

EXTREME DATA MINING: THE KILLER APP FOR METALEARNING?



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MAP-I 2007

Trading in the Stock Exchange: The Machine Learning Way

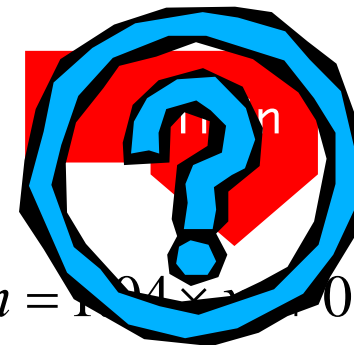
- Goal: decide whether to buy or sell shares

$$f : \text{FinancialVariablesAndOthers} \rightarrow \{1 = \text{buy}, -1 = \text{sell}\}$$

- Table of data

i	$x_{i,1}$	$x_{i,1}$	$x_{i,1}$	$x_{i,1}$	decision
1	0.7	327.2	0	5	-1
2	-0.6	1234.2	1	4	1
3

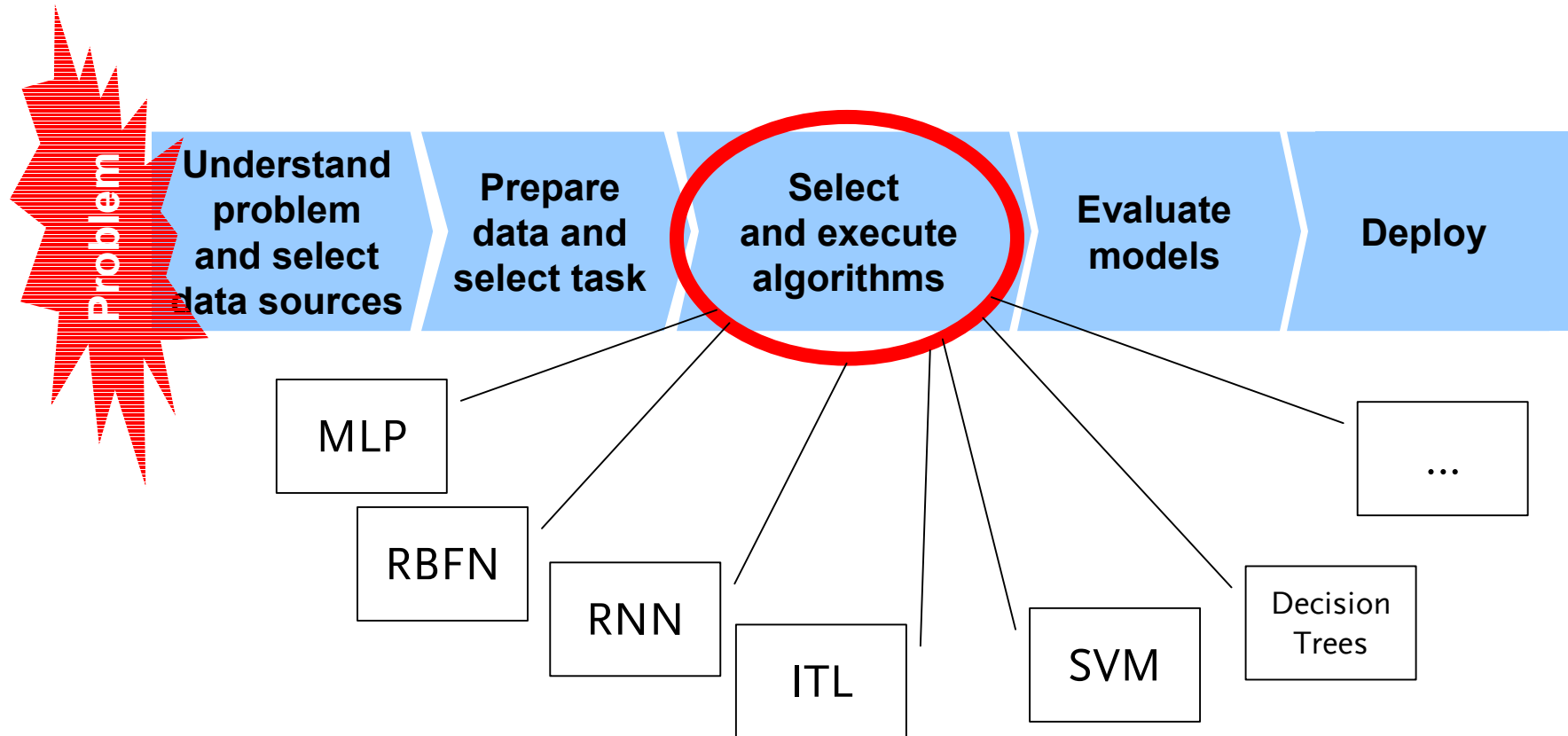
-0.8	37.2	1	15	?
0.2	14.32	1	9	?
...



$$\text{decision} = 1.94 \times x_0 + 0.38 \times x_1 + \dots$$



Problem of Algorithm Selection



WHICH ONE TO USE?

and then some...

Plan: Part I

PART I

- Background: why is this a problem?
 - approximating functions with machine learning
 - algorithm selection and bias
 - a few solutions
- Meta-Learning: **THE** solution

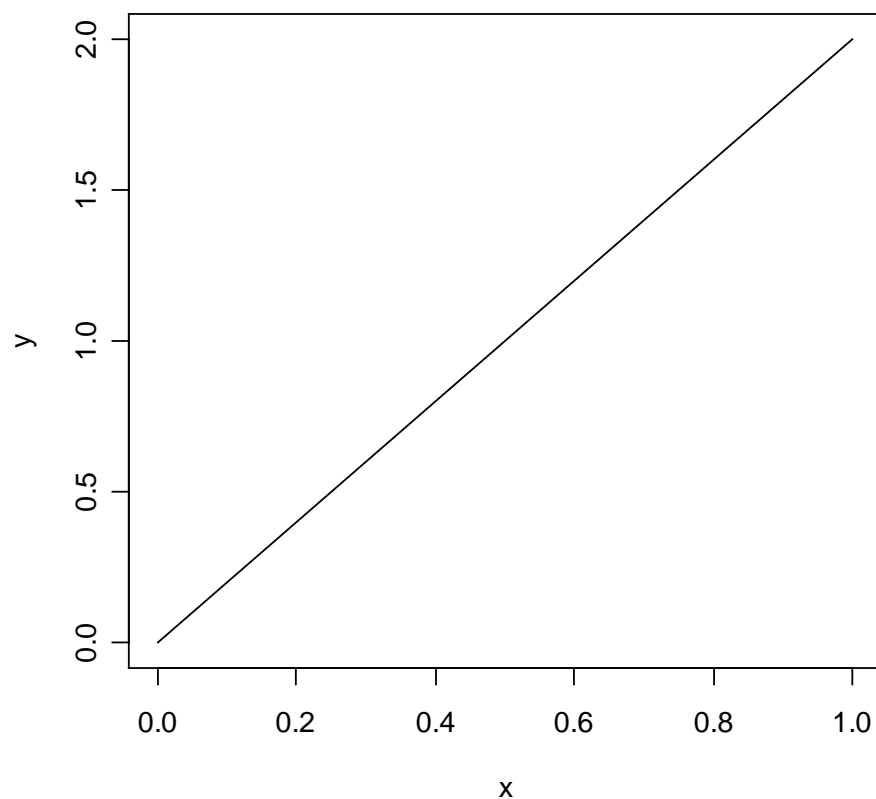
PART II

- Meta-learning for Algorithm Recommendation

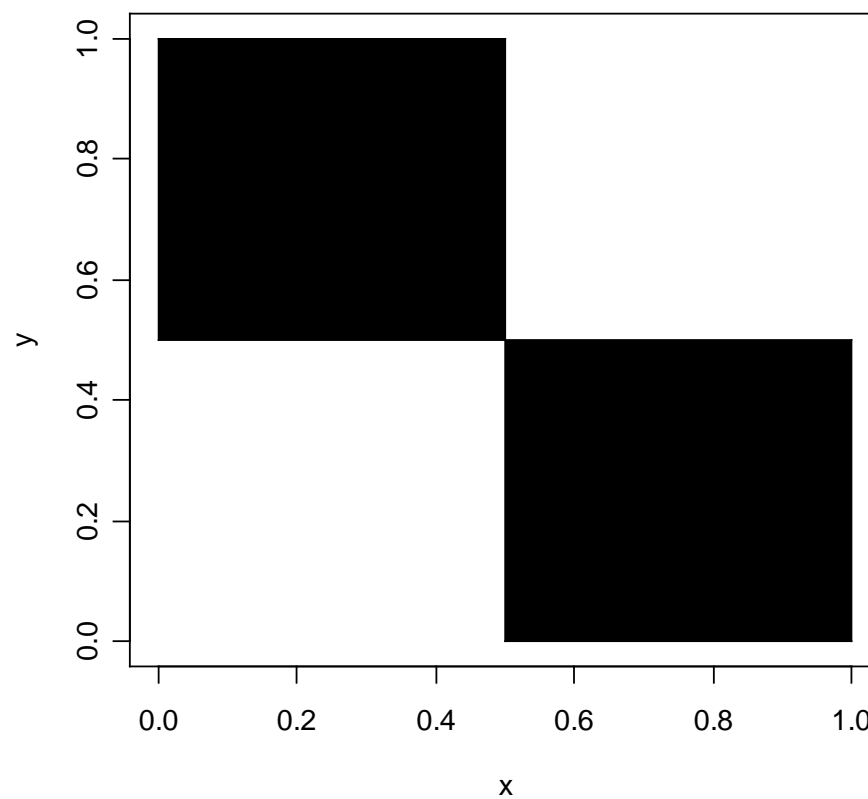
Problem (1/2)

- Quantifiable phenomena...

$y=2*x$



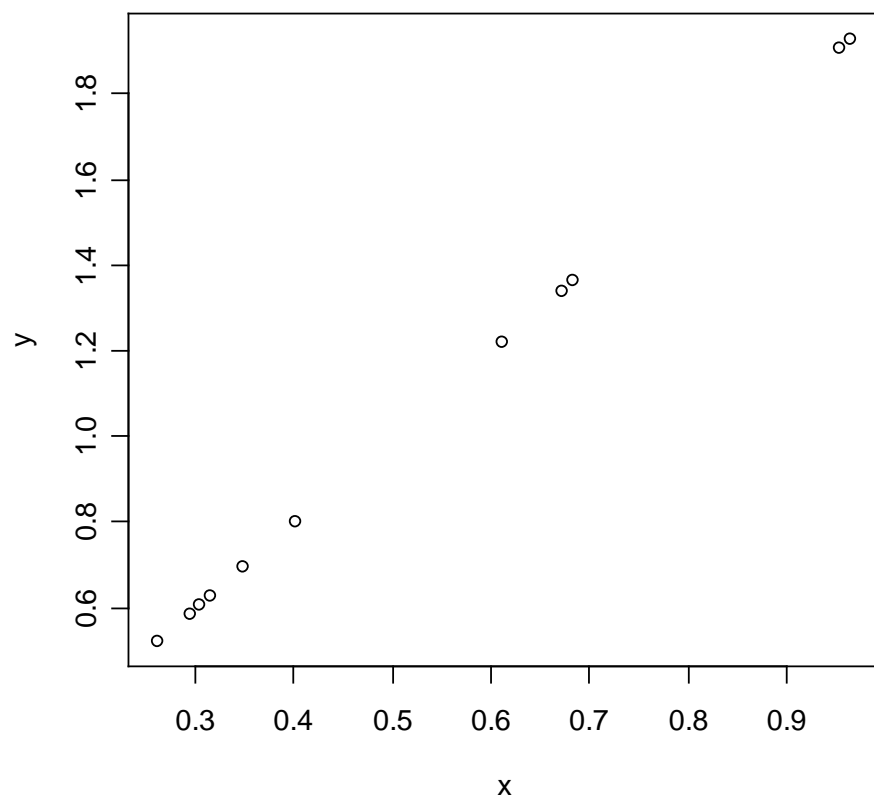
black: $(x > 0.5) \text{ XOR } (y > 0.5)$



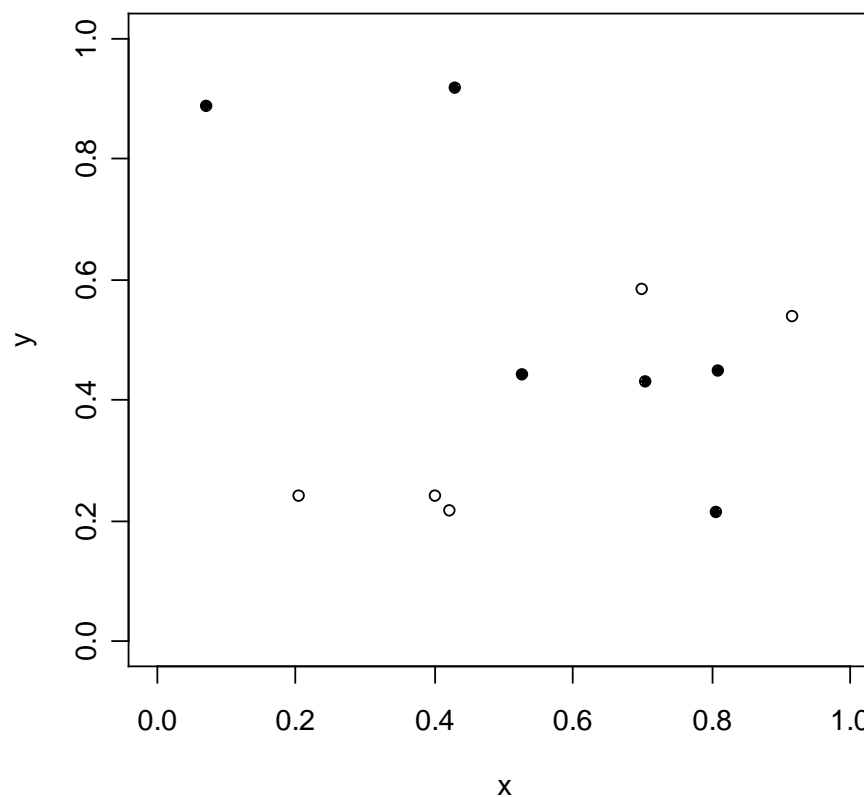
Problem (2/2)

- ... known only through samples

$y=?(x)$



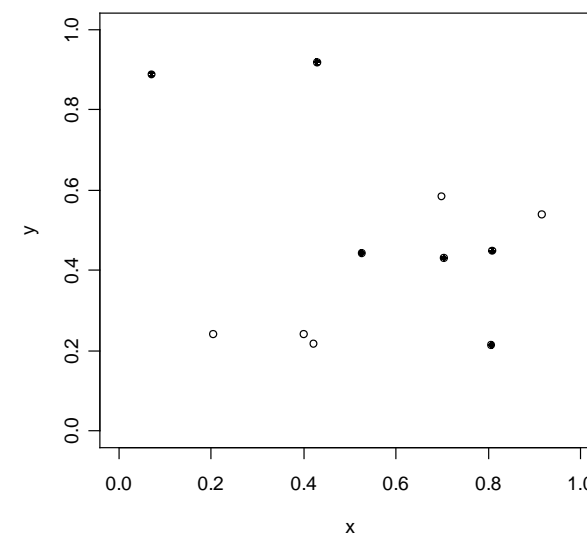
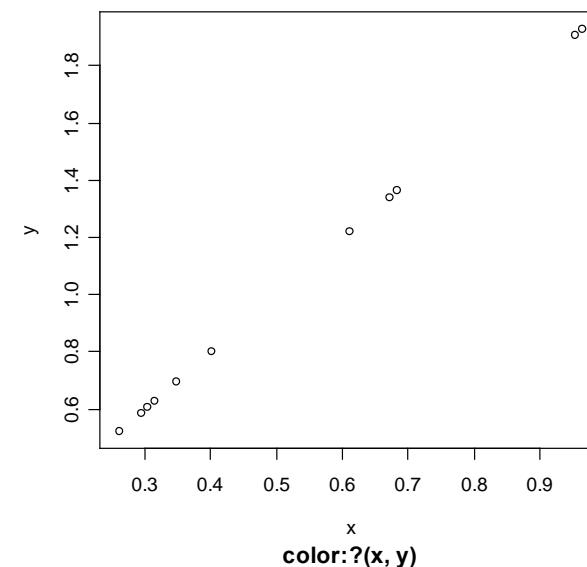
color:?(x, y)



Applications of Machine Learning

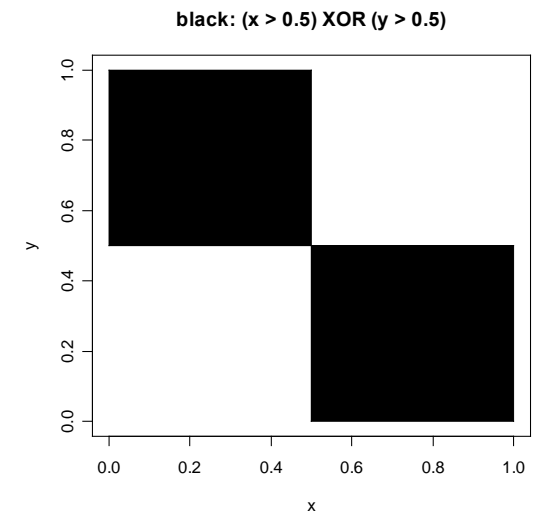
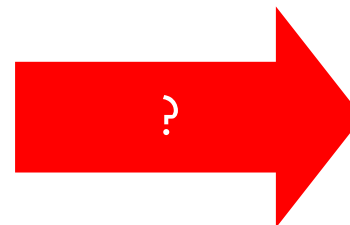
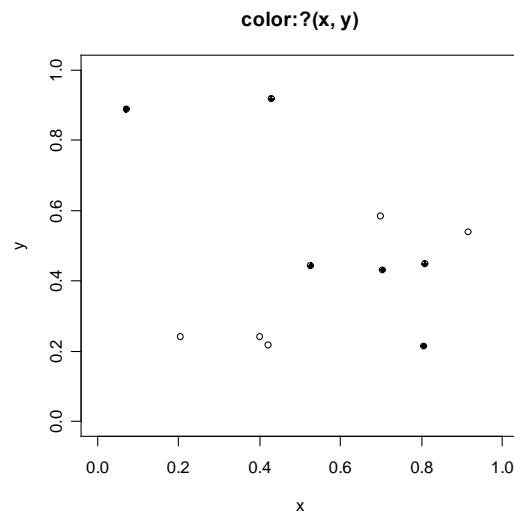
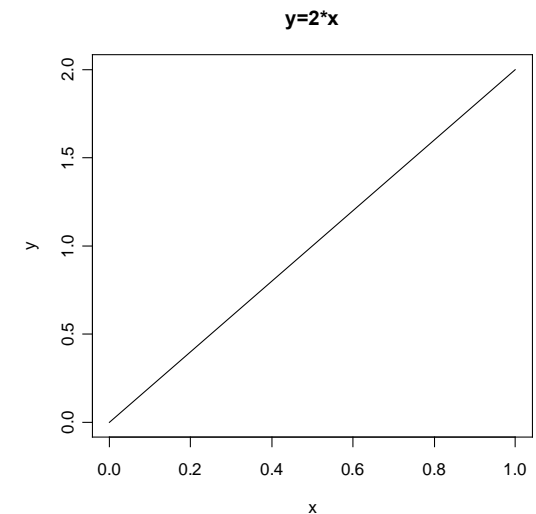
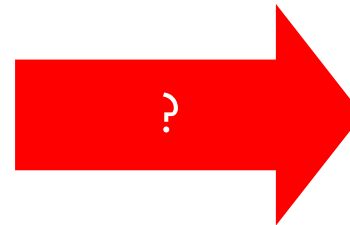
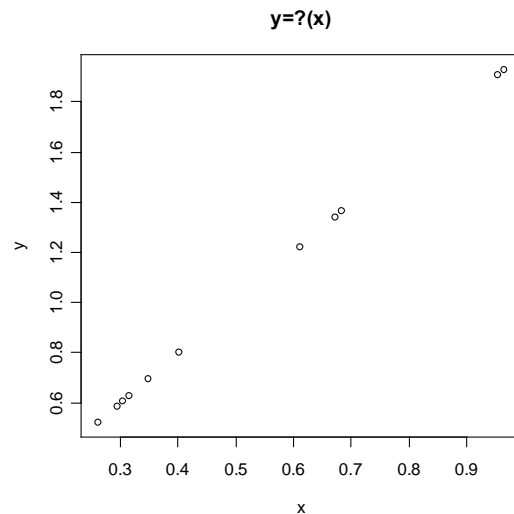
$y=?(x)$

- Based on data samples
- ... model
 - which function describes the relationship between x and y ?
 - how to describe the area in black as a function of x and y ?
- ... predict
 - which is the value of y given $x=0.35$?
 - which is the color of the point ($x=0.3$, $y=0.7$)?



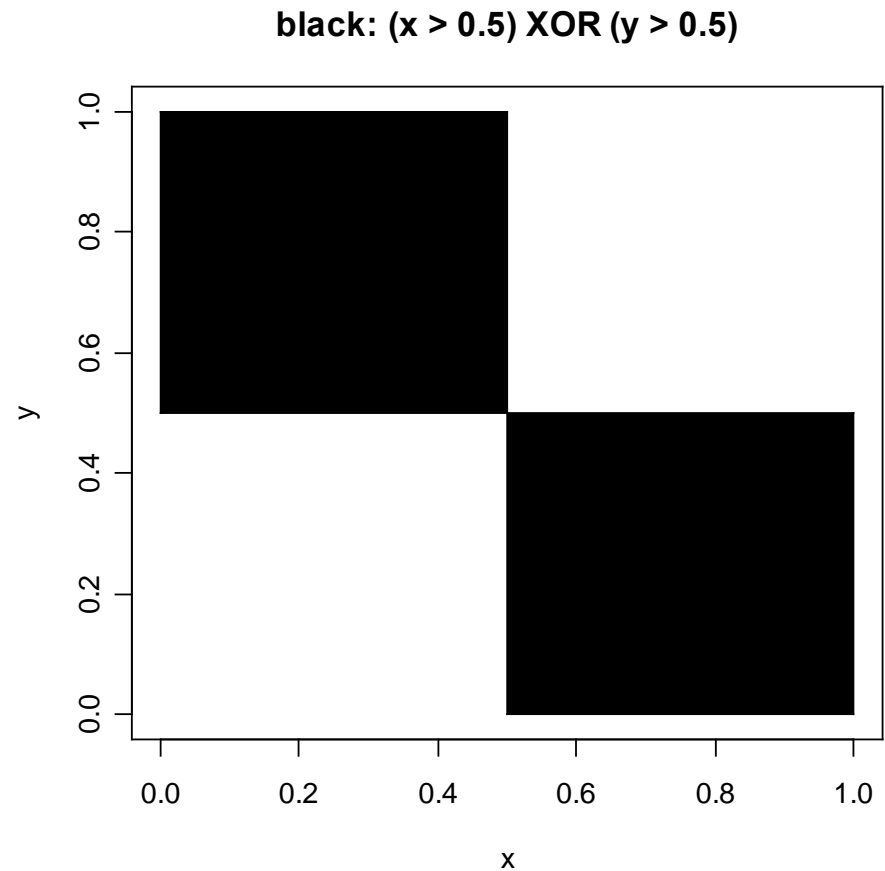
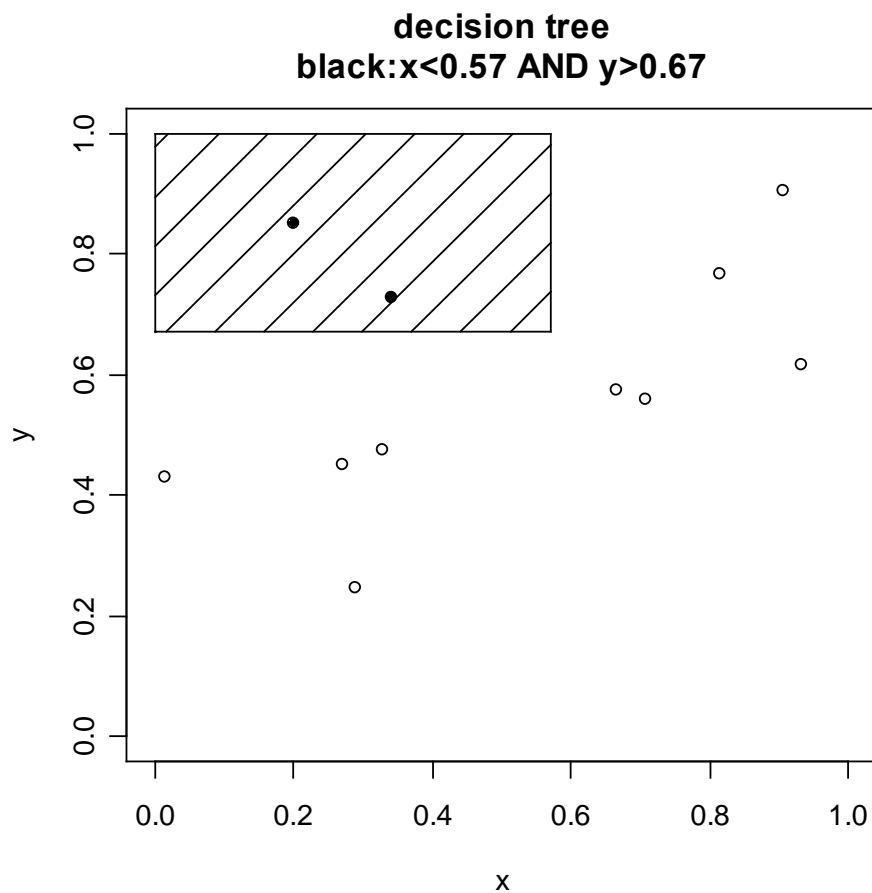
Learning: Summary

- Find the function (model) that best fits the data sample



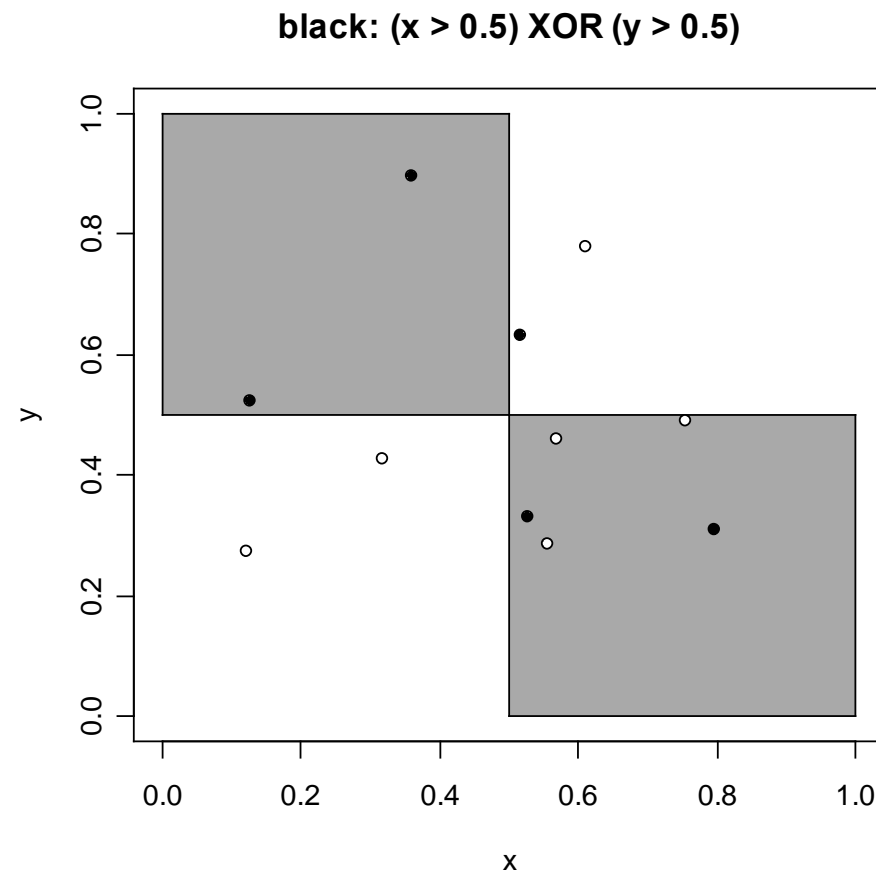
Issues (1/2)

- Representativeness of sample



Issues (2/2)

- Noise



Machine Learning Algorithms: Examples

- Neural Networks
- Support Vector Machines
- Decision trees
- Rule induction
- Linear Discriminants
- Naive Bayes
- k-Nearest Neighbors

WHAT IS THE DIFFERENCE?

Bias

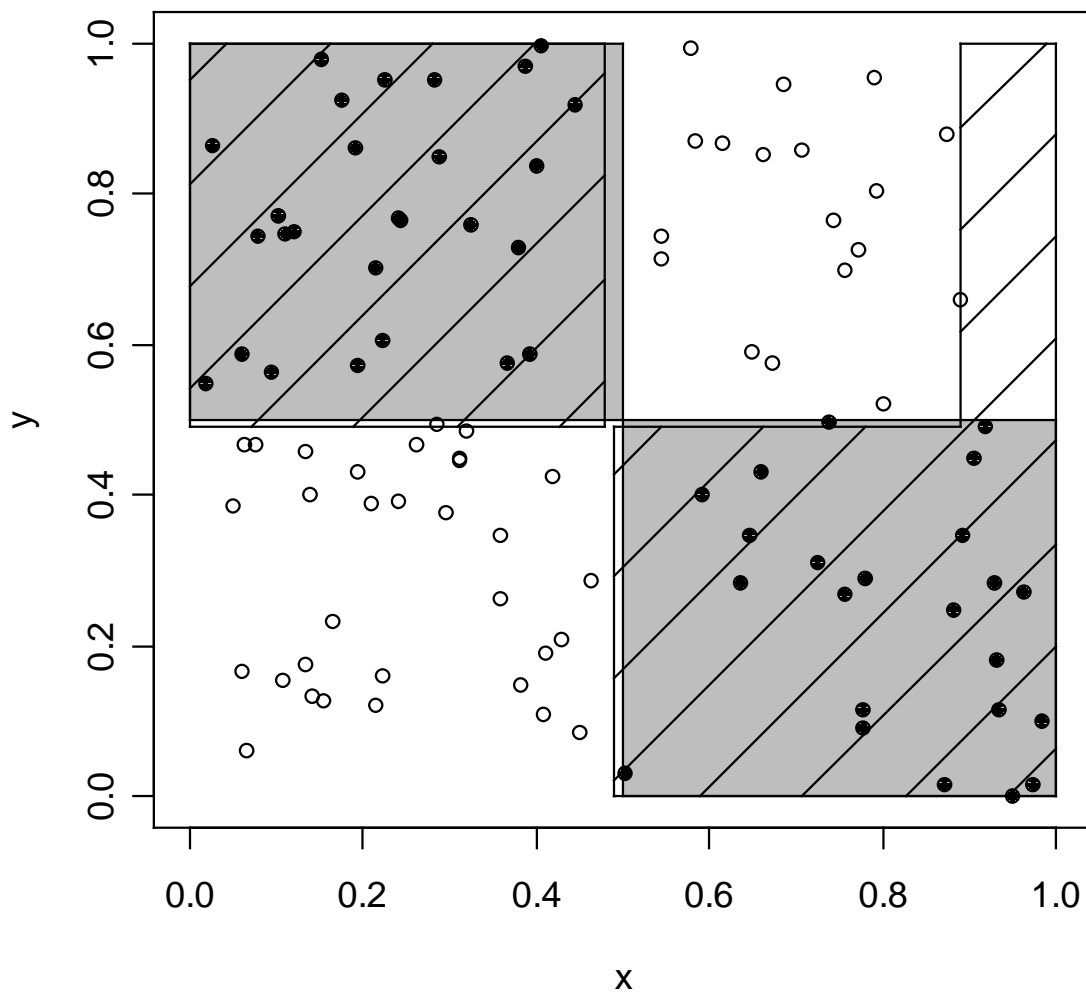
- Criteria to select one from a set of models
 - adapted from des Jardins e Gordon (95)
 - which is extended from Mitchell (80, 90), which did not include error
- Types of bias
 - representation: hypotheses space
 - procedural: search algorithm
- Corollary
 - given a data sample and a learning algorithm
 - ... not every model is possible

Example: Bias of ID₃

- Top-Down Induction of Decision Trees
 - Quinlan (86)
- Hypotheses space: DNF expressions
 - disjunction of conjunctions
 - ... defining hyperplanes that are orthogonal to the axes
- Search algorithm: Top-Down Induction
 - start with simple models (large hyperplanes)
 - increase complexity gradually (smaller hyperplanes)

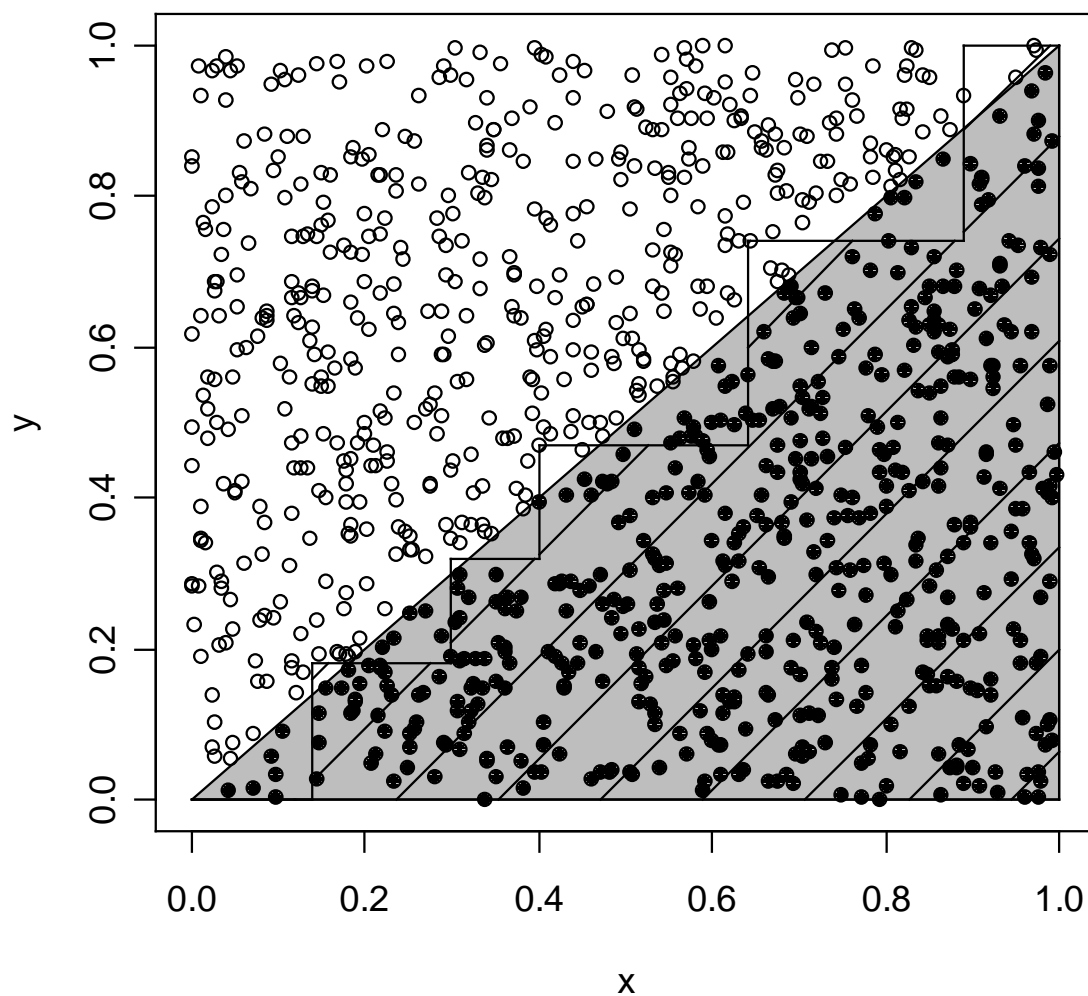
Example: ID₃ is Suitable

sample: 100 examples



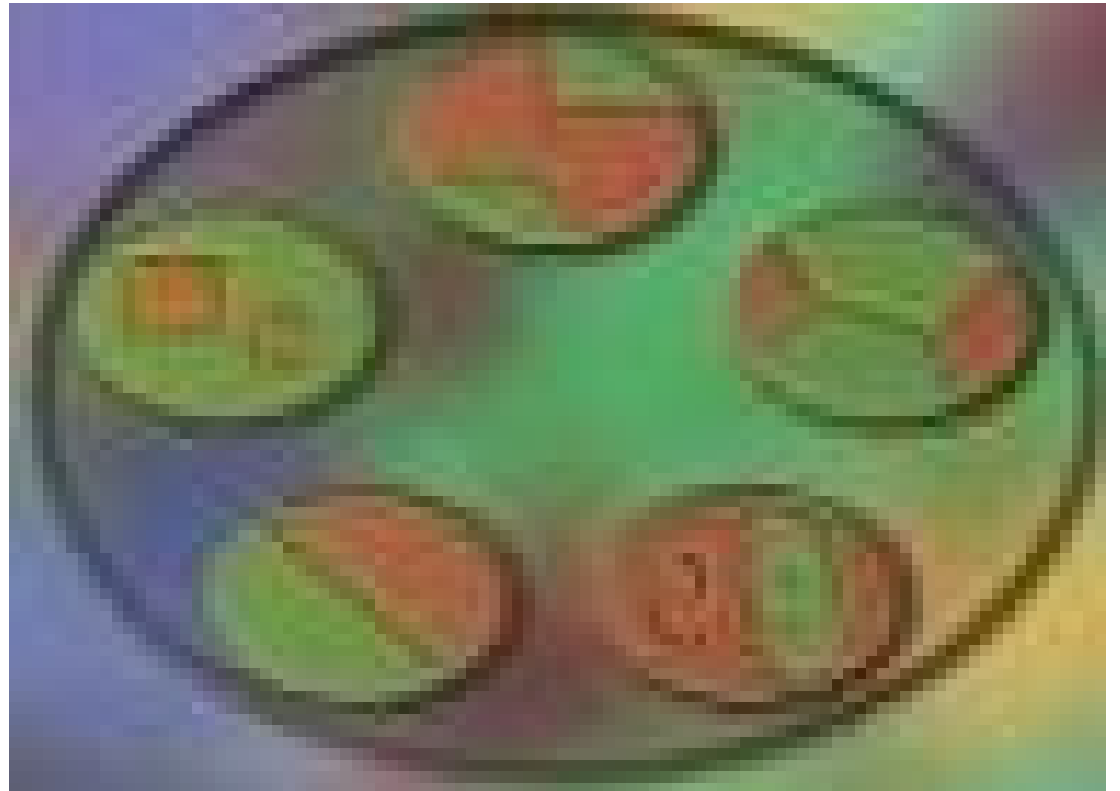
Example: ID₃ is Not Suitable

sample: 1000 examples



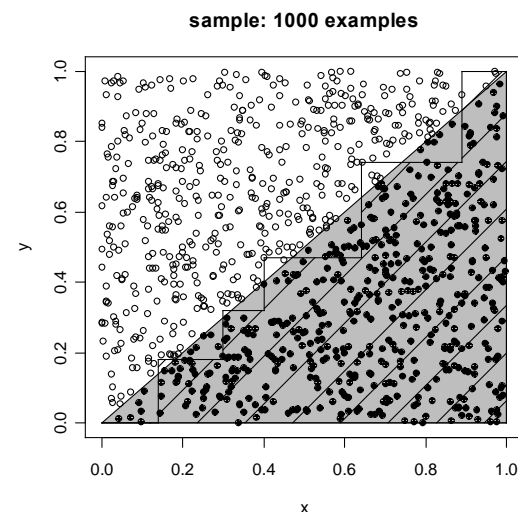
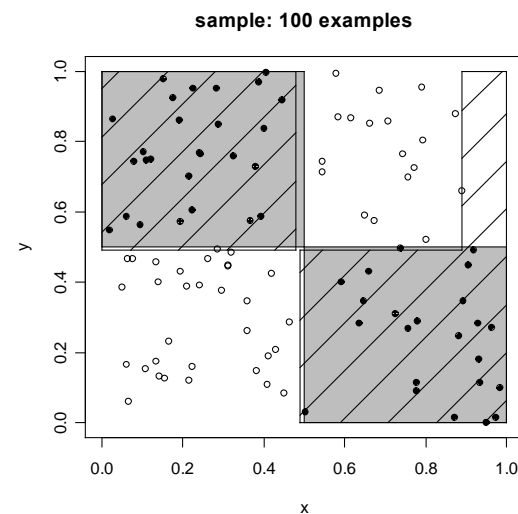
Types of Hypotheses Spaces (According to Langley - 2000)

- Decision trees
- Logical rules
- Cases
- Neural networks
- Probabilistic descriptions



Choice of Algorithm: Summary

- Limits to the models that may be obtained from a data sample using any algorithm
 - can be successful
 - ... or not



Solution I: Bias-Free Algorithm

- Bias-free learning is futile (Mitchell 97, Ch. 2)
 - an algorithm that assumes nothing concerning the function it is trying to learn has no rational basis to classify unknown cases
- Going back to the definition of bias
 - criteria to prefer one model relative to another
- ... and the goal of learning
 - find function (model) that best fits a data sample
- ... how to select the best model if all models are considered equally suitable?

Solution II: The Hard Way

- Test all algorithms
 - pick the one with the best results
- Computationally impossible
 - many algorithms
 - ... most with several parameters
 - ... limited time

Solution III: The Chosen One

- Experimental study
 - a few algorithms (a few parameter settings)
 - ... a few problems
 - ... pick best
 - ... use always
- No-Free Lunch Theorem
 - Wolpert (96)
 - the mean error of all algorithms for all problems in the universe is the same (assuming no information about the problem is used)
- ... limited practical value
- ... but the corollary is verified in practice
 - empirical studies show that “the chosen one” does not exist

Solution IV: Meta-Learning

Learning by experience when different
biases are suitable for particular
problems

Rendell, Seshu e Tcheng (1987)

- Biases, biases... not really
 - ... **implementations** of biases
 - ... or algorithms
- There are other definitions

Solutions for Algorithm Selection: Summary

- Bias is necessary
- Trying all alternatives is not possible
- Choice is important
- Meta-learning: learning models to select which algorithm to use for which problems
 - and more...

Plan: Part I

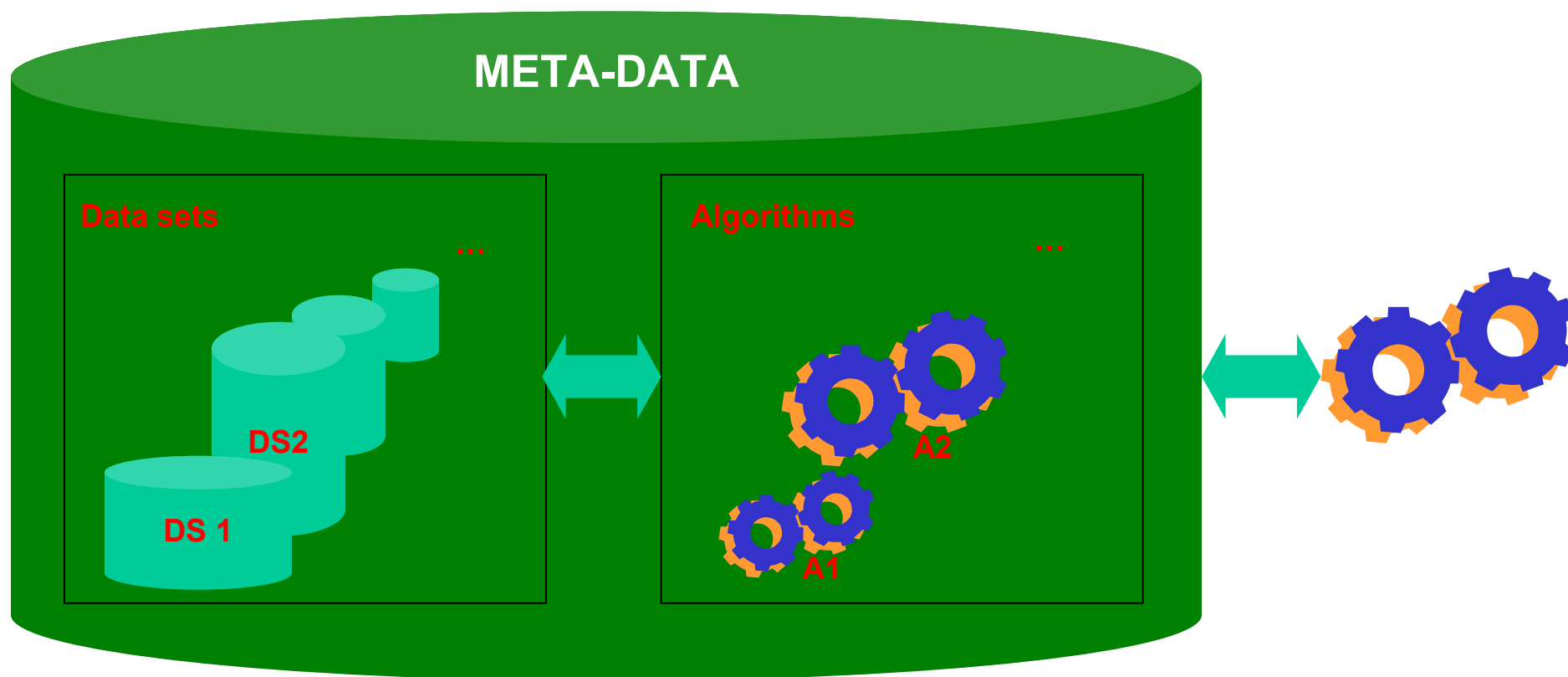
PART I

- Background: why is this a problem?
- Meta-Learning: **THE** solution
 - difference between base-level and meta-level learning
 - different meta-learning approaches

PART II

- Meta-learning for Algorithm Recommendation

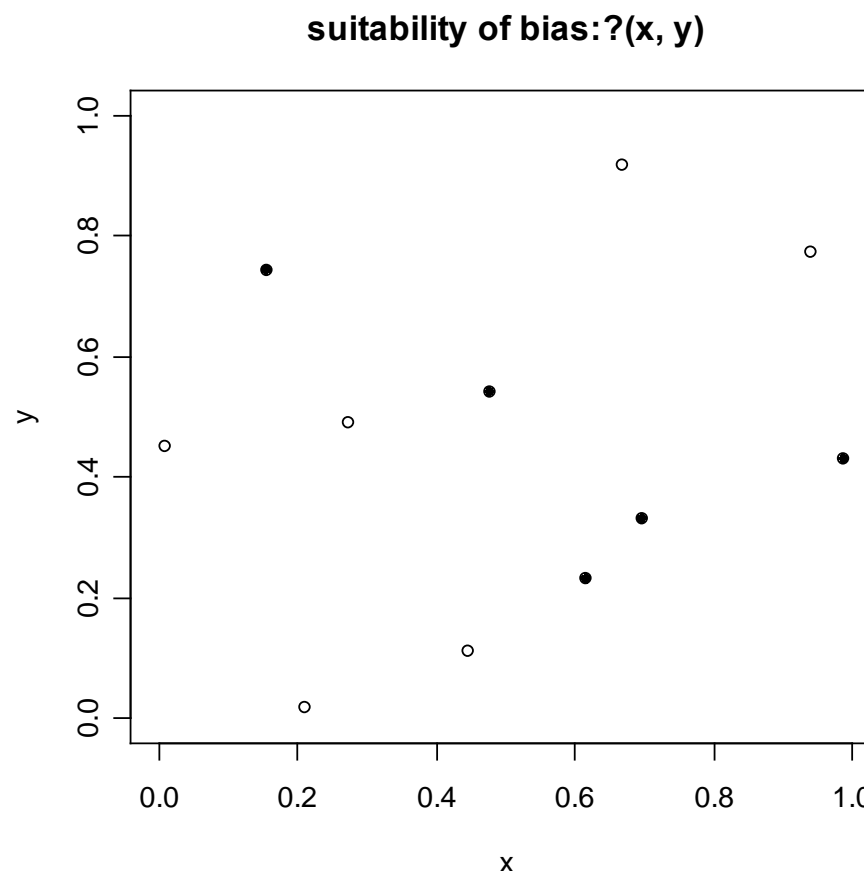
The Meta-Learning Picture



Said Differently, Meta-Learning...

- Applying learning methods to model the relationship between the characteristics of learning problems and the suitability of biases

- [Meta-]data
 - sample: learning problems
 - points
 - problem characteristics
 - x and y
 - suitability of biases
 - black or white



Base vs. Meta: Examples

i	$x_{i,1}$	$x_{i,2}$	$target$
1	.	.	.
2	.	.	.
3	.	.	.

i	$x_{i,1}$	$x_{i,2}$	$target$
1	.	.	?
2	.	.	?
3	.	.	?

Base

Train

$x_{i,1}$	$x_{i,2}$	$target$
.	.	.
.	.	.
.	.	.

i	$x_{i,1}$	$x_{i,2}$	$target$
1	.	.	.
2	.	.	.
3	.	.	.

$$target = 1.04 \times x_1 + 0.38 \times x_2 + \dots$$

Apply

i	$x_{i,1}$	$x_{i,2}$	$target$
1	.	.	.
2	.	.	.
3	.	.	.

Meta

- individuals of interest in the domain
 - e.g. patients; clients

- learning problems
 - e.g. medical diagnosis of disease x in hospital y ; direct marketing for company z

Base vs. Meta: Target Variable

i	$x_{i,1}$	$x_{i,2}$	$target$
1	.	.	.
2	.	.	.
3	.	.	.

.	.	?
.	.	?
.	.	?

Train

$$target = 1.04 \times x_1 + 0.38 \times x_2 + \dots$$

Apply

Base

Meta

- problem-specific decision
 - e.g. diagnosis; send catalog or not
- algorithm
 - e.g. decision trees, MLP

Base vs. Meta: Independent Variables

i	$x_{i,1}$	$x_{i,2}$	$target$
1	.	.	.
2	.	.	.
3	.	.	.

.	.	?
.	.	?
.	.	?

Train

$$target = 1.04 \times x_1 + 0.38 \times x_2 + \dots$$

Apply

Base

Meta

- different characteristics of individuals
 - e.g. job, age and income of person; price and type of product

- problem characteristics and suitability measures
 - e.g. number of variables, number of classes and classification error

Base vs. Meta: Problem

i	$x_{i,1}$	$x_{i,2}$	$target$
1	.	.	.
2	.	.	.
3	.	.	.

Train

$$target = 1.04 \times x_1 + 0.38 \times x_2 + \dots$$

.	.	?
.	.	?
.	.	?

Apply

Base

Meta

- relationships between variables from a domain
 - e.g. individual profile and income; symptoms and diagnosis
- relationship between problem characteristics and suitability of biases
 - e.g. sample morphology and performance of algorithms

Meta-Learning Approaches

- Type of goal
 - continuous adaptation of models/algorithms
 - model construction
 - model combination
 - algorithm selection
- Other classifications are possible

Continuous Adaptation of Models/Algorithms

- Change bias while solving a problem and across different problems
 - also known as “knowledge transfer” or “learning to learn”
- Example: Self-Modifying Policies
 - Schmidhuber, Zhao and Schraudolph (97)
 - parts of the algorithm are able to change other parts of the same algorithm
 - ... even themselves
 - probability of application of a part depends on its past merit
 - illustrated with a reinforcement learning algorithm
 - ... assumes problems are similar

Model Construction

- Build a model made of parts with different biases
- Example: Model Class Selection
 - Brodley (93)
 - recursive partitioning algorithm (decision trees-alike)
 - choice of better bias at each node
 - tested with 3 different biases
 - ... no real learning at the meta-level: choice is based on fixed rules

Model Combination

- Meta-model combining several different base models
- Examples: Stacked Generalization/Cascade Generalization
 - Wolpert (92)/Gama and Brazdil (00)
 - meta-dataset including the predictions made by the base models
 - meta-model obtained by learning with the meta-dataset
 - possibly recursive

Algorithm Selection

- Choosing one (or more) algorithms for a given problem
- Examples: algorithm recommendation
 - Rendell, Seshu and Tcheng (87)
 - Variable Bias Management System
 - Aha (92)
 - generalization from case studies
 - Brazdil, Gama and Henery (94)
 - systematic approach
 - as part of the StatLog Project
 - METAL project (02 – many publications by many authors)
 - follow-up to the work on the StatLog project
 - Data Mining Advisor website
 - www.metal-kdd.org

Plan: Part II

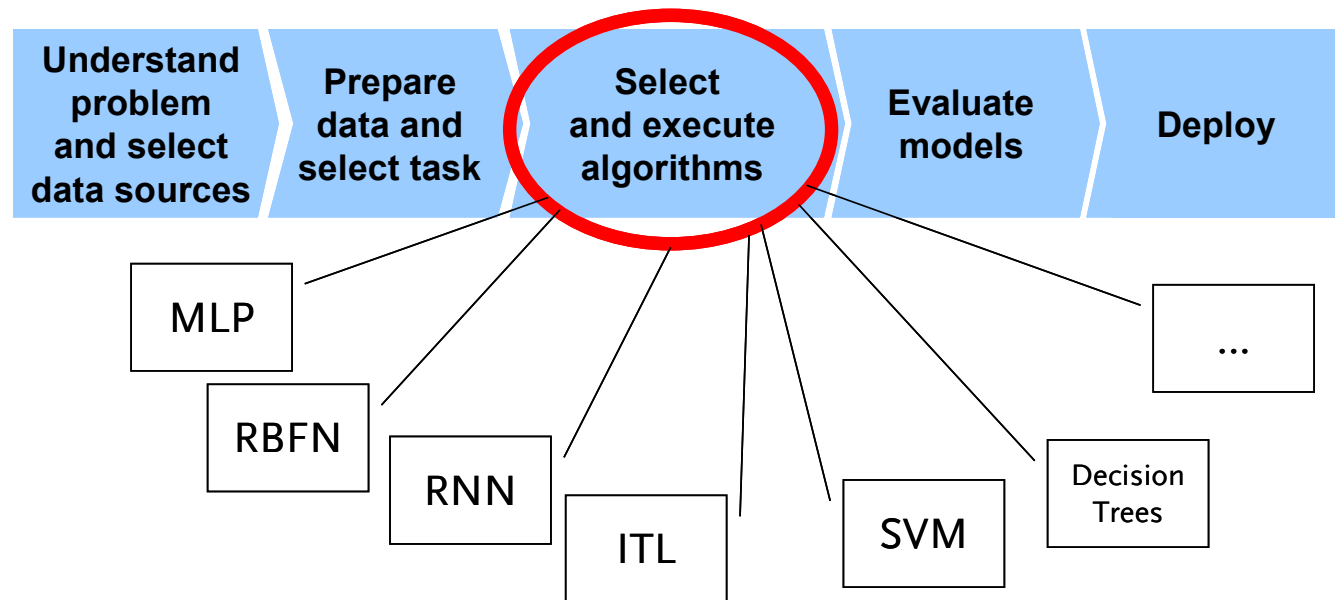
PART I

- Background: why is this a problem?
- Meta-Learning: **THE** solution

PART II

- Meta-learning for Algorithm Recommendation
 - context & goals
 - ranking methodology based on the k-NN
 - evaluation methodology
 - results on the problem of recommending classification algorithms
- Discussion
- Recommendation of Parameter Settings of SVM

Application Context: Data Mining



- Many alternative methods
 - common approach is experimentation

Goal of algorithm recommendation: save time/computational resources with minimal loss in the quality of results

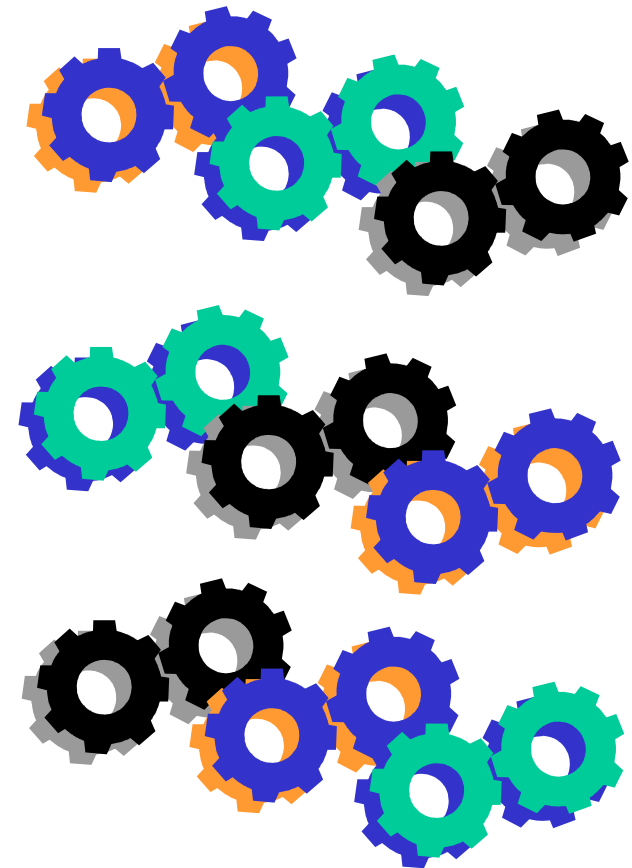
Research Context: Meta-Learning

i	$x_{i,1}$	$x_{i,1}$	$target$
1	.	.	.
2	.	.	.
3	.	.	.

.	.	?
.	.	?
.	.	?

Train

Apply

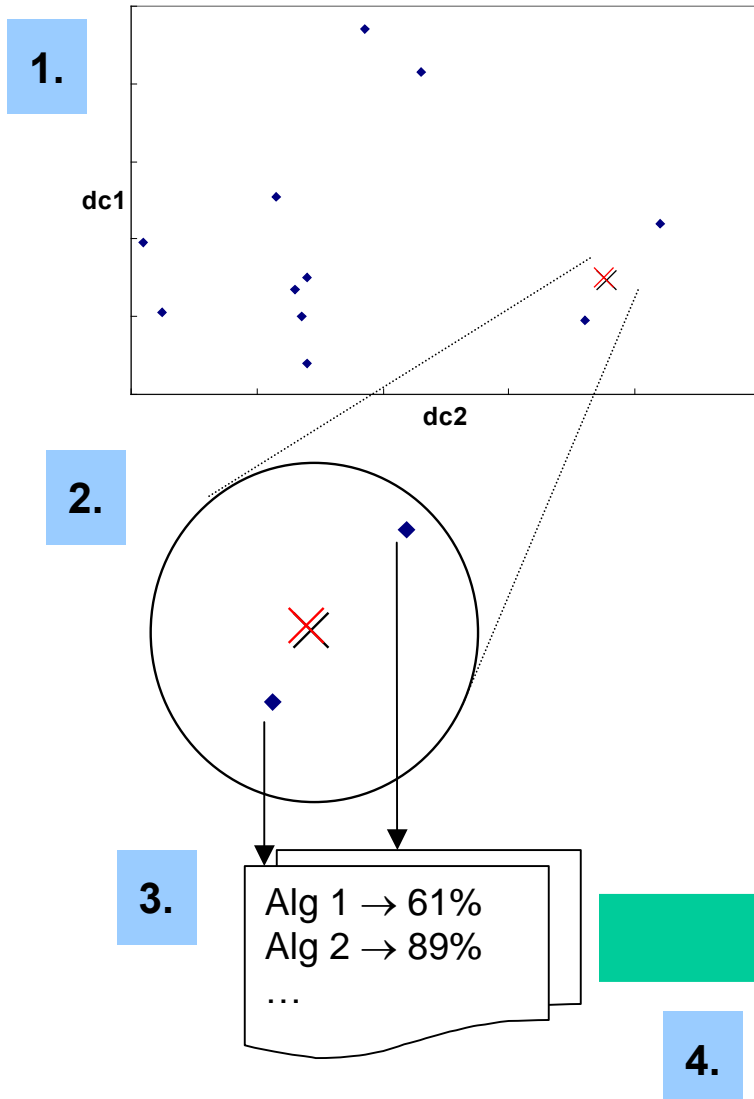


Goal of **meta-learning**: accurately predict the relative performance of algorithms (i.e., **ranking**)

Data Preparation

- Define alternatives
 - 10 classification algorithms
- Define examples
 - 57 problems mostly from the UCI repository
- Obtain performance meta-data
 - run all algorithms on all the data sets
 - computationally intensive...
 - but time to obtain results is not critical
 - measure classification accuracy
- Characterize data sets
 - **meta-features**: # examples, # continuous variables, etc.

k -NN Ranking Method



Given new data set

1. characterize it
 - e.g., # attributes, # examples
2. select k nearest neighbors
3. retrieve performance information
 - e.g., accuracy
4. build **recommended ranking** by aggregating performance information

1. Alg 2
2. Alg 3
...
 n Alg 1

***k*-NN Ranking Method: Ranking Aggregation Method**

- **Solve conflicts between the *k* selected rankings**
- **For instance, Average Ranks**
 - for each selected data set *p*, calculate ranking of algorithms
 - average rank of each algorithm *i* across all selected data sets

$$\overline{R}_i = \frac{\sum_{p=1}^k R_{p,i}}{k}$$

- rank algorithms according to their average rank

k-NN Ranking Method: Example

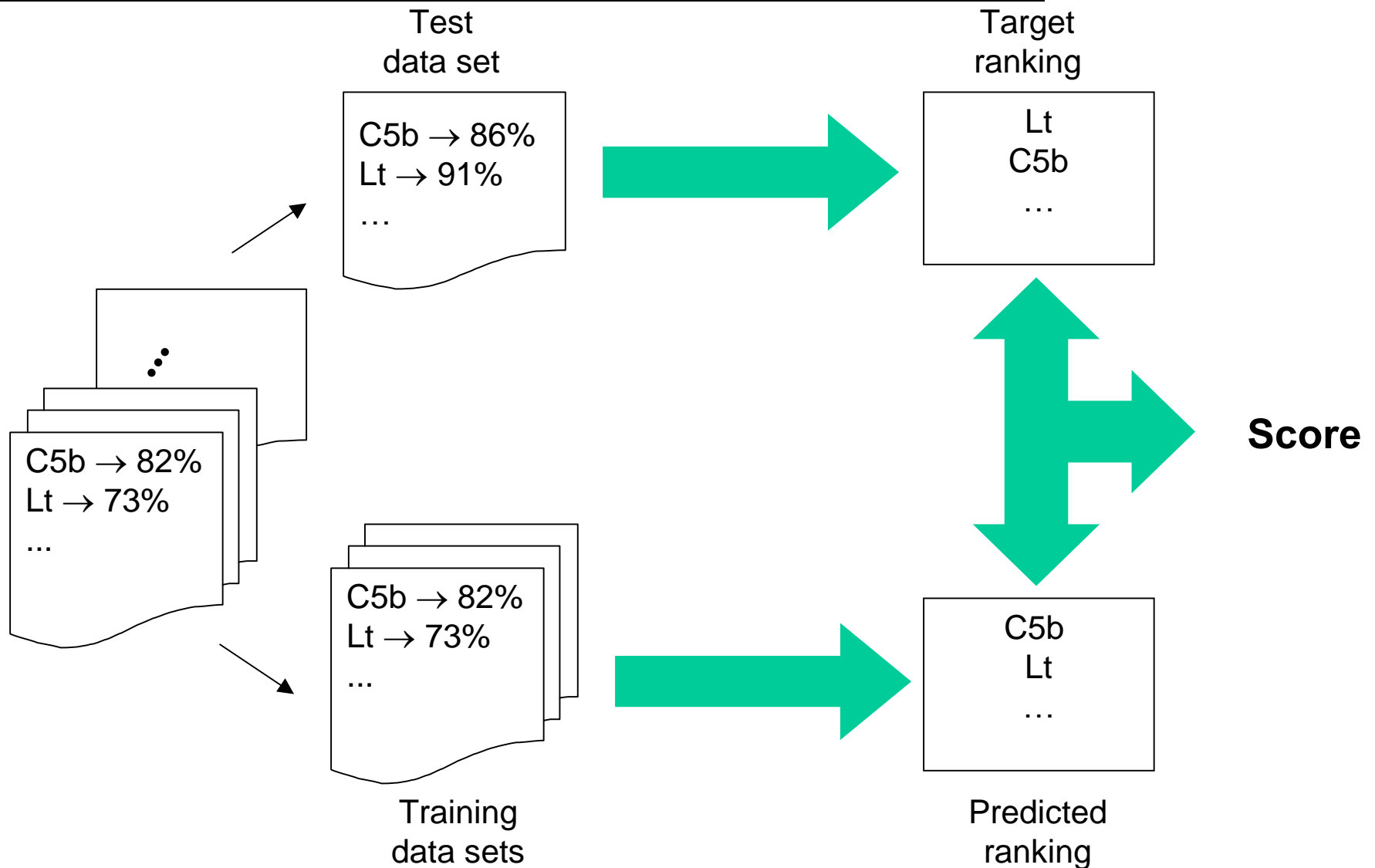
- Recommendation for the letter data set using 3-NN

algorithms

data sets

ranks	bC ₅	C ₅ r	C ₅ t	MLP	RBFN	LD	Lt	IB ₁	NB	RIP
byzantine	2	6	7	10	9	5	4	1	3	8
isolet	2	5	7	10	9	1	6	4	3	8
pendigits	2	4	6	7	10	8	3	1	9	5
predicted	1	5	7	9	10	4	3	1	5	8

Evaluation of Methods to Predict Rankings



Measuring Ranking Accuracy

- **Target ranking**

- representing performance of algorithms on the “new” data set

- **Spearman's Rank Correlation Coefficient**

- values range from -1 to 1

$$r_S = 1 - \frac{6 \sum_{i=1}^n (\hat{R}_i - R_i)^2}{n^3 - n}$$

ranks	bC5	C5r	C5t	MLP	RBFN	LD	Lt	IB1	NB	RIP
predicted	1.5	5.5	7	9	10	4	3	1.5	5.5	8
target	1	3	5	7	10	8	4	2	9	6

$$r_S = 0.709$$

Default Ranking

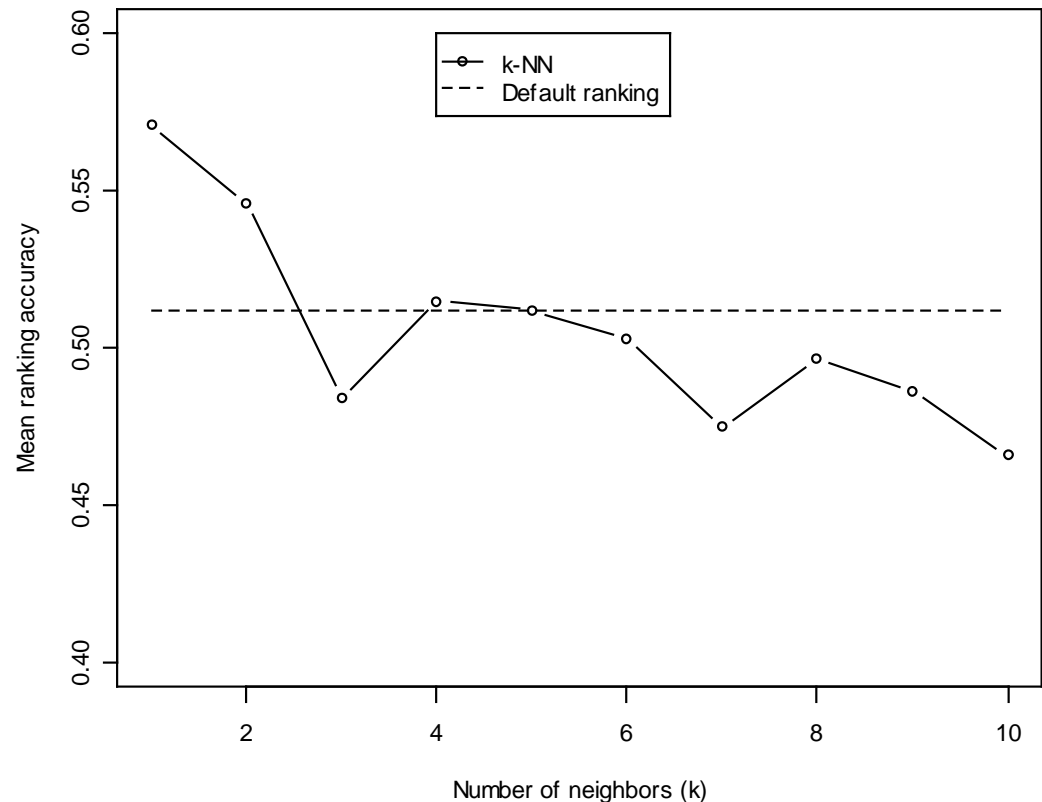
- **Baseline**
 - simple method
 - assess whether ranking method is finding useful patterns
- **Default ranking**
 - apply ranking aggregation method on all the rankings

Ranks	bC5	C5r	C5t	MLP	RBFN	LD	Lt	IB1	NB	RIP
default	1	2	4	7	10	8	3	6	9	5
target	1	3	5	7	10	8	4	2	9	6

$$r_S = 0.879 > 0.709$$

k -NN vs. Default Ranking: Ranking Accuracy Results

- **Baseline default ranking**
 - fixed prediction...
 - but quite accurate
- **k -NN more accurate than DR**
 - small k
- **Significance of differences between methods**
 - Friedman's and Dunn's tests



Possible to predict the relative performance of algorithms

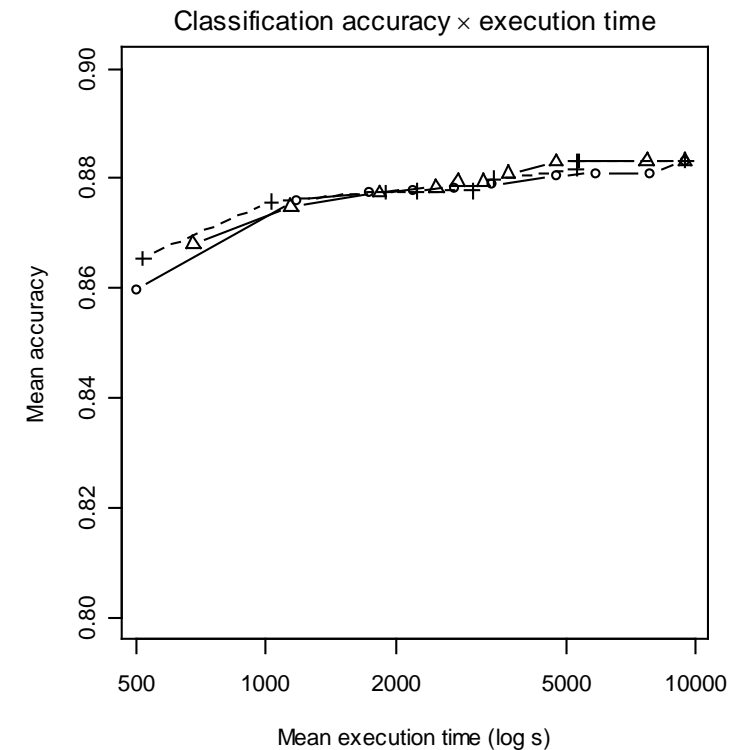
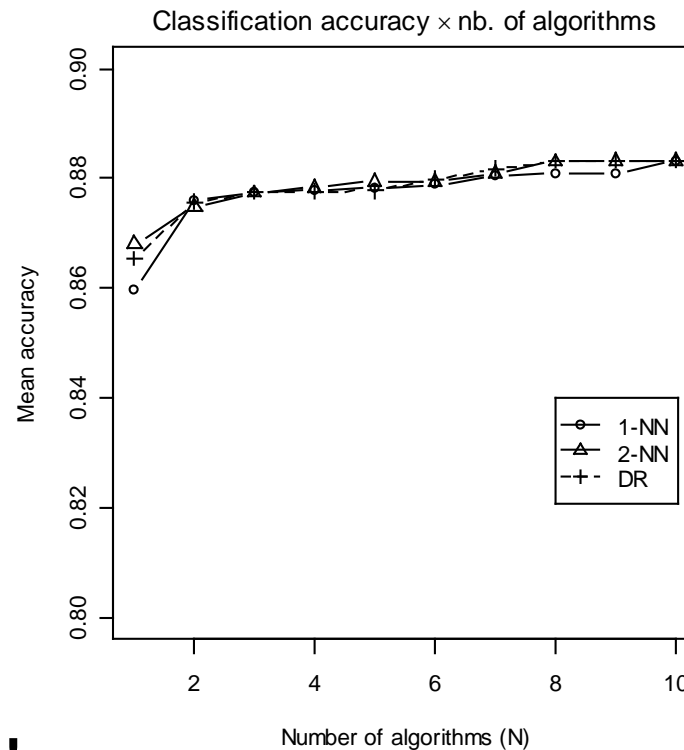
Measuring Value of Recommended Rankings

- **Accurate rankings are not necessarily useful**
 - goal is to save time with minimal loss in (classification) accuracy
- **Value depends on the use**
 - order defined by ranking is followed...
 - but number of algorithms executed is not known beforehand
- **Top-N evaluation**
 - best accuracy of top-N algorithms in the ranking
 - total cost of executing them

recommendation for letter	bC5	IB1	LT	LD	C5R	NB	...	RBFN
	81%/56s	87%/81s						88%/478s

k -NN vs. Default Ranking: Top-N Results

	Acc. (%)	Time
All	88.3	2.5 h
Top-1	86.8 (-1.5)	11 min
Top-2	87.5 (-0.8)	20 min
bC5	86.5 (-1.8)	8 min



• Difficult problem!

- Possible to save significant amounts of time with small loss in accuracy
- Ranking is more suitable for algorithm recommendation

Ranking According to Accuracy and Time

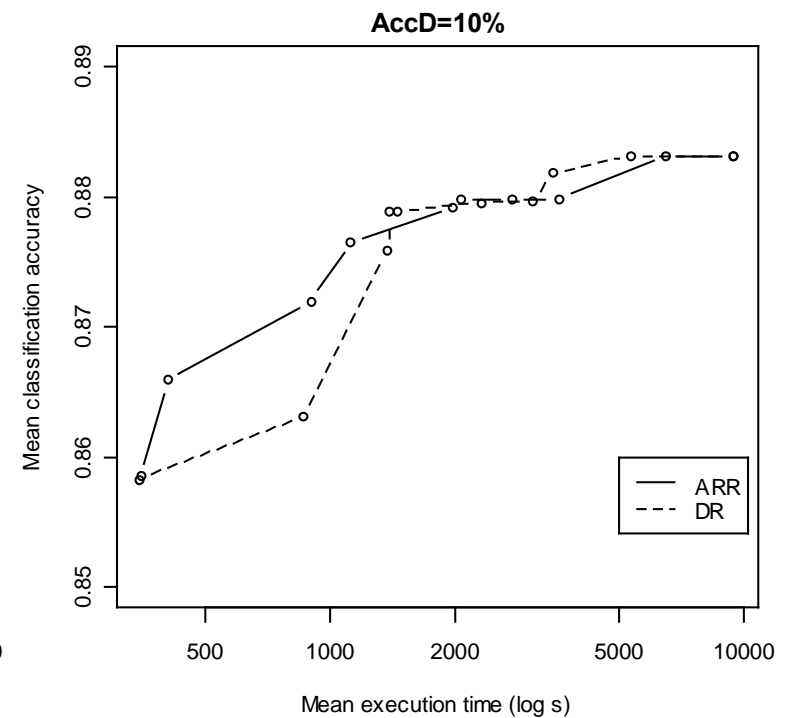
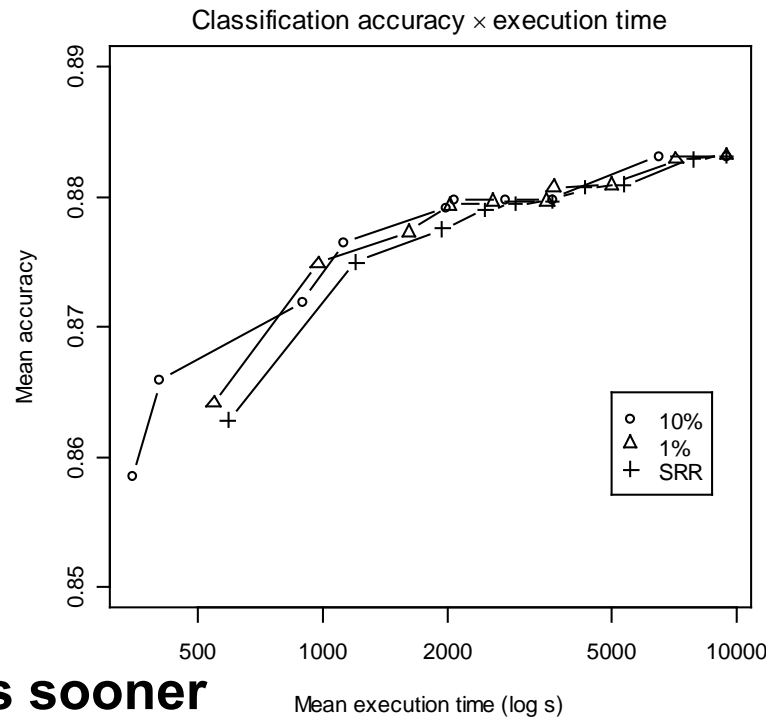
- Incorporate knowledge about the goal into the recommendation method
 - save time with minimal loss in (classification) accuracy

- **Adjusted Ratio of Ratios**

$$ARR_{i,j} = \frac{\frac{SR_i}{SR_j}}{1 + AccD \times \log\left(\frac{T_i}{T_j}\right)}$$

- **Parameter defining relative importance of accuracy and time**
 - AccD= the accuracy the user is willing to trade for a 10 times speedup

k -NN with ARR: Top-N Results



- **Better results sooner**
 - less accurate algorithms at the top...
 - but more algorithms are executed

Problem-specific knowledge is more important than the choice of aggregation method

Plan: Part II

PART I

- Background: why is this a problem?
- Meta-Learning: **THE** solution

PART II

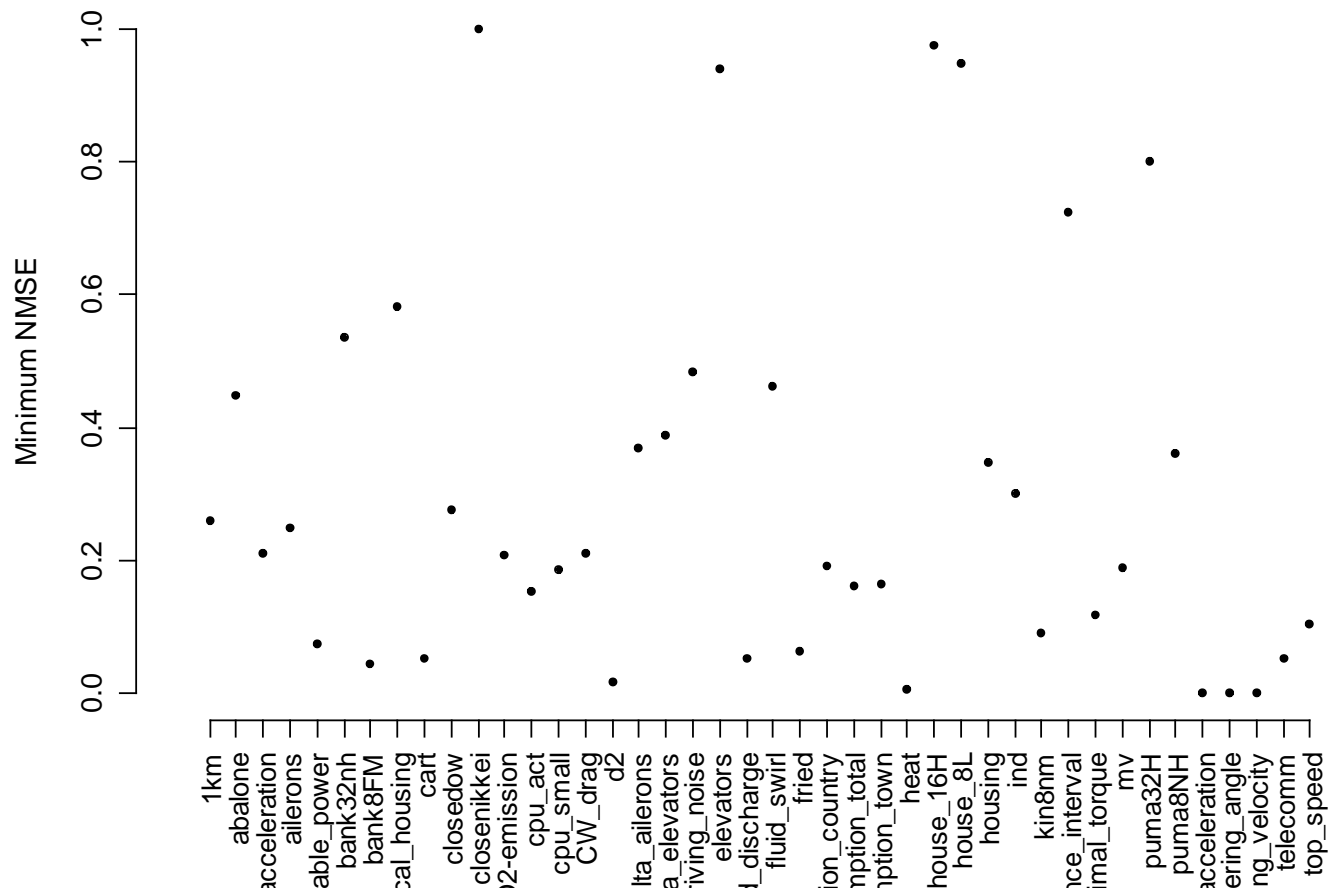
- Meta-learning for Algorithm Recommendation
- Discussion
 - pre-selection of alternatives
 - obtaining problems
 - characterization of problems
 - meta-accuracy
 - other applications
- Recommendation of Parameter Settings of SVM

Pre-selection of Alternatives

- Which algorithms?
 - the ones in available tools
 - constraints on acceptable models
 - e.g. understandability
 - preferences of the data analyst
 - ... or ignorance concerning others
- Which parameters?
 - domains are frequently infinite
 - continuous parameters
- Is the selected set adequate?

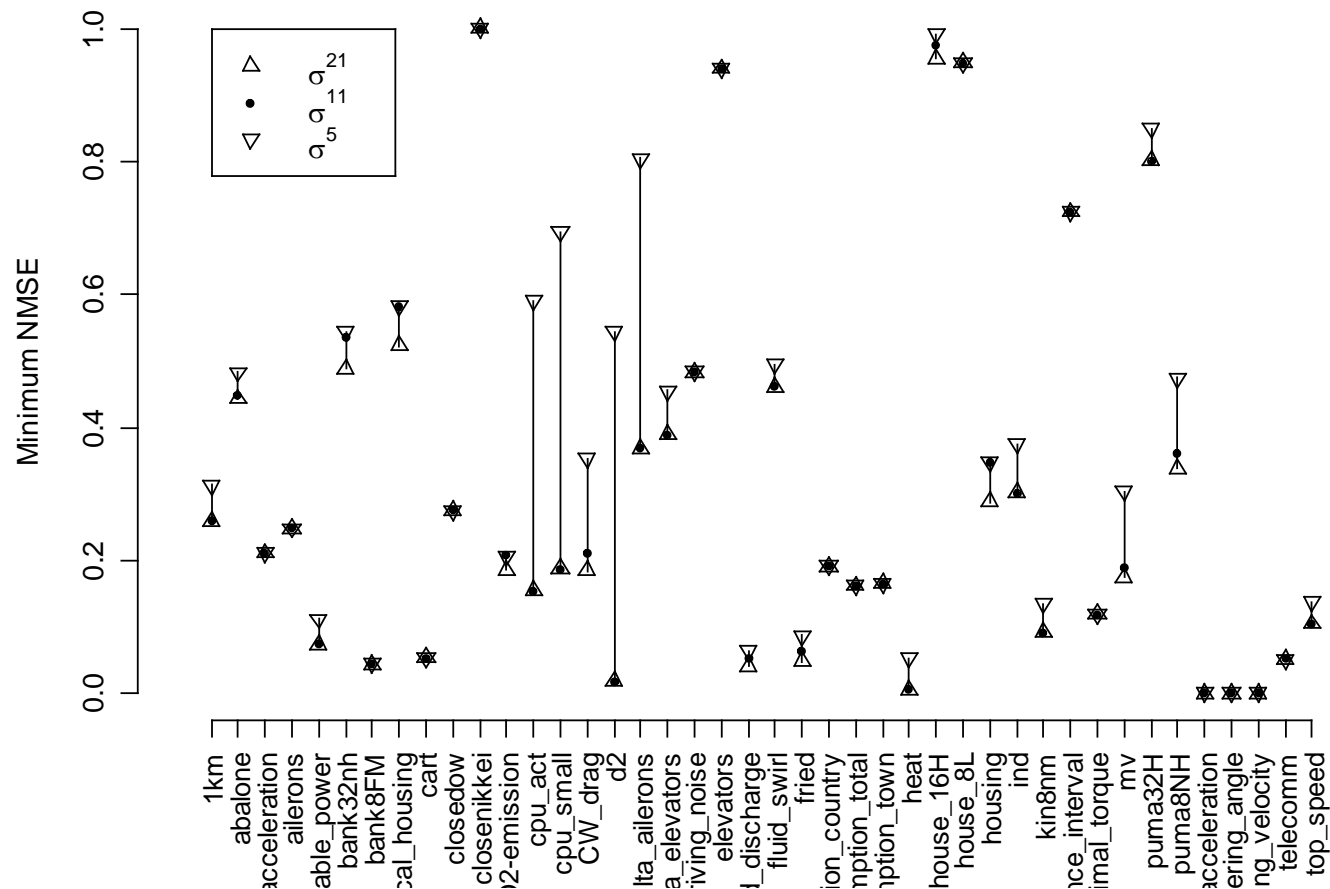
Pre-selection of Alternatives: Overall Relevance

- For most data sets there should be an alternative that obtains an error which is lower than the error of a given baseline



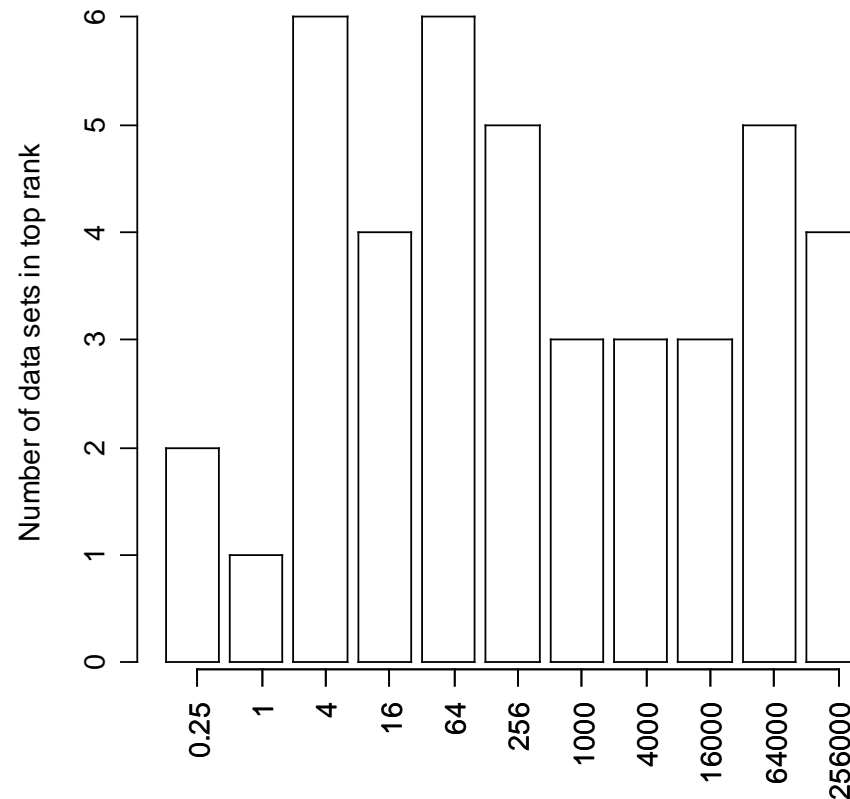
Pre-selection of Alternatives: Overall Competitiveness

- Given some pre-selected set of alternatives, the results cannot be further significantly improved by adding additional ones



Pre-selection of Alternatives: Individual Competitiveness

- For every alternative, we should be able to identify at least one data set for which it is the best one, from the pre-selected set

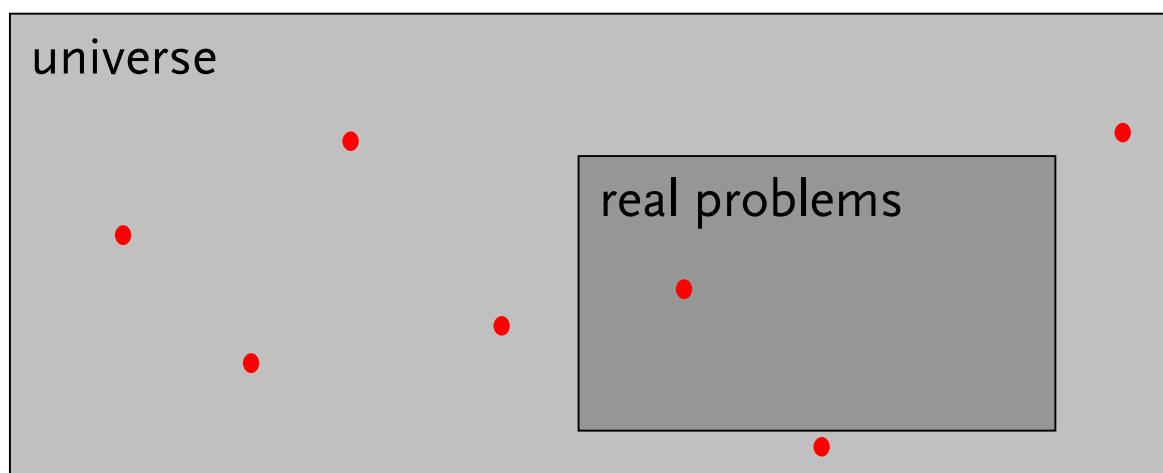


Pre-selection of Alternatives: Individual Relevance

- For every alternative, there should not exist another one such that the performance of former is never significantly better than that of latter for all data sets considered
 - each setting is significantly better than each of the others on at least one data set

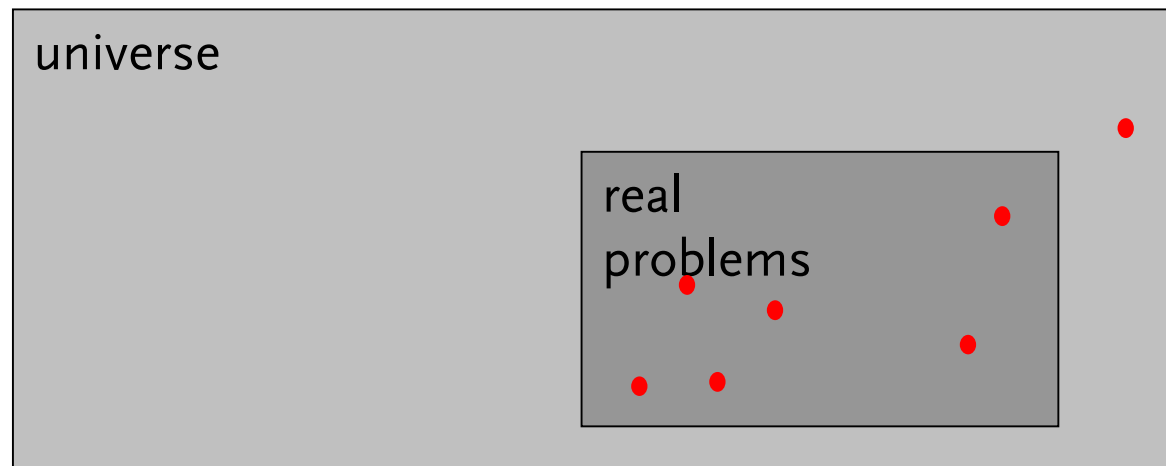
Quantity/Quality of Meta-data

- Meta-models are based on a few dozen problems
 - small sample
 - results are positive but are they stable?
- How to generate more meta-data?
 - **random** methods are not suitable



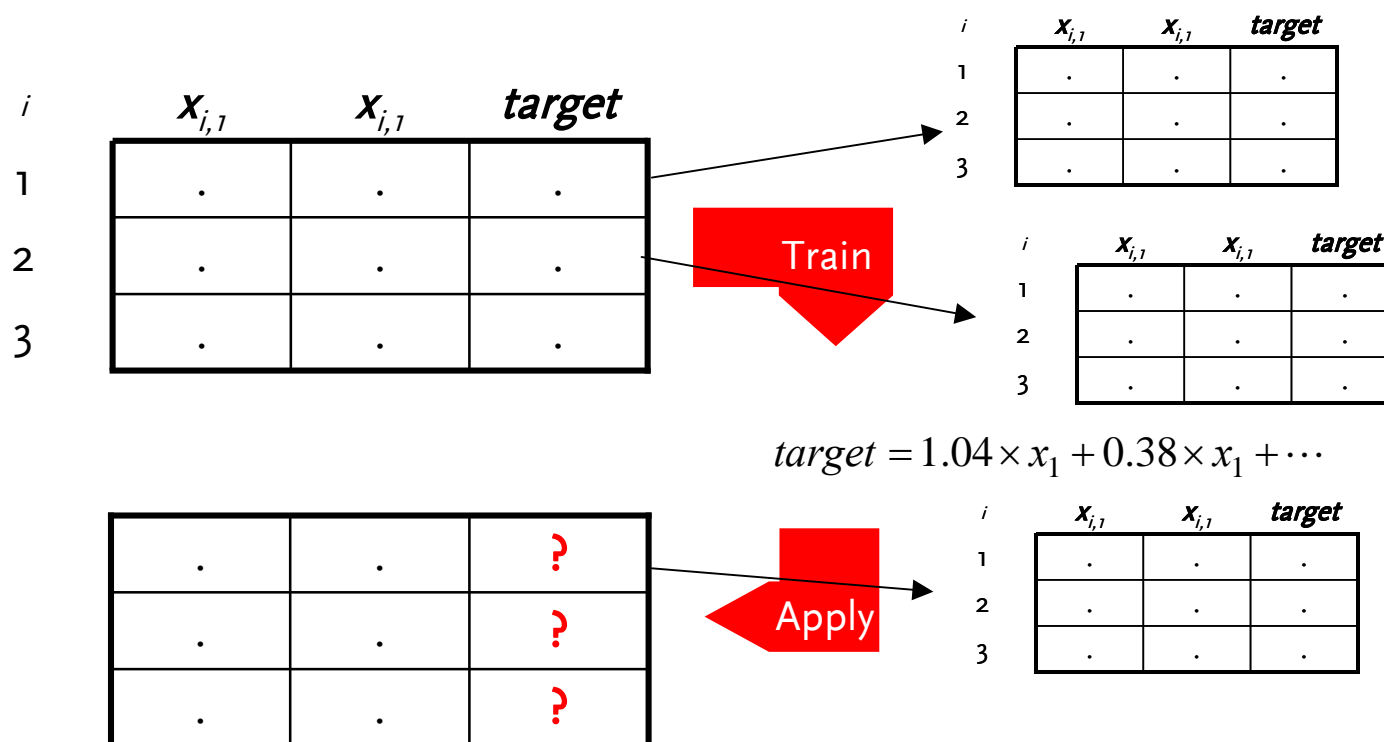
Simulated Applications using Real Data

- Get real data
 - any source is fine
 - e.g. transactions, time between events
- Simulate applications
 - one problem for each variable
 - ... corresponding value may not make any sense
- Goal



Characterization of Datasets

- Meta-Dataset

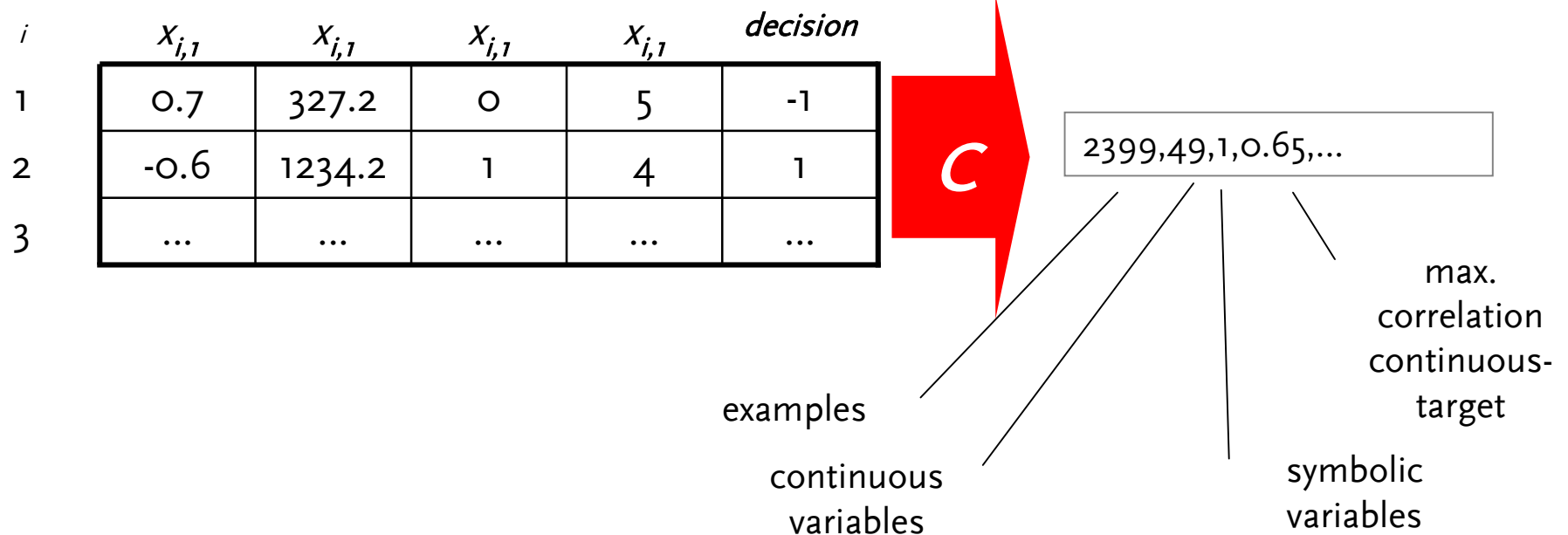


meta – model : DataSets \rightarrow Performance

Meta-Features

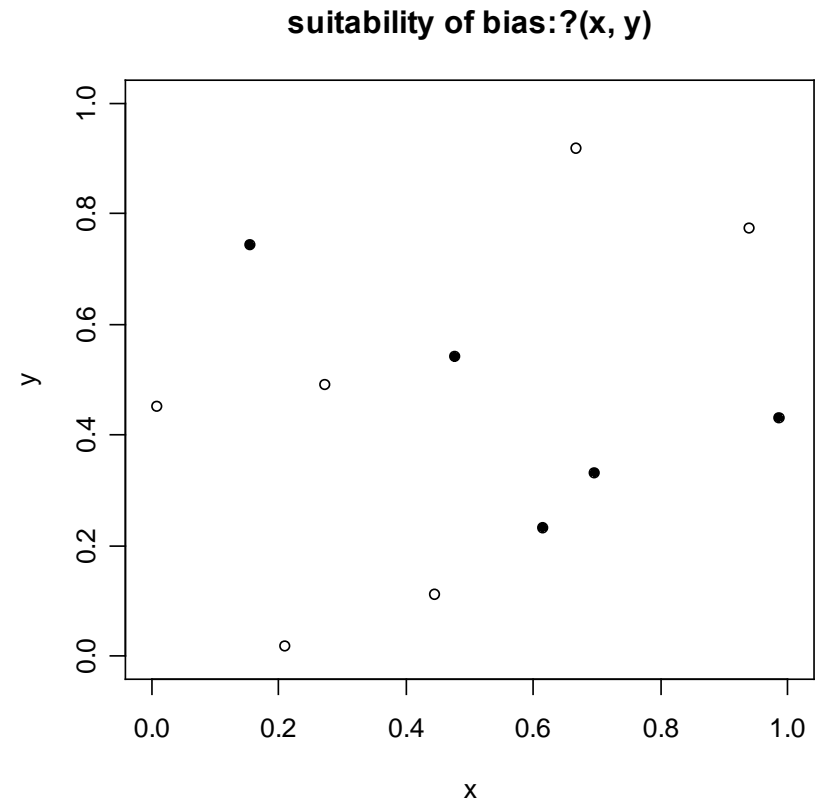
$meta - model : c(DataSets) \rightarrow Performance$

- c is a mapping between a matrix of values of variable size and type and a set of values of fixed size



Good Meta-features

- Measures that potentially contain information about the relative performance of algorithms
- ... but are computationally cheaper than the algorithms
- probably the hardest problem!



?

Approaches to Characterize Problems

- General, Statistical and Information-theoretic meta-features
 - *à la* StatLog
 - ex. # attributes, proportion of numeric attributes with outliers, class entropy
- Landmarkers
 - Bensusan and Giraud-Carrier (2000)
 - results of simple algorithms used to predict the performance of more complex ones
 - subsampling landmarks: results of complex algorithms on subsamples of the data
 - Furnkranz and Petrak (01), Soares, Petrak and Brazdil (01)
- Model-based
 - Bensusan, Giraud-Carrier and Kennedy (2000)
 - properties of an induced model

Meta-Feature Selection

- **Adequate choice of meta-features is essential**
 - k -NN algorithm assigns the same weight to all variables
 - measures that potentially contain information about the **relative performance** of algorithms
- **Knowledge-based approach**
 - identify properties of the data
 - select/design meta-features representing those properties

Meta-Feature Selection: Classification

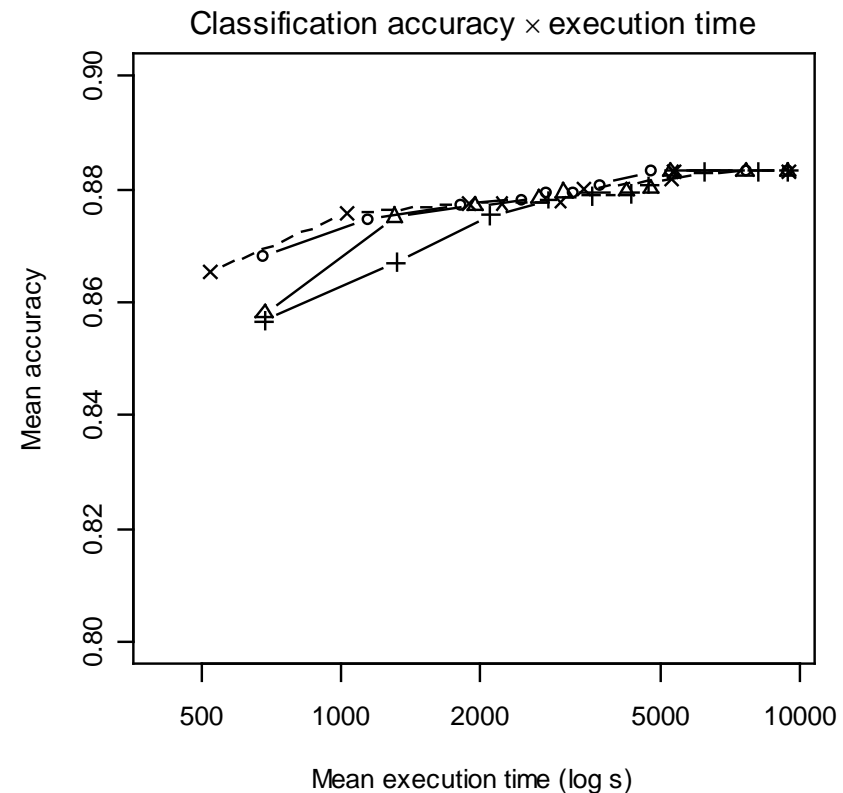
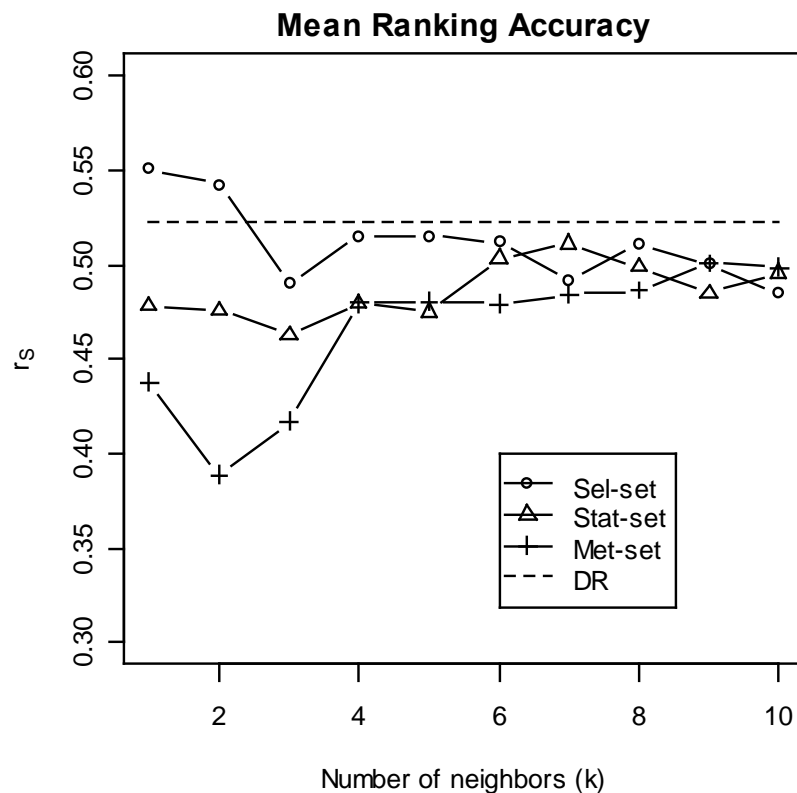
- **Set used so far**

Property	Measure
Scalability	# examples
Nominal vs. numeric attributes	proportion of symbolic attributes
Robustness to missing values	proportion of missing values
Robustness to outliers	proportion of numeric attributes with outliers
Number of classes	
Frequency of classes	class entropy
Information in nominal attributes	mean mutual information of class and attributes
Information in numeric attributes	canonical correlation of the most discriminating single linear combination of numeric attributes and the class distribution

- **Other properties and measures could be used**

Results with Selected Classification Meta-Features

- Significantly better than previous sets of meta-features
- general, statistical and information-theoretic measures

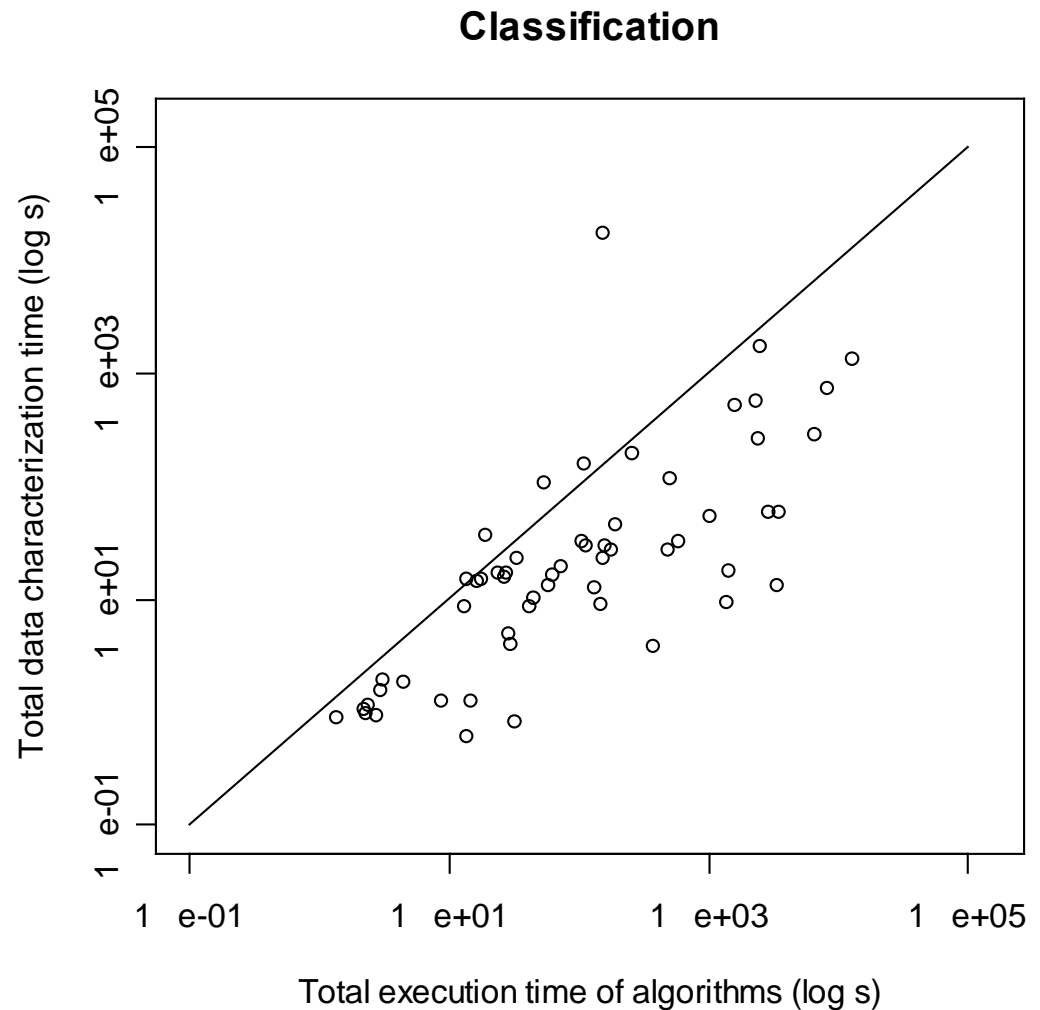


Informal method for meta-feature selection/design

Cost of Data Characterization

- Gains in execution time achieved by executing less alternatives compensate for data characterization time

- approximately mean execution time of single algorithm



Weighted Ranking Accuracy

- The highest the rank, the more harmful the error
 - top-ranked algorithms are selected more often
- **Weighted Rank Correlation Coefficient**

$$r_W(\mathbf{X}, \mathbf{Y}) = 1 - \frac{6 \sum_{i=1}^n (R(X_i) - R(Y_i))^2 (2n + 1 - R(X_i) - R(Y_i))}{n^4 + n^3 - n^2 - n}$$

- r_W yields values quite different from r_s in some cases...
 - up to 0.1 just by swapping a pair of ranks
 - but similar results in the algorithm recommendation problem

Log Ranking Accuracy

- The highest the rank, the more harmful the error
 - top-ranked algorithms are selected more often
- Log Ranking Accuracy Measure

$$r_{\log}(\mathbf{X}, \mathbf{Y}) = 1 - \frac{2 \sum_{i=1}^n \log_{1+R(X_i)} (1 + (R(X_i) - R(Y_i)))^2}{\sum_{i=1}^n \log_{1+i} (1 + (i - (n - 1 + 1)))^2}$$

- Complementary information
 - k -NN makes fewer errors at top ranks than the default ranking

Measure of ranking accuracy that assigns more importance to algorithms that are most likely to be selected

Other Applications

- Tested
 - regression
 - recommendation of parameters for pre-processing methods
- Current work
 - time series
 - outlier detection
 - optimization
- Future work
 - pre-processing methods + algorithm + parameters

Plan: Part II

PART I

- Background: why is this a problem?
- Meta-Learning: **THE** solution

PART II

- Meta-learning for Algorithm Recommendation
- Discussion
- Recommendation of Parameter Settings of SVM

SVM

- Support Vector Machines
 - linear learning machines that maximize the margin
 - duality
 - kernel trick
- According to Bennet & Campbell, “Support Vector Machines: Hype of Hallelujah?”, SIGKDD Explorations, 2000
 - geometrical intuition
 - elegant math
 - theoretical guarantees
 - practical (and successful) algorithms
- Successful but...
 - heavy tuning usually required

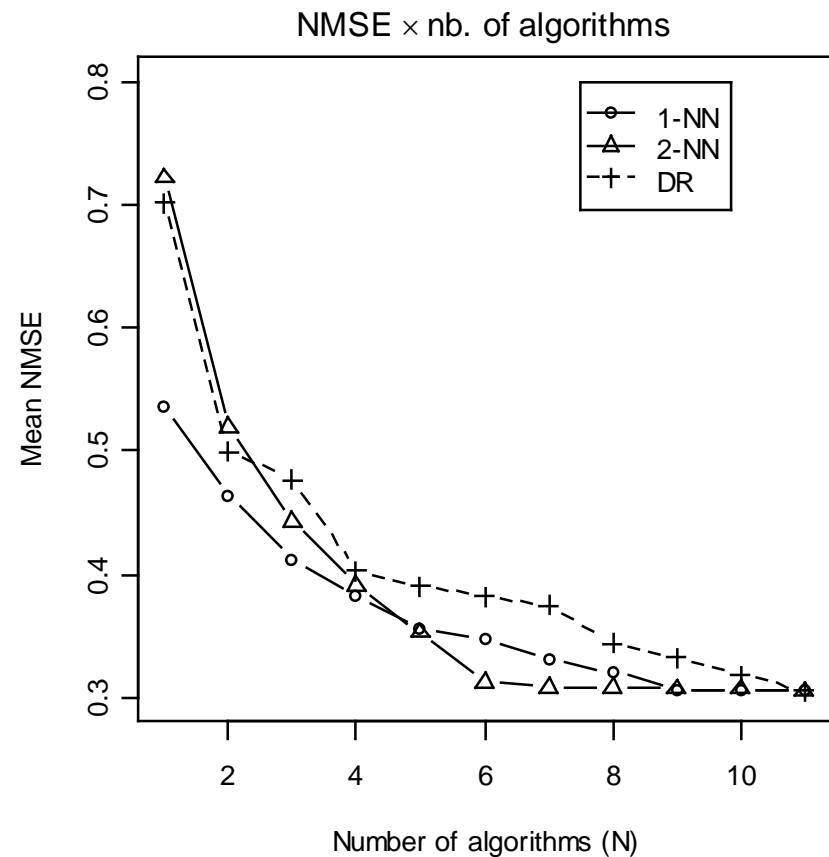
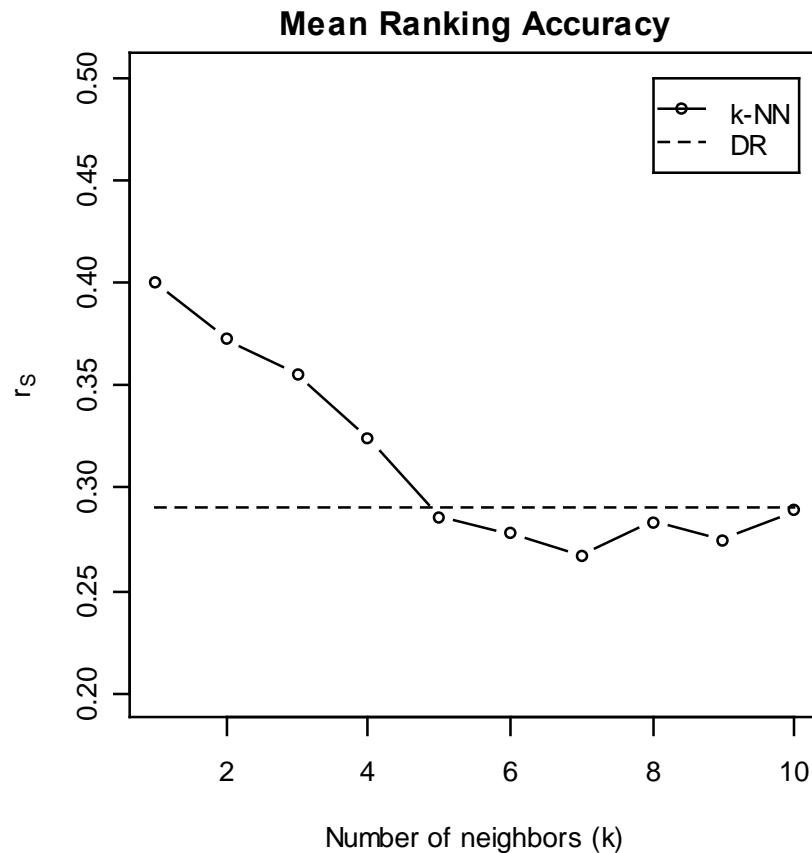
***k*-NN Ranking for Parameter Setting**

- **Goal: test methodology on different problem**
- **Application: Support Vector Machines for regression**
 - width of the Gaussian kernel, σ

$$K(\mathbf{x}_i, \mathbf{x}_j) = e^{\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}}$$

- **Pre-selection of a set values required**
 - continuous parameter
 - set of 11 σ values
- **Pre-selected set valid?**
 - (explained earlier)

k -NN Ranking vs. Default Ranking: Parameter Setting Results



- More accurate rankings than DR
- Significantly more accurate algorithms at the top ranks

k-NN Ranking vs. Jaakkola's Heuristic: Results

- **Heuristic commonly used in SVMs**

- for all examples \mathbf{x}

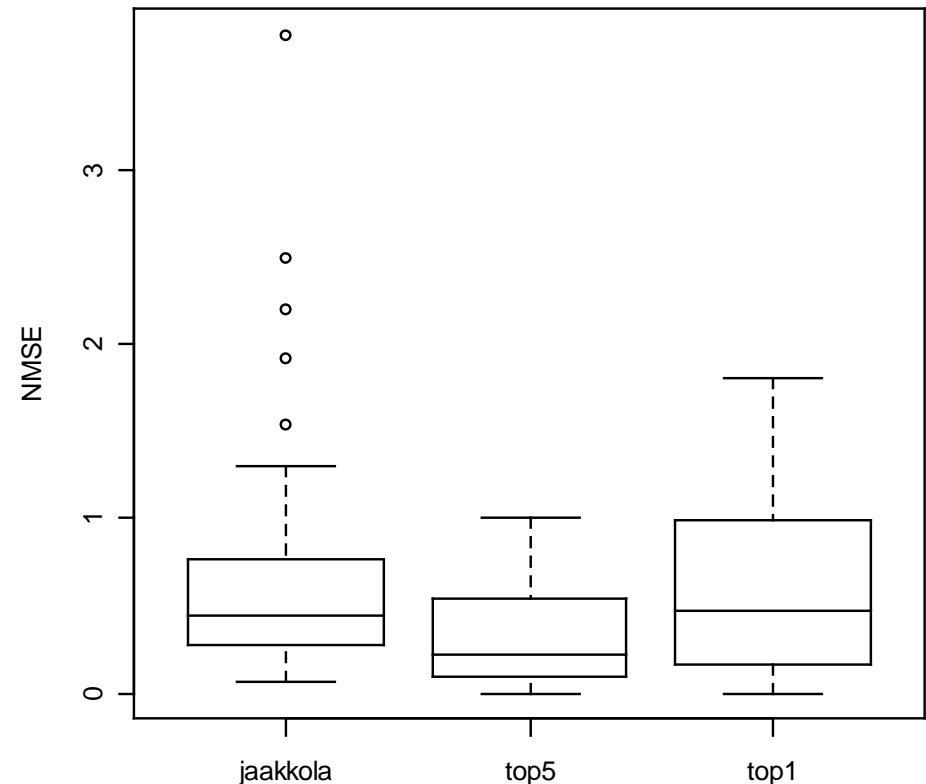
$$d_{\mathbf{x}} = \min_{\mathbf{y}} \left(\sqrt{\sum_i (x_i - y_i)^2} \right)$$

- set width to

$$\sigma = \overline{d_{\mathbf{x}}}$$

- ***k*-NN achieves better results**

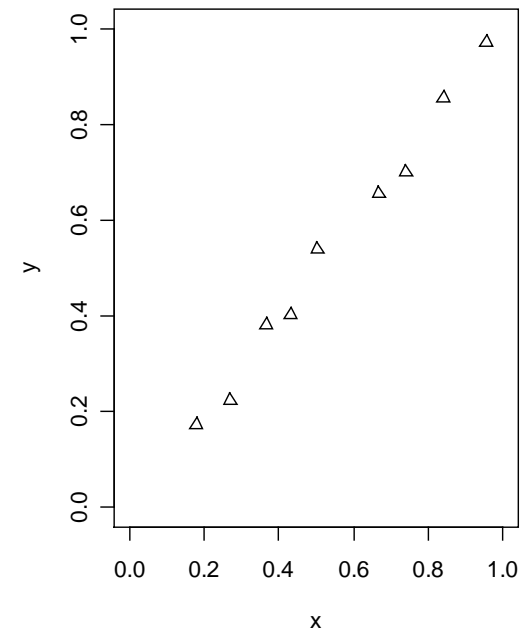
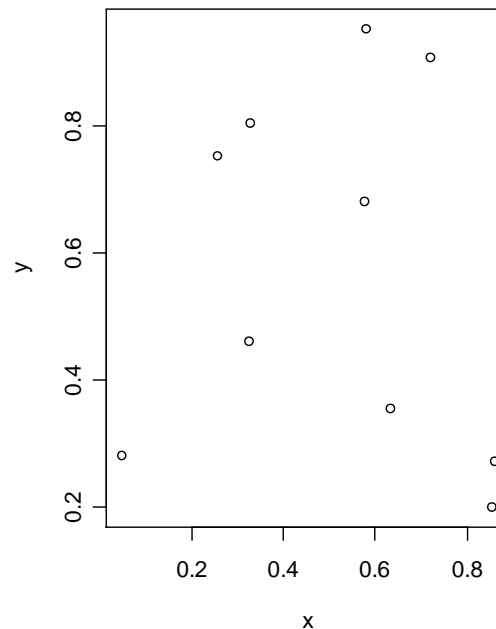
- also more robust
- top-5 results confirms advantage of ranking
- heuristic obtains surprisingly good results



The Kernel Trick

- Kernels project data into a (potentially) higher-dimensionality space
 - potentially infinite
 - a complex pattern-classification problem cast in a high-dimensional space nonlinearly is more likely to be linearly separable than in low-dimensional space (Cover 95)
 - “separable” -> “fit”

$$\Phi : \circ \rightarrow \Delta$$



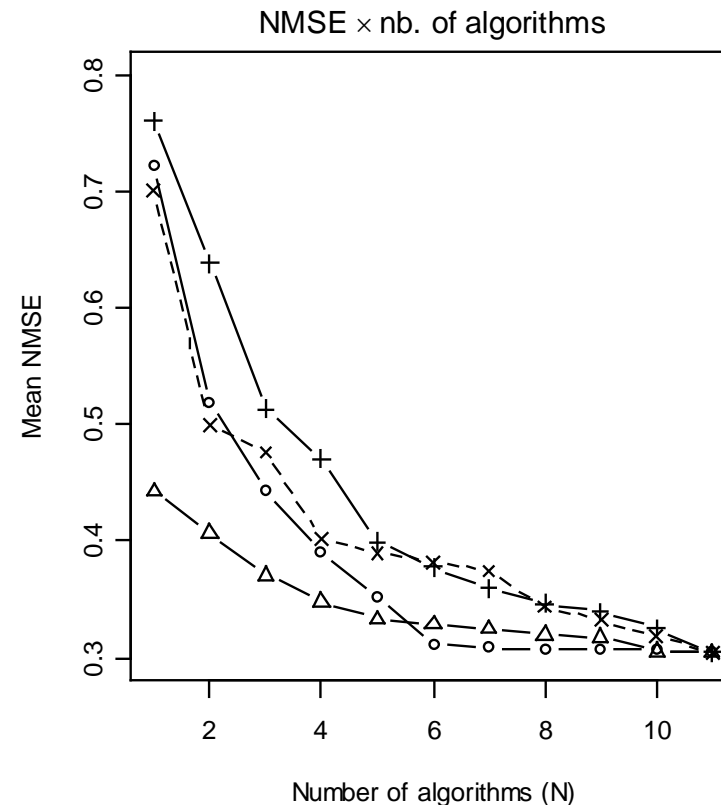
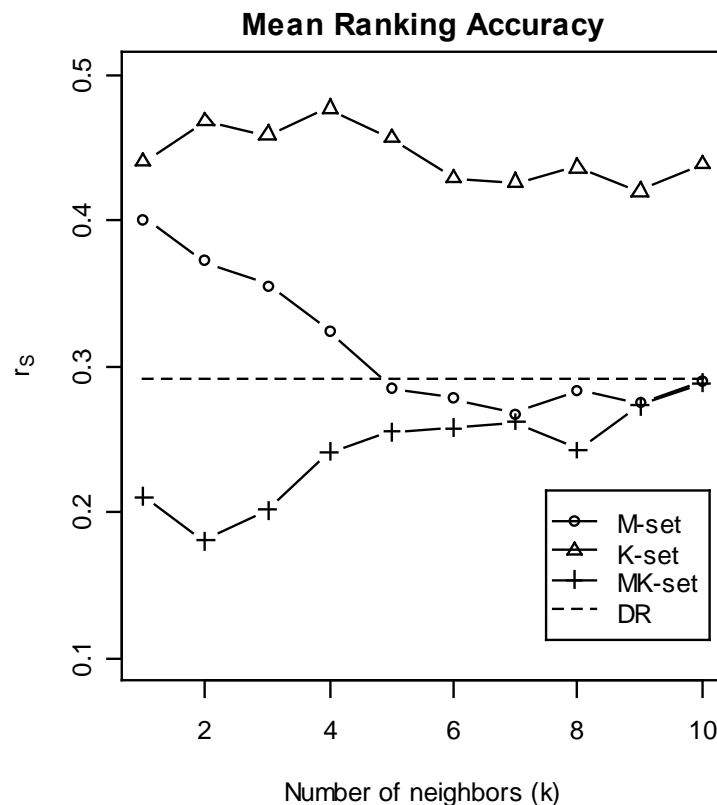
- ... implicitly
 - algorithms use a matrix representing the distances between the examples in projected space

Meta-Features Based on the Kernel Matrix

- Kernel matrix represents distance of examples in projected space
- Design meta-features based on the values of the kernel matrix
 - off-diagonal values are close to 0 when examples are “isolated”
 - MF1: mean of off-diagonal values
 - off-diagonal values should vary when there is structure
 - MF2: variance of off-diagonal values
 - measures “correlation” between a kernel function and ideal kernel
 - MF3: kernel-target alignment
- Calculate for all parameter settings

Results with Selected Kernel Meta-Features

- Significantly improved results with the set of Kernel meta-features
 - unexpected results with the combination of the two sets



- Successful adaptation of the methodology to a different problem
- Successful design of problem-specific meta-features

Conclusions

- Relating characteristics of problems to (relative) performance of learning algorithms is possible
- Recommendation is not the only goal
 - understanding behavior of algorithms
 - insights leading to improvements/new algorithms
- Research on meta-learning is at an early stage
 - data characterization
 - insufficient examples (i.e. data sets)
- Learning to predict rankings is interesting too!

(Very) Short Bibliography

somewhat biased too...

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