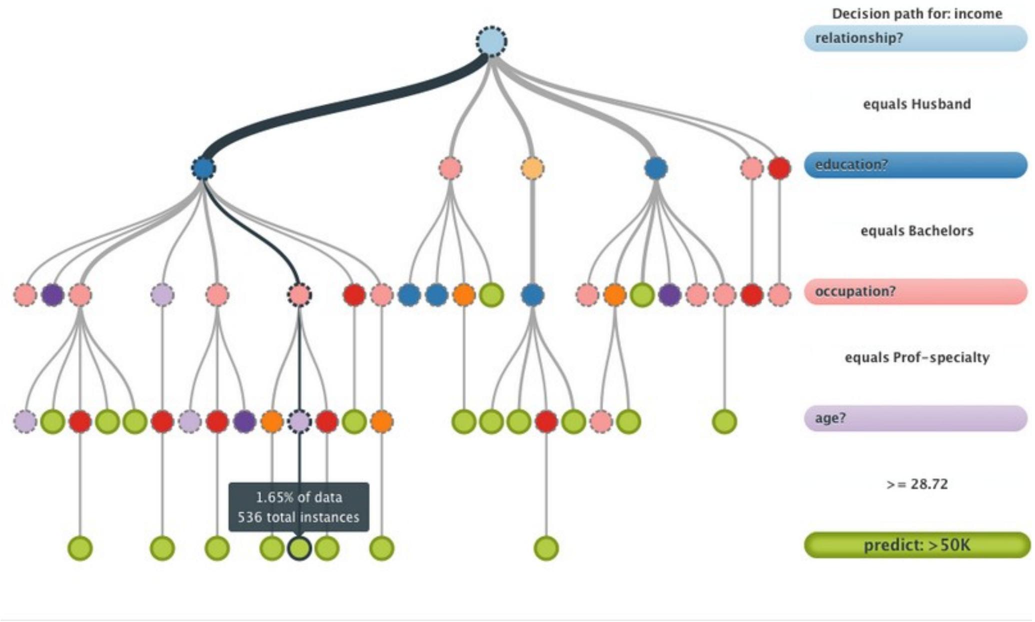
Machine Learning

Lecture 3



Marcin Wolter

IFJ PAN

13 December 2019

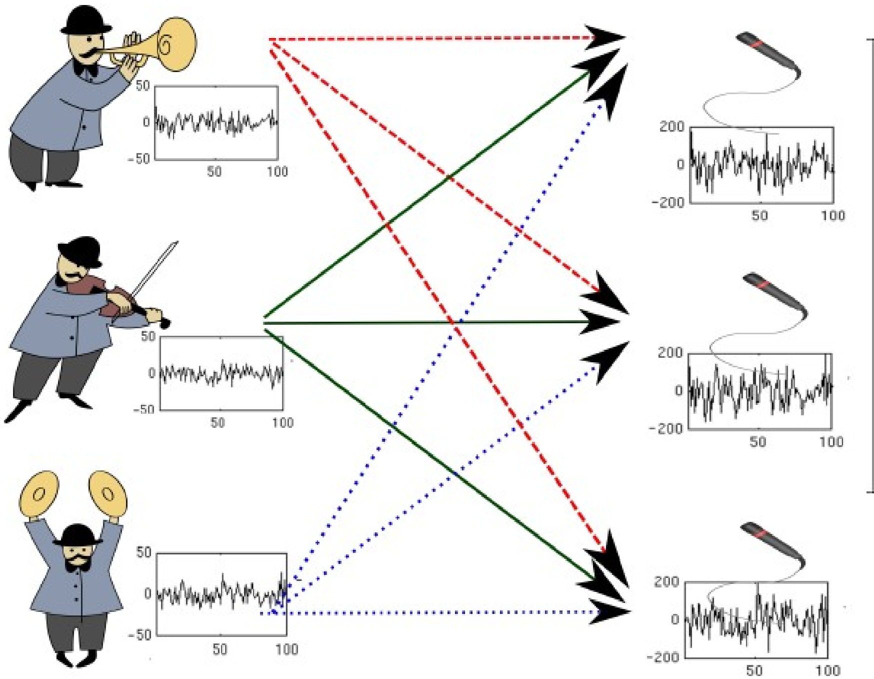
- Independent Component Analysis ICA
- Ensemble learning – Boosted Decision Trees BDT

Independent Component Analysis ICA

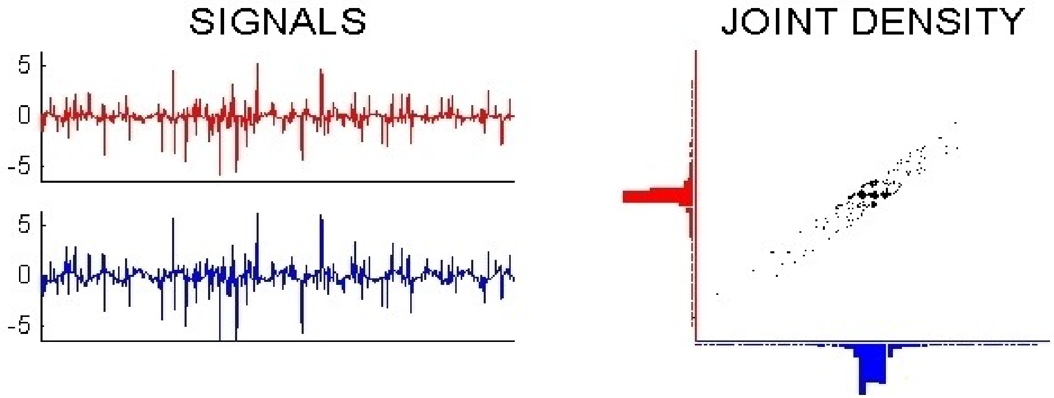
Developed at Helsinki University of Technology *http://www.cis.hut.fi/projects/ica/*

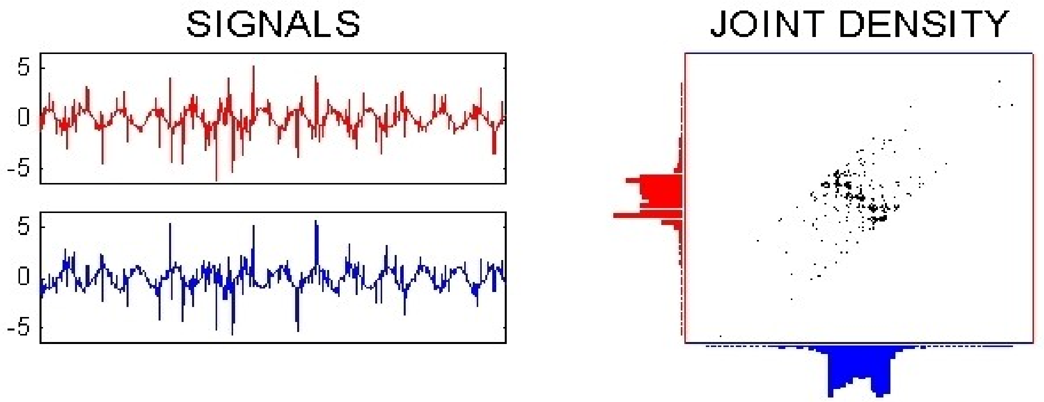
- **Problem:**
  - Assume, that signal **X** is a linear combination **X = AS** of independent sources **S**. The mixing matrix **A** and vector of sources **S** are unknown.
  - **Task:** find a matrix **T (inverted A)**, such that elements of vector **U = TX** are statistically independent. **T** is the matrix returning the original signals.

- **Applications:**
  - Filtering of one source out of many others,
  - Separation of signals in telecommunication,
  - Separation of signals from different regions of brain,
  - Signal separation in astrophysics,
  - Decomposition of signals in accelerator beam analysis in FERMILAB.

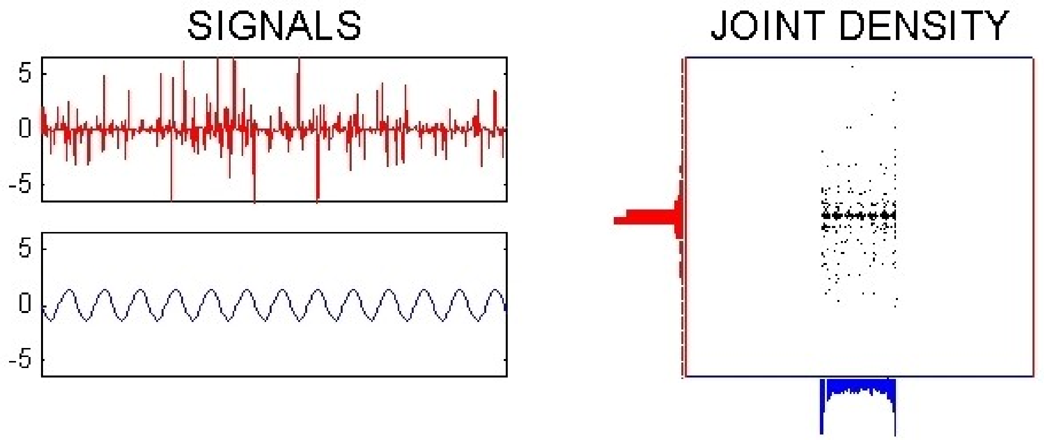


How does ICA work?





Whitened signals and density



Separated signals after 5 steps of FastICA

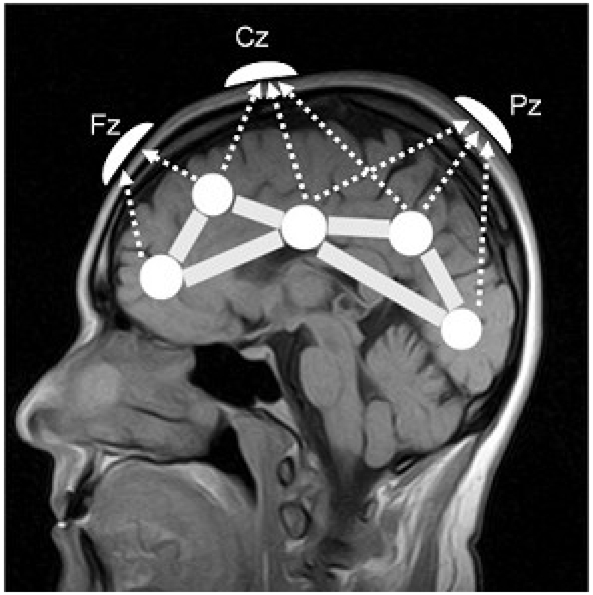
- We have two measured signals and we want to separate them into two independent sources.
- Preparing data - decorrelation (correlation coefficients equal zero, σ=1).

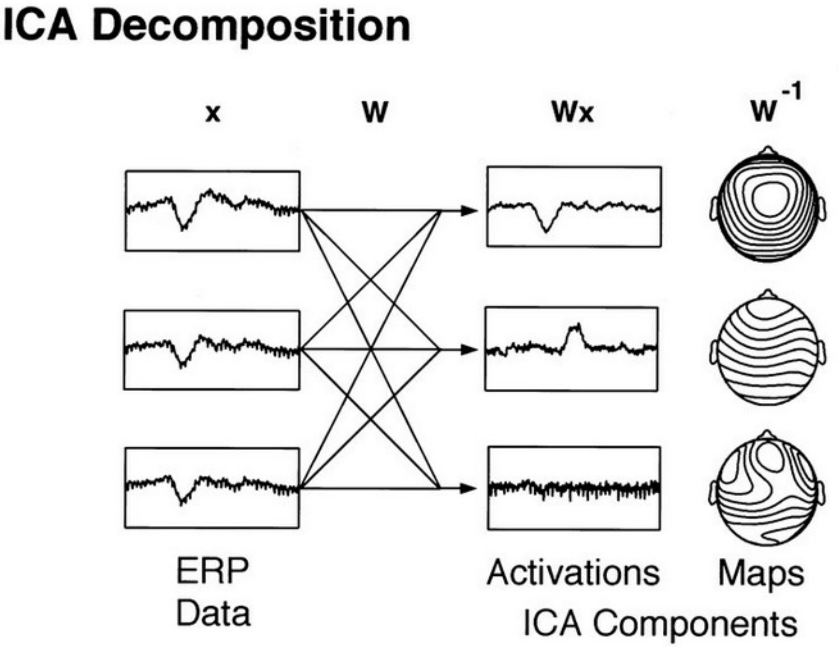
Superposition of many independent distributions gives Gaussian in the limit.

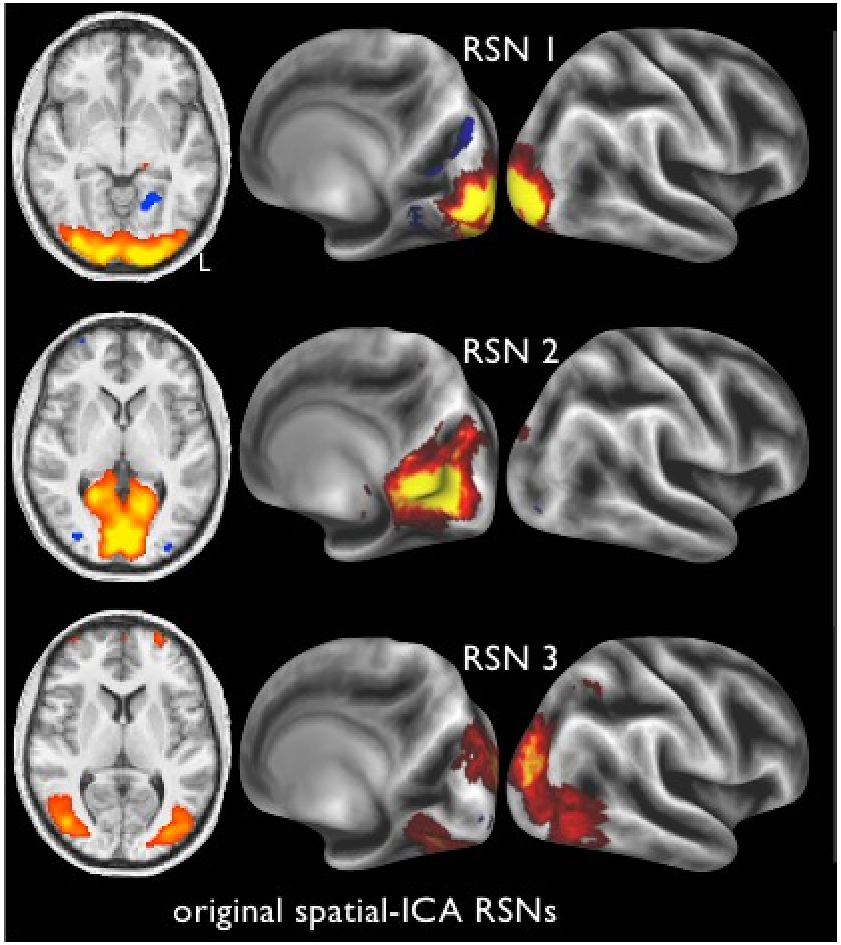
- ICA – rotation, signals should be maximally non-Gaussian (measure of non-Gaussianity might be curtosis).
- *Curtosis:* $\mathrm{Kurt} = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^4}{\sigma^4} - 3$

where μ is the mean of the distribution and σ is a standard deviation.

ICA – brain research, signal separation



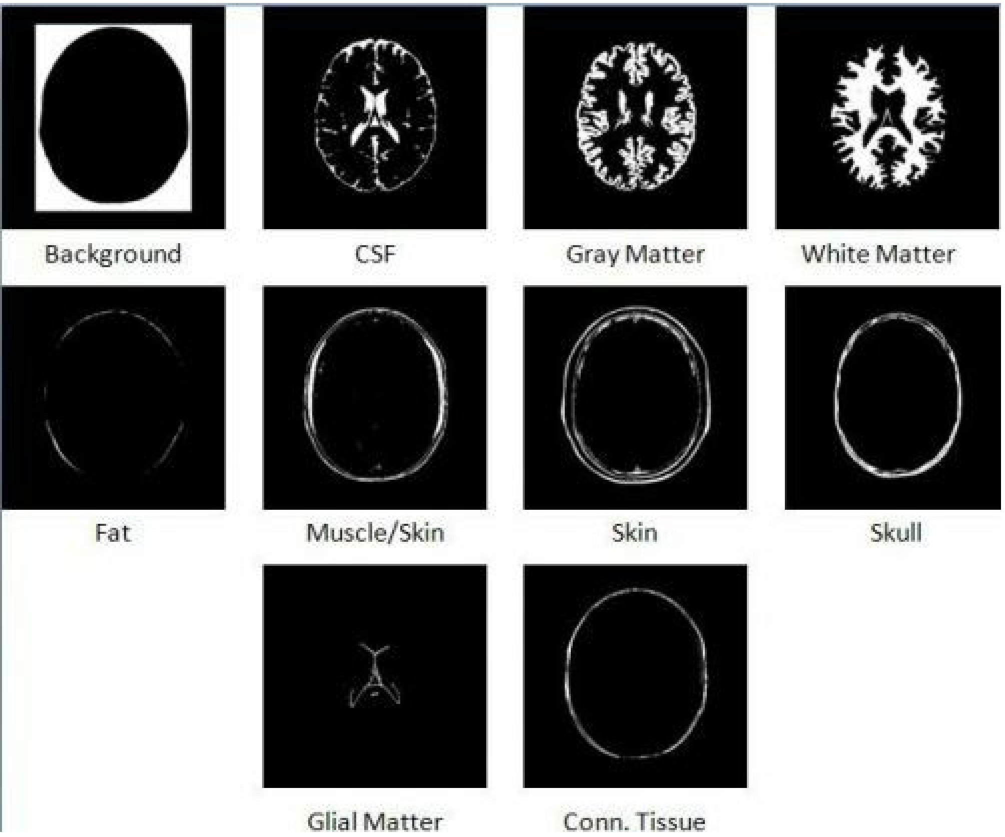




3 components from 21-dimensional decomposition using the “spatial-ICA'' algorithm.

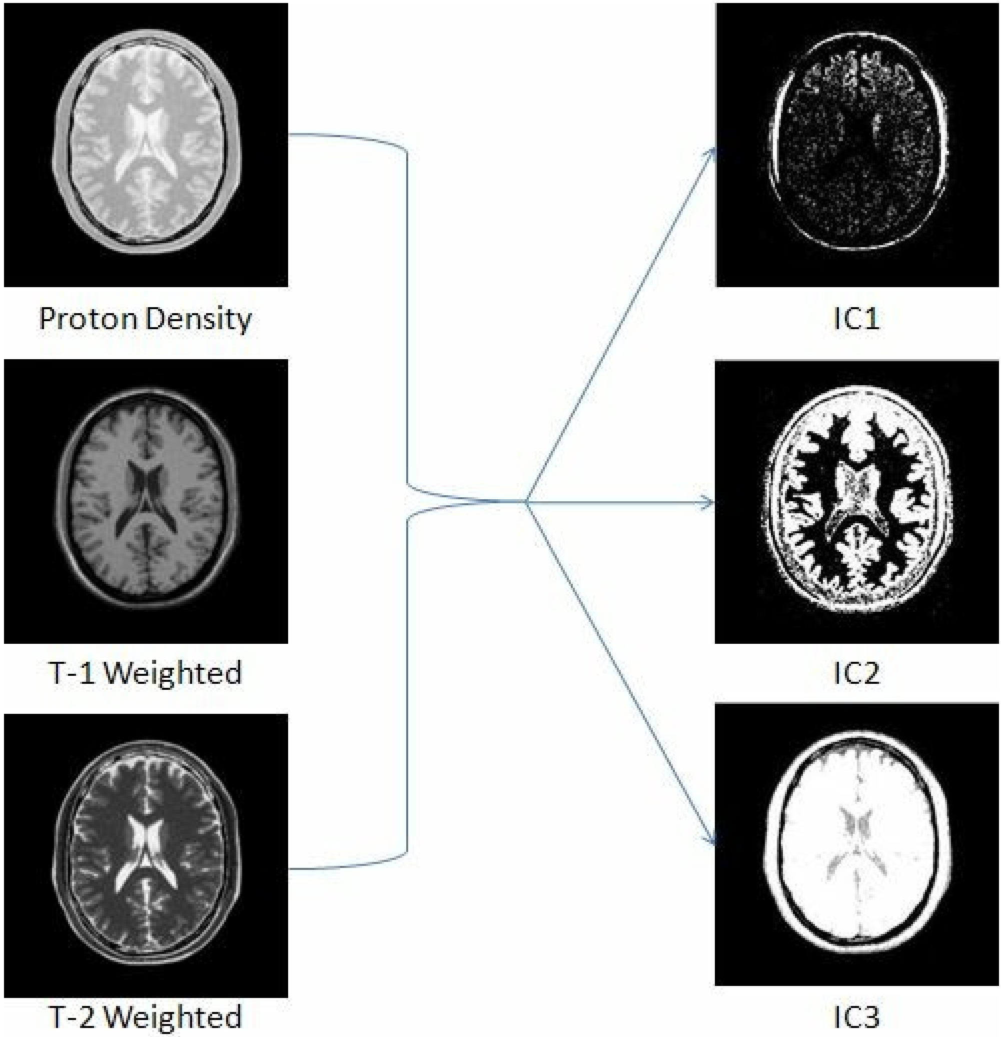
PNAS February 21, 2012 vol. 109 no. 8 3131-3136

ICA and magnetic resonance



Sources of signals

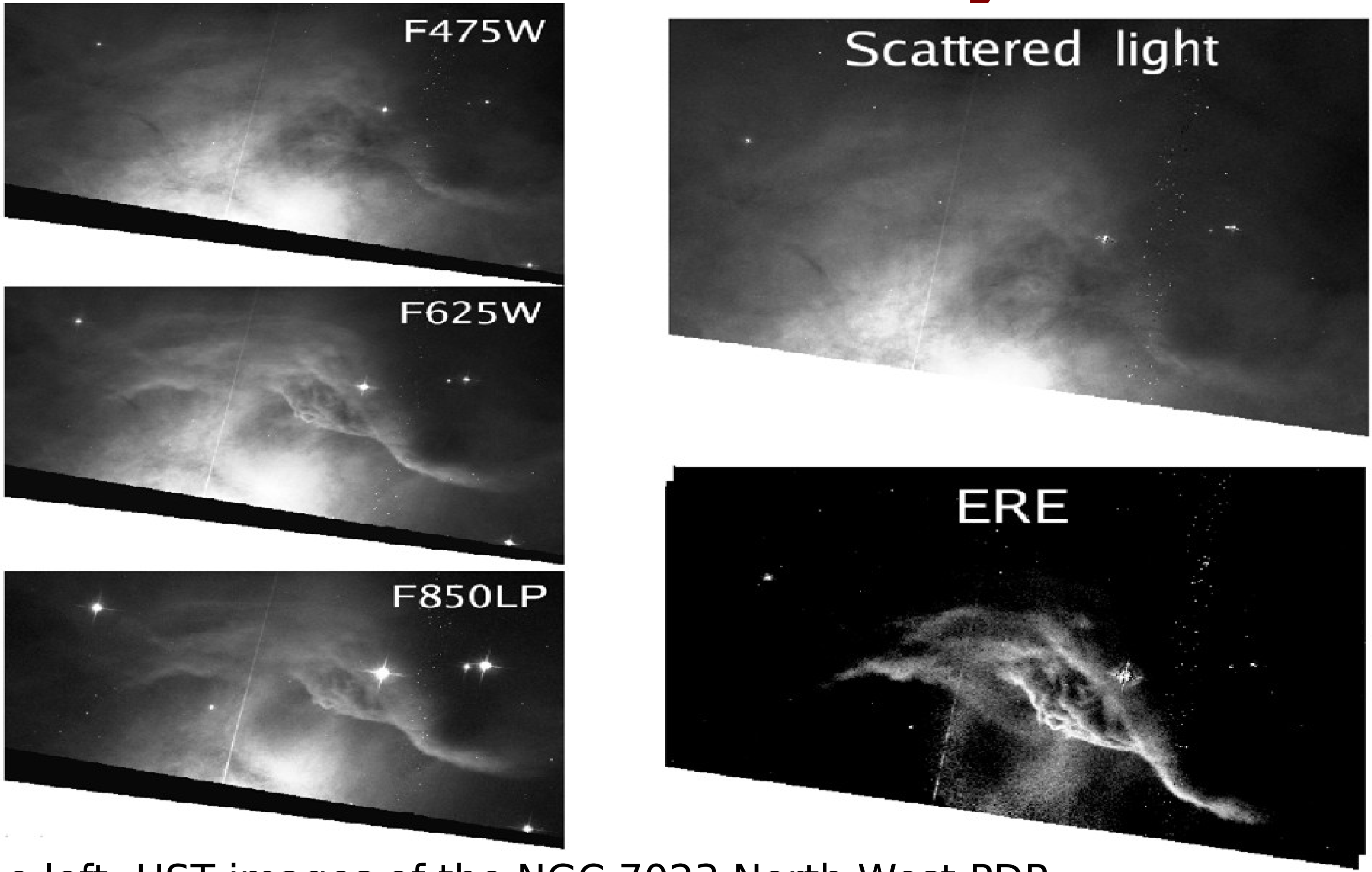
Blind Source Separation in Magnetic Resonance Images
January 30, 2010 by Shubhendu Trivedi



Measured

Separated components

ICA – astronomy



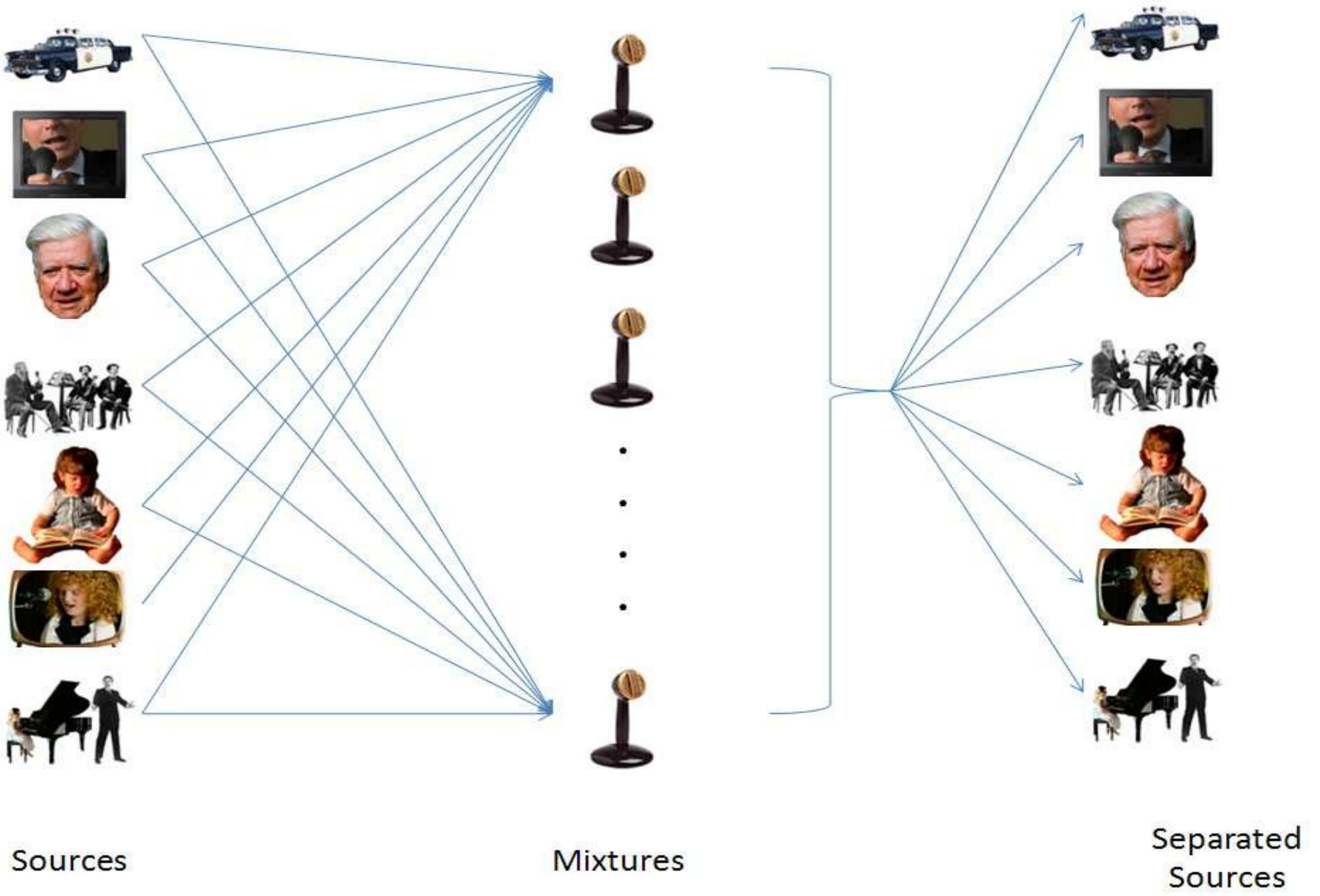
On the left: HST images of the NGC 7023 North-West PDR in three SDSS wide-band filters. On the right: scattered light and ERE (Extended Red Emission) images extracted with FastICA from the observations.

A&A 479, L41-L44 (2008)
DOI: 10.1051/0004-6361:20079158

Desert

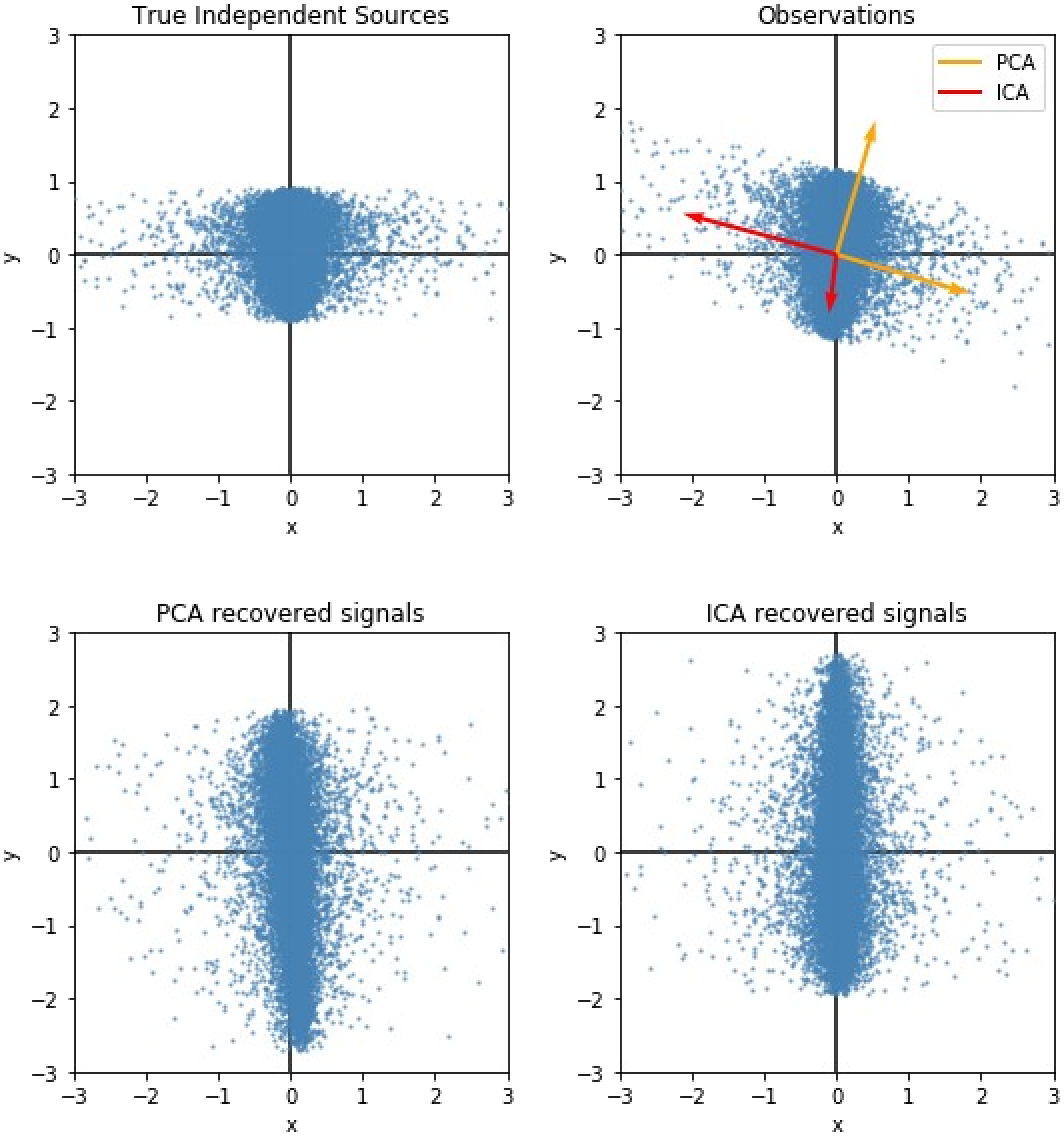
http://cnl.salk.edu/~tewon/Blind/blind_audio.html

- Cocktail Party Demo   - applet showing how the the ICA algorithm works – blind separation of sound sources.



ICA example

- https://github.com/marcinwolter/MachineLearnin2019/blob/master/plot_ica_vs_pca.ipynb



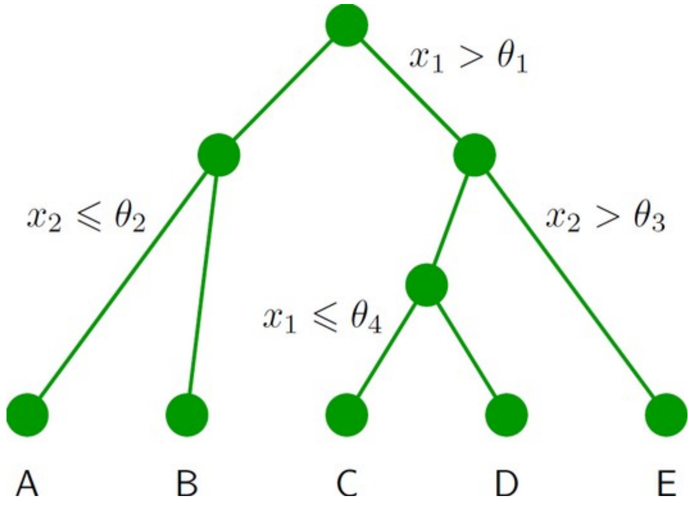
Boosting, bagging, BDT... Ensemble learning

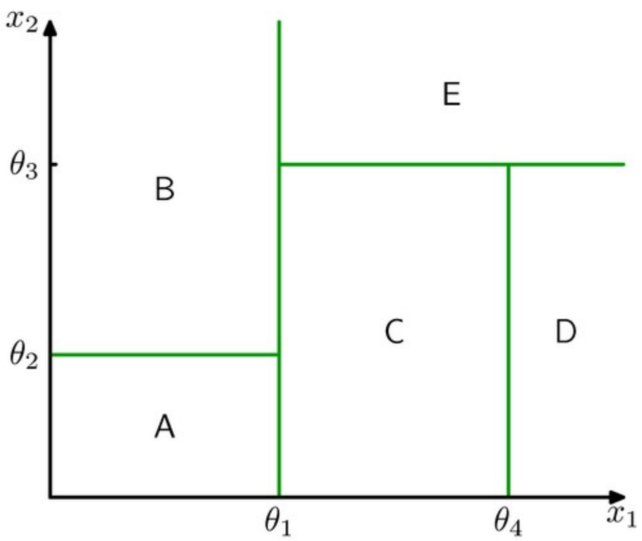
What does BDT mean???

- **BDT – Boosted Decision Tree:**
  - **Decision Tree** – an algorithm know for a long time, used in most of the expert systems. For example, the first aid manual is frequently written in the form of a decision tree: if (condition) do something, else do something different, then check another condition...
  - **Boosted** - a method of joining many weak classifiers in an ensemble to get one strong classifiers. It is not limited to decision trees, however with them it is most commonly used.

Decision trees

- Decision tree – a series of cuts, each „leaf” (A,B,C,D,E) has a label, for example ”signal” and “background”.

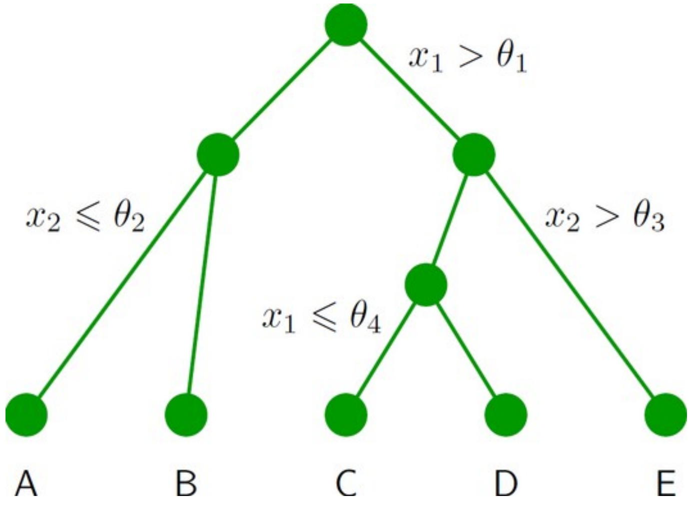




- Easy in visualization and interpretation
- Resistant for *outliers*.
- Weak variables are ignored.
- Fast training and classification.
- Unfortunately: **sensitive for fluctuations, unstable**.

Building the tree

- We start from the root.
- We divide the training sample by the best separating cut on the best variable.
- We repeat the procedure until the stopping conditions are fulfilled, for example: number of leafs, number of events in a leaf etc.
- The ratio S/B in a leaf defines the classification (binary signal or background, or a real number giving the probability, that a given event is a signal).



Definitions of separation:

- Gini inpurity: (*Corrado Gini 1912, invented the Gini index used to measure the inequality of incomes*)

  p (1-p) : p= P(signal), *purity*
- Cross-entropy:

  -(p ln p + (1-p)ln(1-p))
- Missidentification:

  1-max(p,1-p)

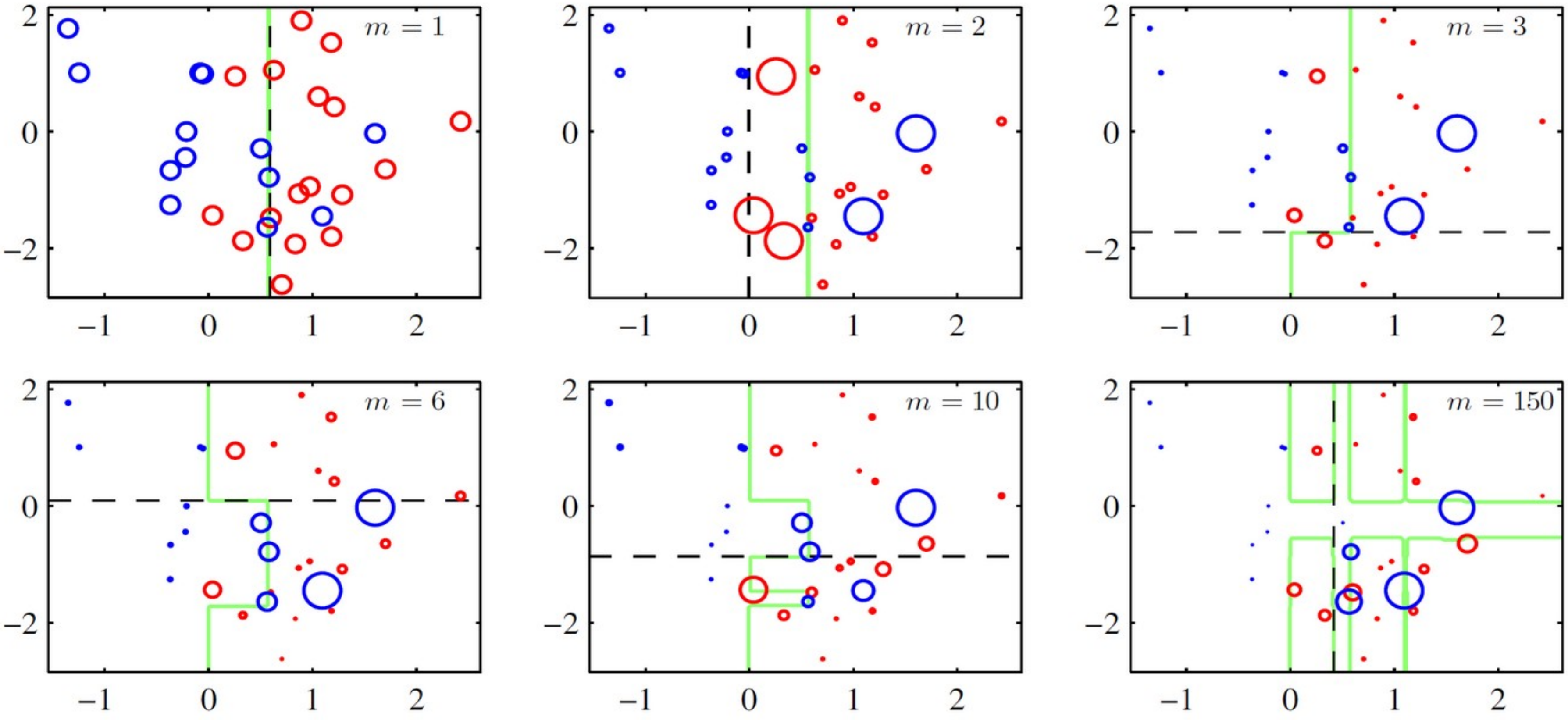
AdaBoost – ensemble of classifiers

Problem: could we improve a weak classifier?

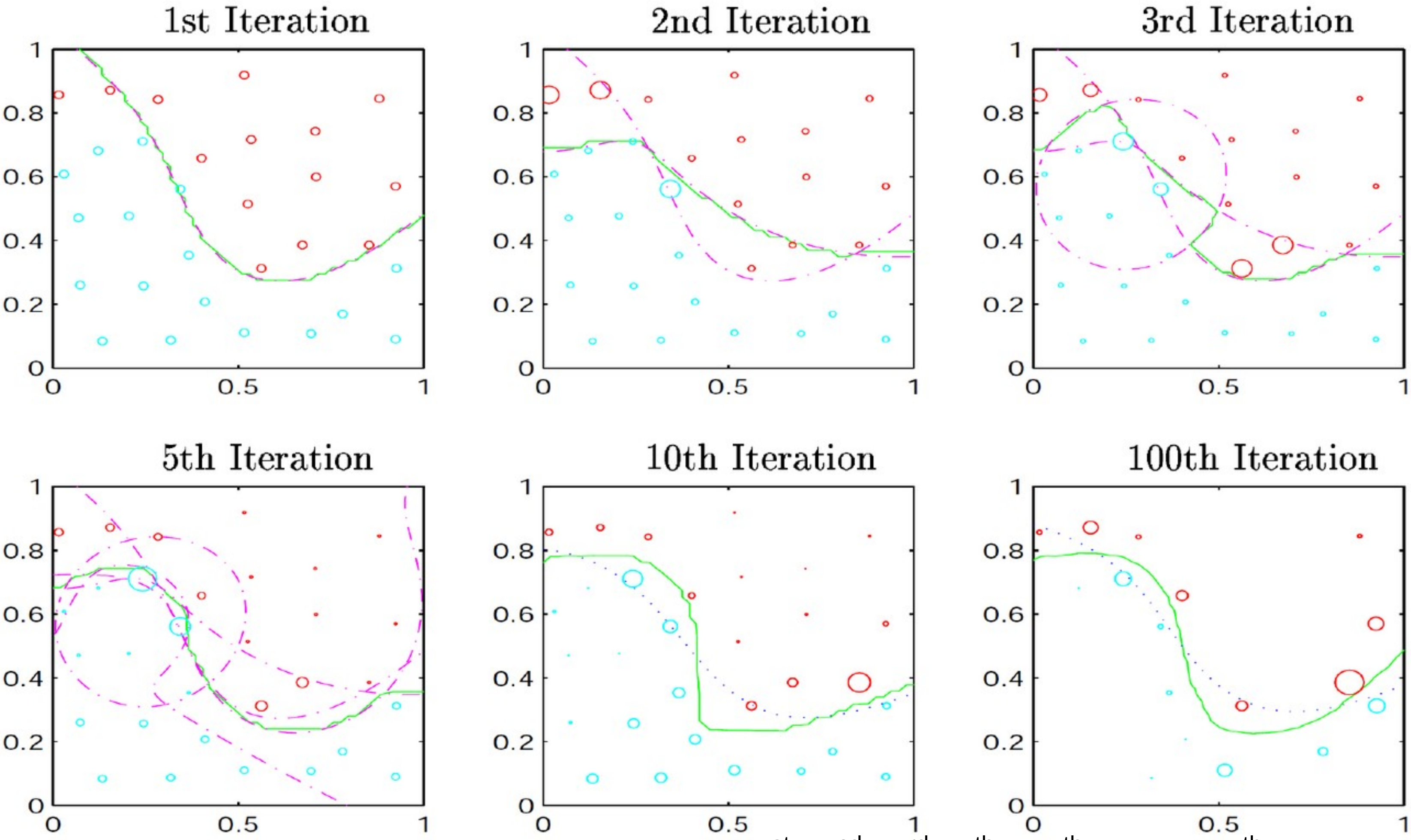
Answer: yes, by applying it many times.

- An algorithm used most frequently: **AdaBoost** (Freund & Schapire 1996 – Gödel prize)

- Build a decision tree.
- Increase the weights of wrongly classified events.
- Repeat many times (typically 100-1000)
- Classify the events by “voting” by all the trees.



AdaBoost



AdaBoost for 2-dimensional data – results after 1st, 2nd, 3rd, 5th, 10th and 100th iteration. The solid green line shows the results of the combined classifier, the dashed line the borders between classes obtained after each step. For the last two plots the dotted line marks the class borders obtained from the bagging algorithm (we will talk about bagging soon).

AdaBoost

- Five years after publication of AdaBoost Friedman proved, that the algorithm in fact minimizes the exponential loss function:

$$E = \sum_{n=1}^{N} \exp\left(-t_n f_m(x_n)\right)$$

where *f(x)* is the answer of the algorithm

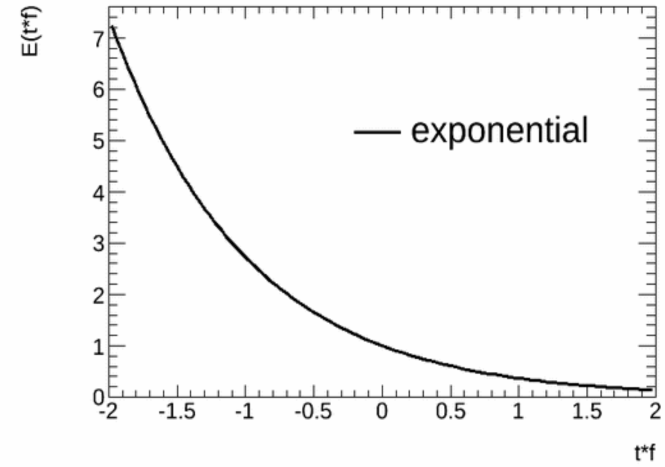
t = 1 signal, *t = -1* background

$t_n \cdot f_m(x_n) > 0$ – correctly classified

$t_n \cdot f_m(x_n) < 0$ – incorrectly classified

- Exponential function goes up quickly => huge punishment for wrongly classified events, so the algorithm is sensitive for single, outstanding points. Classification becomes worse, when data are hardly separable.

  - Another loss function?
  - Friedman in year 2000 proposed few other loss functions, but AdaBoost is still the most popular (we will talk about).



AdaBoost in action

AdaBoost algorithm in detail

1. Give all vectors from the training set a weight w_i=1/N.

2. For m = 1,...,M:

a) Train classifiers y_m(x) on the training sample minimizing:

$$J_m = \sum_{n=1}^{N} w_n^m I\left(y_m(x_n) \neq t_n\right)$$

b) Evaluate the quantities:

$$\epsilon_m = \frac{\sum_{n=1}^{N} w_n^m I\left(y_m(x_n) \neq t_n\right)}{\sum_{n=1}^{N} w_n^m}$$

$$\alpha_m = \frac{1}{2} \ln \frac{1-\epsilon_m}{\epsilon_m}$$

c) Update the weights of the vectors in the training sample:

$$w_n^{m+1} = \begin{cases} \frac{w_n^m}{Z_m} e^{\alpha_m} & \mathrm{dla} \quad y_m(x_n) \neq t_n \\ \frac{w_n^m}{Z_m} e^{-\alpha_m} & \mathrm{dla} \quad y_m(x_n) = t_n \end{cases}$$

3.The result of voting is given as:

$$Y_M(\mathbf{x}) = sign\left[\sum_{m=1}^{M} \alpha_m y_m(\mathbf{x})\right]$$

All the classifiers are trained on the same training sample, but with different weights. These weights depend on the results of the preceding training, so it’s difficult to train many classifiers in parallel.

Classifier boosting

- Boosting, bagging – in a “magical” way we get a strong classifier out of weak ones

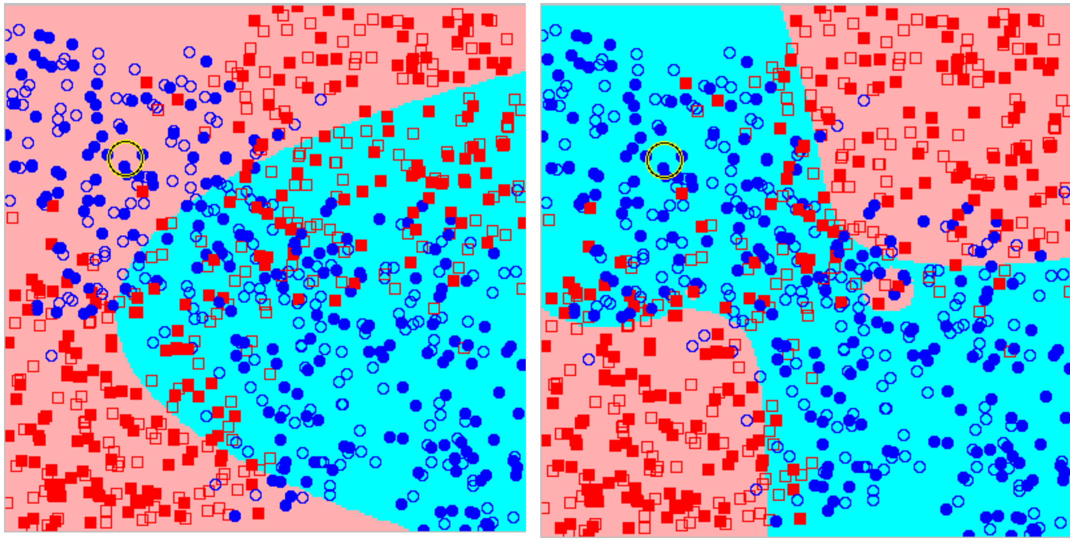
- **Typically boosting used on decision trees – Boosted Decision Trees BDT.**

- Good results without time consuming tuning of parameters:

  „*the best out-of-box classification algorithm*”.

- Relatively resistant on overtraining.

- Quite frequently used nowadays. And with good results!



Naive Bayes classifier

Boosted Naive Bayes classifier

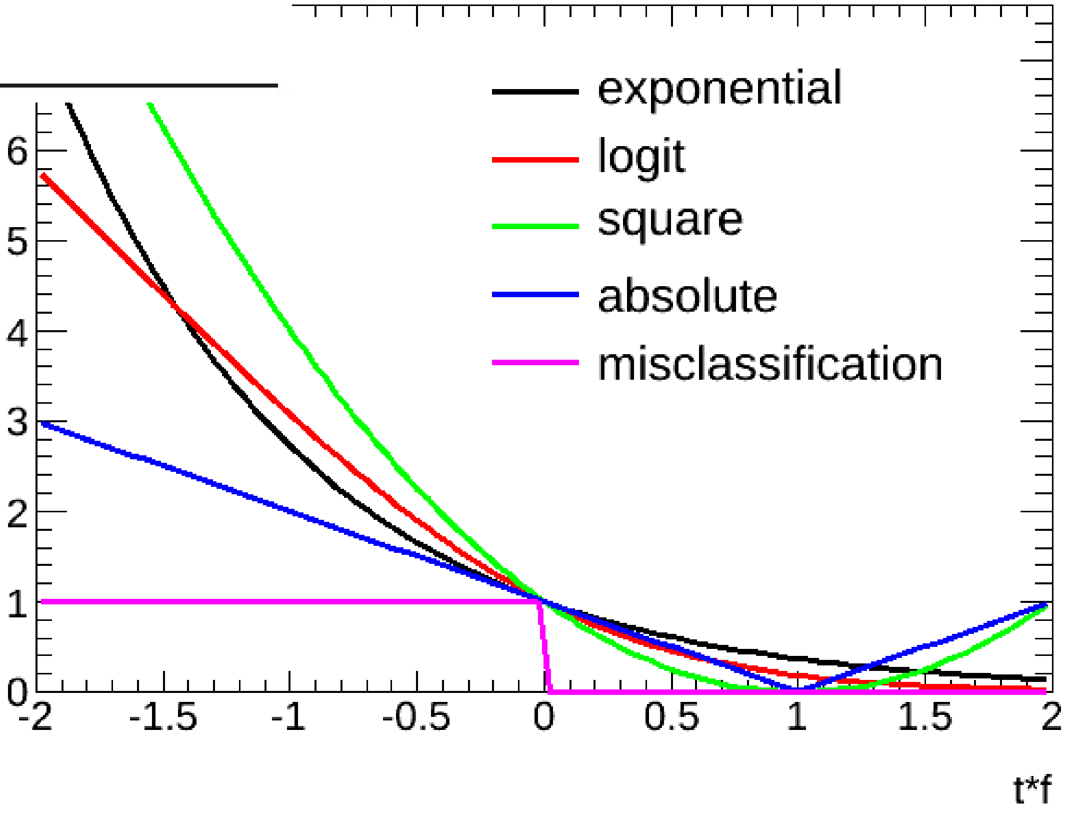
Application of a boosting algorithm (5 iterations) for Naive Bayes classifier.

Boosting – different loss functions

- Another loss functions:

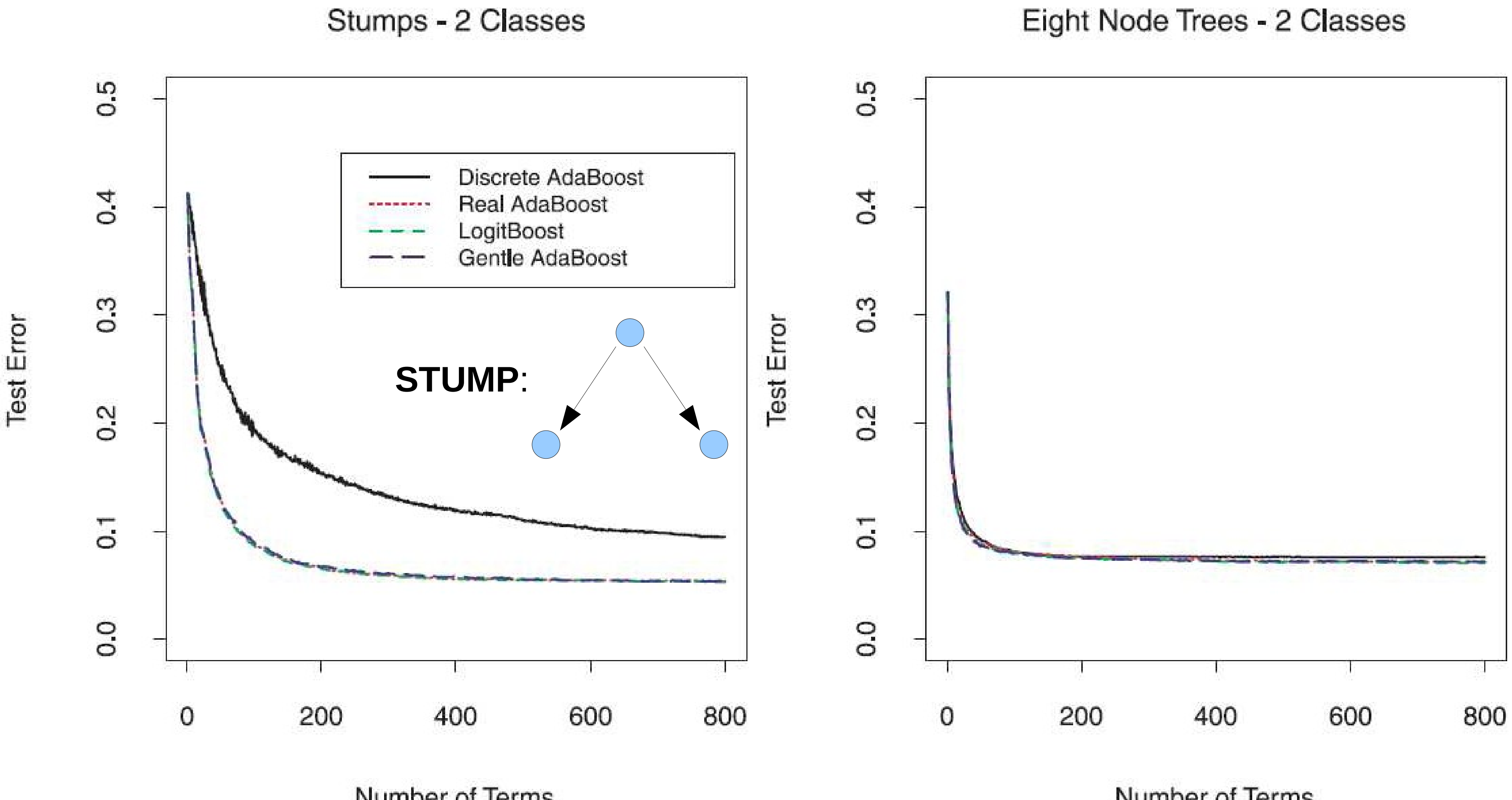
Nazwa funkcji	Równanie	Nazwa algorytmu
Exponential	$\exp\left(-t_n f_m(x_n)\right)$	*AdaBoost*
Probability	$\log\left(1+\exp(-2t_n f_m(x_n)\right)$	*LogitBoost*
Error squared	$(t_n - f_m(x_n))^2$	*SquareBoost*
Absolute error	$\lvert t_n - f_m(x_n)\rvert$	
Zero-one	$\begin{cases} 0 & sign(f_m(x_n)) \neq t_n \\ 1 & sign(f_m(x_n)) = t_n \end{cases}$	

Pro:
Not so sensitive for outliers.
The properly chosen “sensitivity” is important, when there are regions with mixed signal and background.
Contra:
There is no fast and simple minimization algorithm like AdaBoost => minimization using general algorithms, like for function fit.



Boosting – different loss functions

- Discrete AdaBoost – the basic AdaBoost described on previous slides
- Real AdaBoost, LogitBoost, Gentle AdaBoost- modifications (different loss functions and minimization algorithms) proposed by Friedman.
- For bigger trees the results are identical.

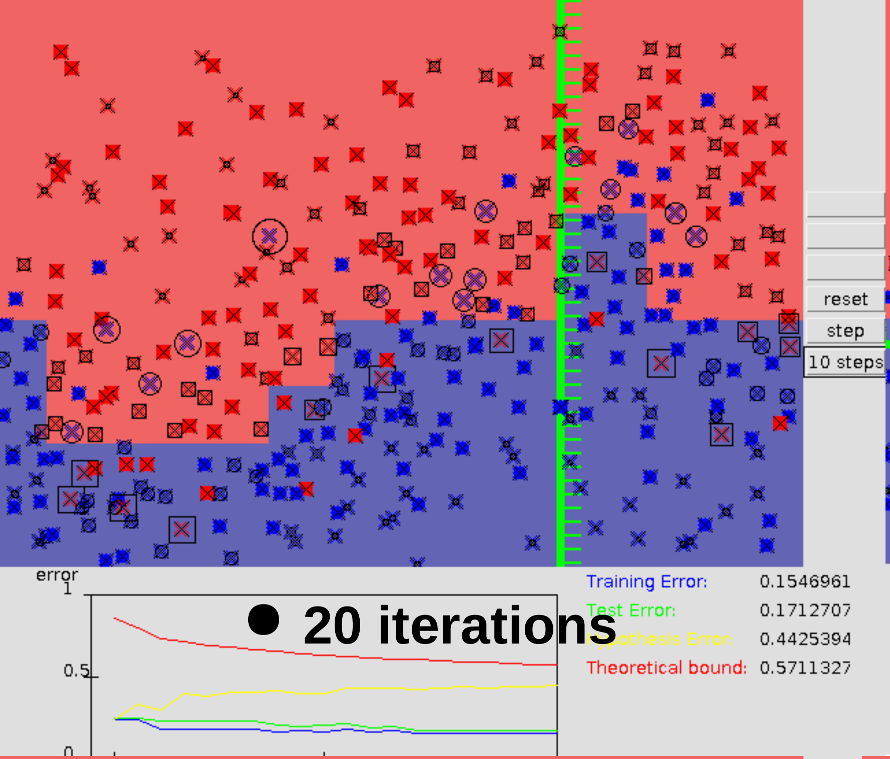


STUMP:

Overtraing of the Boosted Decision Tree (BDT)

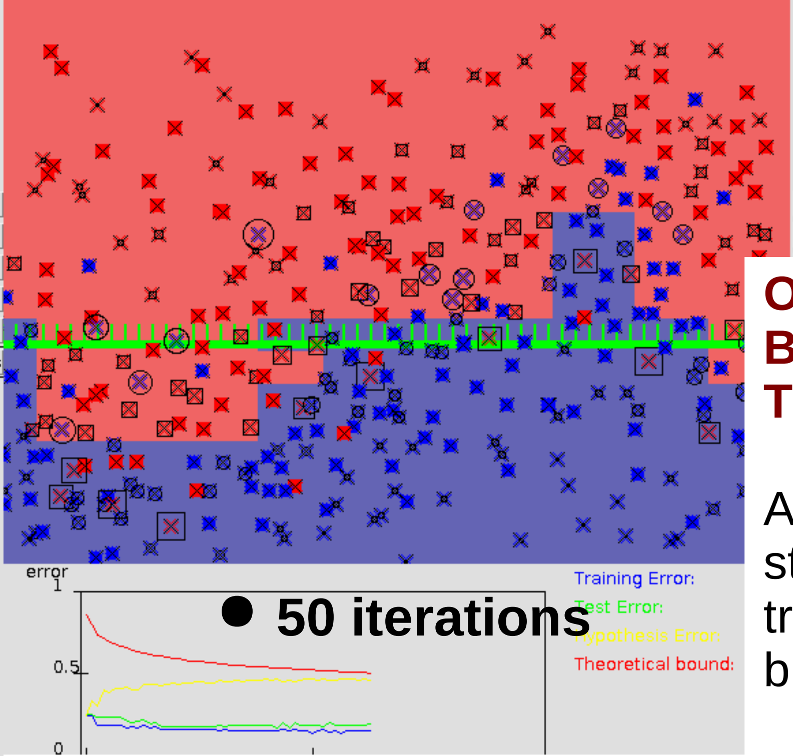
Algorithm uses stumps – decision trees with two branches.

At the end the space is divided into very small areas - overtraining.



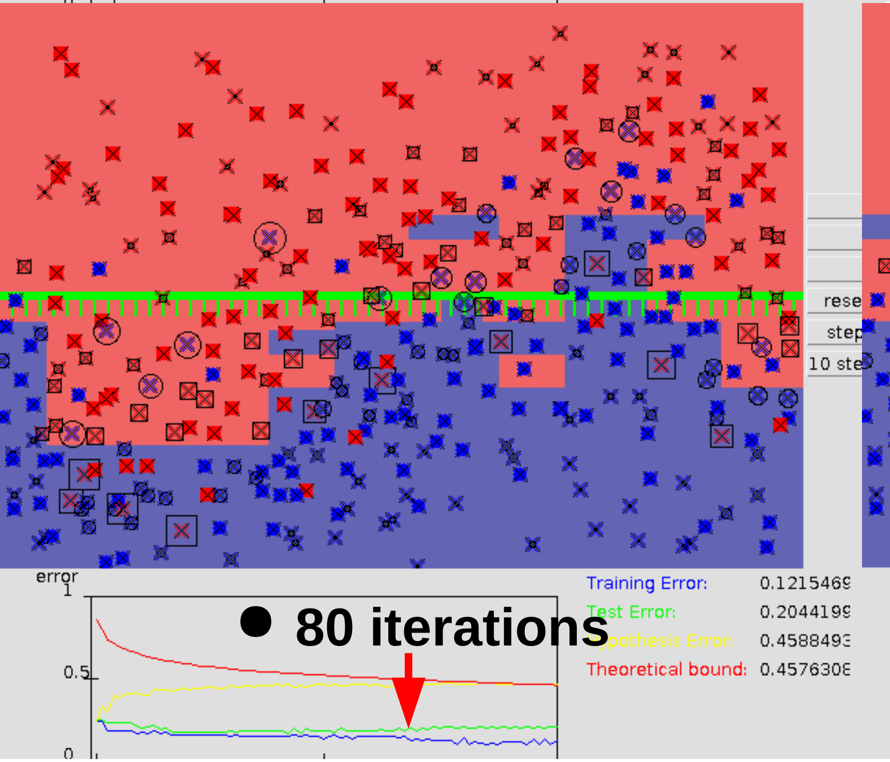
- 20 iterations

Training Error: 0.1546961
Test Error: 0.1712707
Hypothesis Error: 0.4425394
Theoretical bound: 0.5711327



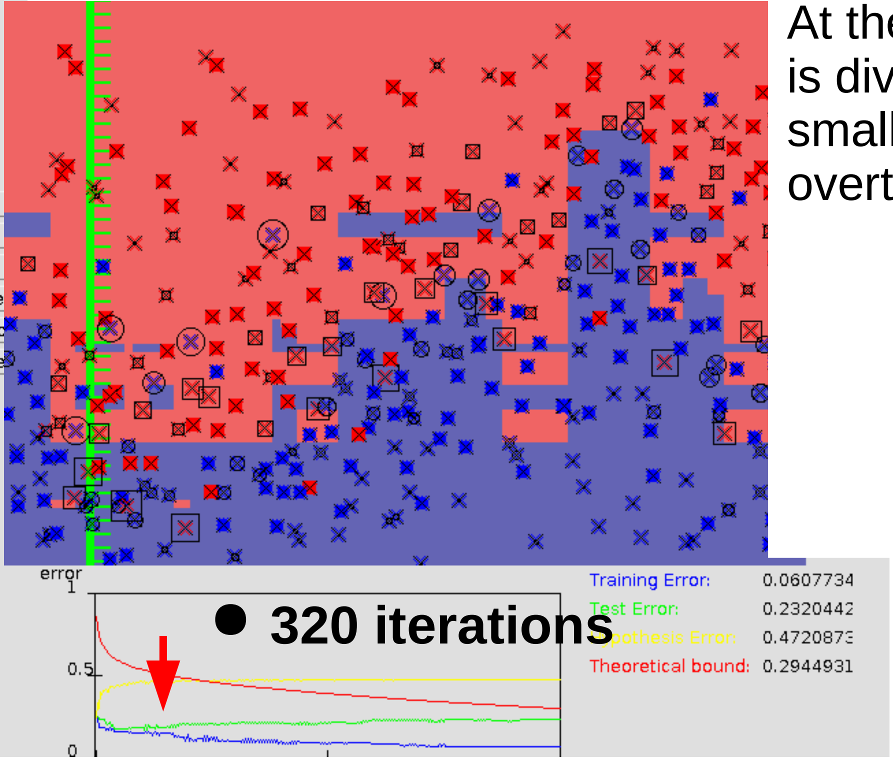
- 50 iterations

Training Error:
Test Error:
Hypothesis Error:
Theoretical bound:



- 80 iterations

Training Error: 0.1215469
Test Error: 0.2044199
Hypothesis Error: 0.4588493
Theoretical bound: 0.4576308

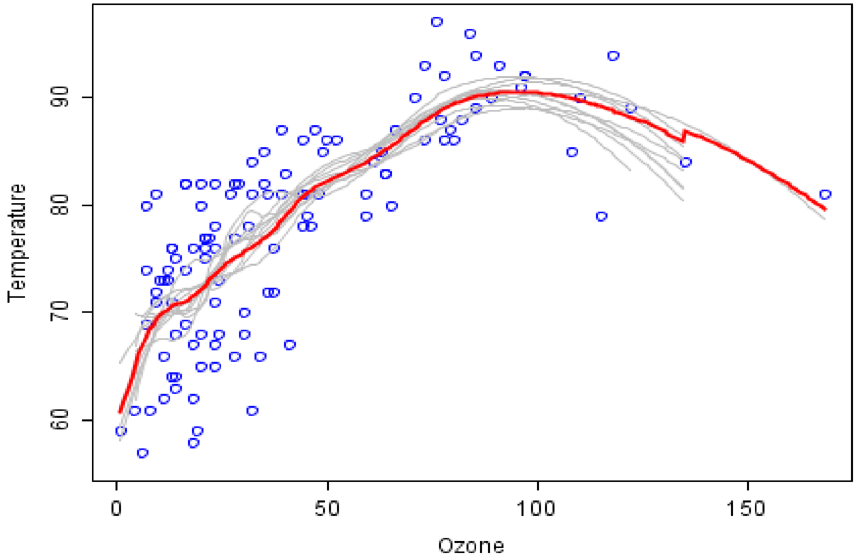


- 320 iterations

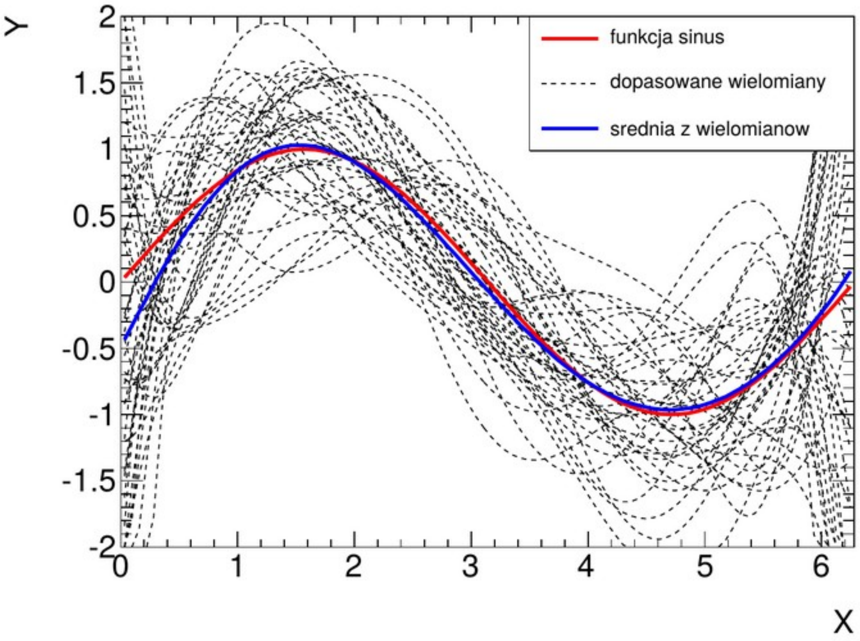
Training Error: 0.0607734
Test Error: 0.2320442
Hypothesis Error: 0.4720873
Theoretical bound: 0.2944931

Bagging (Bootstrap AGGregatING)

- **Algorithm proposed by Leo Breiman in 1994:**
  - Take N events from N-element training set, but with repetitions.
  - Train the classifier on this set.
  - Repeat many times
  - Classify new events by voting of all the classifiers.



For this data the red line (mean of 100 classifiers) is smoother, more stable and more resistant for overtraining the any of the single classifiers.



Analogy: mean of many poorly fitting functions gives a good fitting function.

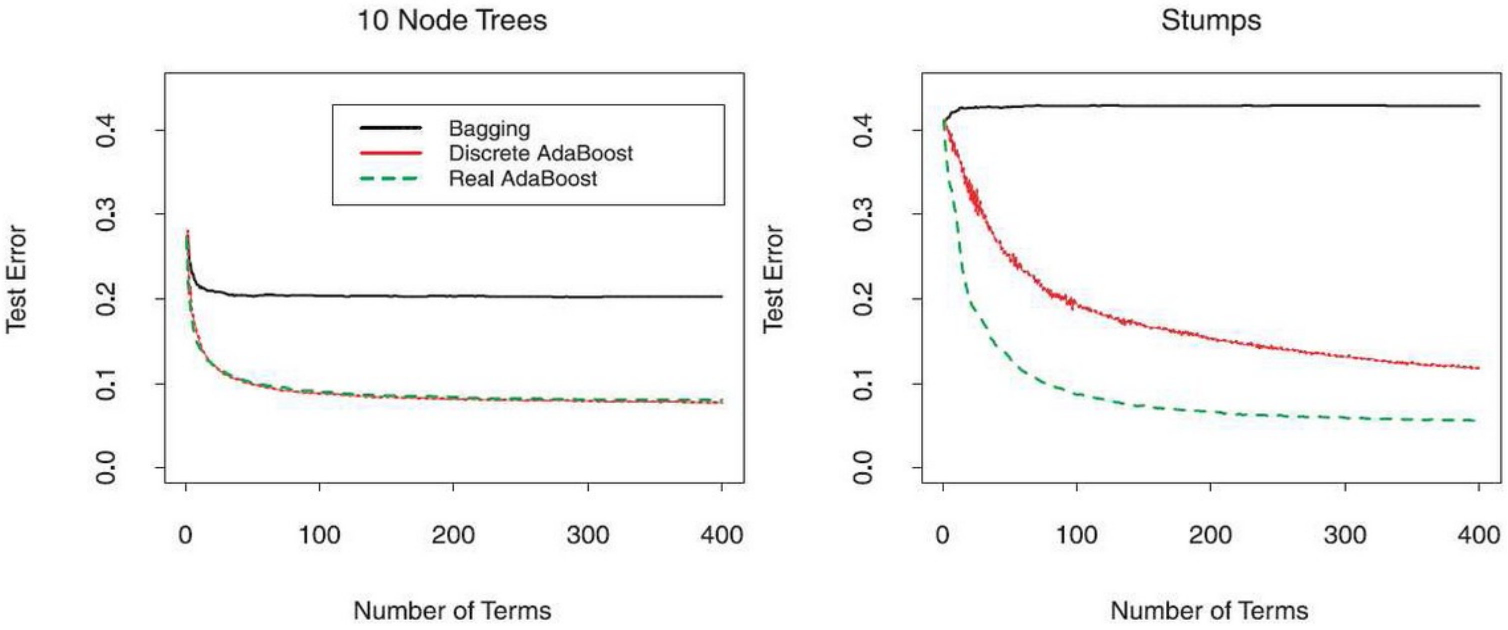
Random Forest

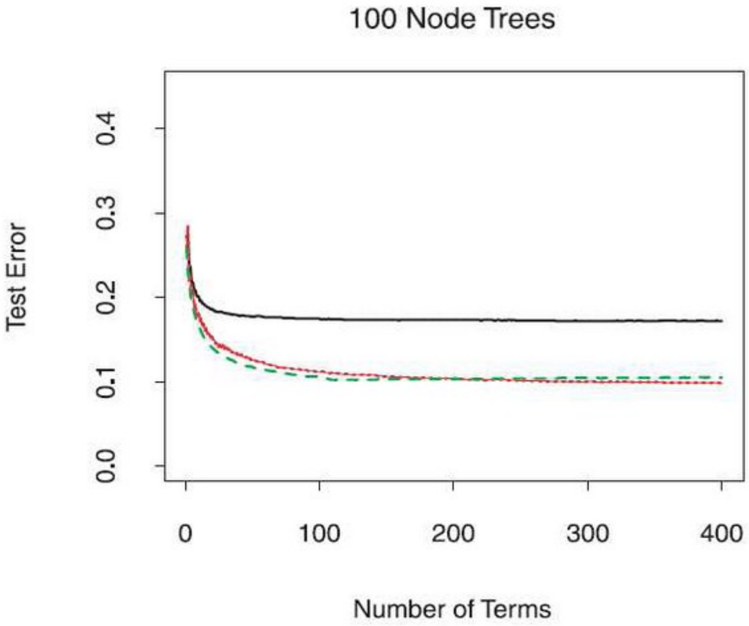
- **Random Forest** – further development of bagging:
  - K times pick N elements from the N element sample.
  - For each sample train a decision tree.
  - Building the tree in every decision point use only m randomly chosen variables

- Typically boosting gives better results, but bagging has a tendency to be more stable at high noise or when there are many “outliers”.
- Bagging is a parallel algorithm, boosting a sequential one.

Bauer and Kohavi, “An empirical comparison of voting classification algorithms”, Machine Learning 36 (1999)

Bagging vs. boosting





Test error for Bagging, Discrete AdaBoost and Real AdaBoost on a simulated two-class nested spheres problem. There are 2000 training data points in ten dimensions.
[Friedman 2000].

Ensemble Learning example

Example code to run various classification tasks, also with ensemble learning:

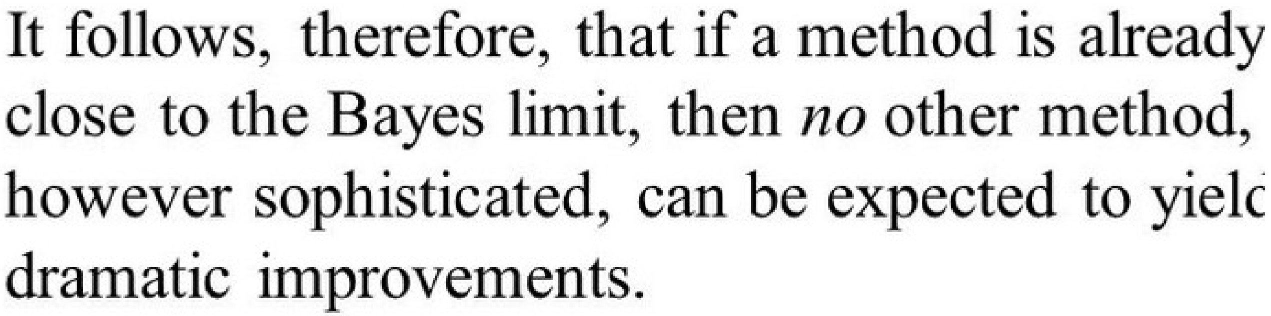
https://github.com/marcinwolter/MachineLearnin2019/blob/master/EnsambleLearningExample.ipynb

Summary

- Boosting, bagging – in a magic way we can build a strong classifier out of weak ones.
- Commonly used for decision trees, because they are simple and fast.
- Gives good results:

  - „the best out-of-box classification algorithm”.
- Very popular in high energy physics
- Or maybe just fancy?...

Should we use BDT only:



It follows, therefore, that if a method is already close to the Bayes limit, then *no* other method, however sophisticated, can be expected to yielc dramatic improvements.

Harrison B. Prosper