Classification 2

IE500 Data Mining

Outline

- Decision Trees
- Overfitting
- Evaluation Metrics
- **Naïve Bayes**
- **Support Vector Machines**
- **Artificial Neural Networks**
- **Evaluation Methods**
- **Hyperparameter Selection**

Naïve Bayes

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- Probabilistic classification technique based on Bayes theorem
  - successful, old-school method for various tasks: NLP, recommendation, …
- Goal: Estimate the most probable class label for a given record
- Probabilistic formulation of the classification task:
  - consider each attribute and class label as random variables
  - given a record with attributes $(A_1, A_2, \dots, A_n)$
    the goal is to find the class C that maximizes the conditional probability
    $\boldsymbol{P(C \mid A_1, A_2, \dots, A_n)}$
- Example: Should we play golf?
  - P(Play=yes | Outlook=rainy, Temperature=cool)
  - P(Play=no | Outlook=rainy, Temperature=cool)
- Question: How to estimate these probabilities given training data?

Bayes Classifier

- Thomas Bayes (1701-1761)
  - British mathematician and priest
  - tried to formally prove the existence of God
- Bayes Theorem
  - important theorem in probability theory
  - was only published after Bayes' death

Bayes Classifier

- Question:
  - How likely is class C, given that we observe attributes A
  - This is called a conditional probability, denoted $P(C|A)$
    - e.g.: Given some attributes A, what is the likelihood of a certain class C?
- Bayes Theorem

$$P(C|A) = \frac{P(A|C)\,P(C)}{P(A)}$$

  - Computes one conditional probability $P(C|A)$ out of another $P(A|C)$
  - given that the base probabilities $P(A)$ and $P(C)$ are known
- Useful in situations where P(C|A) is unknown
  - while P(A|C), P(A) and P(C) are known or easy to determine/estimate?

Bayes Classifier

- **Prior probability** of class C:
  - probability of class C before attributes are seen
  - we play golf in 70% of all cases -> $P(C) = 0.7$
- **Posterior probability** of class C:
  - probability of class C after attributes A is seen
  - evidence: It is windy and raining -> $P(C|A) = 0.2$

Estimating the Prior Probability $P(C)$

- The prior probability $P(C_j)$ for each class is estimated by
  - counting the records in the training set that are labeled with class $P(C_j)$
  - dividing the count by the overall number of records
- Example:
  - P(Play=no) = **5**/14
  - P(Play=yes) = **9**/14

Training Data

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

Estimating the Class-Conditional Probability $P(A|C)$

- Naïve Bayes assumes that all attributes are **statistically independent**
  - knowing the value of one attribute says nothing about the value of another
  - this independence assumption is almost never correct!
  - but … this scheme works well in practice
- The **independence assumption** allows the joint probability $P(A|C)$ to be reformulated as the product of the individual probabilities $P(A_i|C_j)$

$$P(A_1, A_2, \ldots, A_n|C_j) = P(A_1|C_j) * P(A_2|C_j) * \ldots * P(A_3|C_j) = \prod_{i=1}^{n} P(A_i|C_j)$$

$$P(\text{Outlook=rainy, Temperature=cool} \mid \text{Play=yes}) = \mathrm{P}(\mathrm{Outlook} = \mathrm{rainy} \mid \mathrm{Play} = \mathrm{yes}) * \mathrm{P}(\text{Temperature=cool} \mid \mathrm{Play} = \mathrm{yes})$$

- Result: The probabilities $P(A_i|C_j)$ for all A_i and C_j can be estimated directly from the training data

Estimating the Probabilities $P(A_i|C_j)$

Outlook			Temperature			Humidity			Windy			Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	2	Cool	3	1								
Sunny	**2/9**	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5		
Rainy	3/9	2/5	Cool	3/9	1/5								

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	**Yes**
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	**Yes**
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

- The probabilities $P(A_i|C_j)$ are estimated by
  - Count how often an attribute value co-occurs with class C_j
  - Divide by the overall number of examples belonging to class C_j

Example:

“Outlook=sunny” occurs on 2/9 examples in class “Yes”

P(Outlook=sunny|Yes) = 2/9

Classifying a New Record

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- Unseen record

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

Class-conditional probability of the record

$$P(yes|A) = P(Outlook = Sunny|yes)$$
$$\times P(Temperature = Cool|yes)$$
$$\times P(Humidity = High|yes)$$
$$\times P(Windy = True|yes)$$
$$\times \frac{P(yes)}{P(A)}$$

Prior probability of class “yes”

Prior probability of record

Probability of class “yes” given the evidence

$$= \frac{\frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{9}{14}}{P(A)}$$

Classifying a New Record

Outlook			Temperature			Humidity			Windy			Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	2	Cool	3	1								
Sunny	**2/9**	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5		
Rainy	3/9	2/5	Cool	3/9	1/5								

- A new day:

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

Class conditional probability

Prior probability

Likelihood of the two classes

For "yes" = 2/9 × 3/9 × 3/9 × 3/9 × 9/14 = 0.0053

For "no" = 3/5 × 1/5 × 4/5 × 3/5 × 5/14 = 0.0206

Conversion into a probability by normalization:

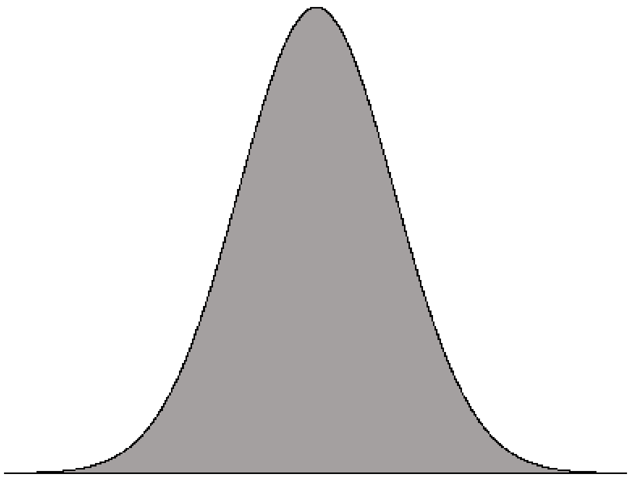
Choose Maximum

P("yes") = 0.0053 / (0.0053 + 0.0206) = 0.205

P("no") = 0.0206 / (0.0053 + 0.0206) = 0.795

Handling Numerical Attributes

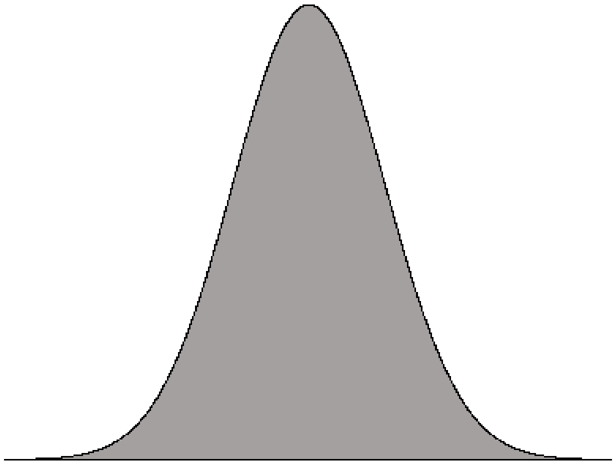
- Option 1:
  Discretize numerical attributes before learning classifier.
  - Temp= 37°C -> "Hot"
  - Temp= 21°C -> "Mild"
- Option 2:
  Make assumption that numerical attributes have a **normal distribution** given the class.
  - use training data to estimate parameters of the distribution (e.g., mean and standard deviation)
  - once the probability distribution is known, it can be used to estimate the conditional probability $P(A_i|C_j)$



Handling Numerical Attributes

- The probability density function for the normal distribution is

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$



- It is defined by two parameters:
  - Sample mean $\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$
  - Standard deviation $\sigma = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \mu)^2}$

- Both parameters can be estimated from the training data

Handling Numerical Attributes

Outlook			Temperature		Humidity		Windy			Play	
	Yes	*No*	*Yes*	*No*	*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	64, 68,	65, 71,	65, 70,	70, 85,	False	6	2	9	5
Overcast	4	0	69, 70,	72, 80,	70, 75,	90, 91,	True	3	3		
Rainy	3	2	72, …	85, …	80, …	95, …					
Sunny	2/9	3/5	μ =73	μ =75	μ =79	μ =86	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	σ =6.2	σ =7.9	σ =10.2	σ =9.7	True	3/9	3/5		
Rainy	3/9	2/5									

- Example calculation:

$$f(temp = 66 \mid yes) = \frac{1}{\sqrt{2\pi} * 6.2} e^{-\frac{(66-73)^2}{2*(6.2)^2}} = 0.034$$

Classifying a New Day

- Unseen record

Outlook	Temp.	Humidity	Windy	Play
Sunny	66	90	true	?

Likelihood of "yes" = 2/9 × 0.0340 × 0.0221 × 3/9 × 9/14 = 0.000036

Likelihood of "no" = 3/5 × 0.0291 × 0.0380 × 3/5 × 5/14 = 0.000136

P("yes") = 0.000036 / (0.000036 + 0. 000136) = 20.9%

P("no") = 0.000136 / (0.000036 + 0. 000136) = 79.1%

- **But note:** Some numeric attributes are not normally distributed, and you may thus need to choose a different probability density function or use discretization

Handling Missing Values

- Missing values may occur in training and in unseen classification records
- **Training:** Record is not included into frequency count for attribute value-class combination
- **Classification:** Attribute will be omitted from calculation
  - Example: Unseen record

Outlook	Temp.	Humidity	Windy	Play
?	Cool	High	True	?

Likelihood of “yes” = 3/9 × 3/9 × 3/9 × 9/14 = 0.0238

Likelihood of “no” = 1/5 × 4/5 × 3/5 × 5/14 = 0.0343

P(“yes”) = 0.0238 / (0.0238 + 0.0343) = 41%

P(“no”) = 0.0343 / (0.0238 + 0.0343) = 59%

The Zero-Frequency Problem

- What if an attribute value doesn't occur with every class value? (e.g. no "Outlook = overcast" for class "no")
  - class-conditional probability will be zero! $P(Outlook = Overcast|no) = \frac{0}{5} = 0$
- Problem: Posterior probability will also be zero! $P(no|A) = 0$
  No matter how likely the other values are!
- Remedy: Add 1 to the count for every attribute value-class combination (**Laplace Estimator**)
- Result: Probabilities will never be zero!
  also: stabilizes probability estimates
- Original: $P(\mathrm{A_i}|\mathrm{C}) = \frac{N_{ic}}{N_c}$ Laplace: $P(\mathrm{A_i}|\mathrm{C}) = \frac{N_{ic}+1}{N_c+c}$

c = number of attribute values of A

Using Conditional Probabilities for Naïve Bayes

Result Overview | ExampleSet (Retrieve Golf-Testset)

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

ExampleSet (14 examples, 4 special attributes, 4 regular attributes) View Filter (14 / 14):

Row No.	Play	confidence(no)	confidence(yes)	prediction(Play)	Outlook	Temperature	Humidity	Wind
1	yes	0.711	0.289	no	sunny	85	85	false
2	no	0.058	0.942	yes	overcast	80	90	true
3	yes	0.014	0.986	yes	overcast	83	78	false
4	yes	0.412	0.588	[illegible]	[illegible]	[illegible]	96	false
5	yes	0.460	0.540	[illegible]	[illegible]	[illegible]	80	true
6	no	0.336	0.664	[illegible]	[illegible]	[illegible]	70	true
7	yes	0.010	0.990	yes	overcast	64	65	true
8	no	0.596	0.404	no	sunny	72	95	false
9	yes	0.248	0.752	yes	sunny	69	70	false
10	no	0.407	0.593	yes	sunny	75	80	false
11	yes	0.496	0.504	yes	sunny	68	70	true
12	yes	0.038	0.962	[illegible]	[illegible]	[illegible]	90	true
13	no	0.027	0.973	[illegible]	[illegible]	[illegible]	75	true
14	yes	0.453	0.547	[illegible]	[illegible]	[illegible]	80	true

Classifier is **quite** sure

Classifier is **not** sure

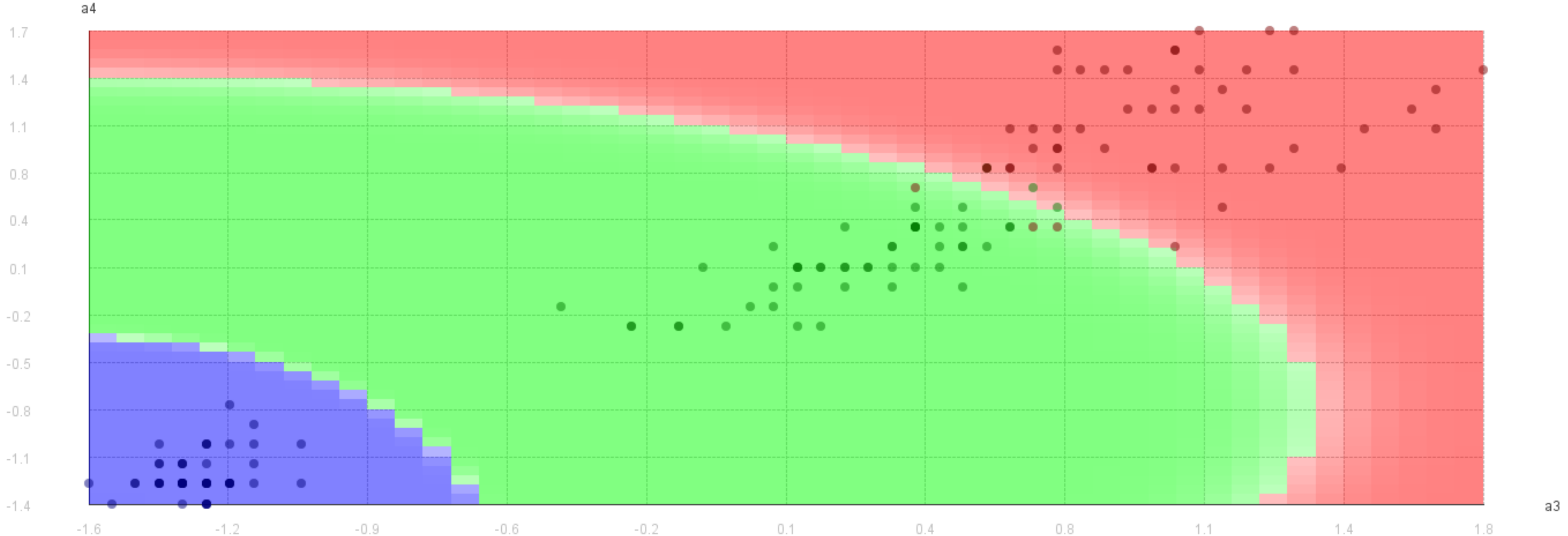
Python

```python
from sklearn.naive_bayes import MultinomialNB
from sklearn.naive_bayes import GaussianNB

# Train classifier
estimator = MultinomialNB(alpha=1.0)
estimator.fit(preprocessed_training_data, training_labels)
```

Decision Boundary of Naive Bayes Classifier

- Usually larger coherent areas
- Soft margins with uncertain regions
- Arbitrary (often curved) shapes



Naïve Bayes Discussion

- Naïve Bayes **works surprisingly well**
  - Even if independence assumption is clearly violated
  - Classification doesn't require accurate probability estimates as long as maximum probability is assigned to correct class
- Robust to **isolated noise points** as they will be averaged out
- Robust to **irrelevant attributes** as $P(\mathrm{A_i}|\mathrm{C})$ distributed uniformly for A_i
- Adding too many redundant attributes can cause problems
  - Solution: Select attribute subset as Naïve Bayes often works better with just a fraction of all attributes
- Technical advantages
  - learning Naïve Bayes classifiers is computationally cheap (probabilities can be estimated doing one pass over the training data)
  - Storing the probabilities does not require a lot of memory

Support Vector Machines

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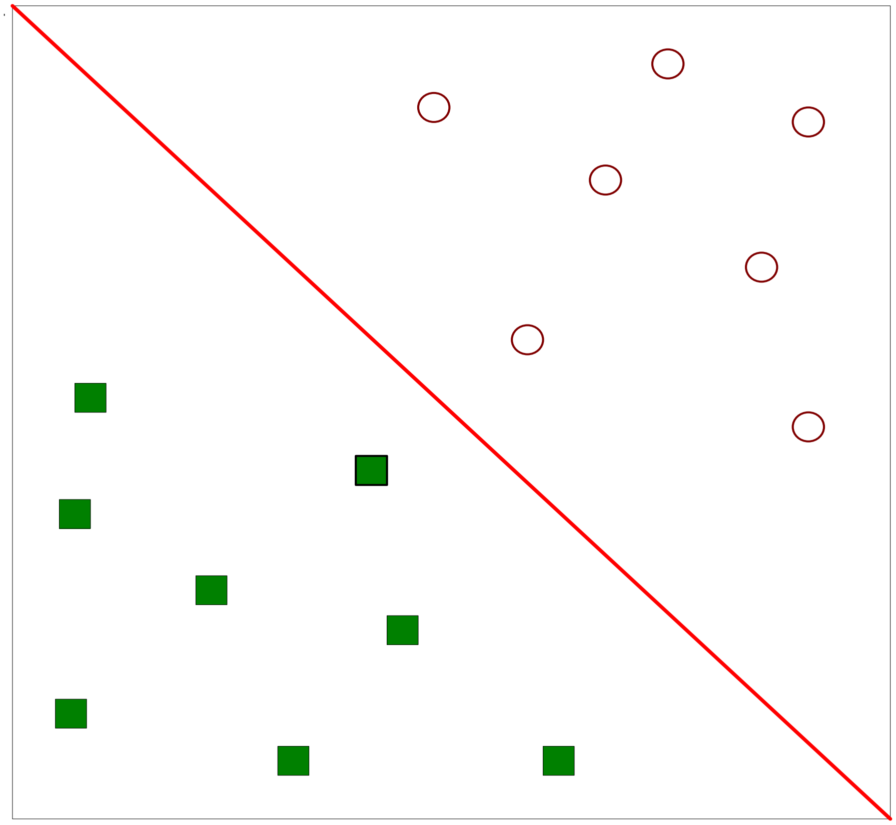
- Support vector machines (SVMs) are algorithms for learning linear classifiers for
  - **Two class problems** (a positive and a negative class)
  - From examples described by continuous attributes
- SVMs
  - achieve **very good results** especially for high dimensional data
  - invented by V. Vapnik and his co-workers in 1970s in Russia and became known to the West in 1992

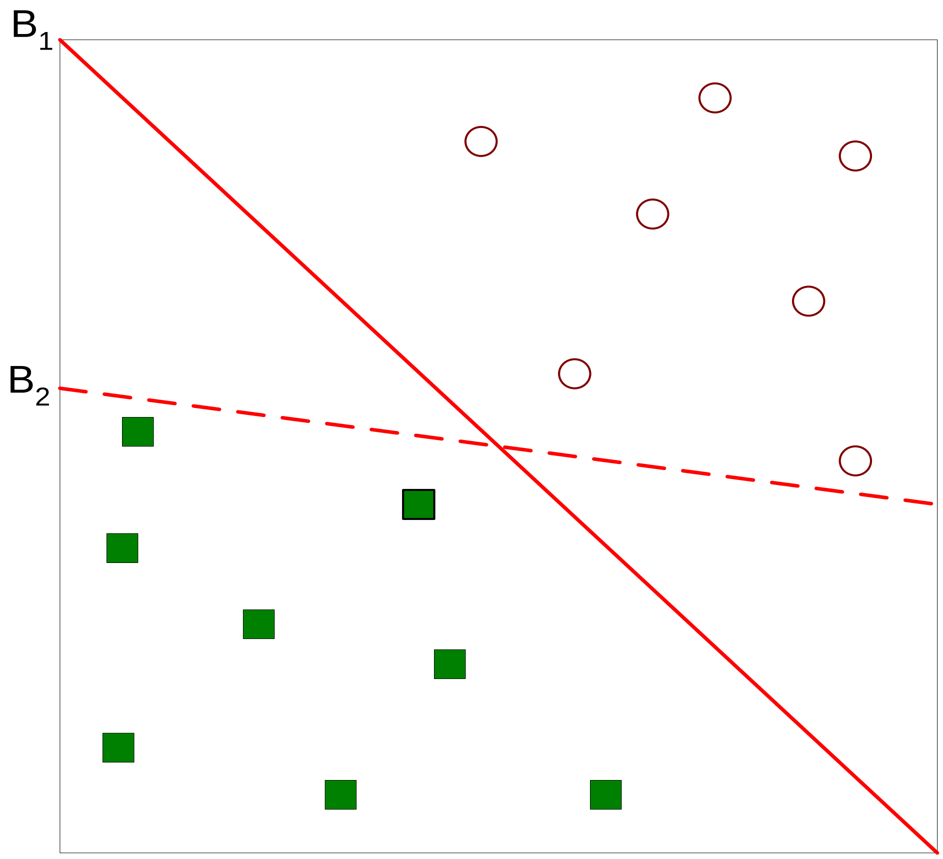
Support Vector Machines

- Find a linear hyperplane (decision boundary) that will separate the data



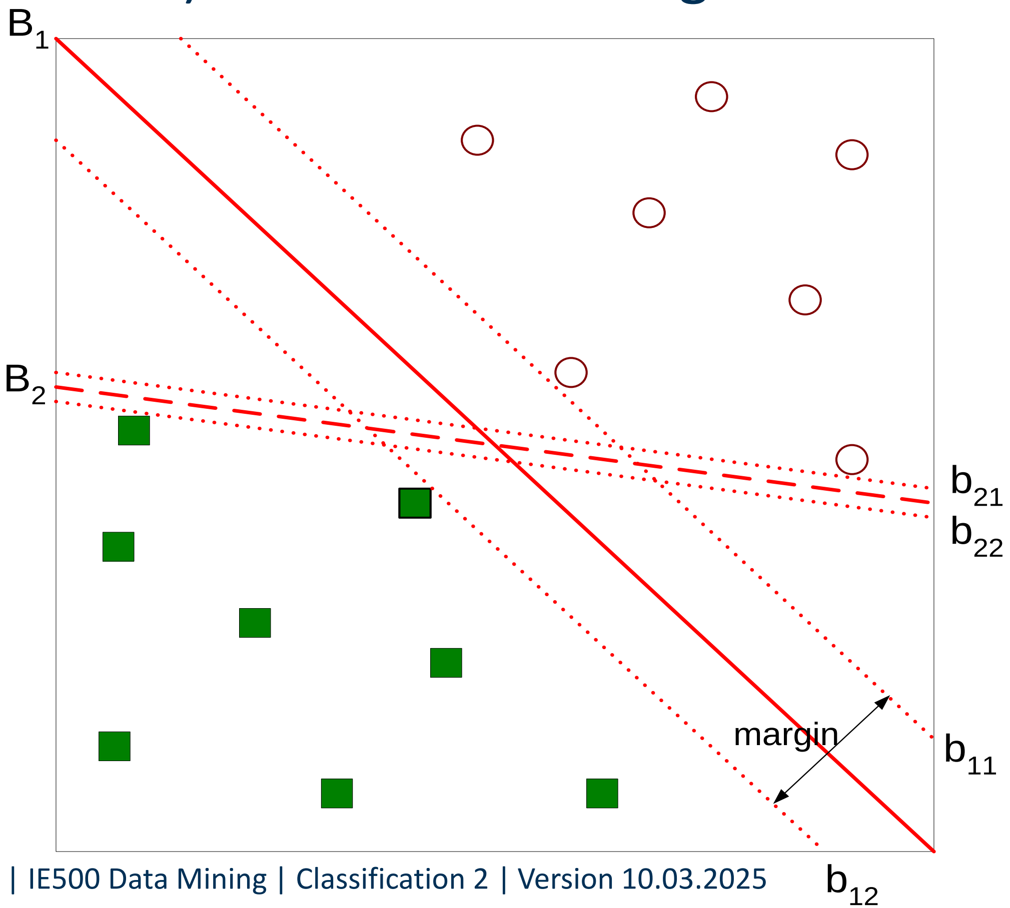
Which Hyperplane is better?

- Which one is better? B1 or B2? How do you define “better”?



Which Hyperplane is better?

- Find hyperplane **maximizes** the margin to the closest points (support vectors) to avoid overfitting => B1 is better than B2



Which Hyperplane is better?

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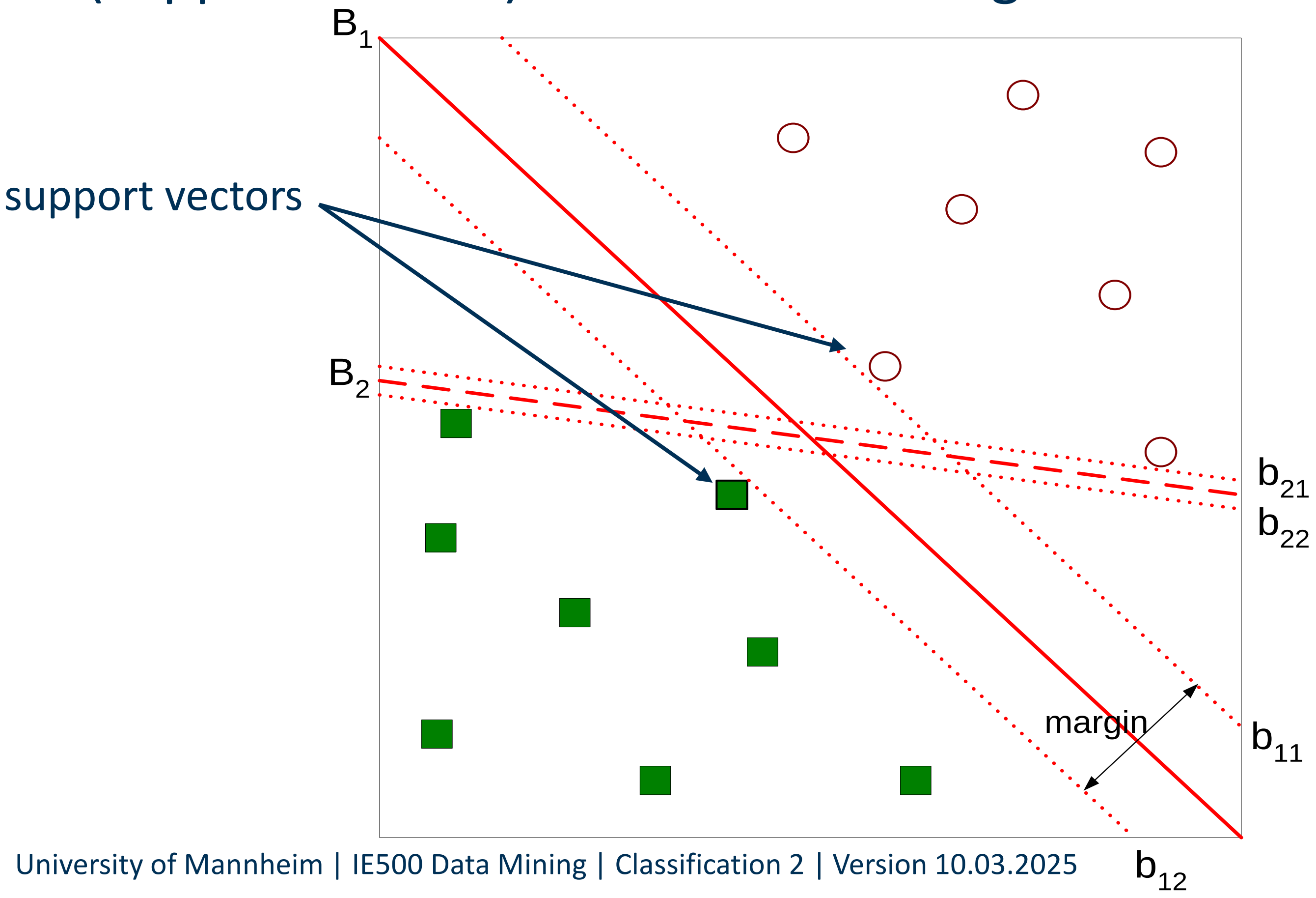
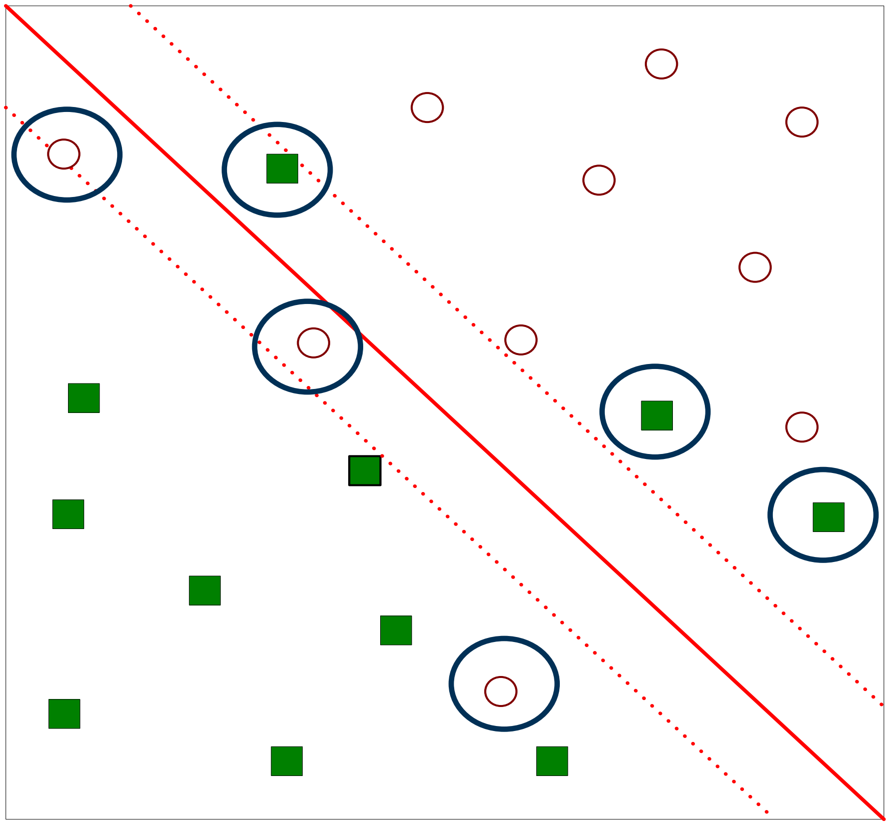


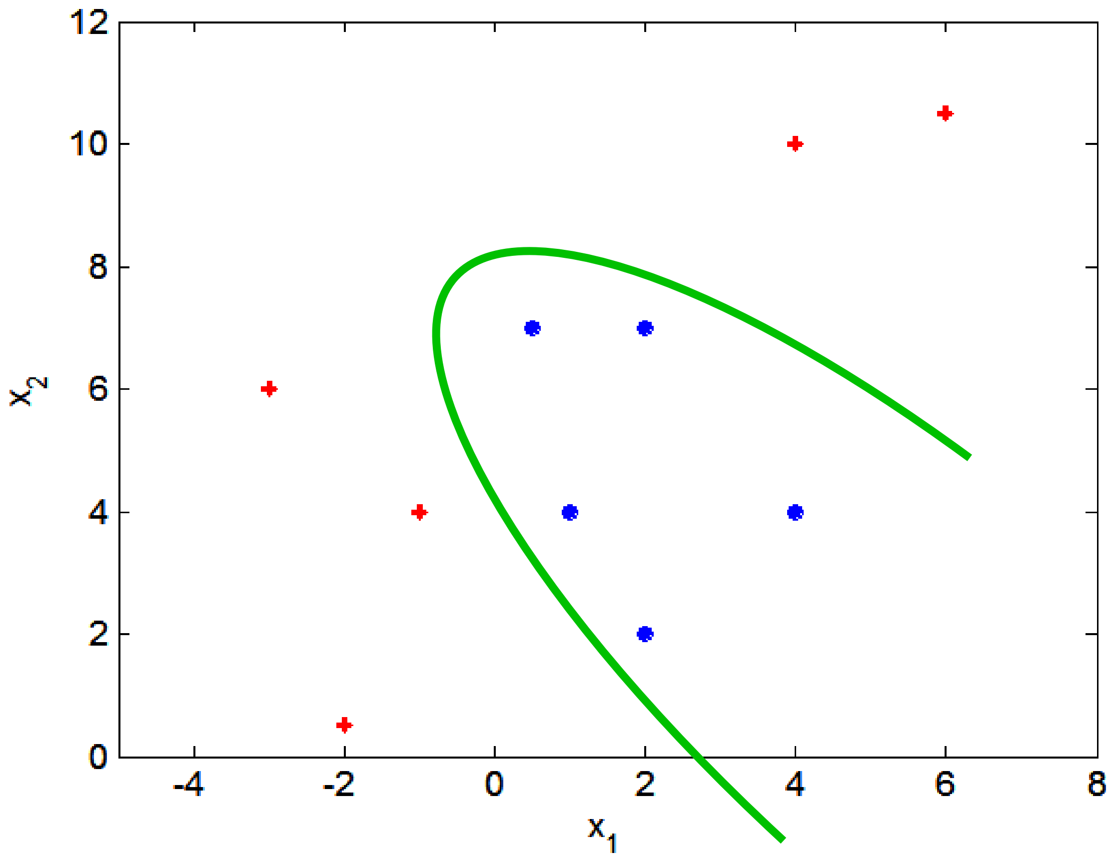
Dealing with
Not Linearly Separable Data

- Introduce **slack variables** in margin computation which result in a penalty for each data point that violates decision boundary



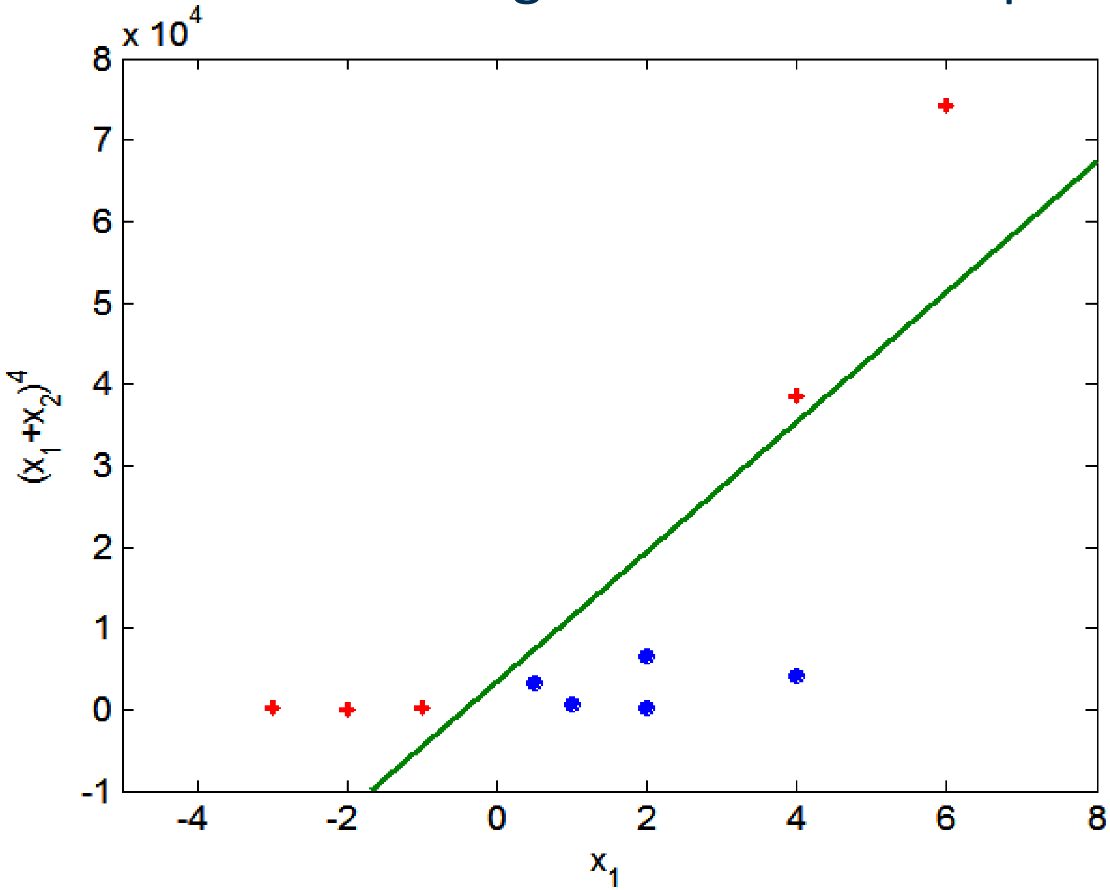
Nonlinear Support Vector Machines

- What if decision boundary is not linear?



Nonlinear Support Vector Machines

- Transform data into higher dimensional space



Nonlinear Support Vector Machines

- Transformation in higher dimensional space
  - Uses so-called Kernel function
  - Different variants: polynomial function, radial basis function, …

- Finding a hyperplane in higher dimensional space
  - is computationally expensive
  - Kernel trick: expensive parts of the calculation can be performed in lower dimensional space
- Python:

```
from sklearn.svm import SVC

# Train classifier
estimator = SVC(C=1.0, kernel='rbf')
estimator.fit(scaled_training_data, training_labels)
```

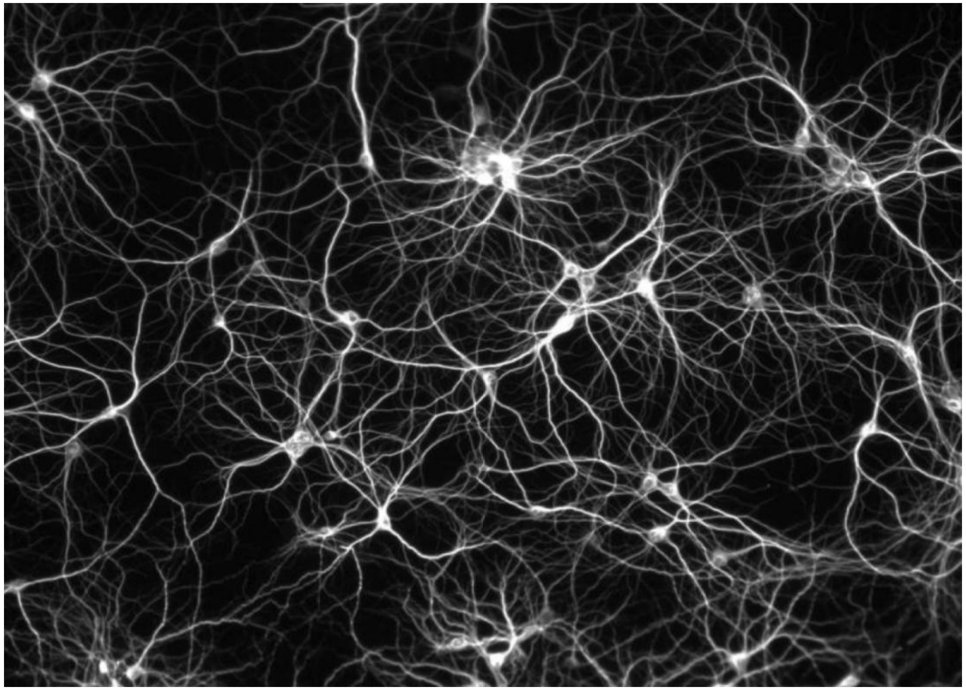
Tuning of SVM

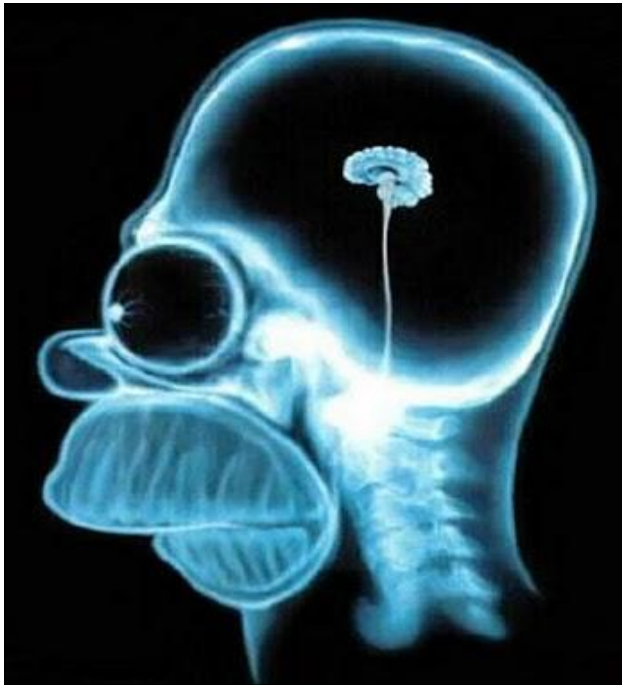
- Instead of randomly trying a few kernel and parameters Hsu et al. proposes a systematic method
  1. Linearly **scaling** each attribute to the range [−1, +1] or [0, 1]
  2. Use **RBF Kernel**
  3. Use **cross-validation** to find the best parameter C and γ
     - trying exponentially growing sequences of C and γ
       e.g. $C = 2^{-5}, 2^{-3}, \ldots, 2^{15}$ γ=$2^{-15}, 2^{-13}, \ldots, 2^{3}$
  4. Use the best parameter C and γ to **train the whole training set**
  5. **Test**

Chih-Wei Hsu, Chih-Chung Chang, and Chih-Jen Lin:
A Practical Guide to Support Vector Classification

Artificial Neural Networks (ANN)

- Inspiration
  - one of the most powerful super computers in the world

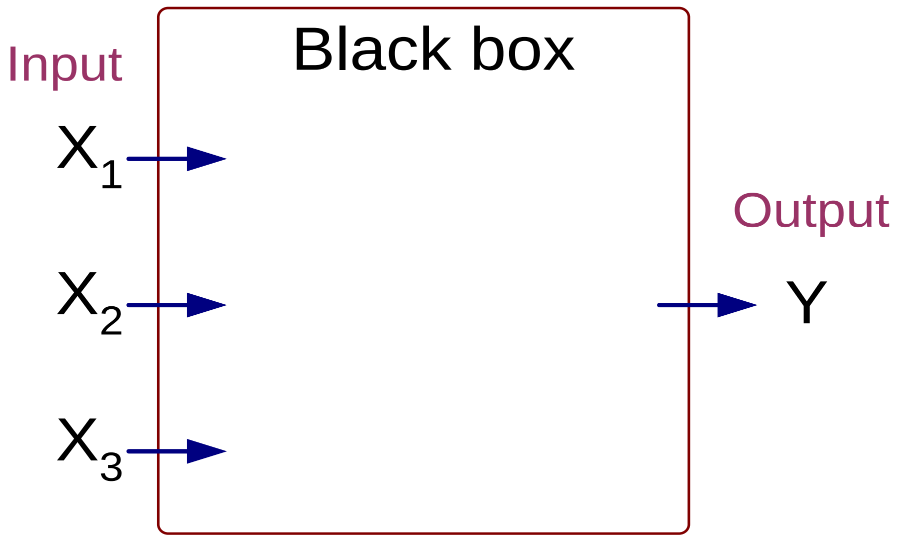




Artificial Neural Networks (ANN)

- Function fitting the training data:
  Output Y is 1 if at least two of the three inputs are equal to 1

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

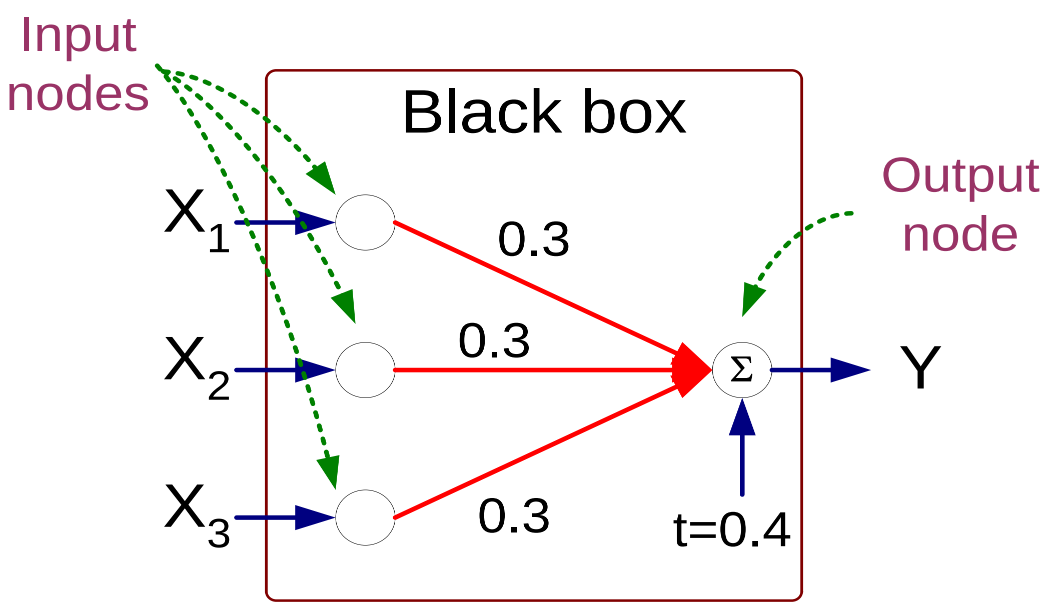


Artificial Neural Networks (ANN)

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

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

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

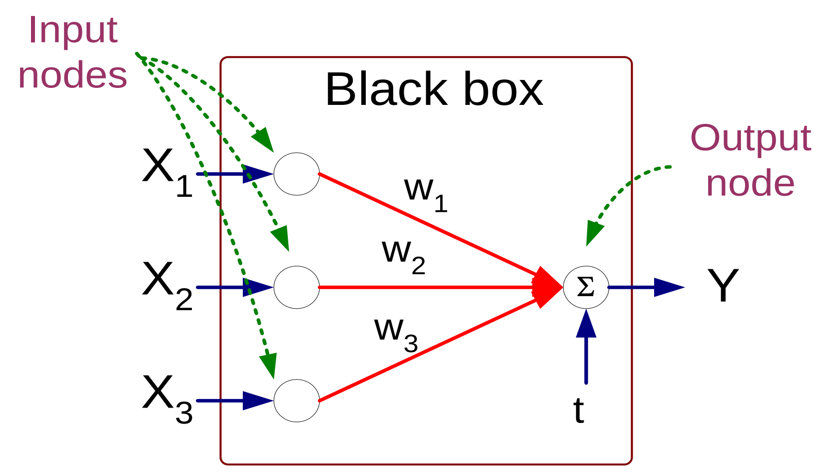


Artificial Neural Networks (ANN)

- Model is an assembly of inter-connected nodes (called neurons) and weighted links

- Output node sums up each of its input values according to the weights of its links

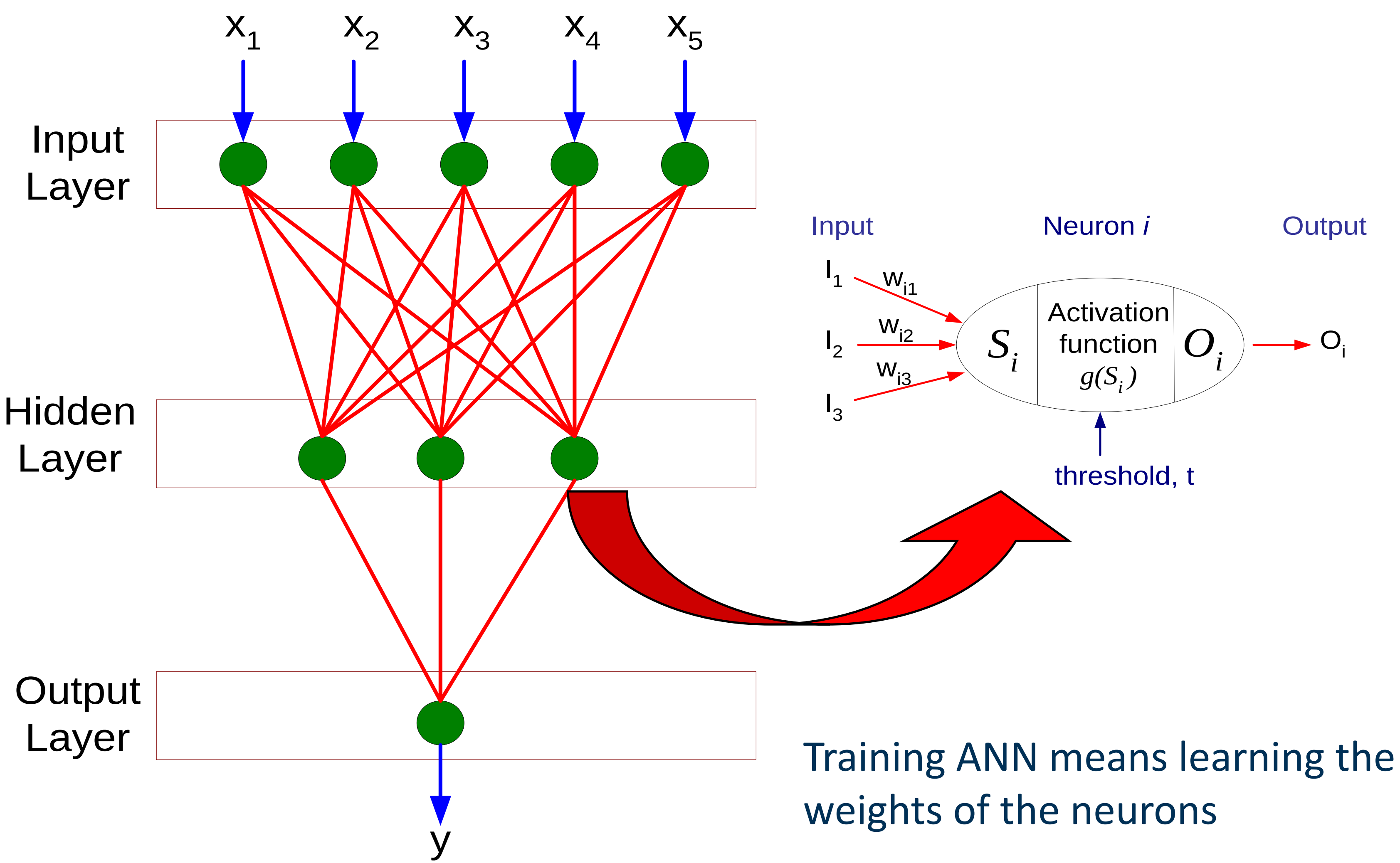
- Classification decision: Compare output node against some threshold t



Perceptron Model

$$Y = I\left(\sum w_i X_i - t > 0\right)$$

Multi-Layer Artificial Neural Networks

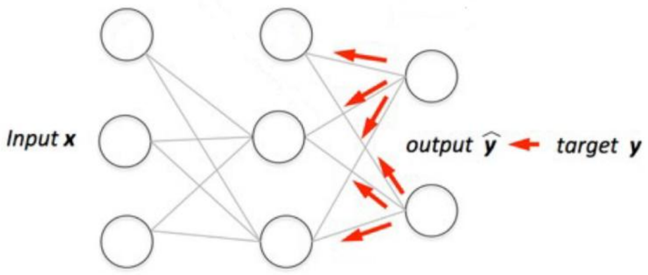


Training ANN means learning the weights of the neurons

Algorithm for Training ANNs

1. Initialize the weights (w_0, w_1, …, w_k), e.g., random or pre-trained

2. Adjust the weights in such a way that the output of ANN is as consistent as possible with class labels of the training examples
   - Objective function: $E = \sum_i [Y_i - f(w_i, X_i)]^2$
   - Find the weights w_i's that minimize the sum of squared error E
   - using the **back propagation algorithm** (see Tan/Steinbach: Chapter 6.7, Gemulla: Machine Learning)
   - Adjustment factor: learning rate



Python

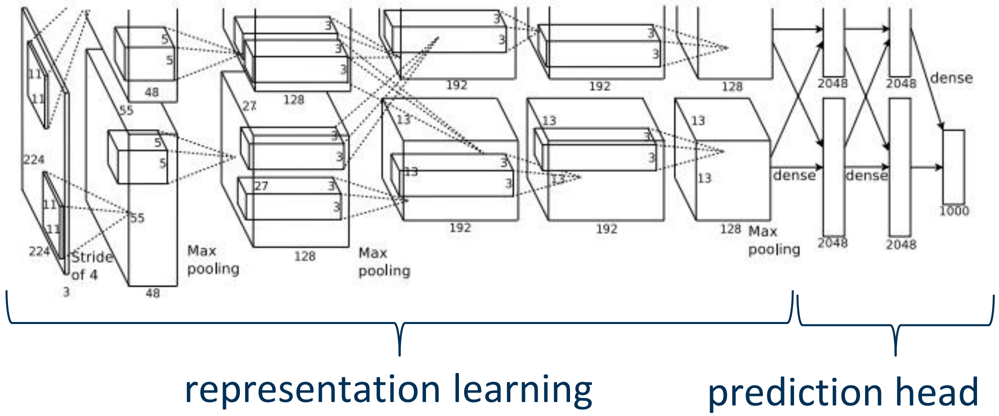
```
from sklearn.neural_network import MLPClassifier

# Train classifier
neuralnet = MLPClassifier(hidden_layer_sizes=(100, ), learning_rate_init=.1)
neuralnet.fit(training_data, training_labels)
```

Overview: Types of Deep Learning Models

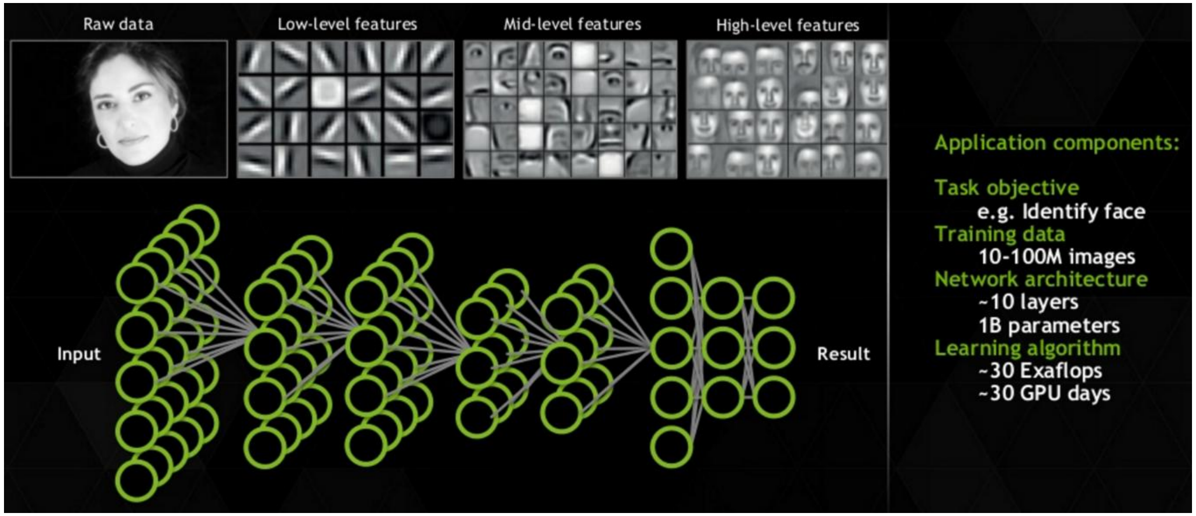
- Convolutional Neural Networks
- Pre-Trained Language Models: BERT
- Generative Models: T5, GPT3, DALL·E
- Instruct Models: ChatGPT, LaMDA

Convolutional Neural Networks (CNNs)

- Invented in computer vision
- Combine
  1. Representation learning (convolutions and pooling)
  2. Prediction head (densely connected layers)

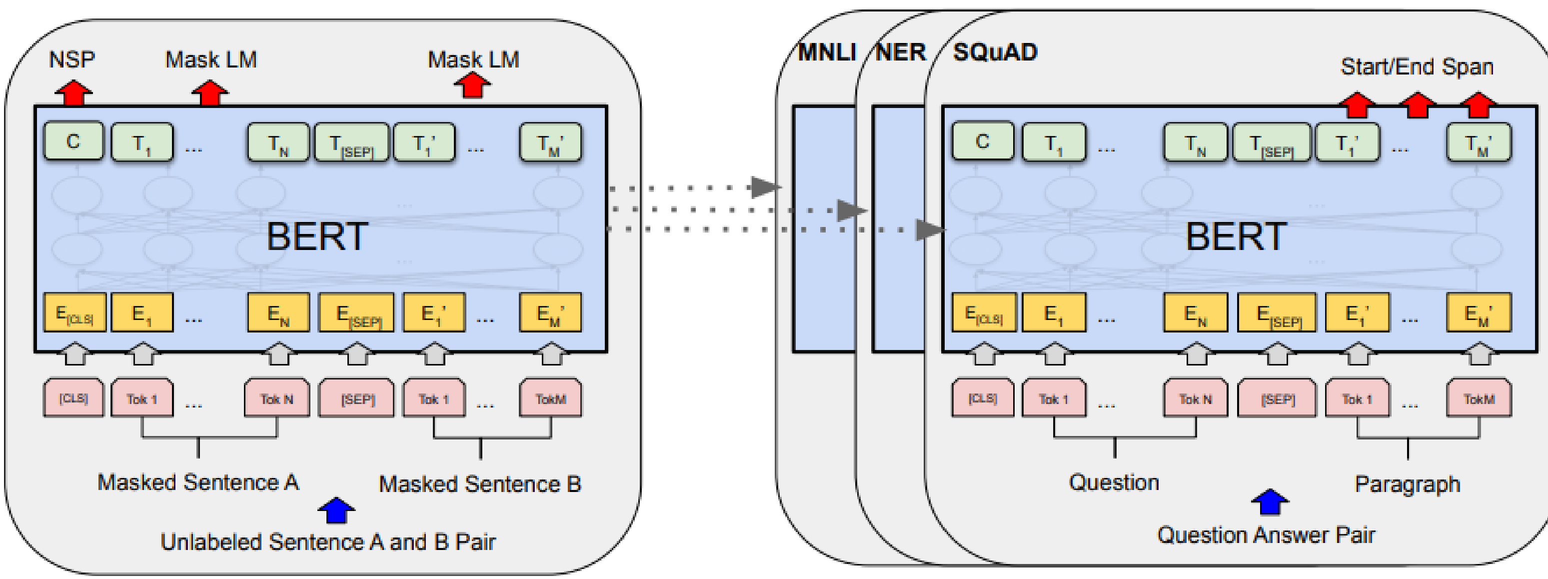


- Reduce number of input features via convolutions and pooling
- High capacity of models requires
  - Lots of training data
  - Lots of GPU time



Pre-Trained Language Models

- Introduce pre-training, fine-tuning paradigm
  - Pre-trained on large text corpora
  - Model size: BERT-base 110 million parameters
- Outperform previous models on most NLP tasks

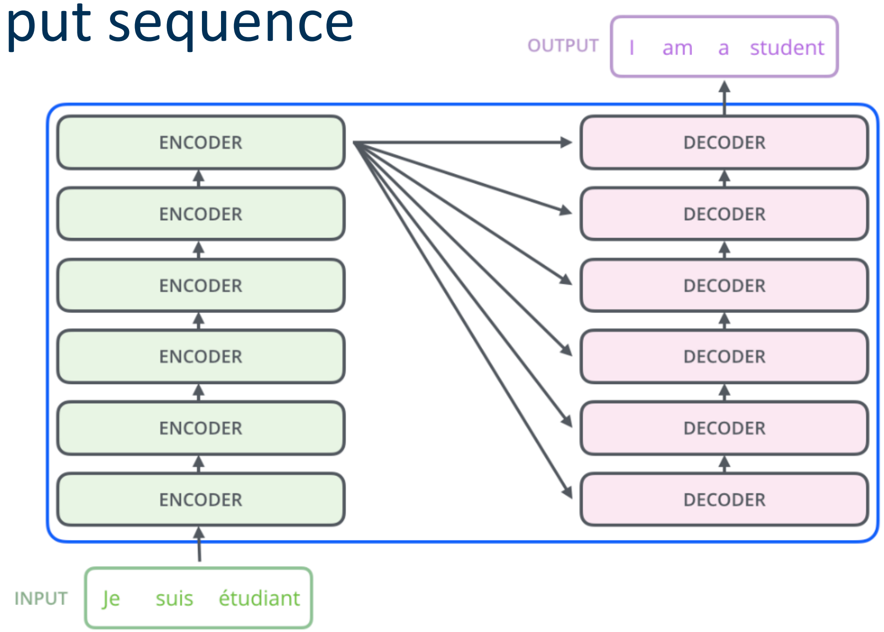


Pre-training

Fine-Tuning

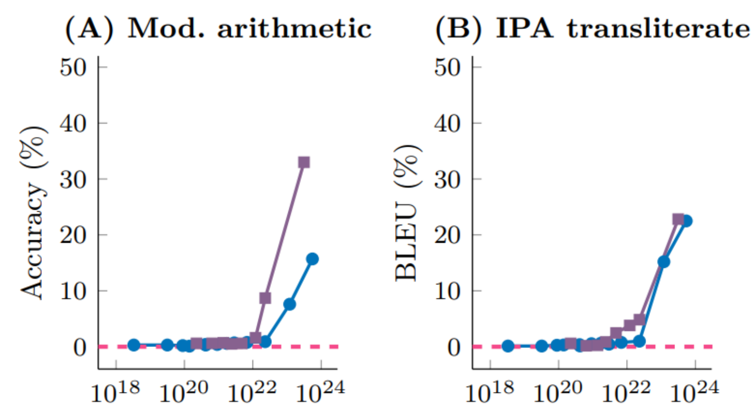
Generative Models

- Use transformer architecture to generate text or images based on embeddings of input sequence
- Models for Text
  - T5, GPT3
- Models for Images
  - DALL·E, Stable Diffusion
- Pretrained on large text and image corpora
  - Web crawls
  - ImageNet, LAION-5B
- Model sizes: 5 to 175 billion parameters
  - accessible mostly via APIs



Instruct Language Models

- After being pre-trained on large text corpora, instruct models are fine-tuned with instruction/output pairs
- Show good few-shot performance on wide range of task
  - BIG-bench collects 200+ tasks
- Models show emergent abilities
  - Can perform tasks they were not directly trained for
- Prompt design and in-context learning determine performance of frozen models



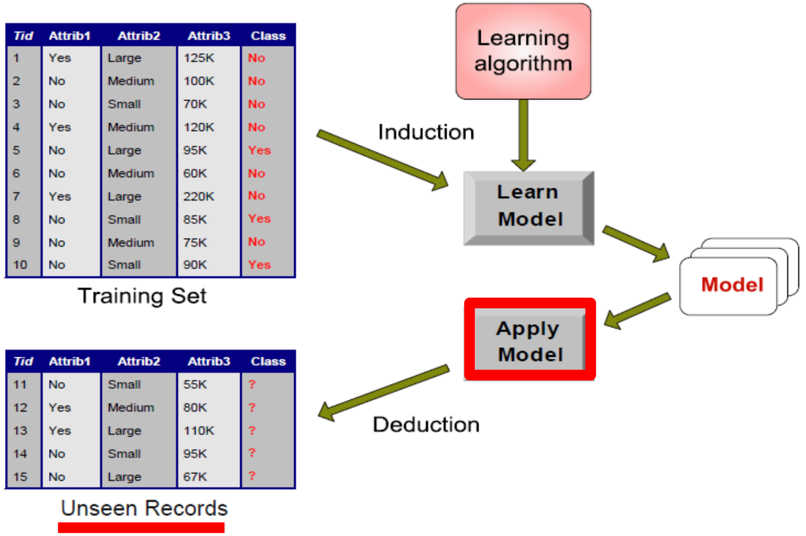
Wei: Emergent Abilities of Large Language Models. TMLR 2022.

Model Evaluation

- Central Question:
  - How good is a model at classifying unseen records? (generalization performance)

- Last week: **Evaluation Metrics**
  - How to measure the performance of a model?

- **This week: Evaluation Methods**
  - How to obtain reliable estimates?



Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

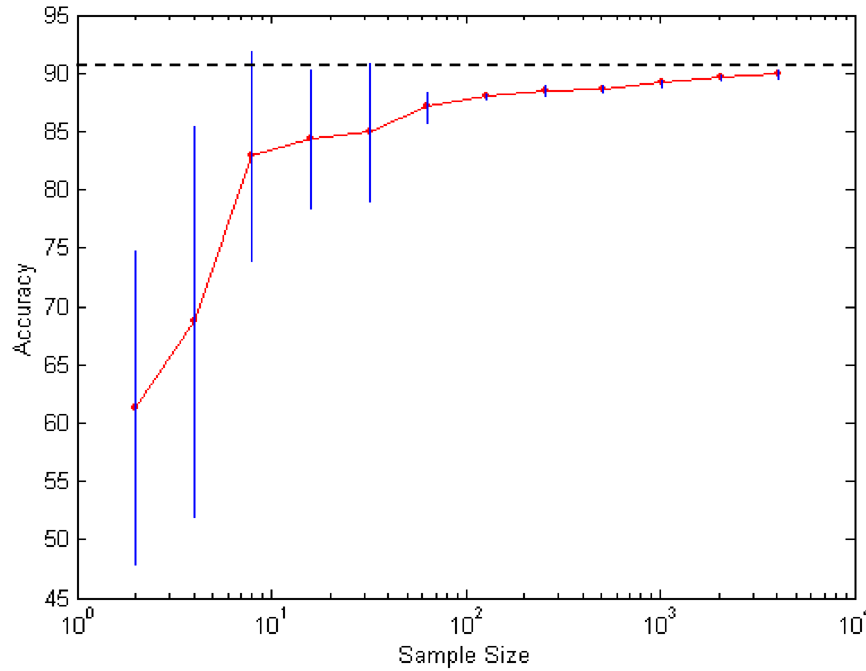
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Model Evaluation

- How to obtain a reliable estimate of the generalization performance?
- General approach: Split labeled records into
  a training set and a test set
- **Never ever test a model on data that was used for training!**
  - Because model has been fit to training data, evaluating on training data does not result in a suitable estimate of the performance on unseen data
  - We need to keep training set and test set strictly separate
- Which labeled records to use for training and which for testing?
- Alternative splitting approaches:
  - Holdout Method
  - Random Subsampling
  - Cross Validation

Learning Curve

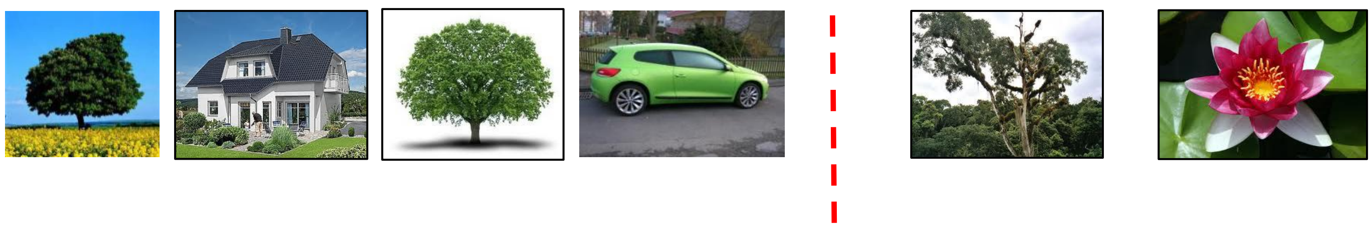
- The learning curve shows how accuracy changes with growing training set size
- Conclusion:
  - If model performance is low and unstable, get more training data
  - Use labeled data rather for training than testing
- Problem:
  - Labeling additional data is often expensive due to manual effort involved



Holdout Method

- The **holdout method** reserves a certain amount of the labeled data for testing and uses the remainder for training
  - applied when **lots of sample data** is available
- Usually: 2/3 for training , 1/3 for testing (or even better 80% / 20%)

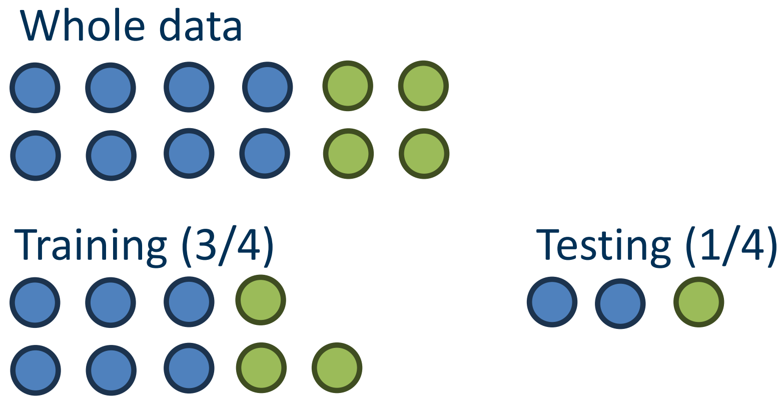
Training Set Test Set



- For imbalanced datasets, random samples might not be representative
  - few or no records of the minority class (aka positive class) in training or test set

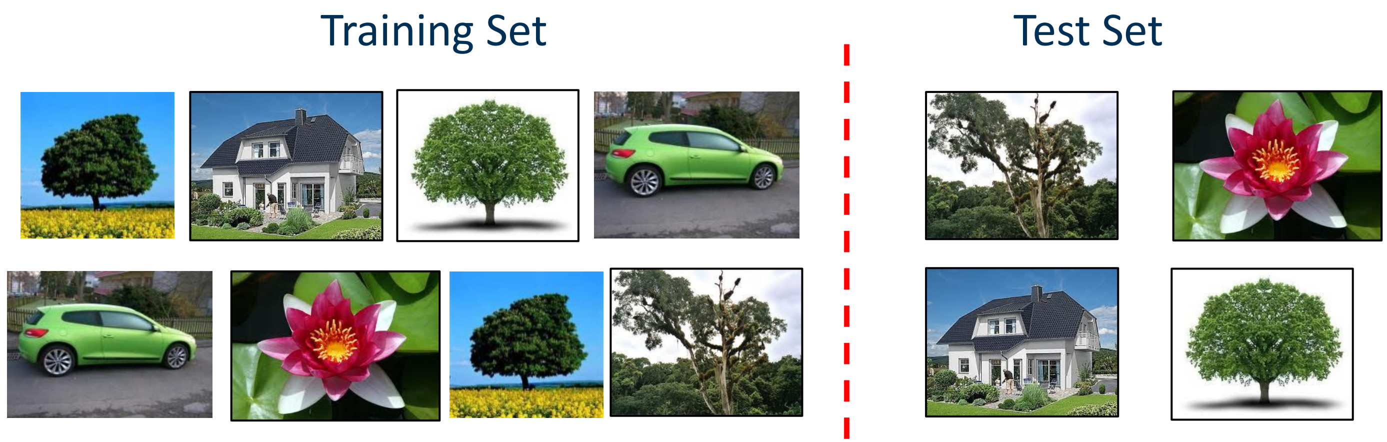
Stratified Sampling

- **Stratified sample:** Sample each class independently, so that records of the minority class are present in each sample
  - Make sure that each class is represented with approximately equal proportions in both subsets
  - Other attributes may also be considered for stratification
    - e.g., gender, age, …



Random Subsampling

- Holdout estimate can be made more reliable by repeating the process with different subsamples
  - In each iteration, a certain proportion is randomly selected for training
  - The performance of the different iterations is averaged



- Still not optimal as the different test sets may overlap
  - Problem: some outliers might always end up in the test sets
  - Problem: important records for learning (red tree) might always be in test sets

Leave One Out

- Iterate over all examples
  - Train a model on all examples but the current one
  - Evaluate on the current one

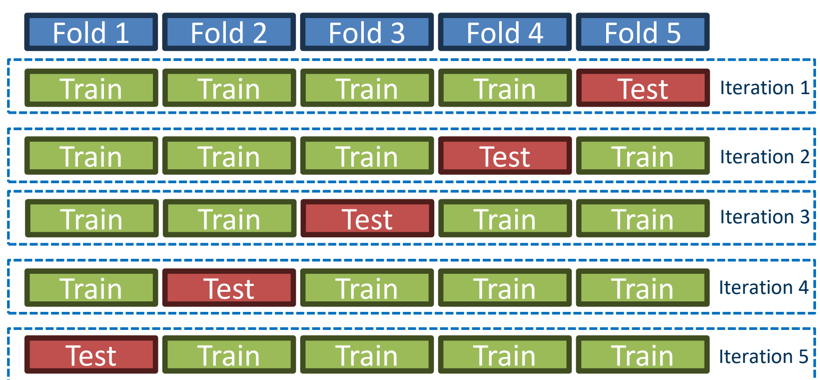
- Yields a very accurate estimate
- Uses as much data for training as possible
  - But is computationally infeasible in most cases

- Imagine: a dataset with a million instances
  - One minute to train a single model
  - Leave one out would take almost two years

Cross-Validation

- Compromise of Leave One Out and decent runtime
- Cross-validation avoids overlapping test sets
  - First step: data is split into k subsets of equal size
    - Stratification may be applied
  - Second step: each subset in turn is used for testing and the remainder for training
- This is called k-fold cross-validation
- The error estimates are averaged to yield an overall error estimate

5-fold cross-validation



Cross-Validation

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- Frequently used value for k : 10
  - Why ten? Extensive experiments have shown that this is a good choice to get an accurate estimate
  - Often the subsets are generated using stratified sampling (to deal with class imbalance)
  - Recent works on very large models have lead to a tendency of lowering that value (default value in scikit-learn is 5)

Python

```
from sklearn.model_selection import StratifiedKFold
from sklearn.model_selection import cross_val_score

# Specify how examples are split
cross_val = StratifiedKFold(n_splits=10, shuffle=True, random_state=42)

# Run cross-validation and caclulate performance metric
accuracy = cross_val_score(estimator, data, target, cv=cross_val, scoring='accuracy')
```

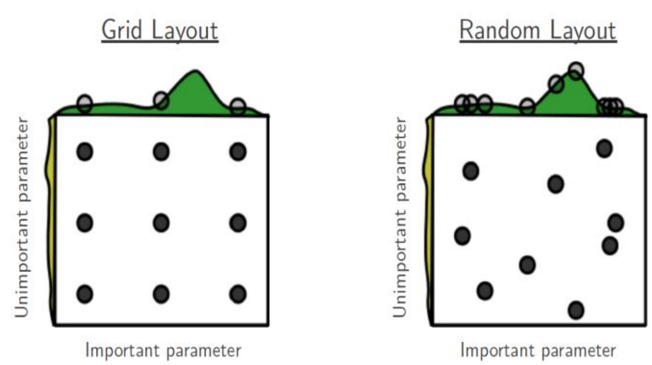
Hyperparameter Selection

- A **hyperparameter** is a parameter which influences the learning process and whose value is set **before the learning begins**
  - pruning thresholds for trees and rules
  - gamma and C for SVMs
  - learning rate, hidden layers for ANNs
- By contrast, **parameters** are learned during training / from training data
  - weights in an ANN, probabilities in Naïve Bayes, splits in a tree
- Many methods work poorly with the default hyperparameters ☹
- How to determine good hyperparameters?
  - Manually play around with different hyperparameter settings
  - Have your machine automatically test many different settings (hyperparameter optimization)

Hyperparameter Optimization

- Goal: Find the combination of hyperparameter values that results in learning the model with the lowest generalization error
- How to determine the parameter value combinations to be tested?
  - **Grid Search**: Test all combinations in user-defined ranges
  - **Random Search**: Test combinations of random parameter values

- Paper from 2012 (Bergstra and Bengio):
  - Grid search may easily miss best parameters
    - some hyperparameters are pretty sensitive e.g., 0.02 is a good value, but 0 and 0.05 are not
  - Random search often yields better results

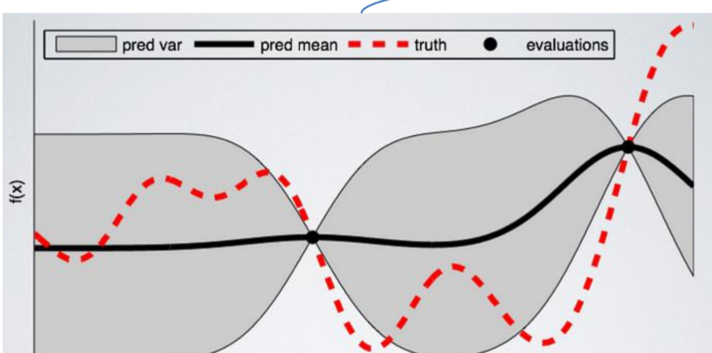


Bergstra & Bengio: Random Search for Hyper-Parameter Optimization, JMLR, 2012

Hyperparameter Optimization

- **Evolutionary Search**
  - Keep specific parameter values that worked well
- **Bayesian optimization**
  - Hyperparameter tuning as a learning problem:
    - Given a set of hyperparameters p, predict evaluation score s of model
    - The prediction model is referred to as a **surrogate model** or oracle
  - Training and evaluating an actual model is costly

“test these hyperparameters, please”



“here’s the performance of those hyperparameters”

Surrogate Model

Actual Model

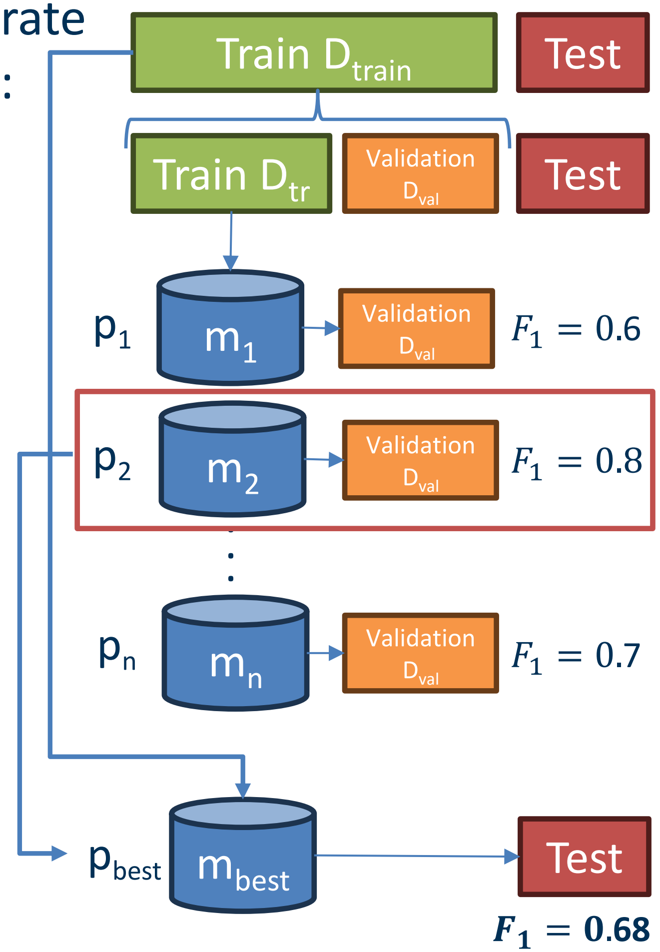
https://www.cs.toronto.edu/~rgrosse/courses/csc411_f18/tutorials/tut8_adams_slides.pdf

Hyperparameter Optimization

- Done:
  - Which hyperparameter combinations should be tested
  - Often hundreds of combinations are tested
    - reason for cloud computing
- Now:
  - **Model Selection**: From all learned models M, select the model m_{best} that is expected to generalize best to unseen records
    - On which data should the model be tested?

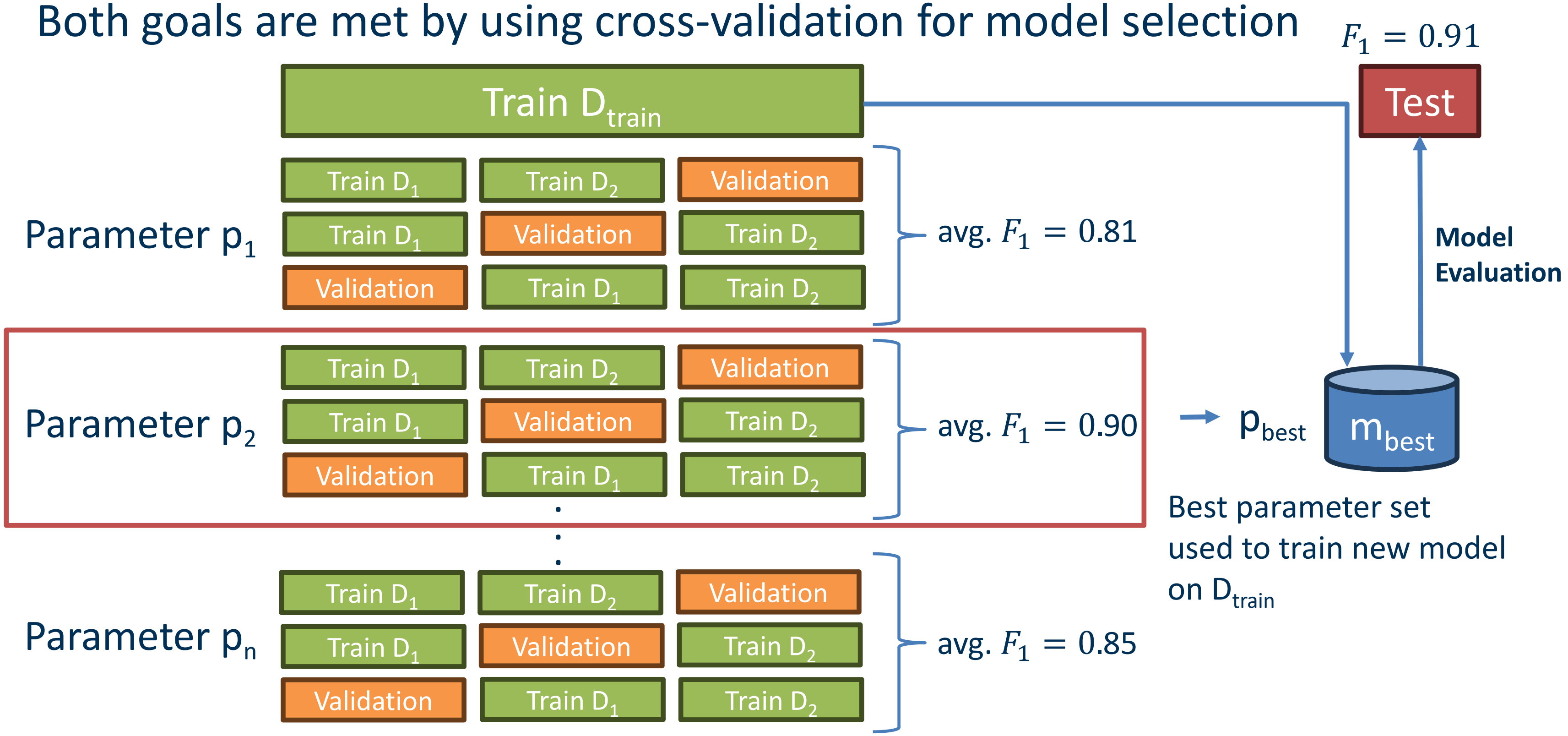
Model Selection Using a Validation Set

- Keep data used for model selection strictly separate from data used for model evaluation, otherwise:
  - Selected model m_{best} will overfit to test set
  - Estimate of generalization error is too optimistic
- Method to find the best model:
  1. Split training set D_{train} into validation set D_{val} and training set D_{tr}
  2. Learn models m_i on D_{tr} using different hyperparameter value combinations p_i
  3. Select best parameter values p_{best} by testing each model m_i on the validation set D_{val}
  4. Learn final model m_{best} on complete D_{train} using the parameter values p_{best}
  5. Evaluate m_{best} on test set in order to get an unbiased estimate of its generalization performance



Model Selection Using Cross-Validation

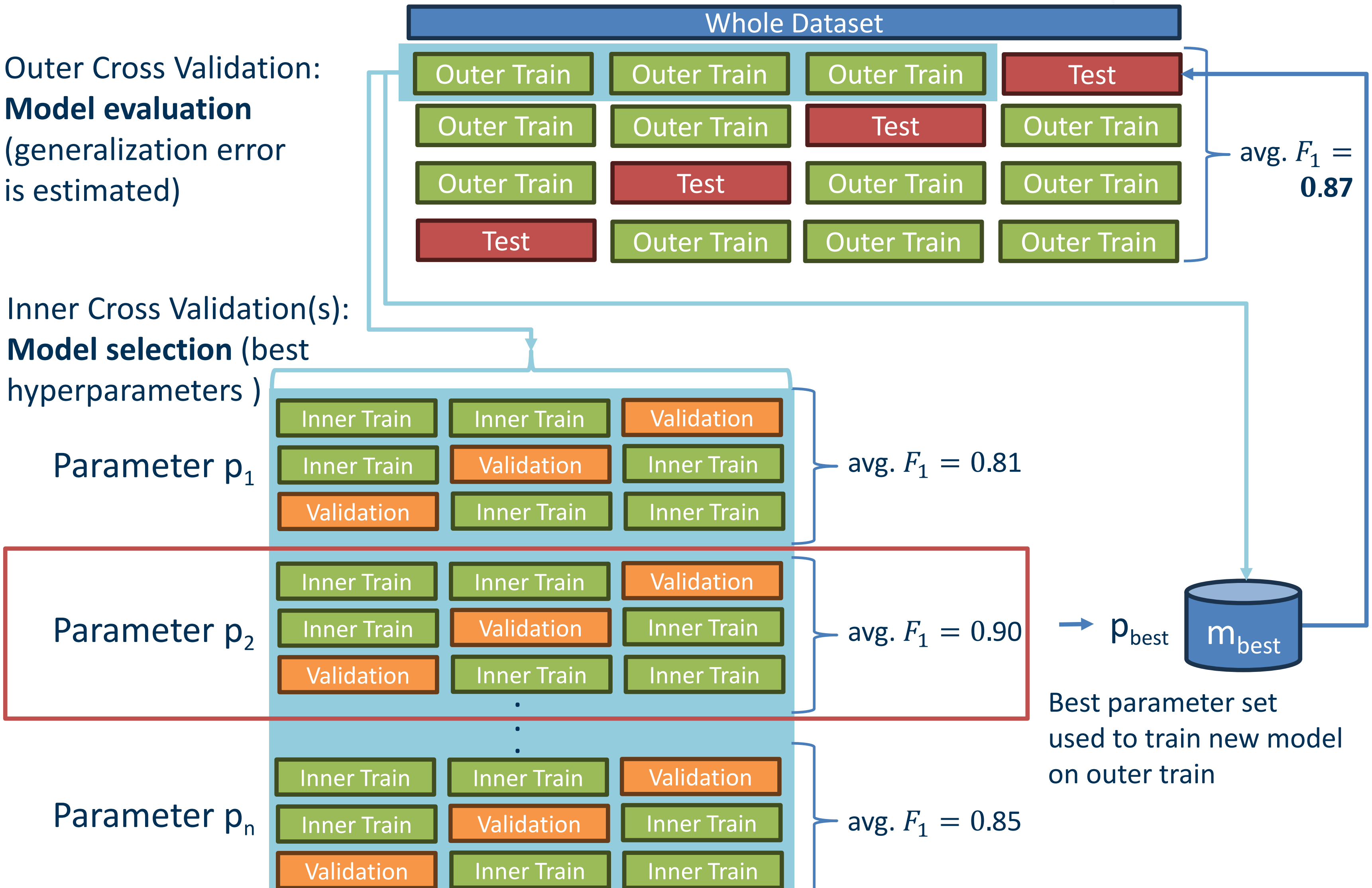
- But wait, we want to
  1. Make sure that all examples are used for validation once
  2. Use as much labeled data as possible for training
- Both goals are met by using cross-validation for model selection



Nested Cross-Validation

Outer Cross Validation:
Model evaluation
(generalization error
is estimated)

Inner Cross Validation(s):
Model selection (best
hyperparameters)



Best parameter set
used to train new model
on outer train

Nested Cross-Validation in Python

Python

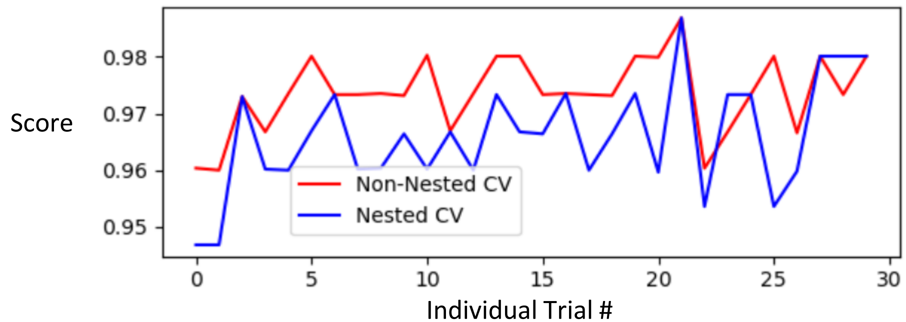
```
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import cross_val_score
from sklearn.svm import SVC

# Specify hyperparameter combinations for search
parameter_grid = {"C": [1, 10, 100, 1000], "gamma": [.001, .01, .1, 1]}

# Create SVM
estimator_svm = SVC(kernel='rbf')

# Create the grid search for model selection
estimator_gs = GridSearchCV(estimator_svm, parameter_grid, scoring='accuracy', cv=5)

# Run nested cross-validation for model evaluation
accuracy_cv = cross_val_score(estimator_gs, dataset, labels, cv=5, scoring='accuracy')
```

scikit-learn Documentation: Tuning the hyper-parameters of an estimator
https://scikit-learn.org/stable/modules/grid_search.html

scikit-learn Documentation: Nested versus non-nested cross-validation
https://scikit-learn.org/stable/auto_examples/model_selection/plot_nested_cross_validation_iris.html

Model Selection - Overview

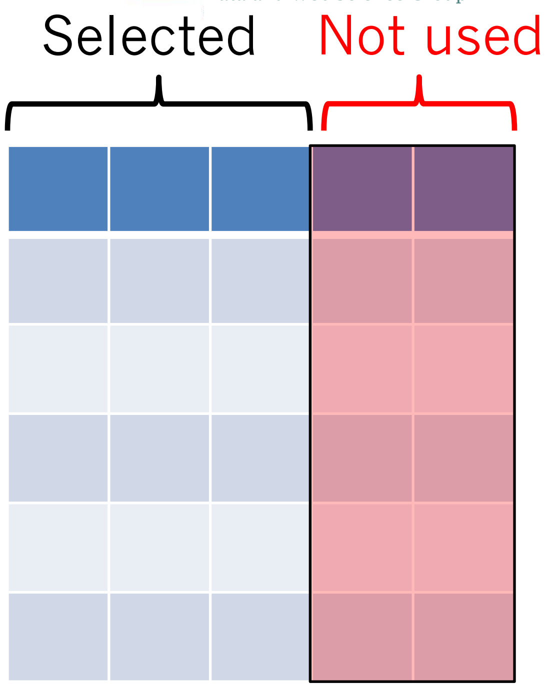
- For model evaluation with validation set and cross validation
  - Use the test set only once to get one final estimate of the error!
- The more models you train, the better estimate of the error



- Setting: 100 parameter combinations, 5 fold cross validation (inner and outer)
  - Validation set: |P|+ 1 = 101 models learned
  - Cross Validation: |folds| * |P| + 1 = 5 * 100 + 1 = 501 models learned
  - Nested Cross Validation: $|\text{folds}_{\text{Outer}}| * ((|\text{folds}_{\text{Inner}}| * |P|) + 1) =$
    $5*((5*100)+1) = 2505$ models learned

https://scikit-learn.org/stable/auto_examples/model_selection/plot_nested_cross_validation_iris.html

Feature Selection



- Some classification methods automatically select the relevant feature subset as part of the learning process
  - e.g. Decision Trees, Random Forests, ANNs, SVMs
- The performance of other methods depends on the subset of the features provided
  - e.g. KNN, Naïve Bayes
- Automated feature selection approaches
  - **Backward selection**: start using all features, remove features, test again
  - **Forward selection**: Find best single feature, add further features, test again
- Use nested cross-validation to estimate the generalization error

Summary: Hyperparameter and Feature Selection

- Hyperparameter selection
  - Default: **Always run hyperparameter optimization!**
  - Otherwise you cannot say that a method does not work for a task
- Feature selection
  - Default: **Check if classification method requires feature selection**
  - If yes, run automated feature selection
- Model selection
  - Default: **Use nested cross-validation**
  - If computation takes too long: use better hardware, reduce number of folds, reduce parameter search space, sample data to reduce size
  - If exact replicability of results is required: Use single train, validation, test split
- If your dataset is imbalanced
  - don’t forget to **balance your training set**, not your test set!

Online Lectures

- This week additional material is about comparing classifiers

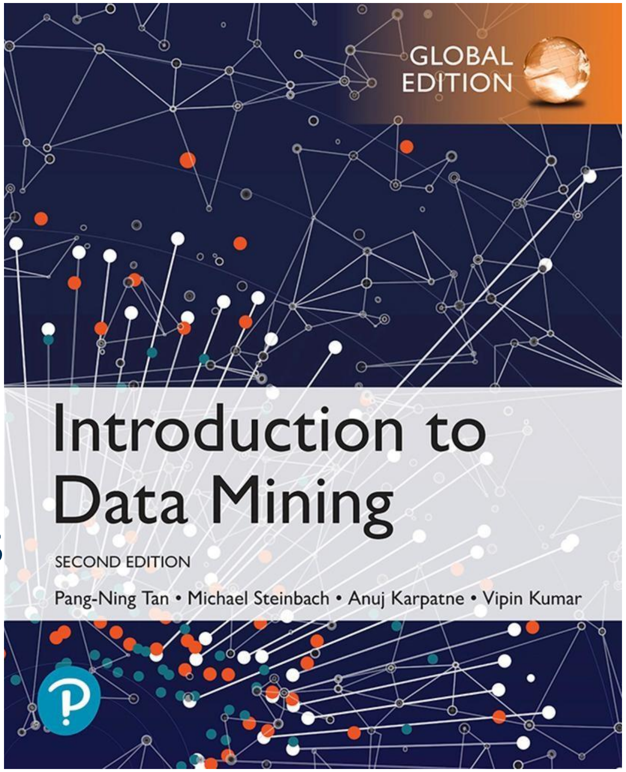
- Online lectures are exercise and exam relevant

Week	Wednesday (Offline Lecture)	Online Lecture (see Ilias Course)	Thursday (Exercise)
10.02.2025	no lecture		Introduction to Python (13:45–15:15)
17.02.2025	Introduction to Data Mining		Intro
24.02.2025	Preprocessing		Preprocessing
03.03.2025	Classification 1	Nearest Centroids	Classification 1
10.03.2025	Classification 2	Comparing Classifiers	Classification 2
17.03.2025	Regression	Ensembles	Regression
24.03.2025	Clustering and Anomalies	Hierarchical Clustering	Clustering
31.03.2025	Feedback on project outlines	Time Series	Time Series
07.04.2025	Association Analysis and Subgroup Discovery		Association Analysis

Questions?

Literature for this Slideset

- Pang-Ning Tan, Michael Steinbach, Anuj Karpatne,Vipin Kumar: Introduction to Data Mining. 2nd Edition. Pearson.



- Chapter 6.4: Naïve Bayes
- Chapter 6.9: Support Vector Machines
- Chapter 6.7 and 6.8: Artificial Neural Networks
- Chapter 3.5: Model Selection
- Chapter 3.7: Presence of Hyper-Parameters