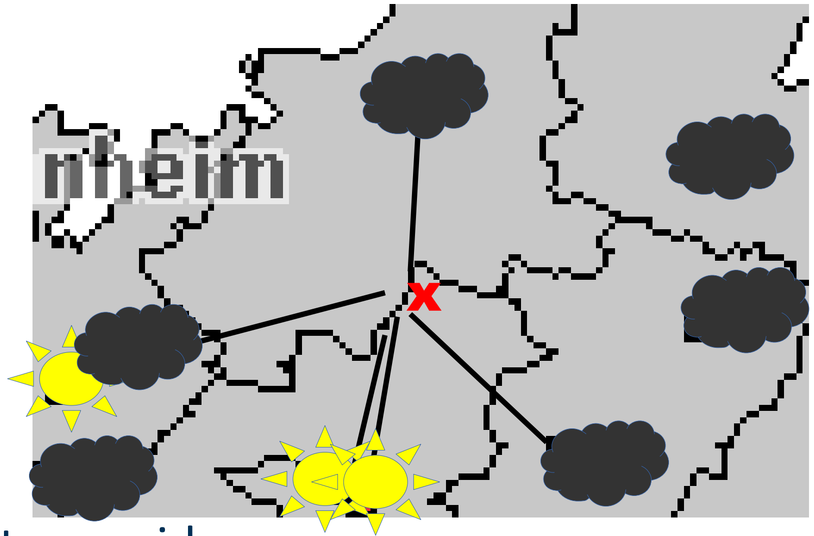
- Problem
  - Predict the **temperature** in a certain place
  - Where there is no weather station
  - How could you do that?





Recap: K-Nearest-Neighbors Classification

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



- Approach is called
  - "k nearest neighbors"
  - where k is the number of neighbors to consider
  - in the example: k=5
  - in the example: "near" denotes geographical proximity

K-Nearest-Neighbors Regression

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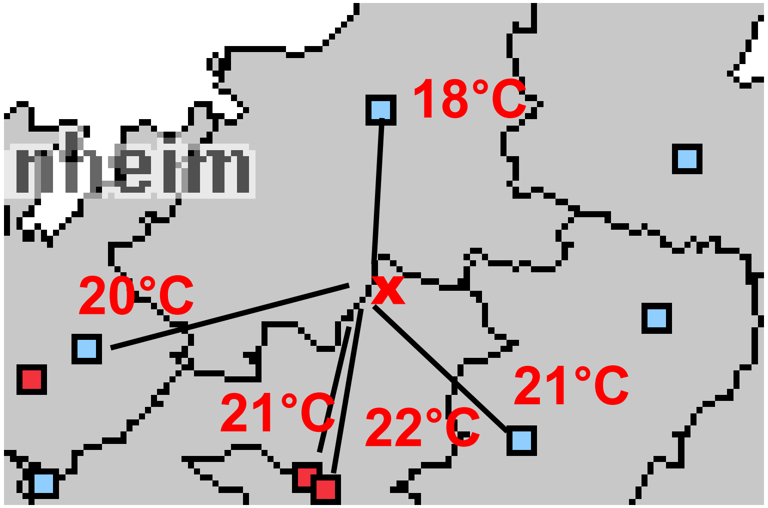
- Idea: **Use the numeric average of the nearest stations**
- Example:
  - 18°C, 20°C, 21°C, 22°C, 21°C
- Compute the average
  - again: k=5
  - average = (18+20+21+22+21) / 5
  - prediction: $\hat{y}$ = 20.4°C



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

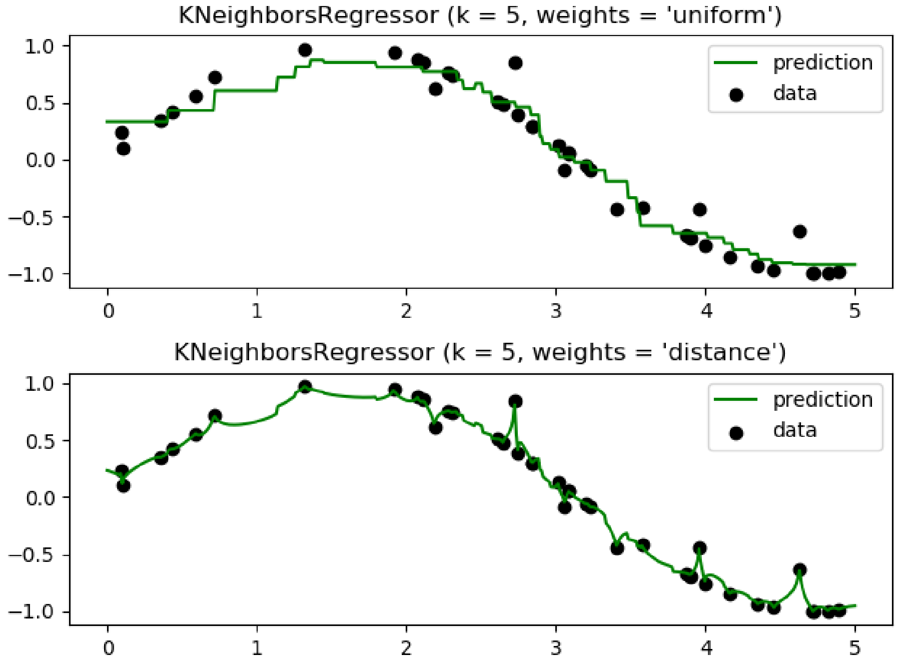
K-NN Regression in Python

Python

```
from sklearn.neighbors import KNeighborsRegressor

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

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



Evaluation Metrics

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

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

Same scale as the domain
e.g. temperature

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

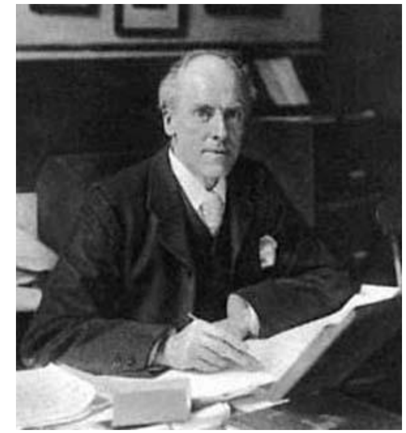
$$MSE = \frac{1}{n}\sum_{i=1}^{n} (p_i - a_i)^2$$

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

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

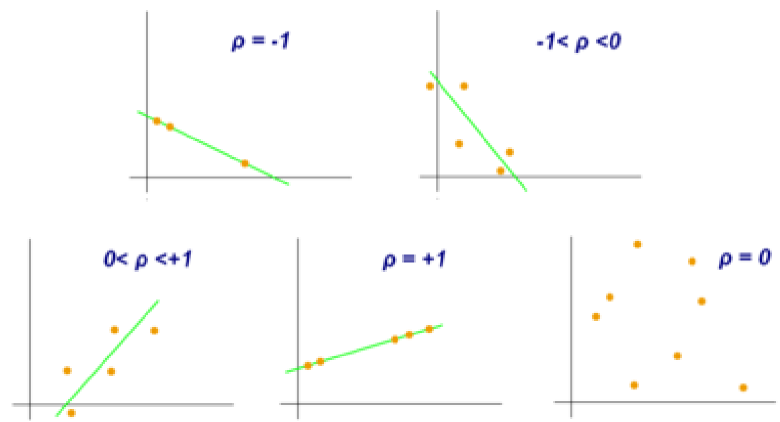
Same scale as the domain
e.g. temperature

Evaluation Metrics



- **Pearson's correlation coefficient**
  - Normalized value [-1, 1]
- 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

$$\text{PCC} = \frac{\sum_{i=1}^{n}(p_i - \bar{p}) * (a_i - \bar{a})}{\sqrt{\sum_{i=1}^{n}(p_i - \bar{p})^2} * \sqrt{\sum_{i=1}^{n}(a_i - \bar{a})^2}}$$



Evaluation Metrics

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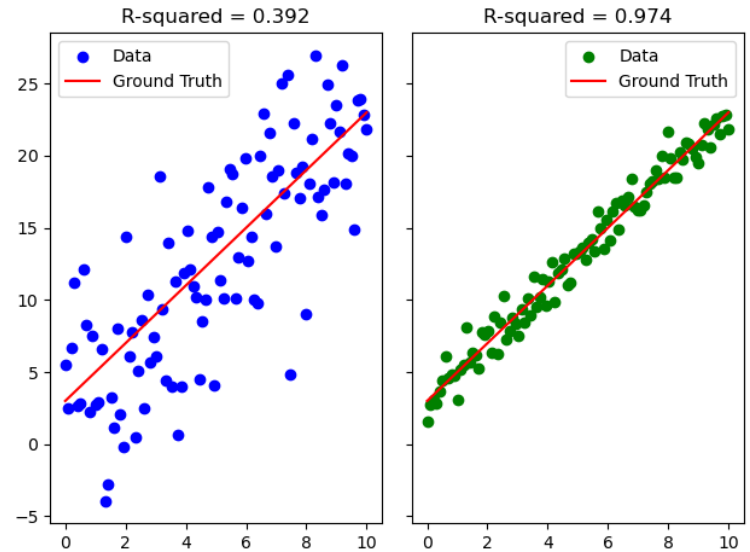
- **R Squared** (also called **Coefficient of Determination**)
  – Normalized value [0, 1]
  – Measures the part of the total variation in the dependent variable y that is predictable (explainable) from the explanatory variables X
  – $R^2 = 1$: Perfect model as total variation of y can be completely explained from X

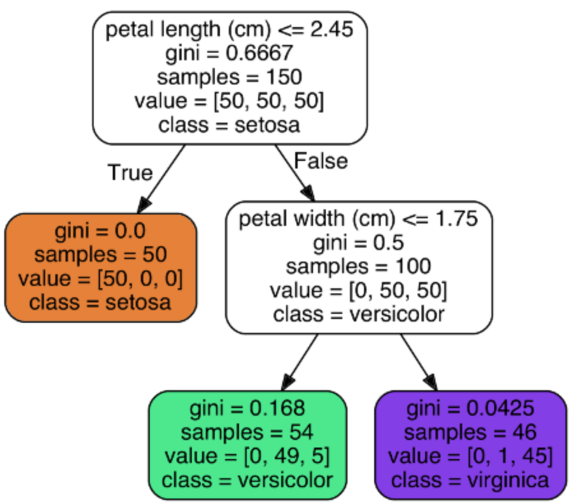
$$R^2 = \frac{\overbrace{\sum_{i=1}^{n}(p_i - \bar{a})^2}^{\text{explained sum of squares}}}{\underbrace{\sum_{i=1}^{n}(a_i - \bar{a})^2}_{\text{total sum of squares}}}$$



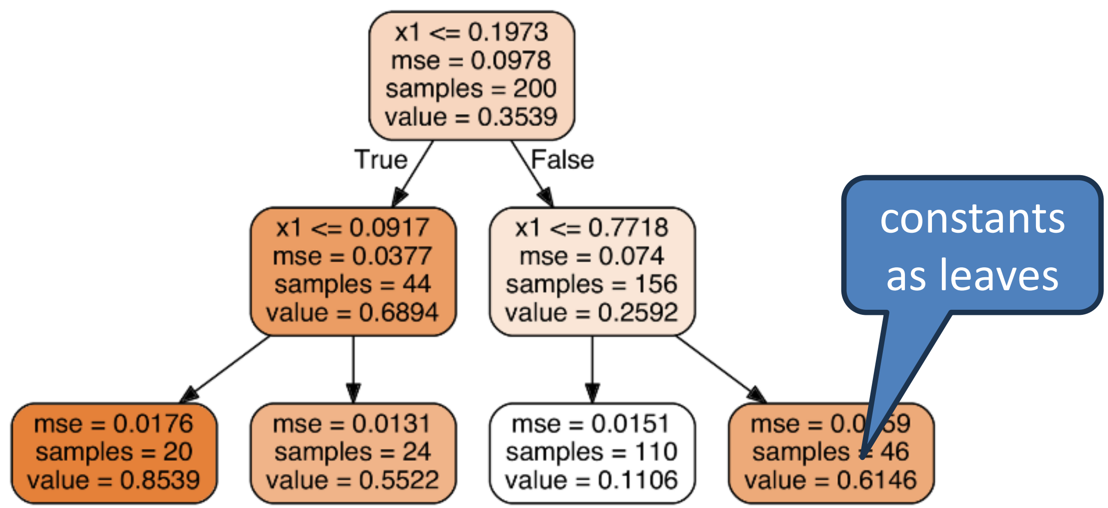
Regression Trees

- 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)
  2. Prediction is average value of the training examples in a specific leaf

Decision Tree

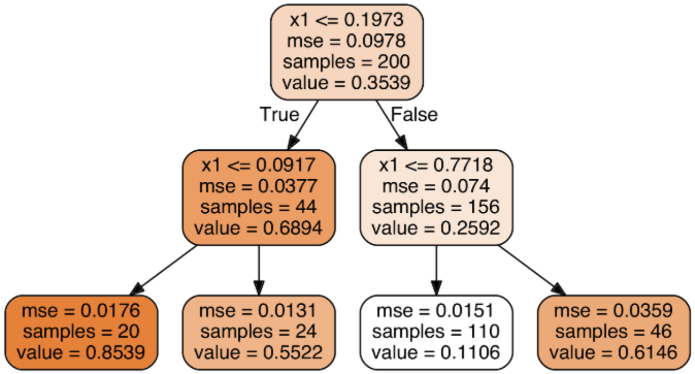


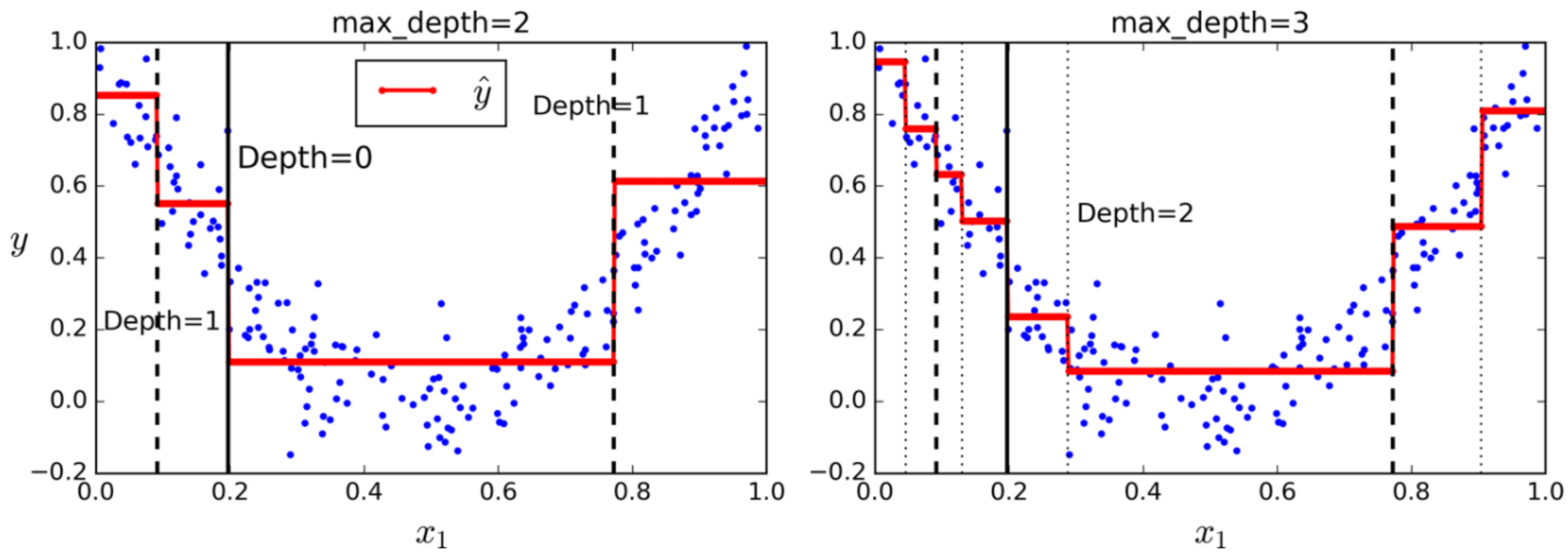
Regression Tree



Regression Trees

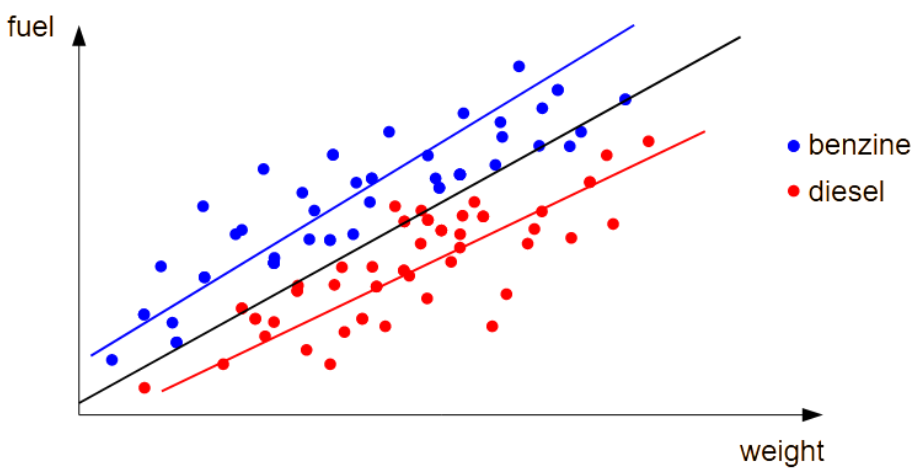
- Pre-pruning parameters determine how closely the tree fits the training data
  - E.g. max_depth parameter
- Resulting model: piecewise constant function

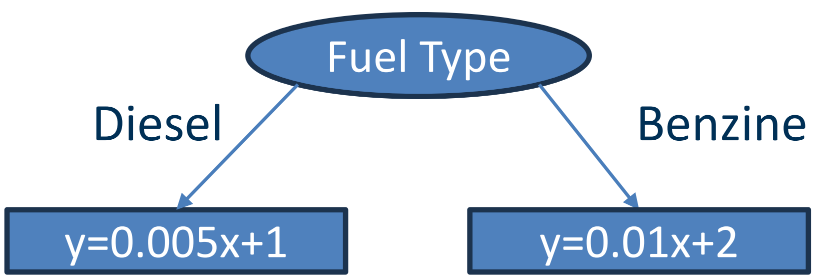




Model Trees

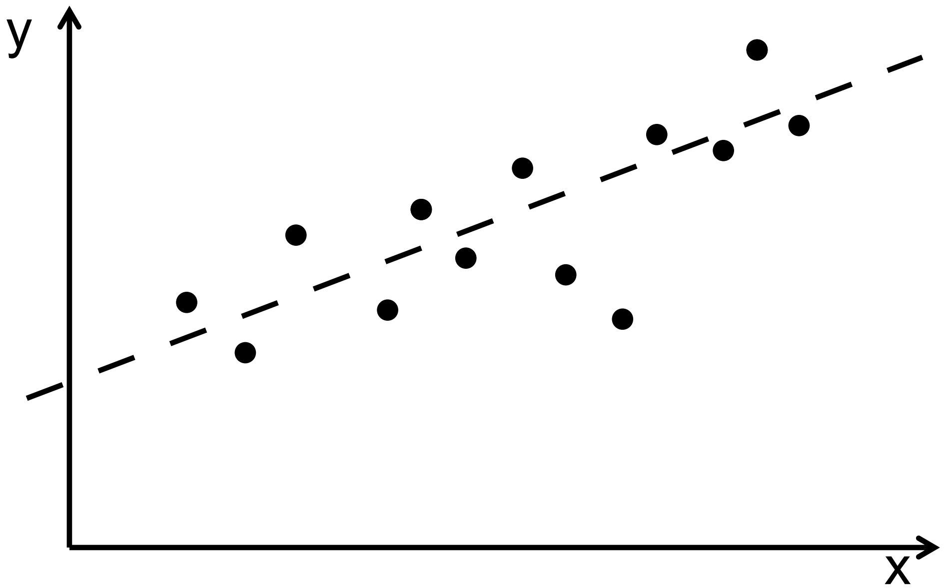
- Idea: split data first so that it becomes "more linear"
  - Example: fuel consumption by car weight
- Instead of a constant in each leave, learn a **linear regression function**
- Prediction: go down tree, then apply function
- Resulting model: piecewise **linear** function





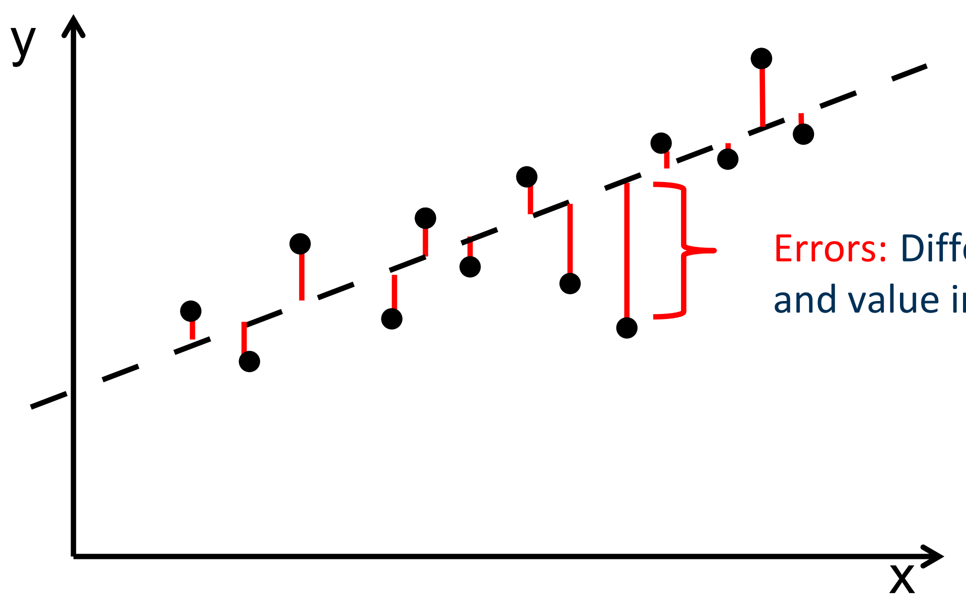
Linear Regression

- How to learn a linear regression function?
- Assumption: 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 $X = x_1, x_2, \ldots, x_n$ (multiple linear regression)



Fitting a Regression Function

- Least-Squares Approach (simple linear regression):
  - Find the weight vector $W = w_0, w_1$
    of a linear function $f(x) = w_0 + w_1 x_1$
    that minimizes the sum of squared error $SSE = \sum_{i=1}^{n} (y_i - f(x_i))^2$

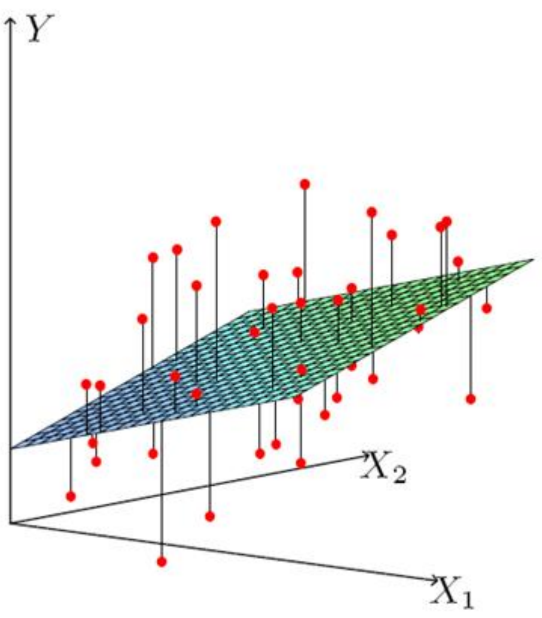


Errors: Differences between estimated value and value in training data, also called residuals.

Fitting a Regression Function

- Least-Squares Approach (multiple linear regression):
  - Find the weight vector $\mathrm{W} = w_0, w_1, \dots, w_n$ of a linear function $\hat{y}(X) = w_0 + w_1 x_1 + w_2 x_2 + \ \dots + w_n x_n$ that minimizes the sum of squared error

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



Linear Regression and Overfitting

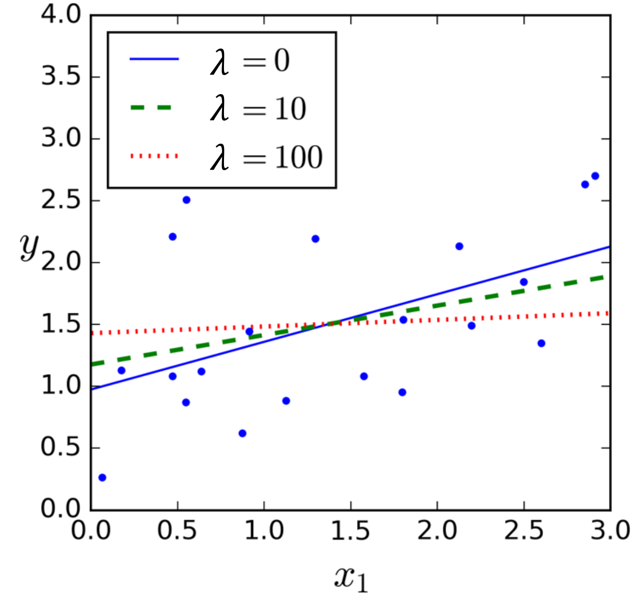
- Given two regression models
  - One using five variables to explain a phenomenon
  - Another one using 100 variables
- Which one do you prefer?

- Recap: Occam’s Razor
  - Out of two theories explaining the same phenomenon, prefer the smaller one

Ridge Regression

- Variation of least squares approach which tries to avoid overfitting by keeping the weights W small
- Ridge Regression:
  - introduces *regularization*
  - create a simpler model by favoring larger factors, minimize

$$\underbrace{\sum_{\mathrm{i}=1}^{\mathrm{n}} (\mathrm{y_i} - \hat{y}(X_i, W)))^2}_{\text{Linear regression}} + \underbrace{\lambda \sum_{\mathrm{i}=1}^{\mathrm{n}} w_i^2}_{\text{Regularization}}$$



Lasso Regression

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

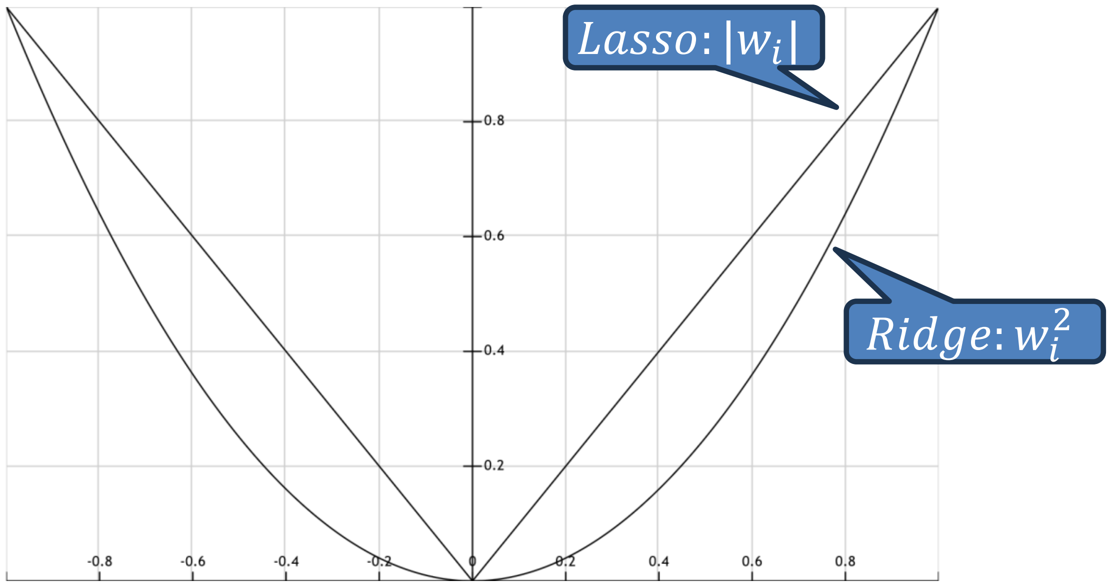
- Lasso Regression optimizes

$$\underbrace{\sum_{\mathrm{i}=1}^{\mathrm{n}} (\mathrm{y}_\mathrm{i} - \hat{y}(X_i, W)))^2}_{\text{Linear regression}} + \lambda \underbrace{\sum_{\mathrm{i}=1}^{\mathrm{n}} |w_i|}_{\text{Regularization}}$$

Lasso: $|w_i|$ vs. Ridge: w_i^2

Lasso vs. Ridge Regression

- Lasso: 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



Interpolation vs. Extrapolation

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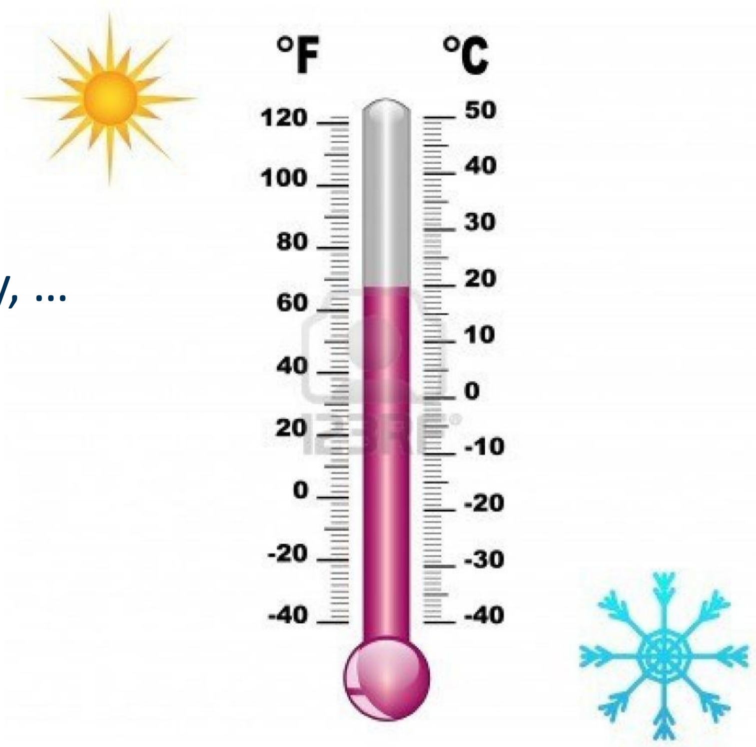
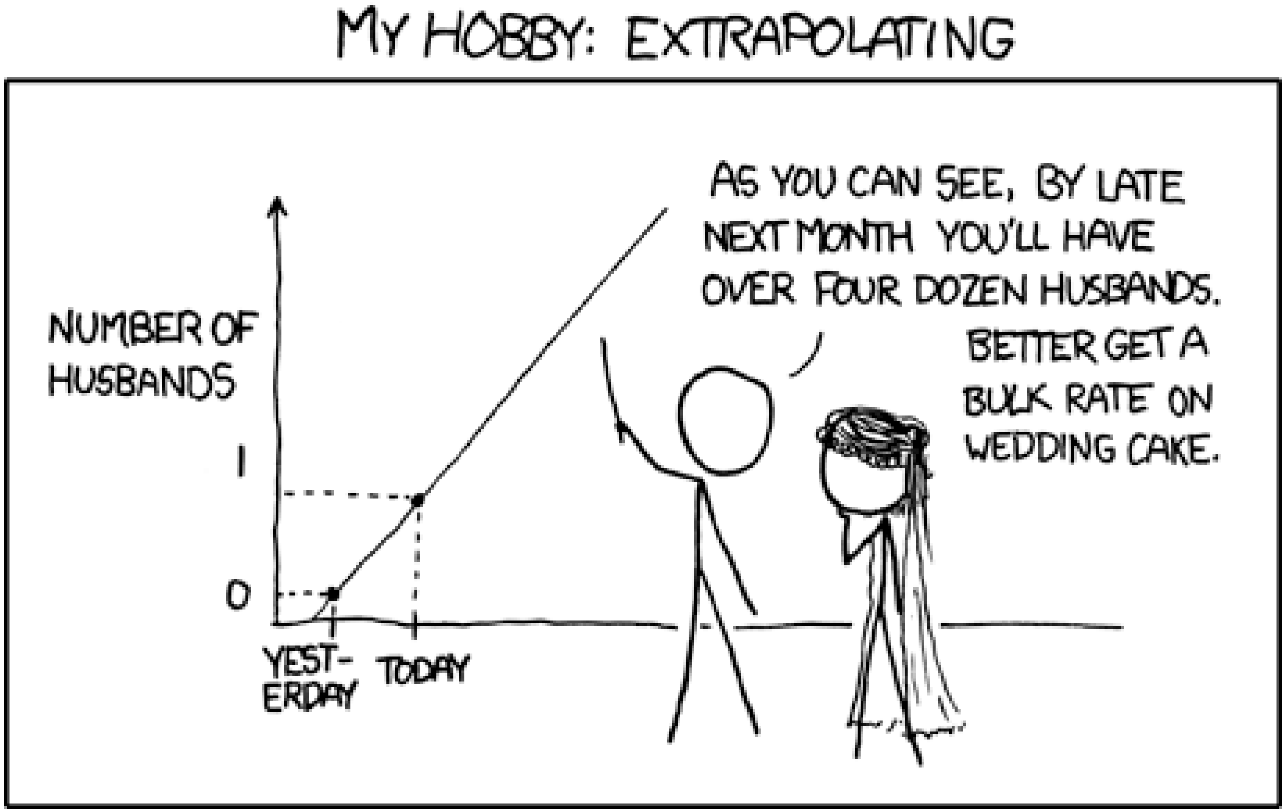


- Training data:
  - Weather observations for current day
  - E.g., temperature, wind speed, humidity, …
  - Target: temperature on the next day
  - Training values between -15°C and 32°C
- Interpolating regression
  - Only predicts values
    from the training interval [-15°C,32°C]
- Extrapolating regression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

Interpolation vs. Extrapolation

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



http://xkcd.com/605/

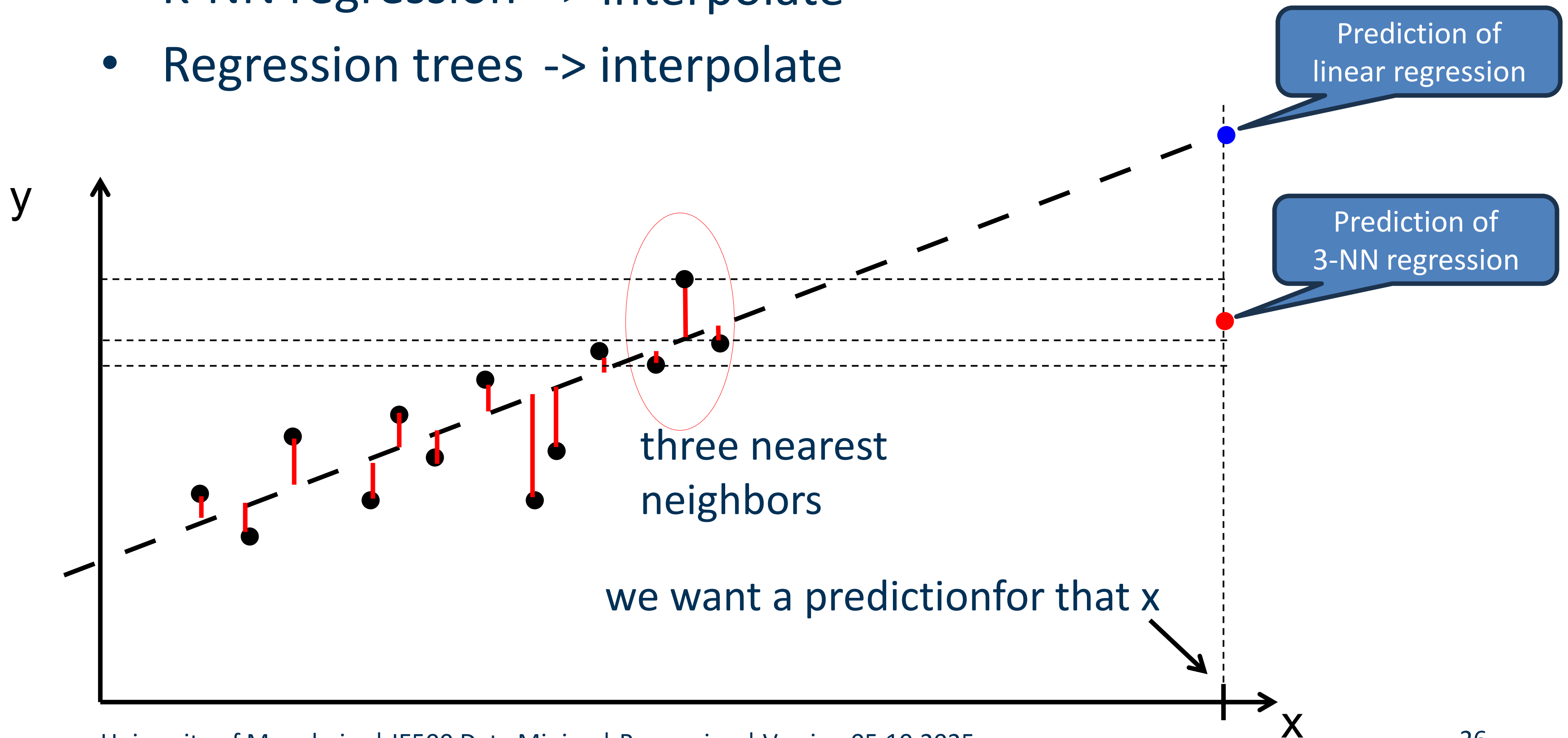
Interpolation vs. Extrapolation

- 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 regression -> interpolate
- Regression trees -> interpolate



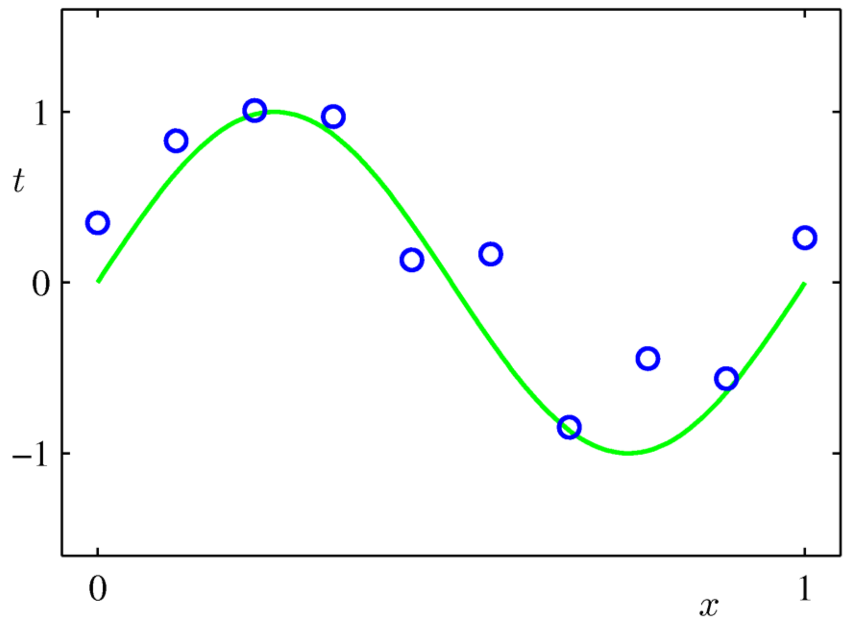
Baseline Prediction

- 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

THE PROBLEM WITH AVERAGING STAR RATINGS

http://xkcd.com/937/

..but what about Non-linear Problems?



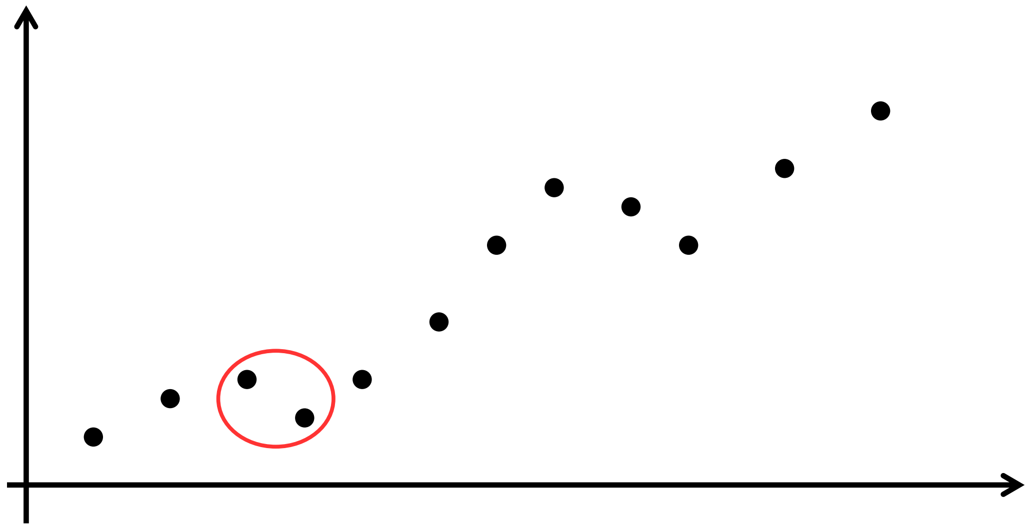
- Possible Solutions:
  - Isotonic Regression
  - Polynomial Regression

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., $f(x_i) > f(x_{i+1})$
- 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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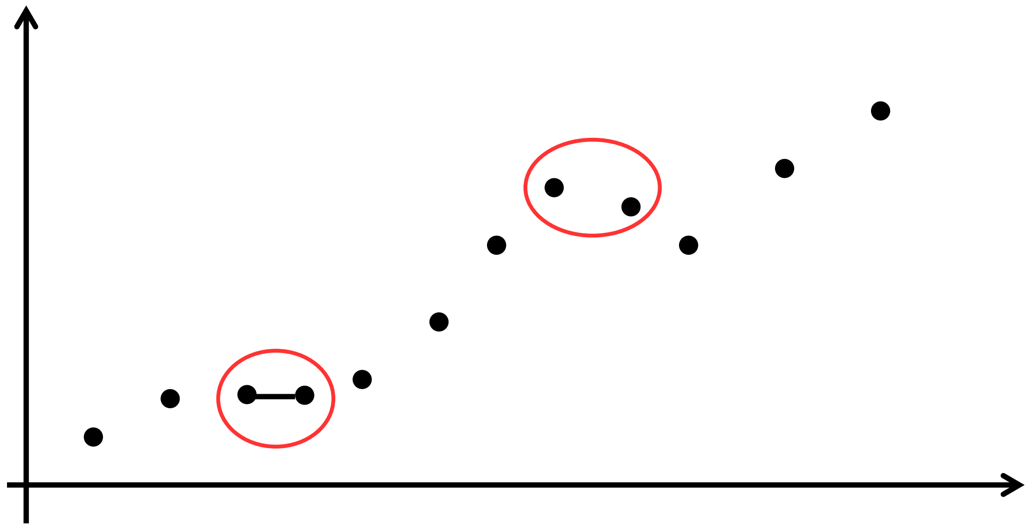

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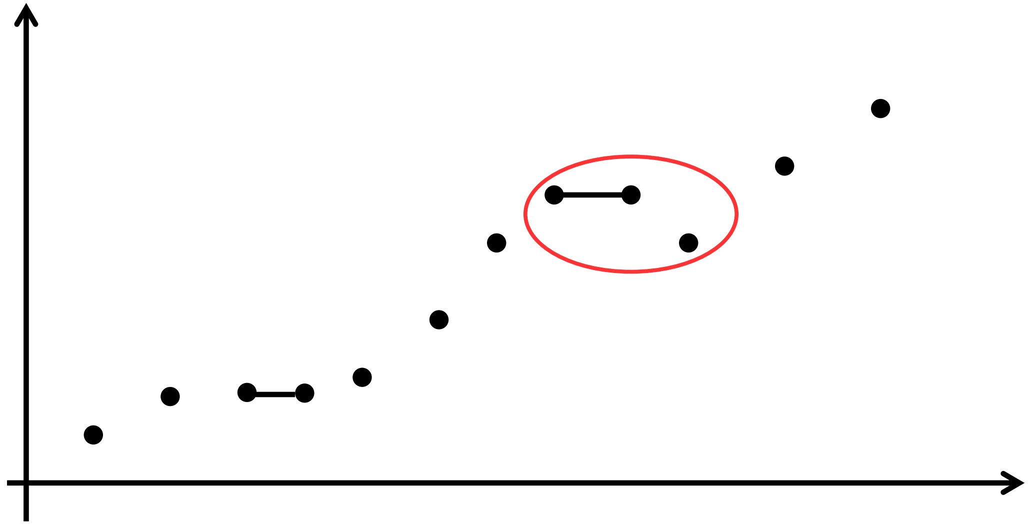

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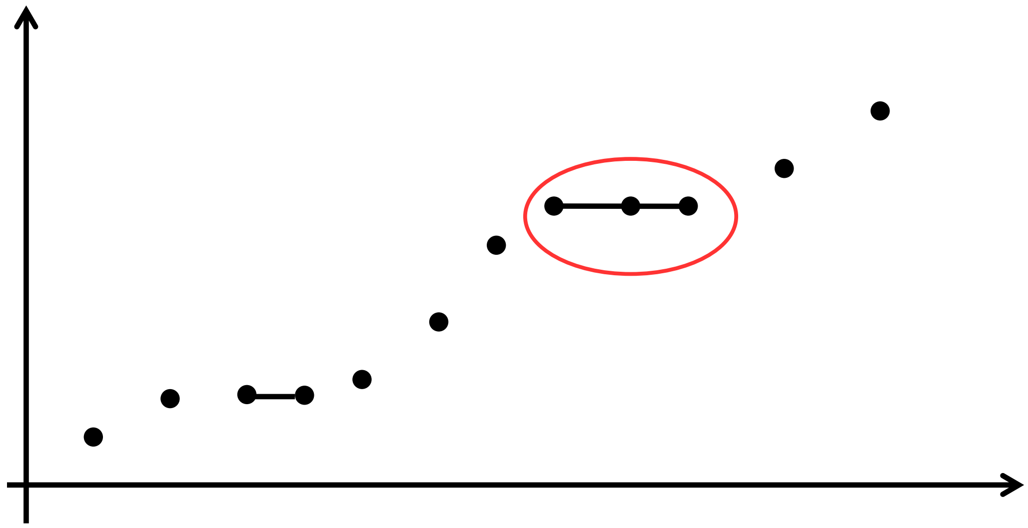
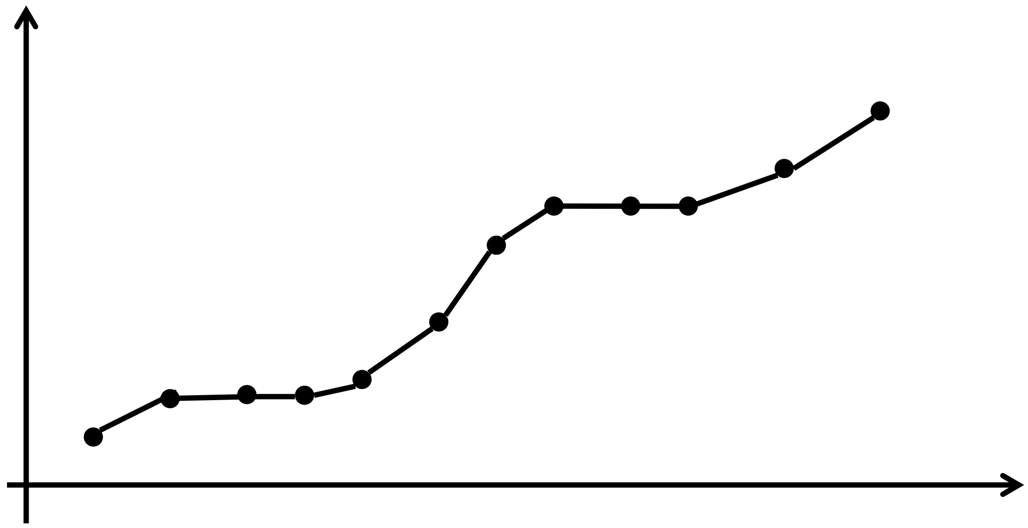


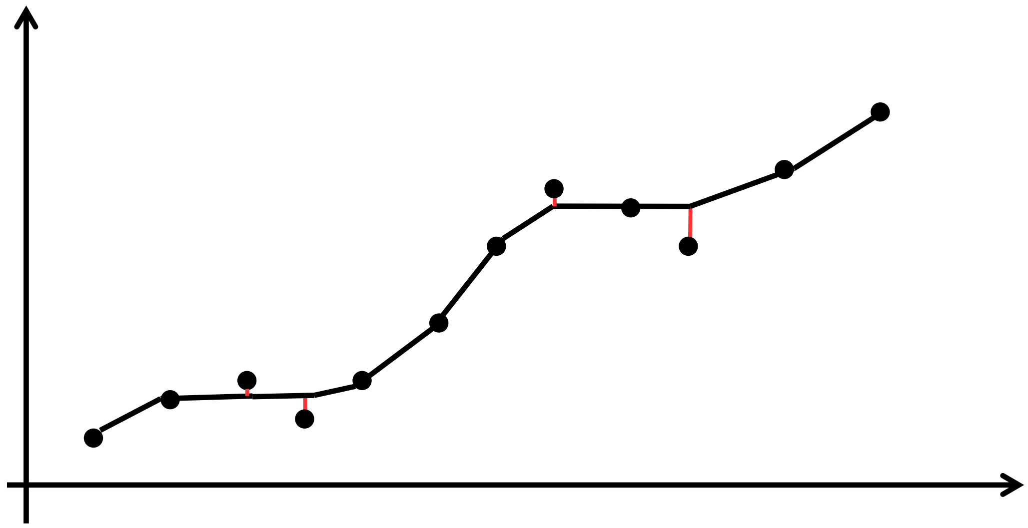
Isotonic Regression

- 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

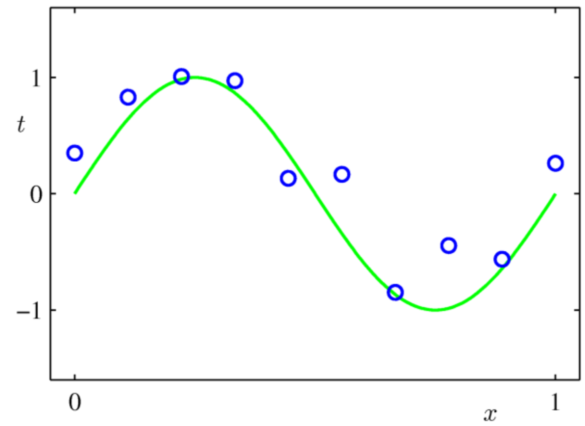
- Comparison to the original points
  - Plateaus exist where the points are not monotonous
  - Overall, the mean squared error is minimized



Isotonic Regression

- Python:
  - `IsotonicRegression`
- Parameter *increasing*
  - Can be constrained to increasing (true) or decreasing (false)
  - *auto* finds the best setting
- Parameter *out_of_bounds* (how to handle unseen x values)
  - *clip* uses the smallest/largest y value in the training data
  - *nan* assigns NaN
  - *raise* creates an error

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

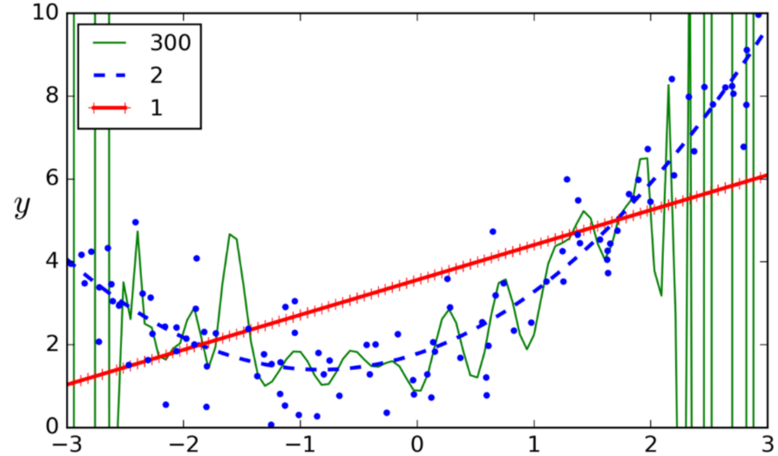


- One possibility is to apply transformations to the explanatory variables X within the regression function
  - e.g. log, exp, square root, square, etc.
  - polynomial transformation
    - example: $y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$

Polynomial Regression

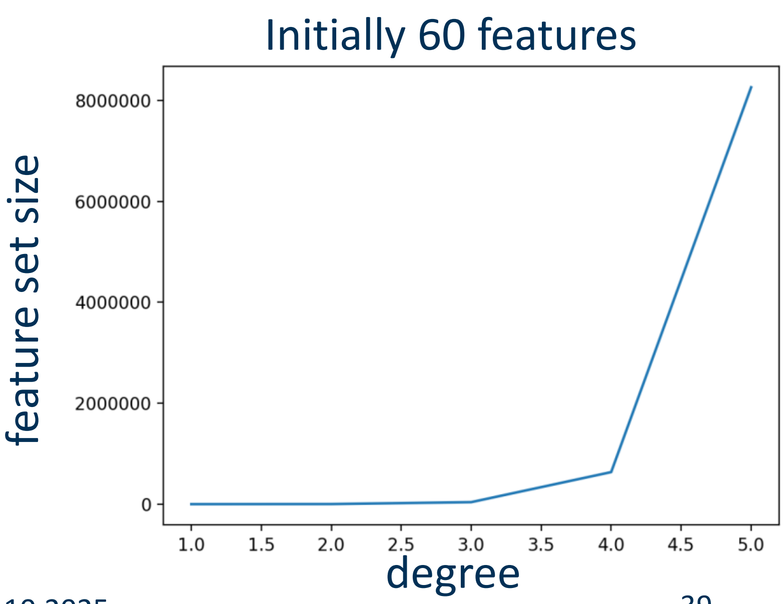
$$\hat{y}(x, \boldsymbol{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_d x^d = \sum_{j=0}^{d} w_j x^j$$

- Widely used extension of linear regression
- Can also be fitted using the least squares method
- has tendency to over-fit training data for large degrees d
- Workarounds:
  - Decrease d
  - Increase amount of training data



Polynomial Regression – Multiple Features

- Number of 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

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- 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!

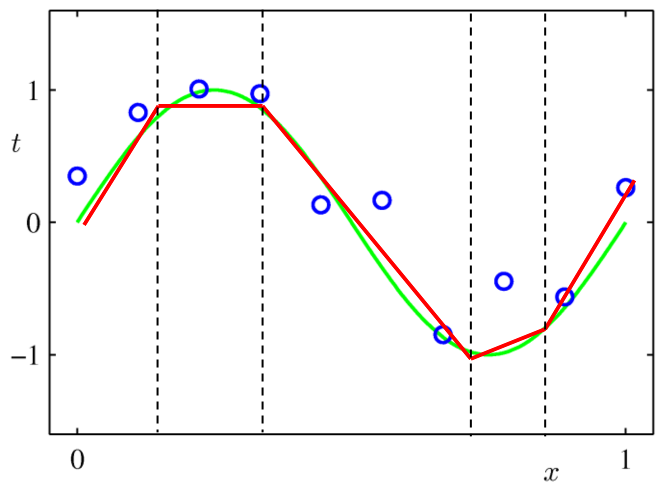
Python

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

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

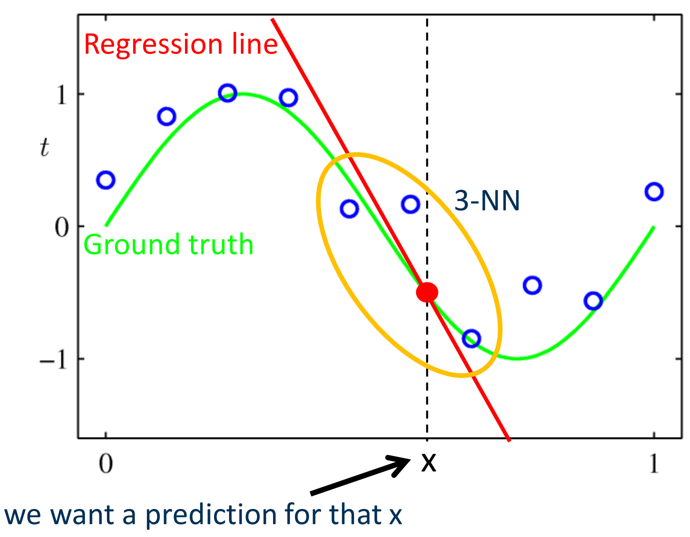
Local Regression

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



Discussion of Local Regression

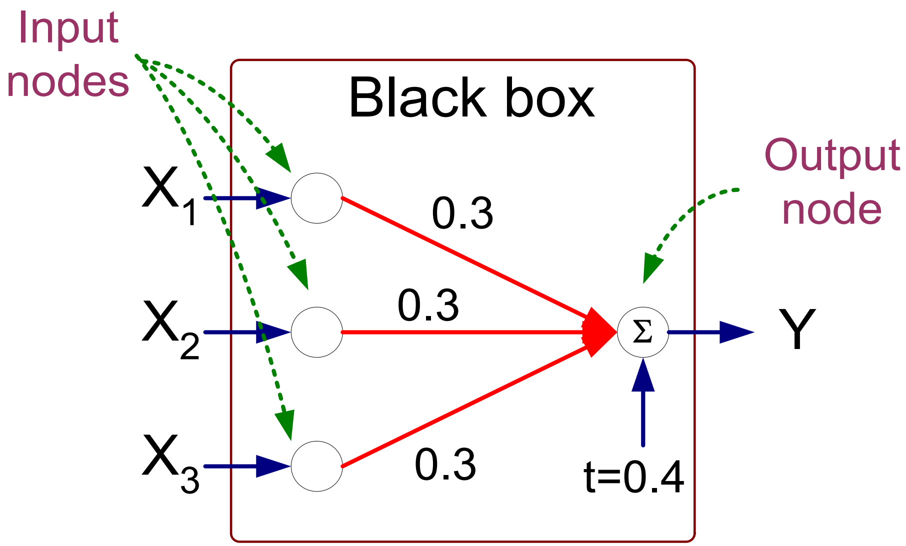
- Advantage: fits non-linear models well
  - Good local approximation
  - Often better than pure k-NN

- Disadvantage
  - Slow at runtime
  - For each test example:
    - Find k nearest neighbors
    - Compute a local model

Artificial Neural Networks (ANNs) for Regression

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

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



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

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

Artificial Neural Networks (ANNs) for Regression

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

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

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

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

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

Artificial Neural Networks (ANNs) 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 e.g. mean squared error

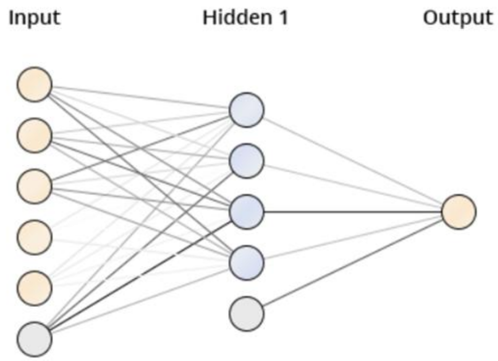
Artificial Neural Networks (ANNs) for Regression

- 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**

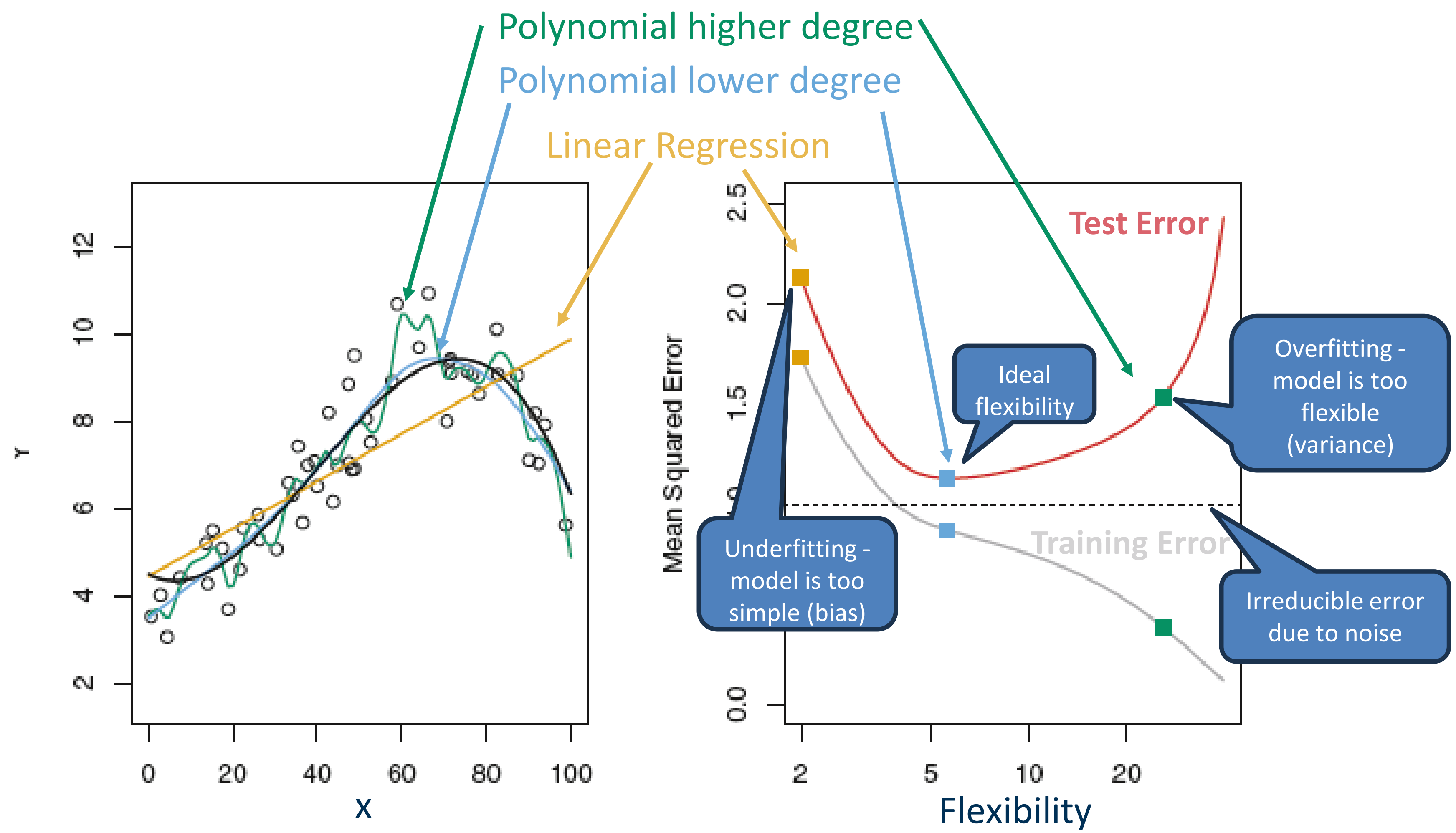


The Bias/Variance-Tradeoff

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

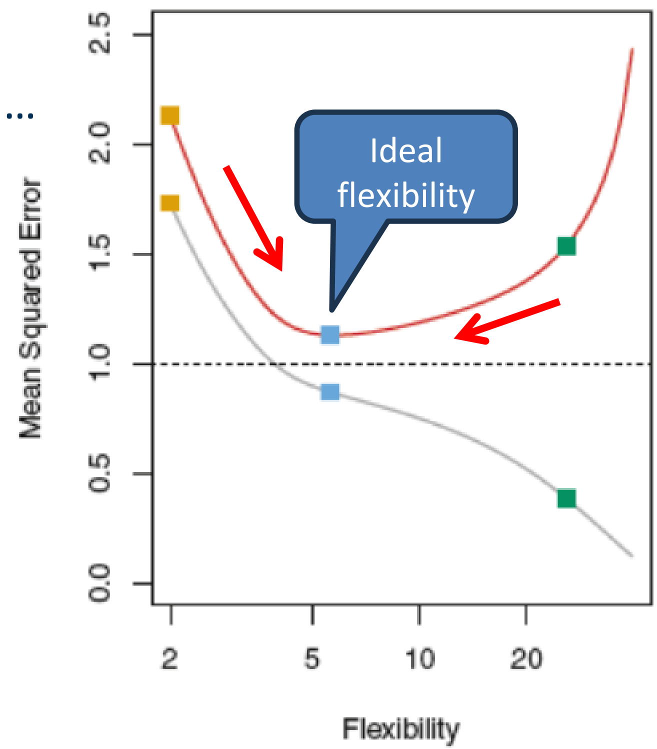
The Bias/Variance-Tradeoff

- Three models with different flexibility trying to fit a function



Learning Method and Hyperparameter Selection

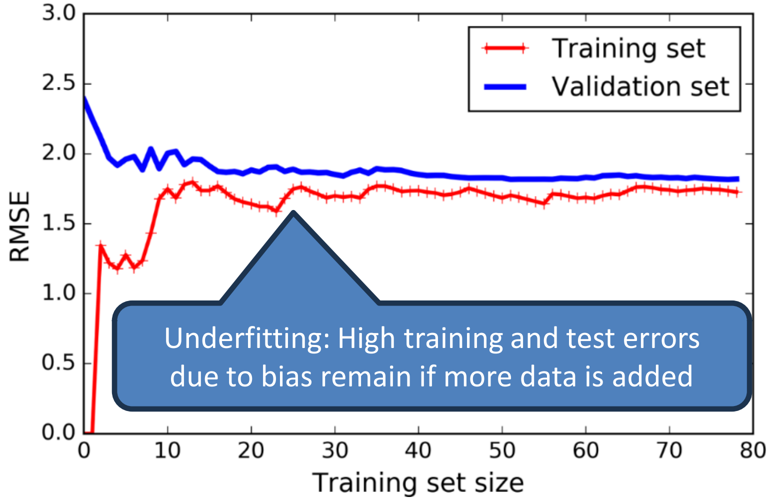
- We try to find the **ideal flexibility** (bias/variance-tradeoff) by
  - Testing different learning methods
    - Linear regression, polynomial regression, …
    - Decision Trees, ANNs, Naïve Bayes, …
  - Testing different hyperparameters
    - degree of polynomial, ridge
    - max depth of tree, min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



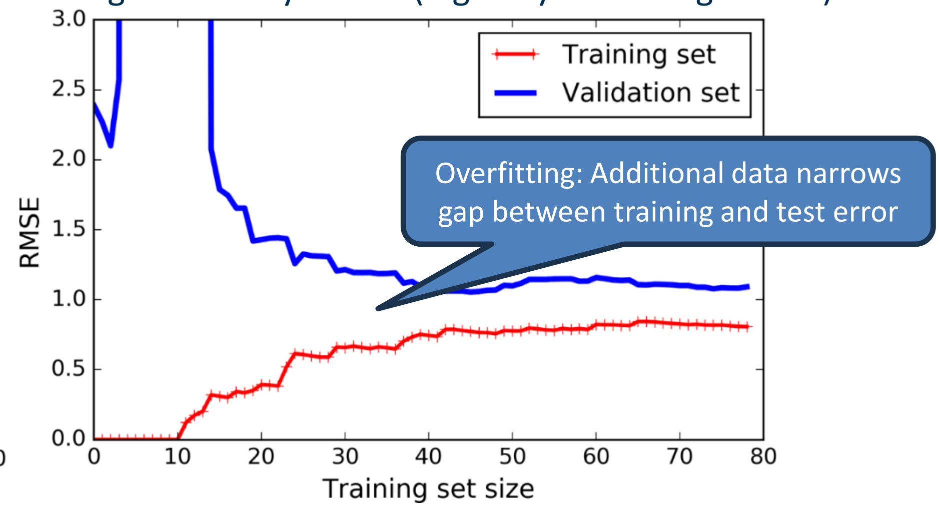
Learning Curves for Under- and Overfitting Models

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

Low Flexibility Model (e.g. Linear regression)



High Flexibility Model (e.g. Polynomial regression)



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

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 false for $(-\infty,0.5]$ and true for $(0.5,\infty)$
  - Similarly for ordinal (e.g., good, medium, bad)
  - Non-ordinal multi-class problems are trickier

Summary

- Regression
  - Predict numerical values instead of classes
- Model evaluation
  - Metrics: (root) mean squared error, R squared, …
- Methods
  - K nearest neighbors, regression trees, model trees
  - Linear regression (ridge, lasso)
  - Isotonic regression, polynomial regression, local regression
  - Artificial neural networks for regression
- For good performance on unseen data
  - Choose learning method having the right flexibility (bias/variance-tradeoff)
  - Use large quantities of interesting training data

Online Lectures

- This week additional material is about Ensembles

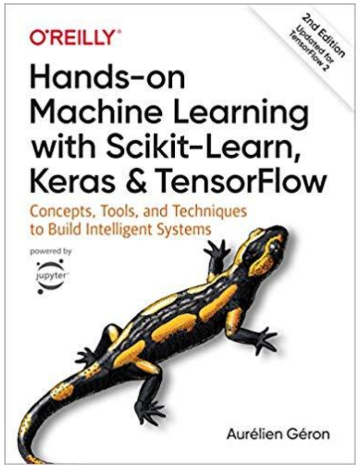
- Online lectures are exercise and exam relevant

Week	Monday(Offline Lecture)	Online Lecture (see Ilias Course)	Thursday (Exercise)
01.09.2025	no lecture		Introduction to Python (13:45–15:15)
08.09.2025	Introduction to Data Mining (PDF, 3 MB)		Intro
15.09.2025	Preprocessing (PDF, 2 MB)		Preprocessing
22.09.2025	Classification 1 (PDF, 2 MB) + Intro to Student Project	Nearest Centroids	Classification 1
29.09.2025	Classification 2	Comparing Classifiers	Classification 2
06.10.2025	Regression	Ensembles	Regression
13.10.2025	Clustering and Anomalies	Hierarchical Clustering	Clustering
20.10.2025	Feedback on project outlines	Time Series	Time Series
27.10.2025	Association Analysis and Subgroup Discovery	Multi Modal Data	Association Analysis
03.11.2025	Project feedback session		Project Work
10.11.2025	Project feedback session		Project Work
17.11.2025	Project feedback session		Project Work
24.11.2025	Project feedback session		Project Work
01.12.2025	Q&A		**Project Presentations**

Questions?

Literature for this Slideset

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



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