Institute of Bioinformatics Johannes Kepler University Linz



Unit 1

Introduction to Machine Learning



Finding solutions of a system of equations



- Finding solutions of a system of equations
- Prediction of trajectory of a space shuttle

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- Prediction of trajectory of a space shuttle
- Diagnosis whether a patient has a certain disease



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- Prediction of outcome of election



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- Recognition of handwritten characters
- Identification of customer target groups
- Prediction of function of protein from its amino acid sequence







- Traditional disciplines like physics, chemistry, and biology are usually aiming at *exact explicit models*, i.e. to know how (and why) things work in a particular way; then a solution to a new problem can be found *deductively* using explicit knowledge
- That goal, however, is sometimes too difficult to achieve; reasons may be computational complexity, insufficient knowledge, insufficient information, etc.

Machine Learning = Inductive Learning

- Machine learning tries to elicit models/knowledge from previously observed data with the following two main goals:
 - 1. Getting insight
 - 2. Being able to predict future outcomes
- Putting it simple, machine learning is about *learning from data* (often called *inductive learning*)

What Do We See Here?



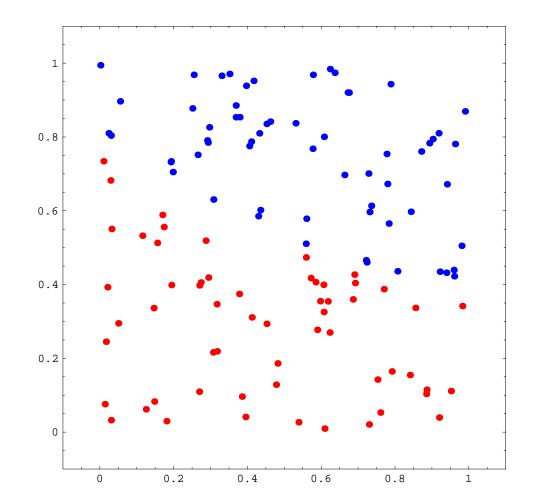
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0.972187	0.0802574	+1
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0.807075	0.872155	-1
0.240068	0.801159	-1
0.206602	0.562109	+1
0.581611	0.335561	+1
0.944329	0.026344	+1
0.569412	0.30145	+1
0.552694	0.864825	-1
0.700995	0.517267	-1
0.209818	0.342484	+1
0.94141	0.928017	-1
0.148546	0.198177	+1
0.872544	0.50608	-1
0.371062	0.272064	+1

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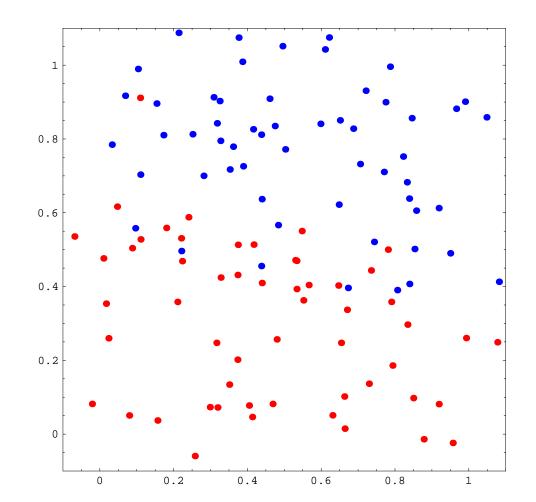
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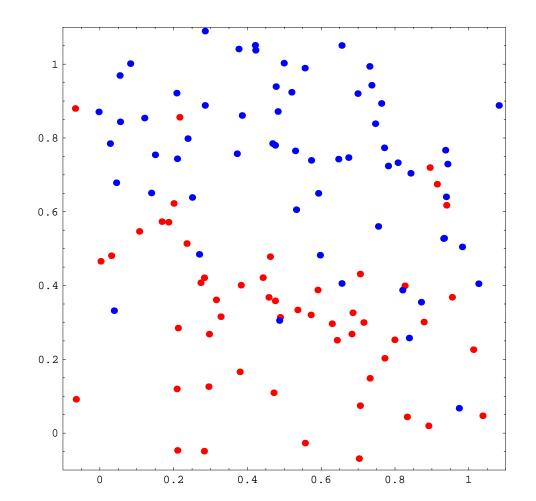




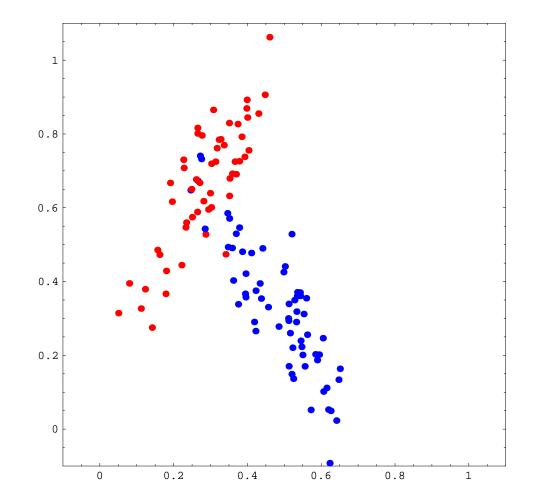




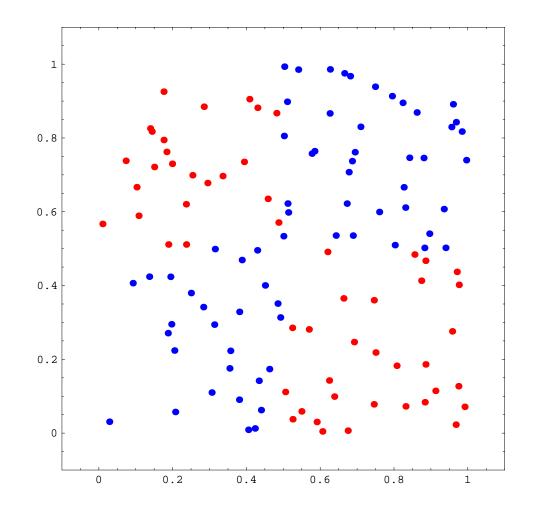














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0.733515	0.640438	1.19068	0.639685	0.0793674	0.160503	+1
0.274817	0.261054	1.20056	0.689895	0.401913	0.277955	-1
0.329943	0.241299	0.848705	0.721673	0.973852	0.795238	-1
0.334784	0.350487	0.315131	0.928277	0.816343	0.558292	-1
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0.360569	0.638554	1.0307	0.260456	0.00658296	0.380672	+1
0.0857518	0.3775	0.386551	0.570562	0.15437	0.102717	+1
0.755808	0.1362	0.544536	0.848888	0.874862	0.307479	-1
0.421025	0.785714	0.449038	0.920612	0.420418	0.749187	-1
0.939446	0.0468747	0.15846	0.625944	0.198894	0.176125	+1
0.845362	0.767883	0.824993	0.725803	0.808218	0.63495	-1
0.484793	0.129329	0.0783719	0.465347	0.291457	0.254278	+1
0.399041	0.751829	0.763511	0.894785	0.47902	0.15156	-1
0.643232	0.615629	0.430261	0.0458972	0.446513	0.844081	+1
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Supervised ML: an explicit target (output) value is given for each (input) data item; the goal is to identify the relationship between input and output

Unsupervised ML: no target value is given, the goal is to identify structure in the data



Classification: the output value is a class label

Regression: the output value is numerical

Supervised ML is sometimes called *predictive modeling*. This is due to the fact that the goal is most often to predict the output value for future input values.



- **Projection methods:** down-projection of data to lowerdimensional space in order to concentrate on the essence of the data
- **Clustering:** grouping of similar data objects
- **Density estimation:** estimate the probability distribution of the data
- **Generative model:** building a model that produces data that are distributed as the observed data



Reinforcement learning: learning by feedback from the environment in an online process

- Feature extraction: computation of features from data prior to machine learning (e.g. signal and image processing)
- Feature selection: selection of those features that are relevant/sufficient to solve a given learning task
- Feature construction: construction of new features as part of the learning process





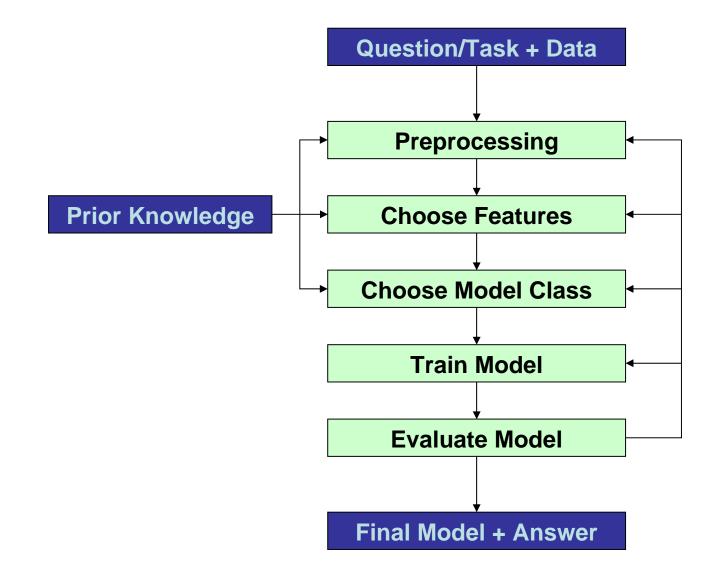
Model: the specific relationship/representation we are aiming at

Model class: the class of models in which we search for the model

- **Parameters:** representations of concrete models inside the given model class
- **Model selection/training:** process of finding that model from the model class that fits/explains the observed data in the best way
- **Hyperparameters:** parameters controlling the model complexity or the training procedure

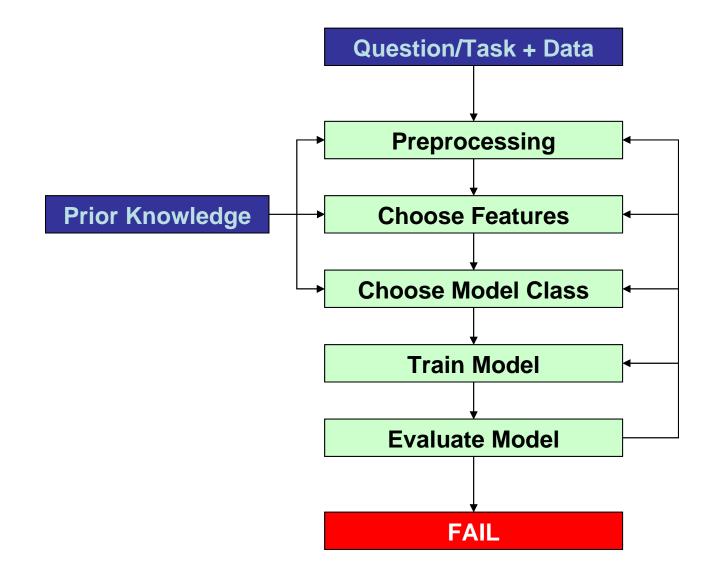
Basic Data Analysis Workflow





Basic Data Analysis Workflow





Some Words of Enthusiasm



- Machine learning methods are able to solve some tasks for which explicit models will never exist
- Machine learning methods have become standard tools in a variety of disciplines (e.g. signal and image processing, bioinformatics)

But ... Some Words of Caution

BIOINF

- Machine learning is not a universal remedy
- Quality of models is depending on quality and quantity of data
- What cannot be measured/observed can never be identified by machine learning
- Machine learning complements explicit/deductive models instead of replacing them
- Machine learning is often applied in a naive way

Goals of This Course



- To understand the underlying principles of machine learning
- To understand what can go wrong in machine learning
- To be able to evaluate the quality of a model created by machine learning
- To gain deeper insight to the fields of support vector machines and neural networks

Introductory Example: Fish Recognition

Example borrowed from

R. O. Duda, P. E. Hart, and D. G. Stork. *Pattern Classification*. Second edition. John Wiley & Sons, 2001. ISBN 0-471-05669-3.

 Automated system to sort fish in a fish-packing company: salmons must be distinguished from sea bass optically

- **Given:** a set of pictures with known fish, the training set
- Goal: automatically distinguish between salmons and sea bass for future pictures

Two Sample Images



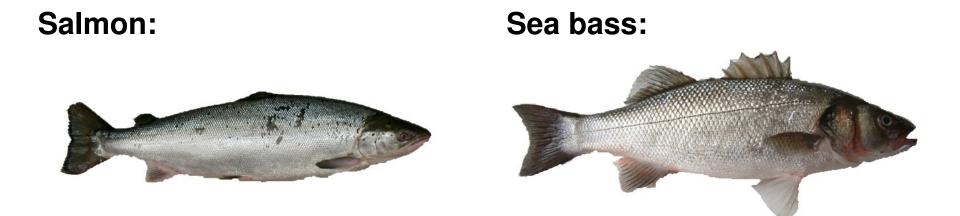
Salmon:



Sea bass:

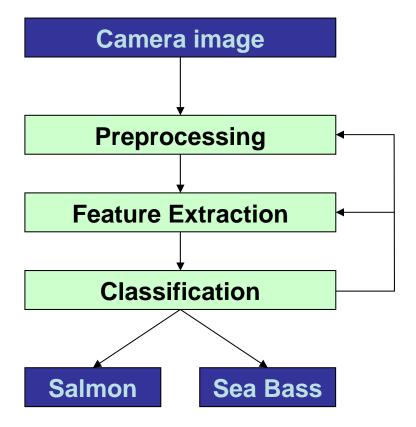




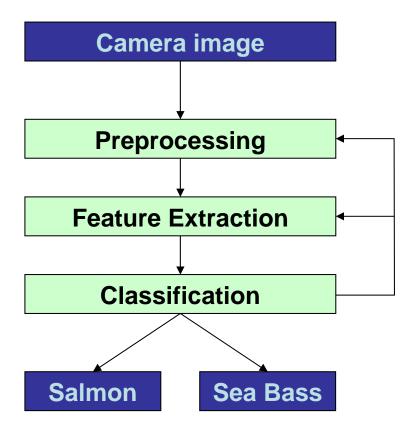


How can we distinguish these two kinds of fish visually?









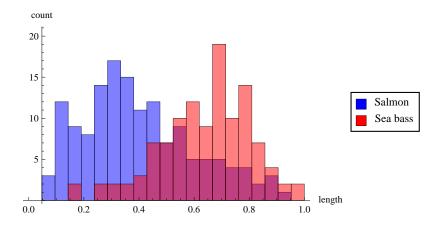
Preprocessing: contrast and brightness correction, segmentation, alignment

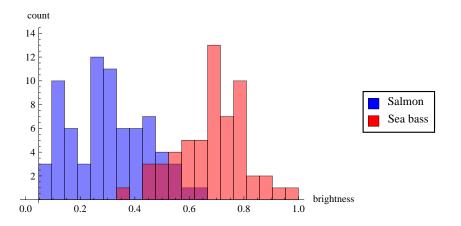
Features:

- 1. Length
- 2. Brightness

Using One Feature

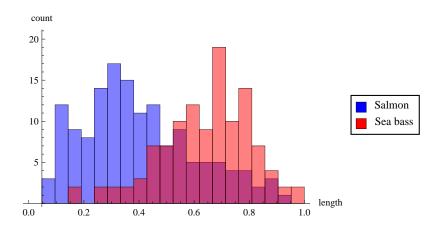


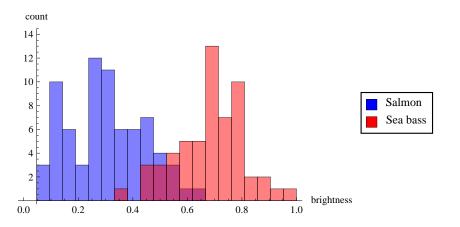




Using One Feature





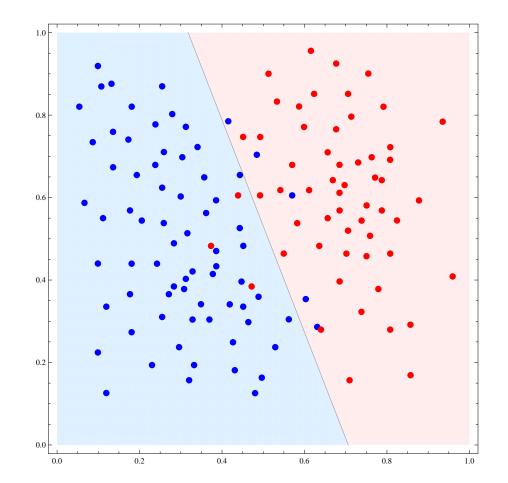


Questions:

- 1. Which is the better feature?
- 2. Where should we put the threshold?

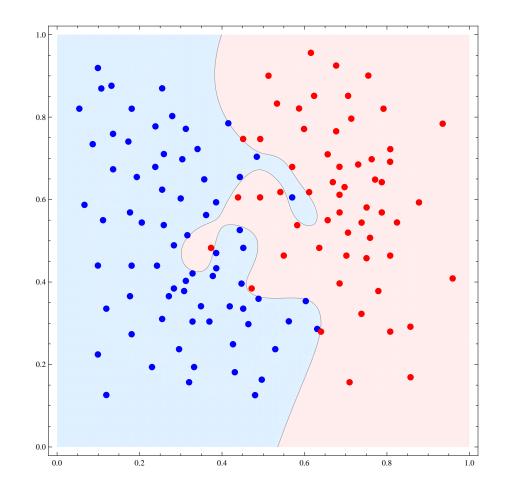
Using Two Features: Linear Separation





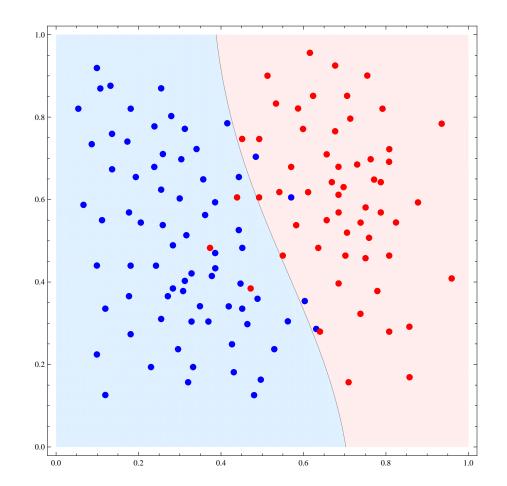
Using Two Features: Highly Nonlinear Separation





Using Two Features: Moderately Nonlinear Separation









- Which is the best result and why?
- What is the best way to measure the quality of a classifier?
- Which methods for constructing classifiers are available?
- Is there a theoretical basis (instead of a purely intuitive one) to answer these questions?





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These questions will be the point of departure of this course.