PhD thesis:

New models and algorithms for semi-naive Bayesian classification focused on the AODE paradigm

PhD defense on 19/06/2012 Ana M. Martínez

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New models and algorithms for semi-naive Bayesian classification focused on the AODE paradigm

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I New BNCs to overcome AODE's limitations

Hidden One-Dependence Estimator

Gaussian AODE and hybrid AODE

The MTE-AODE classifier

II Discretization techniques for semi-naive BNCs

Disjoint discretization techniques

Non-disjoint discretization techniques

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Classification

 $f: X^n \to \{c_1, \ldots, c_k\}$ 

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### Naive Bayes classifier

• The attributes are conditionally independent given the class value  $I(A_i, A_j | C)$ .

$$c_{MAP} = argmax_{c \in \Omega_C} p(c) \prod_{i=1}^n p(a_i|c)$$

- Time complexity:
  - Training:  $\mathcal{O}(mn)$
  - Classification: O(cn)

- Space complexity:
  - Training:  $\mathcal{O}(cnv)$
  - Classification:
    \$\mathcal{O}(cnv)\$

- Limitations:
  - × : It does not work properly in certain datasets.
  - × : Dependencies between attributes reduce, unavoidably, the prediction capability of NB.
  - Not only interesting to be right in the classification in certain applications.

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## AODE classifier I (Averaged One-Dependence Estimators)

 AODE is significantly better in terms of error reduction compared to the rest of semi-naive techniques.



• MAP hypothesis:

$$argmax_{c\in\Omega_{C}}\left(\sum_{j=1,N(a_{j})>m}^{n}p(c,a_{j})\prod_{i=1,i\neq j}^{n}p(a_{i}|c,a_{j})\right)$$

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- Space complexity:
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## Limitations:

- × : Quadratic order time in classification.
- × : High demand of RAM memory.

- Time complexity:
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- $\times$  : Only discrete variables.

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- Limitations:
  - × : Quadratic order time in classification.
  - × : High demand of RAM memory.
  - $\times$  : Only discrete variables.
- Attempts to improve AODE's accuracy
  - Two algorithms based on EM and constrained optimization for learning MAP weights for the SPODEs [Cerquides & de Mántaras, 2005]
  - To select or to weight: A comparative study of model selection and model weighing for SPODE ensembles [Yang et al., 2006].
  - WAODE: Model weighting with *MI*(*C*, *A<sub>j</sub>*) [Jiang & Zhang, 2006].

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## **Objectives**

- Reduce AODE's computational needs in terms of memory storage and classification time.
- Propose different alternatives for handling numeric attributes, commonly present in real databases:
  - Gaussian distributions.
  - Ø Mixtures of truncated exponentials.
  - Oifferent discretization techniques (disjoint vs non-disjoint).
- Study the domain of competence for several semi-naive classifiers according to different complexity measures [Ho & Basu, 2002].

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- AODE is quadratic in training and classification time.
  - Can be a handicap in some real applications where the **response time** is **critical**.
- AODE needs to store the *n* models.
  - Can be problematic when the size of the database (mainly the number of attributes or attribute labels) is very large.
  - Real examples: microarrays or DNA chips or large marketing databases (Orange)
- <u>Our solution</u>: new classifier which **estimates a new variable** which gathers the dependencies represented by every superparent in AODE in *a single model*.

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 $A_1$   $\cdots$   $A_n$ 

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 $\begin{array}{c} C \rightarrow A_n \\ \hline A_1 & A_2 & \cdots & A_{n-1} \end{array}$ 

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 $A_1$   $A_2$   $\cdots$   $A_{n-1}$  n models

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 $(C, H) = \operatorname{argmax}_{c \in \Omega_{C}} \left( \sum_{j=1}^{\#H} p(c, h_{j}) \prod_{i=1}^{n} p(a_{i}|c, h_{j}) \right)$ 

- Necessary to estimate the probability of every attribute value conditioned by the class and *H*.
  - Expectation-Maximization algorithm.

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### Number of states for the *H* variable

### Greedy technique:

- First step: #*H* = 1 (NB).
- Execution of EM algorithm and build models: #H = #H + 1.
- Evaluate model: if worse than previous model then stop process.
- How is the fitness of the model evaluated?
  - Log-likelihood (LL):

$$LL = \sum_{i=1}^{l} \log \left( \sum_{t=1}^{\#H} p(c^{i}, a_{1}^{i}, \cdots, a_{n}^{i}, h_{t}) \right) = \sum_{i=1}^{l} \log \left( \sum_{t=1}^{\#H} p(c^{i}, h_{t}) \prod_{r=1}^{n} p(a_{r}^{i} | c^{i}, h_{t}) \right)$$

• Penalization: Akaike Information Criterion or AIC:

$$AIC = LL - C(M)$$

• **Results:** (*w*/*t*/*l*): 16/6/14.

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## What could make us vote for one or the other? Time complexity

- At training time HODE is quadratic in the worst case:
  - $1mn + 2mn + \cdots + nmn$
  - AODE is usually faster in model construction (because of EM).
- At classification time:



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### What could make us vote for one or the other? Space complexity

- Lower than AODE's, it needs to store less CPTs.
  - $\mathcal{O}(cn \# Hv)$  for HODE vs  $\mathcal{O}(c(nv)^2)$  for AODE.
- AODE demands more RAM memory, problems in large databases with a high number of attributes or even attributes with too many states.

•	Experiments in 7	datasets	(microarray	s or DN	A chips).
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Dataset	k	n	1	NB	AODE	HODE
colon	2	2000	62	93.5484	91.9355	96.7742
DLBCL-Stanford	2	4026	47	100	100	100
GCM	14	16063	190	60.5263	OutOfMem	70
leukemia	2	7129	72	100	OutOfMem	98.6111
lungCancerHarvard2	2	12533	181	98.895	OutOfMem	99.4475
lymphoma	9	4026	96	96.875	OutOfMem	75
prostate_tumorVS	2	12600	136	80.1471	OutOfMem	95.5882

• OutOfMem: problems of overflow with a maximum of 8 gigabytes.

• HODE terminated without problems, even with a lower need for memory.

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## **HODE's parallelization**



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### Partial conclusions and future work

- HODE: alternative to the AODE classifier (similar accuracy results).
  - Reduction in space complexity and classification time.
- HODE tested in a parallel environment: global optimum for #H.
- $\checkmark$  Direct adaptation for the imputation of **missing values** in the dataset, use of **EM**.
  - Better records (12-0-6) than imputation with the global mean/mode.
  - Future improvements:
    - Average the constructed models.

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### **Motivation**

- A BN assumes all the variables are discrete.
- It is common the coexistence of discrete and continuous variables in the same problem.
- <u>Direct solution</u> → discretization.
  - × : Unavoidable loss of precision.
  - × : Which discretization method should we choose?.
- Some alternative solutions:
  - Kernel-based distributions. Space and temporal undesired restrictions for AODE (concerning the number of instances).
  - **2** Conditional Gaussian Networks.
  - 8 Mixtures of truncated exponentials.

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### **Conditional Gaussian Networks**

• Every continuous variable X is modeled with a conditional Gaussian distribution.

$$f(X|\mathbf{Y} = y, \mathbf{Z} = z; \Theta) = \mathcal{N}\left(x: \mu_X(y) + \sum_{j=1}^s b_{XZ_j}(y)(z_j - \mu_{Z_j}(y)), \sigma_{X|\mathbf{Z}}^2(y)\right)$$

- b<sub>XZ<sub>j</sub></sub>(y), regression term that measures the strength of the connection between X and every continuous parent.
- $\sigma_{X|\mathbf{Z}}^2(y)$  is the **conditional variance** of X over its continuous parents.

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 $\begin{array}{c} C \\ A_{j} \\ A_{1} \\ A_{2} \\ A_{j-1} \\ A_{j+1} \\ A_{j+1} \\ A_{n} \end{array}$ 

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### - Conditional Gaussian Distribution -

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- Time complexity:
  - The same as AODE (incremental computation of parameters).
- Space complexity:
  - Training & Classification:  $\mathcal{O}(kn^2)$  (independent from v).
- Probabilities estimated can be more reliable comparing to the multinomial version as they are modeled from more samples.
- Not possible to define the corresponding probability function for a discrete variable conditioned to a numeric attribute. Restricted to Numerical datasets.

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### - Multinomial distribution -



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### - Multinomial distribution -



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### - Multinomial distribution -



# - Univariate Gaussian distribution - (Multinomial distribution)

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- Time complexity:
  - The same as AODE (incremental computation of parameters).
- Space complexity:
  - Training & Classification: The same as AODE  $\mathcal{O}(k(nv)^2)$  in the worst case.
- $\sqrt{}$  Able to deal with **hybrid datasets** too.

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### Results

### Datasets with only continuous attributes

- ✓ Both of our classifiers are significantly better than NB.
- ✓ GAODE obtains competitive results comparing to AODE.
- HAODE offers an even higher advantage, HAODE significantly improves AODE in numeric datasets.

### Hybrid datasets?

- Wilcoxon test: No statistical difference.
- No significant pattern found when the percentage of numerical variables with respect to discrete ones was analysed.
- Apparent tendency of HAODE to **penalize datasets with missing values**. Statistical difference (Wilcoxon) when only datasets with missing values are considered.

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### Partial conclusions and future work

- GAODE: applies CGNs.
  - $\checkmark$  Competitive results comparing to AODE (5 16 5).
  - Reduction in the space complexity.
  - Maintains AODE's time complexity.
  - × : Restricted to continuous datasets.
- HAODE: discretizes the superparents.
  - ✓ Significantly better than AODE in continuous datasets (6 19 1).
  - $\checkmark$  Able to deal with **all kind of datasets**.
  - × : Clear preference for datasets with continuous attributes and absence of missing data.
- Reconsider Gaussian assumption.

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### The MTE model (Moral et al., 01)

#### **Definition (MTE potential)**

• X: mixed *n*-dimensional random vector.  $\mathbf{Y} = (Y_1, \ldots, Y_d)$ ,  $\mathbf{Z} = (Z_1, \ldots, Z_c)$  its discrete and continuous parts. A function  $f : \Omega_{\mathbf{X}} \mapsto \mathbb{R}^+_0$  is a Mixture of Truncated Exponentials potential (MTE potential) if for each fixed value  $\mathbf{y} \in \Omega_{\mathbf{Y}}$  of the discrete variables  $\mathbf{Y}$ , the potential over the continuous variables  $\mathbf{Z}$  is defined as:

$$f(\mathbf{z}) = a_0 + \sum_{i=1}^m a_i \exp\left\{\sum_{j=1}^c b_i^{(j)} z_j
ight\}$$

for all  $\mathbf{z} \in \Omega_{\mathbf{Z}}$ , where  $a_i$ ,  $b_i^{(j)}$  are real numbers.

Also, *f* is an MTE potential if there is a partition D<sub>1</sub>,..., D<sub>k</sub> of Ω<sub>z</sub> into hypercubes and in each D<sub>i</sub>, *f* is defined as above.

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**Univariate case** 

Learning a univariate MTE density involves three basic steps:

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#### **Univariate case**

Learning a univariate MTE density involves three basic steps:

 Determination of the splits into which Ω<sub>X</sub> will be partitioned (Convexity/Concavity). New models and algorithms for semi-naive Bayesian classification focused on the AODE paradigm

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#### **Univariate case**

Learning a univariate MTE density involves three basic steps:

- Determination of the splits into which Ω<sub>X</sub> will be partitioned (Convexity/Concavity).
- Determination of the number of exponential terms in the mixture for each split (usually 2).

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- Determination of the splits into which Ω<sub>X</sub> will be partitioned (Convexity/Concavity).
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#### Alternatives explored in literature

- Least squared estimation (LS).
- Maximum likelihood estimation (ML).

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- Determination of the number of exponential terms in the mixture for each split (usually 2).
- Estimation of the parameters.

#### Alternatives explored in literature

- Least squared estimation (LS).
- Maximum likelihood estimation (ML).

#### **Conditional case**

• Mixed tree: efficient data structure for dealing with conditional MTE densities.

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### **MTE-AODE** classifier

#### Definition

An **MTE-AODE classifier** classifies an individual as in AODE, where all the probability functions involved are of class MTE.

### Advantages:

- (over GAODE) the underlying distribution is not assumed to be of Gaussian type, as MTEs are able to accurately represent the most common distributions.
- (over HAODE) there is no need to discretize the super-parent nodes, as the MTE mode allows discrete variables with continuous parents.
- Disadvantage: the learning phase is slower.
- We can trivially extend this definition to the MTE-NB classifier as a particular case of MTE-AODE.

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### Accuracy comparisons

- Study the application of MTEs over a large group of datasets without individual parametrization.
  - 16 hybrid datasets.

	Naive Bayes		AODE	
	MTE vs G	MTE vs D	MTE vs H	MTE vs D
EF10	10-6	5-11	8-8	•5-11
EF5	11-5	7-9	9-7	7-9
F&I	10-6	9-7	8-8	8-8

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## Estimation of MTEs when selecting different number of cutpoints





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### Partial conclusions and future work

- Generalization of AODE to all kind of datasets through MTEs.
  - $\checkmark$  Extensible to NB and other semi-naive classifiers.
- The selection of the number of intervals is not trivial:
  - It is advisable to find the optimum for every data set, but also,
  - To find the optimum for every domain to partition in each leaf of the mixed tree independently, requiring a more sophisticated supervised "discretization" technique oriented to the estimation of MTEs.
- 2 Time complexity:
  - The estimation of MTEs requires more time than EF discretization.
  - This time can be controlled: limiting the number of exponential terms and the maximum number of intervals into which divide the domain.
  - Good alternative to CGs and discretization for some datasets.

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### **Motivation**

- Discretization is probably one of the pre-processing techniques most broadly used in machine learning.
- The real distribution of the data is replaced with a mixture of uniform distributions.
- Discretization methods: unavoidable loss of information.
- Appropriate discretization can outperform straightforward use of common, but often unrealistic parametric distribution (e.g. Gaussian).
- Many distinct techniques for discretization can be found in literature.
- Should we worry about the discretization method applied when designing the set of experiments?.
  - HAODE vs AODE's results with F&I can be generalized.

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#### Study in terms of accuracy



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## Before we go: discretization bias and variance

## In practice:

- Discretization Bias: Intuitively, discretization resulting in large interval numbers tends to have low bias (any given interval is less likely to include a decision boundary of the original numeric attribute).
- Discretization Variance: discretization resulting in *intervals* with a large number of instances tends to have low variance (as the probability estimations are more stable and reliable).
- Problem: assuming there is a fixed dataset size, the larger the number of intervals, the smaller the number of instances per interval is.

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## Study in terms of bias/variance







NB



KDB1







AODE

HAODE

**BNHC** 

#### NB-tailored discretization techniques Study in terms of accuracy



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## Partial conclusions and future work

#### Outcomes:

- Can the use of a particular discretization method alter the ranking between classifiers?
  - Not for HAODE, AODE and BNHC.
  - As NB, TAN and KDB obtain very similar results, their position in the ranking can vary in a particular case
- Ocmparison between AODE and HAODE with several discretization methods:
  - In all cases HAODE's average accuracy is higher than AODE's (significantly better except for EF10).
- If discretization technique tailored to NB not extensible to other classifiers of the same family.
- Future work: considering a wider range of discretization techniques (e.g. multivariate discretization).

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## **Motivation**

- For AODE and HAODE, previous studies have shown its robustness towards the discretization method applied.
  - **Only disjoint discretization** techniques taken into account so far.
- Non-Disjoint discretization:
  - Good performance in Naive Bayes [Yang & Webb, 2002].
  - Are disjoint intervals appropriate for AODE and/or HAODE?

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## **Disjoint vs Non-Disjoint Discretization**

- Given x<sub>i</sub>, x<sub>j</sub> ∈ ℝ, any disjoint discretization (DD) method would create a unique interval (a, b] ∋ x<sub>i</sub> and (d, e] ∋ x<sub>j</sub> for every value.
- In DD (EF, EW, MDL): every numeric sample belongs to a single interval:
  - If x<sub>i</sub> or x<sub>j</sub> falls around the **center of the interval** assigned, we could expect more **distinguishing information** than when it falls near one of the boundaries of the interval.
- In NDD: with an odd number of intervals (in training time) every numeric value will always be located toward the middle of the final interval when classifying each test instance (e.g. three intervals).

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 $\lfloor \sqrt{m} \rfloor$  intervals with  $\lfloor \sqrt{m} \rfloor$  samples

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Hidden One-Dependence Estimator

Gaussian AODE and hybrid AODE

The MTE-AODE classifier

II Discretization techniques for semi-naive BNCs

Disjoint discretization techniques

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 $\lfloor \sqrt{m} \rfloor$  intervals with  $\lfloor \sqrt{m} \rfloor$  samples



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## **MODIFICATIONS:**

A threshold to mark the minimum frequency from which an atomic interval will not be merged with its neighbours. New models and algorithms for semi-naive Bayesian classification focused on the AODE paradigm

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## **MODIFICATIONS:**

- A threshold to mark the **minimum frequency** from which an atomic interval will not be merged with its neighbours.
- 2 The interval size is not equal to the interval number  $(\approx \lfloor \sqrt{m} \rfloor)$ .

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- A threshold to mark the **minimum frequency** from which an atomic interval will not be merged with its neighbours.
- 2 The interval size is not equal to the interval number  $(\approx \lfloor \sqrt{m} \rfloor)$ .
- When the number of cut-points is lower than 3 → Equal Frequency discretization will be kept.

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## **MODIFICATIONS:**

- A threshold to mark the **minimum frequency** from which an atomic interval will not be merged with its neighbours.
- 2 The interval size is not equal to the interval number  $(\approx \lfloor \sqrt{m} \rfloor)$ .
- When the number of cut-points is lower than 3 → Equal Frequency discretization will be kept.
- Weighting importance (wNDD): samples to be placed in its corresponding interval (when classification) are given more importance when training.

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## **Experiments**

- Group of 28 hybrid datasets (same as in [Yang & Webb, 2002]).
- Parameters: #atomic\_bins= 15 (with equal frequency) min\_freq\_not\_merging= 100 (per operational int.)

	non-we	eighted	weighted	
	AODE	HAODE	AODE	HAODE
	NDD vs EF5	NDD vs EF5	NDDw vs EF5	NDDw vs EF5
Accuracy	23-0-5	21-1-6	22-1-5	18-2-8
Bias	14-3-11	21-1-6	15-3-10	22-0-6
Variance	18-2-8	14-4-10	13-2-13	10-0-14

### Win-Draw-Lose

#### **Average Values**

	AODE		HAODE					
	EF5	NDD	EF5	NDD				
Accuracy	82.4169	83.5873	82.2658	82.4935				
Bias	0.1298	0.1250	0.1348	0.1275				
Variance	0.0395	0.0355	0.0440	0.0435				

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## Partial conclusions and future work

- Main conclusion: whereas some of the most common disjoint discretization techniques have failed to demonstrate consistent improvement relative to alternatives, NDD demonstrates better win-draw-loss records and significant overall improvement.
- Test wNDD in high-dimensional datasets (variance component should be reduced).
- NDD will be strengthened when applied to **AnDE** (Aggregating *n*-dependence estimators).
- Drawback of NDD: additional parameters (apart from the number of bins):
  - Number of atomic bins per operational interval.
  - Minimum frequency per interval.

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## **Motivation**

• No clear winners for all problems.



 Can we measure geometrical complexity of classification problems? New models and algorithms for semi-naive Bayesian classification focused on the AODE paradigm

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# Some Useful Measures of Geometric Complexity (Ho&Basu 2002)



New models and

algorithms for semi-naive Bayesian

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## Some Useful Measures of Geometric Complexity

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Туре	ld.	Name	Simpler if	
	F1	Maximum Fisher's discriminant ra-	+	
Overlaps in the feature		tio		
values from different classes	F1v	Directional-vector maximum Fish-	+	
values norn unerent classes		er's discriminant ratio		
	F2	Overlap of the per-class bounding	-	
		boxes		
	F3	Maximum (individual) feature effi-	+	
		ciency		
	F4	Collective feature efficiency	+	
	L1	Minimized sum of the error dis-	-	
Measures of class		tance of a linear classifier		ć
separability	L2	Training error of a linear classifier	-	
Separability	N1	Fraction of points on the class	-	
		boundary		
	N2	Ratio of average intra/inter class	-	
		nearest neighbor distance		
	N3	Leave-one-out error rate of the	-	1
		one-nearest neighbor classifier		1
Measures of geometry	L3	Nonlinearity of a linear classifier	-	
topology and density of	N4	Nonlinearity of the one-nearest	-	
manifolds		neighbor classifier		
maniolus	T1	Fraction of maximum covering	_	
		spheres		
	T2	Average number of points per di-	+	
		mension		

#### NB: Discrete datasets organised according to L2 Good pattern

5e-04 0.022 0.099 0.42 Training 100 8 % Accuracy 80 2 80 0 50 100 150

Data set

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## NB: Discrete datasets organised according to L2 Good pattern



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## NB: Discrete datasets organised according to T2 Bad pattern

3.467 1250 42.553 333.333 Training 100 8 % Accuracy 8 2 8 100 0 50 150

Data set

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## NB characterization in terms of good and bad behaviour by the use of 6 CMs: F1v, F3, F4, L2, N1 and N3

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## Gaussian NB characterization in terms of good and bad behaviour by the use of 6 CMs: F1, L1, N1, N2, N3 and N4



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## GAODE characterization in terms of good and bad behaviour by the use of 6 CMs: F1, L1, N1, N2, N3 and N4



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New dataset -CM's values-Meta-classifier Meta-dataset formation multi-label Calculation of Calculation of Tests to select Best semi-naive accuracy for the CMs for each active class 5 classifiers on BNC predicted dataset labels each dataset

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# Partial conclusions and future work I

# Conclusions

- Easier to characterize datasets in discrete domains.
- ✓ It is possible to characterize both NB and AODE for both domains and obtain disjoint rules to predict if the classifier will perform well or poorly, depending on the values of some of the complexity measures.
- $\checkmark$  Automatic process to advise on the best semi-naive BNC to use for classification.

# Future work

- Datasets from the Landscape contest as test bed (wider range of the complexity measurement space).
- Theoretical way to find the suitability of a measure to characterize a particular classifier.
- Study bivariate/multivariate relationships between the CMs.

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# Summary and contributions to literature

Contribution to the state of the art of semi-naive BNCs, focused on the AODE paradigm.

- New proposals to overcome AODE's limitations.
  - 1 HODE (ECSQARU'09).
  - ② GAODE and HAODE (ICML'09, JFRB'10).
  - **3** MTE-AODE (ISDA'11).
- Impact of several discretization paradigms on the family of semi-naive BNCs:
  - Comparison of disjoint/traditional discretization methods (APPLIED INTELLIGENCE'11, IEA/AIE'10, CAEPIA'09).

2 Non-disjoint discretization for AODE and HAODE (HAIS'12).

- Domains of competence of this family of classifiers.
  - 1 Rules of good and bad behaviour.
  - 2 Meta-classification process to select the best semi-naive BNCs.

(submitted to INFORMATION SCIENCES'12, PGM'12).

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## **Future work**

- HODE: reuse estimations on one step in the EM algorithm used in HODE on posterior steps.
- MTE-AODE: new supervised method to dynamically search for the optimum number in every case into every dataset.
- ODD for {H}AODE: test bed of very high dimensional datasets.
- Obmains of competence: higher dimensionality relations between complexity measures, and datasets created for the Landscape contest.
- 6 AnDE: in high-dimensional datasets.
- Multinets or recursive nets.
- Multi-label classification.
- Multi-instance learning.

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PhD thesis:

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Thank you for your attention

Questions, ideas or comments are welcome





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