

Outline

- Overview
- Foundational Concepts
- Summary

No Free Lunch Theorem

- d_m^y ordered sets of size m of cost values for $y \in Y$
- $f: X \to Y$ a function that is optimized
- $P(d_m^y|f,m,a)$ the conditional probability of getting d_m^y by m times running algorithm a on the function f

Theorem: For any pair of algorithms a_1 and a_2 $\sum_f P(d_m^y|f,m,a_1) = \sum_f P(d_m^y|f,m,a_2)$

All algorithms are equal







Implication of the NFL Theorem



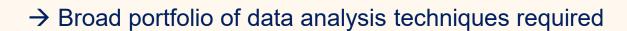
"if an algorithm does particularly well on average for one class of problems then it must do worse on average over the remaining problems"

David H. Wolpert and William G. Macready: No Free Lunch Theorems for Optimization, IEEE Transactions on Evolutionary Computation, 1(1):67-82



No Silver Bullet

- →There is no "one way" to do data analysis
 - But there are some standard techniques that often perform well
- Many factors influence the suitable techniques
 - Data
 - Problem to be solved
 - Available resources
 - ...





Categories of Data Analysis Techniques

| Category | Techniques Covered | Problem to be solved | |
|----------------------|--|---|--|
| Association Rules | Apriori | Relationships between items | |
| Clustering | K-Means Clustering DB Scan | Grouping of similar items Identification of structures | |
| Classification | K-nearest Neighbor Decision Trees Random Forests Logistic Regression Naive Bayes Support Vector Machines Neural Networks | Assignment of labels to objects | |
| Regression | Linear Regression Ridge Lasso | Relationship between outcome and inputs | |
| Time Series Analysis | ARMA | Identification of temporal structures Forecasting of temporal processes | |
| Text Mining | Bag-of-Words Stemming/Lemmatization TF-IDF | Analysis of textual data | |



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Machine Learning

- Definition after Tom M. Mitchel [2]:
 - A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

- Relation to the data analysis techniques
 - Experience *E*: our data
 - Task T: clustering/association mining/classification/...
 - Performance Measure P: depend on tasks



Description of a "Whale" Picture

How would you describe this picture with general concepts?

Has a fin

Blue background

Oval body

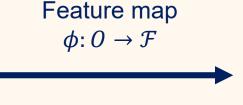
Black top, white bottom



Features of Objects

Object





Features

hasFin = true shape = oval colorTop = black colorBottom = white background = blue

- *O* is the object space
- ϕ is the feature map
- \mathcal{F} is the feature space
 - $\mathcal{F} = \{ \phi(o), o \in O \}$
- Example:
 - Five-dimensional space with dimensions as above
 - ϕ ("whalepicture") = (true, oval, black, white, blue)

Scales of Features

Steven's levels of measurement

| Scale | Property | Allowed Operations | Example |
|----------|------------------------------|----------------------|--|
| Nominal | Classification or membership | =,≠ | Color as "black", "white" and "blue" |
| Ordinal | Comparison or levels | =,≠,>,< | Size in "small", "medium", and "large" |
| Interval | Differences or affinities | =, ≠, >, <, +, - | Dates, temperatures, discrete numeric values |
| Ratio | Magnitudes or amounts | =, ≠, >, <, +, -,·,/ | Size in cm, duration in seconds, continuous numeric values |

S. S. Stevens: On the Theory of Scales of Measurement, Science, 103(2684):677-680



Encoding Categorical Features

- Many algorithms can only work with numeric features
- Encode categorical features as binary numeric features
 - Example: $x \in \{\text{small, medium, large}\}\$
 - Encode as three variables x^{small} , x^{medium} , x^{large}

•
$$x^{small} = \begin{cases} 1 & if \ x = small \\ 0 & otherwise \end{cases}$$
, ...

- · Can also use one variable less, remaining case is encoded by all zeros
- This is called One-Hot-Encoding

Training Data

• Instances of objects described by their features

| hasFin | shape | colorTop | colorBottom | background | value of interest |
|--------|-----------|----------|-------------|------------|-------------------|
| true | oval | black | black | blue | whale |
| false | rectangle | brown | brown | green | bear |
| | | | | | |

- Supervised learning if the value of interest is known
 - → Classification, regression
- Otherwise unsupervised learning
 - → Clustering, Association Rule Mining

The Test Data

- Data for the evaluation of analysis results
 - Same distribution as training data
- Training data ≠ Test data
 - Evaluate generalization
 - Avoid overfitting
 - Analysis results only valid on training data
 - · Different and not working on unseen data
- Test data often difficult to obtain

And where do I get the test data?



Hold-out Data

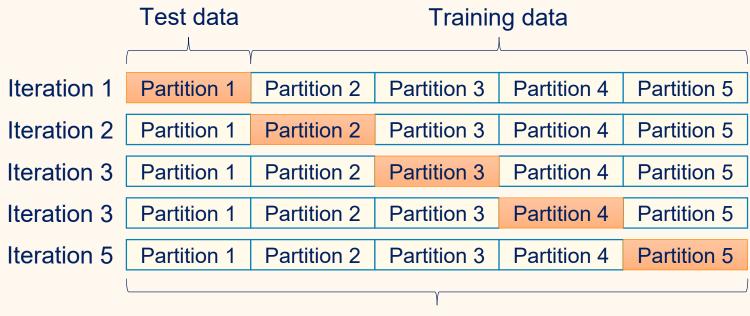
- Data not used for training at all
- Commonly used hold out data sizes

Depends a lot on available data!

- 50% of all data
- 33% of all data
- 25% of all data in case a validation set is used
- Example:
 - Nine months of customer transactions available
 - First six months as training data
 - Last three months as test data

k-fold Cross Validation

- Create k partitions of available data
- One partition for testing, all others for training
- Estimate performance by averaging over the iterations





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- No generic algorithm for all problems
- Objects are described by features
- Features are used for learning about objects
- Data usually split into different sets for different purposes