

# Towards understanding learning behavior

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With Hendrik Blockeel

K.U.Leuven

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# Outline

**Intro: Meta-learning**

**Limitations**

**An integrated solution**

**Conclusion**



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An integrated solution

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# Intro

Discovering structure in data:

- **Data preprocessing**: prepare data for learning (algorithm)
- **Algorithm selection**: find a learning model fitting the data

## Machine Learning Bias

Learn efficiently: make *assumptions* about data structure (*bias*)

- Good learning performance  $\Leftrightarrow$  assumptions hold for data.

Types of bias:

- Representation: data model (*language bias*)
- Hypothesis evaluation: search heuristics (*procedural bias*)
- Data configuration: skewness, discretization, ...



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# Meta-learning: definition

How to know if ML bias matches the given data?

## Meta-Learning

Use experience of previous ML experiments to learn (automatically) how to improve automatic learning.

Goals:

- Gain insight into learning behavior to improve existing algorithms
- Select most promising learning techniques after analysis of new learning tasks



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Algorithm selection: start with looking at given data

- Prior knowledge available about dataset?
- Can we *compute* some data properties?

## Approach

- Compute dataset characteristics (size, corr., entropy, ...)
- Record performance of algorithms on dataset (experiments)
- Predict performance on new datasets (data mining)



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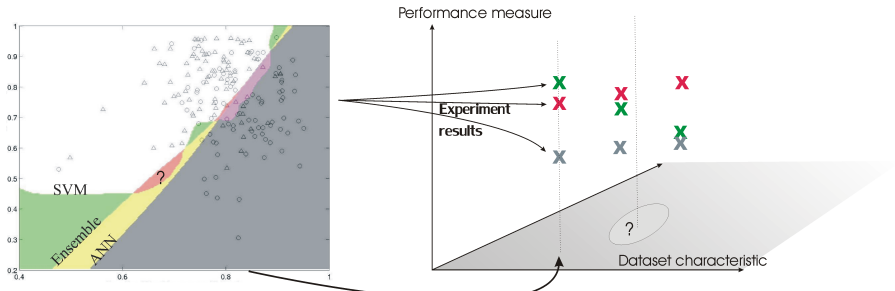
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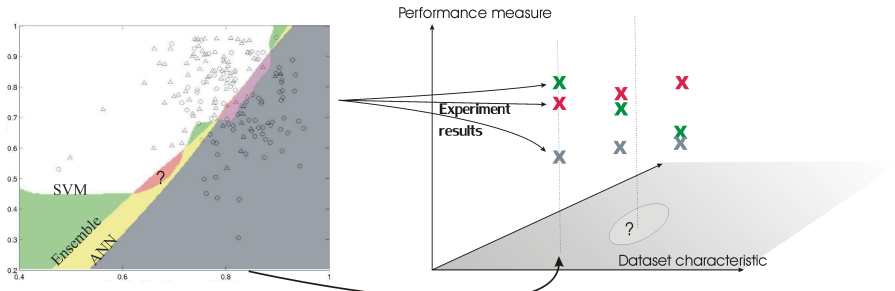
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# Meta-knowledge base

size	#attr.	...	algorithm	accuracy	runtime	...
2300	43		C4.5	.92	43	

Dataset Characteristics
  Algorithm
  Performance measures



Predict performance  
on new datasets

- Characteristics of natural datasets
  - General: size, #attributes, ...
  - Statistical:  $corr(attrX, attrY)$ , skewness, kurtosis, ...
  - Info-theoretic:  $H(class)$ ,  $H(attr)$ ,  $MI(class, attr)$ ,  $N/S, ...$
  - Landmarkers, model-based characterisations
- Algorithm
  - Often default parameters, minimal preprocessing
- Performance measures
  - e.g. predictive accuracy and runtime



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# The curse of dimensionality

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Dataset Characteristics      Algorithm      Performance measures

Curse of dimensionality:

- Many dataset characterizations: high-dimensional space
- Each instance = result of experiment: new dataset
- Limited number of natural datasets: very sparse evidence
- Low generalisability of results

Many more datasets necessary to make good predictions



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Results don't generalise over algorithms:

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  - parameters change ML bias (e.g. under/overfitting)
  - 📄 Hoste & Daelemans, 2005: significant impact on relative performance
- No link to properties of algorithm (eg. *data fragmentation*)

Algorithm characterization needed to generalise results



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Predict performance  
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We can learn *when* an algorithm fails, but not *why*

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- No explanation in terms of algorithm properties

More thorough investigation needed to diagnose failure/success





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# Data transformation

## No link to preprocessing techniques

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Practical advice should include preprocessing steps



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# Descriptive meta-learning

- Goal: Descriptive (vs. comparative) meta-learning
- Investigate specific questions
  - “What would be the effect of increasing parameter  $X$  on runtime?”
  - “Would an algorithm able to model fine-grained concepts perform better (or does it overfit)?”
- Explain reasons behind success/failure
  - Gain insights into why an algorithm behaves a certain way
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# Experiment databases

C4.5 v.1

MLS	heur.	...	Dataset	TP	FP	...
2	gain		DS1	945	84	

Algorithm parameters

Performance measures

-  Blockeel, 2005: improve interpretability of ML experiments
  - Also see Perlich, 2003: ML results ↔ dataset size
- Build database of large number of experiments, such that results are:
  - Generalisable: use large variety of (synthetic) datasets
  - Reusable: store all parameters and measurements (may prove useful later)
  - Reproducible: log all experiment settings (for further tests)
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# ExpDB design

## Dataset

dname	url	properties																			
coepra1	/home/...																				

## Evaluation

eid	auroc	measures																			
1	.84																				

## Experiment

algo_sett	dataset	type	evalmeth	eval	starttime	priority	status	machine
1	coepra1	classif.	10f-CV	1	02:21...	5	done	no-11-23

## Setting

sid	algo	params
1	j48	2

## Machine

mname	factor	properties																			
no-11-23	1.2534																				

## Algorithm

aname	type	properties																			
j48	tree																				

## Parameters

psid	pname	pvalue
2	min LS	2

[Http://www.cs.kuleuven.be/~joaquin/expdb/expdb.php](http://www.cs.kuleuven.be/~joaquin/expdb/expdb.php)



# Experiment databases

Experiment Database

Algo impl.	Par. sett.	Dataset	TP	FP	...
C4.5 v.1	C451 - 1	DS1	945	84	

Dataset characteristics

ID	size	#attr	...
DS1	2300	43	

C4.5 v.1 parameter settings

ID	MLS	heur	...
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General algorithm properties

ID	model	lin?	...
C45v1	DT	no	

Performance measures

TP	FP	...	bias err	var err
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- Experiments not focused on one hypothesis, but to learn about algorithm
- Allows thorough investigation:
  - Test hypothesis by querying expDB
    - “What is the effect of parameter X on runtime for large datasets?”
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    - Rules, decision trees, association rules, ...
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- Maintain validity of meta-learning experiments
- Unbiased: hide large range of different concepts + characterize concept
  - model characteristics
  - concept variation
  - example cohesion,...
- “Natural”: approximate characteristics of natural datasets
  - complex attribute relations
  - complex value distributions
  - noise, missing values,...
- Coverage: control characteristics to cover meta-feature space
  - experiment design



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- Ongoing work
- Underlying concepts: several modules (DT, NN,...)
  - could be combined
- Example generation: multi-tier approach
  - Low-level description
    - initializes *attribute generators* for imposing dependencies, value distributions, noise,...
    - Can be nested
  - High-level description
    - based on dependency model (eg. Bayesian net) and high-level parameters
- Built on WEKA



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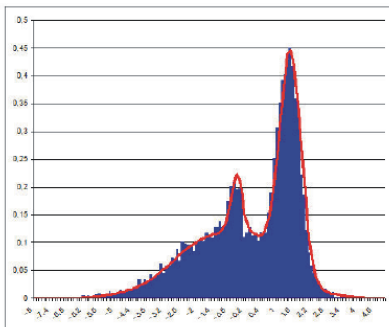
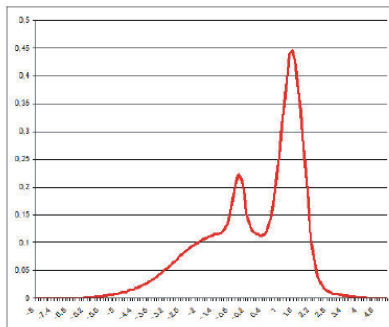


# Attribute generator: value distributions

```

<attgen attname="att1" type="combi">
  <attgen probability=".15" type="normal" mean="0" stddev="1" />
  <attgen probability=".1" type="normal" mean="-2" stddev="1" />
  <attgen probability=".4" type="normal" mean="1.5" stddev=".4" />
  <attgen probability=".05" type="normal" mean="-.5" stddev=".2" />
  <attgen probability=".3" type="normal" mean="-1" stddev="2" />
</attgen>

```

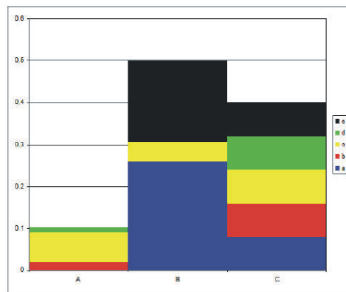
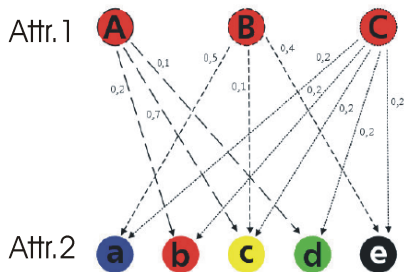


# Attribute generator: dependencies

```

<attgen attname="att1" type="fixedprob"
      values="A;B;C" probabilities=".1;.5;.4"/>
<attgen type="transition" parent="att1" values="a;b;c;d;e" >
<attgen type="fixedprob" values="b;c;d" probs=".2;.7;.1"/>
<attgen type="fixedprob" values="a;c;e" probs=".5;.1;.4"/>
<attgen type="fixedprob"/>
</attgen>

```



# Algorithm characterization

Experiment Database

Algo impl.	Par. sett.	Dataset	TP	FP	...
C4.5 v.1	C451 - 1	DS1	945	84	

Dataset characteristics

ID	size	#attr	...
DS1	2300	43	

C4.5 v.1 parameter settings

ID	MLS	heur	...
C451-1	2	gain	

General algorithm properties

ID	model	lin?	...
C45v1	DT	no	

Performance measures

TP	FP	...	bias err	var err
945	84		43	62

- Algorithm parameters settings
  - Stored as parameter name-value pairs
- General algorithm properties
  - representation model
  - dependency on linear separability, conditional independency, ...
  - use of data fragmentation, attribute summation, ...
  - ability to handle fine-grained concepts, local relevance, ...



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- bias error: systematic error: algorithm underfits target concept
- variance error: variation on different samples (overfitting)

Rep. Bias	Comp. Bias	Bias err	Var. err
appr.	too strong	high	low
appr.	ok	low	low
appr.	too weak	low	high
inappr.	too strong	high	low
inappr.	ok	high	avg
inappr.	too weak	high	high

- Diagnose bad performance and link to dataset/algorithm characteristics:

- bias / : bad representation model
- variance / : bad parameter settings

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ID	size	#attr	...
DS1	2000	18	

C4.5 v.1 parameter settings

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C451	1	amb	

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# Preprocessing steps

Data preprocessing has very large effect on inductive performance

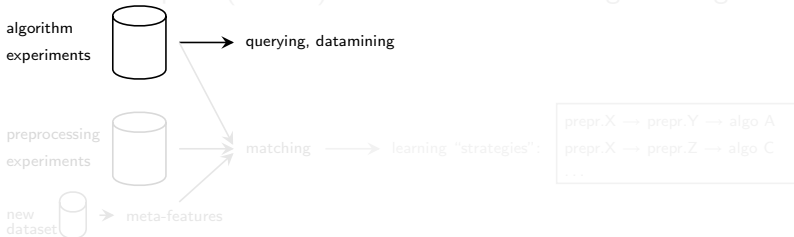
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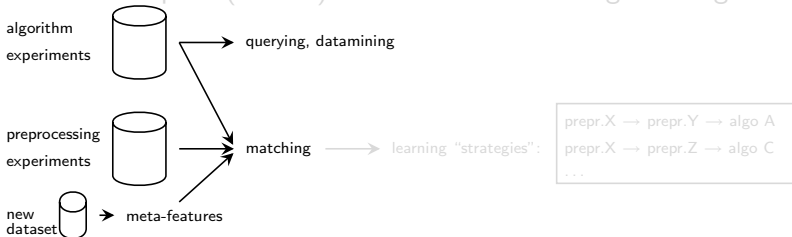




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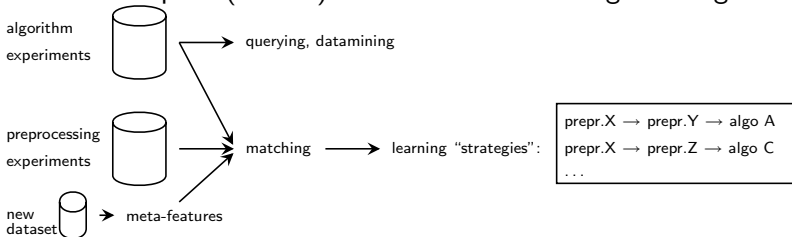
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- Feature construction and transformation
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# Outline

Intro: Meta-learning

Limitations

An integrated solution

**Conclusion**



# Conclusion

- Ideas for a descriptive form of meta-learning
  - thorough investigation of algorithm behavior
  - explain behavior in terms of their properties
- Experiment databases: efficient experimentation
  - synthetic datasets: unbiased, “natural”, covering
  - generalization over algorithms
    - parameter settings
    - general algorithm properties
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# Questions?

