Data Mining in a complex world

Hugues Bersini IRIDIA/CODE

Modelling the data: WHY ??

only if structure and regularities in the data data contains the needed information in a hidden form !!



They might be antagonistic objectives





A compressed model with predictive power







The main techniques of data-mining

- Clustering
- Classification
- Outlier detection
- Association analysis
- Regression
- Forecasting
- Why in business: personalized business, improved prediction, targeted marketing

Data Classification: to understand and/or to predict





Exemple of classification: Decision tree





Clustering and outlier



Market Basket Analysis: Association analysis

Transn.	Juice	Теа	Coffee	Milk	Sugar	Рор
1	0	0	0	0	0	0
2	0	2	2	4	3	0
3	1	0	0	0	0	0
4	0	1	0	0	0	0
5	1	2	1	1	0	0
6	0	2	1	3	2	0
7	0	0	0	0	0	6
8	0	0	0	0	0	0
9	4	0	0	0	0	0
10	0	0	1	1	0	0
11	0	0	0	0	0	6
12	0	0	1	1	0	0
13	0	0	0	0	0	5
14	0	0	0	0	0	0
15	1	2	0	2	0	0
16	0	1	1	1	2	1
17	1	0	1	0	0	0
18	2	0	0	0	0	0
19	0	0	0	0	0	2
20	3	0	0	0	0	3

Quantity bought

Calcul of Improvement

IMPROVEMENT = (N * xij) / (ni * nj)

Improvement	Juice	Tea	Coffee	Milk	Sugar	Рор
Juice	0	0,95	0,82	0,82	0	0,17
Теа	0.95	0	1,9	2.38	3,33	0.56
Coffee	0.82	1,9				
Milk	0,82					
Sugar	0	3,33				
Рор	0,17					

Data Regression and Prediction



spline(x, y, n = 10 * n)\$x

Understand or predict



Important emblematic achievements

1) A new engineering approach



The Darpa Challenge





Games



Min-max







Data mining

2) A new scientific Paradigm: The fourth : Microsoft



Increasingly, scientific breakthroughs will be powered by advanced computing capabilities that help researchers manipulate and explore massive datasets. The speed at which any given scientific discipline advances will depend on how well its researchers collaborate with one another, and with technologists, in areas of eScience such as databases, workflow management, visualization, and cloud computing technologies.



CLIMATE FORECASTING



Figure 1. Upper panel: comparison of observations of global mean temperature (joined points) with model forecasts (grey zone and dotted lines). Lower panel: comparison of observed sea level (joined points) and model forecasts (grey zone and dotted lines). Both panels cover the years 1970 to 2007.



Figure 2. The IPCC model predictions of the extent of ice covering the summer Arctic Ocean (grey zone with a solid line representing the average in its centre) and the observed ice cover (solid line to the left of the figure).



James Lovelock



3) A huge market of business opportunities: IRIDIA's CV

Automatic glass default recognition





Financial prediction

daily stock market index



Santa Fe time series



Task: predict the continuation of the series for the next 100 steps.

Lazy Learning prediction



Automatic image labelling



Cancer diagnosis





Sudden infant death syndrome



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In Silico project: Integration with visualisation and analysis tools



SMART : detection of outlier clinical site

Individuals factor map (PCA)



The future of it: More and more free documents with various contents and various own structuration



Art Mining:

- images
- musics
- movies

23 A	Dostoïevski Crime et châtiment
	Dostoïevski <i>Les pauvres gens</i>
a.	Dostoïevski <i>Le joueur</i>
	Dostoïevski L'idiot
	Turgueniev Roudine —
	Tourgueniev Nid de gentilhommes
2. / Mark	Tourgueniev À la veille
	Tourgueniev Père et Fils
	Tolstoï Jeunesse
	Tolstoï Anna Karénine
	Tolstoï <i>Guerre et Paix</i>
	Gogol Le Portrait
	Gogol La Brouille des deux Ivan
5-18	Gogol Les âmes mortes
	Gogol Tarass Boulba
	Tolstoï <i>Les cosagues</i>
	Bulgakov Le Maître et Marguerite
7	Bulgakov Les œufs fatidiques
	Bulgakov Creur de chien
Sanda Martin	Salgator cara as erren

Exemple of clustering: hierarchical clustering

Algoritm

- → Join the two closest elements.
 - Update the distance matrix.



Distance matrix

Hierarchical clustering

Algoritm

- → Join the two closest elements.
 - Update the distance matrix.



Closest : (1,2) et (3,4,5)


Similarity based on compression algorithm

- Suppose two documents A and B
- Compute length of compressing A: C(A)
- Compute length of compressing B: C(B)
- Compute length of compressing AB: C(AB)
- Similarity (A,B) = 1-[C(A)+C(B)-C(AB)]/C(A)

if $C(A) \ge C(B)$

Simalirity between natural languages



Web Mining

- The Hyperprisme project
- Spy the user and mine his clickstream
- Automatic profiling of users
 - Key words: positif, negatif,...
- Automatic grouping of users on the basis of their profiles



Text Mining: still a lot of possible improvements

Term-document matrix Table III Term Doc1 Doc2 Doc3 Doc4 Doc5 Doc6 Passenger traffic volume Decrease Increase Passengers carried Personal traffic tools Grow up Million Hundred FAST rapid transit system Finished A1 station B1 station C1 station D1 station E1 station Passenger-Kilometers Columniation Check the number Ticket Revenues



Semantic enrichment

Using background knowledge to extend query



Exploit the structure of the documents

Like for XML for instance

<Course> <title> Software technologies </title> <teacher> Bersini </teacher> <themes> <name> programming technique </name> <name> data representation </name> <name> data mining </name> </themes>

Exploit the graph structure of XML + the content between the tags

We are working on Wikipedia

The Nature of Wikipedia

- Wikipedia is a combination of two interconnected graphs
 - A directed graph with the regular pages as nodes and the links between pages as edges
 - An acyclic directed graph with the category pages as nodes and their connections as edges
- The main regular page graph consists of ~ 3 650 000 nodes and the category graph of ~ 700 000 nodes (last count)



Graph Mining

Introduction and Context Betweenness and Covariance Classification of Nodes Conclusion and Perspectives

Introduction Algorithms Experiments

Application to Classification



Let us classify all the nodes.

Introduction and Context Betweenness and Covariance Classification of Nodes Conclusion and Perspectives

Introduction Algorithms Experiments

Application to Classification



Combine different types of information: graph and text

🔁 com	bigraphfeatures04.pd	- Adobe Reader	
Fichier	Edition Affichage	Document Outils Fenêtre Aide	×
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		d1 d2 d1 d1 d1 d1 d1 c3 c36 c20 c20 c1	
		Figure 10: The document nodes has been connected to an external preexisting	
		citation network through inferred k nearest neighbors links (i.e. in blue). The goal	
		is to propagate labels from the citation graph to the just connected documents.	
*			
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Data Warehousing





Source : Le Data Warehouse -Le Data Mining, Eyrolles, Paris, p. 40

Réorganisation des données

- Orientées sujet
- intégrées
- transversales
- historisées
- non volatiles
- Des données productions ---> données décision

	Environnement transactionnel	Data Warehouse
Type d'utilisateurs	Font tourner les roues de l'entreprise	Vérifient si les roues de l'entreprise tournent bien
Définition de système	Système performant = système rapide	Notion de performance est liée au degré de prévisabilité
performant		d'une requête
Volumes manipulés	Faible	Elevé
Type d'accès	Lecture/écriture : la donnée est modifiée en ligne	Chargement par batch, mises à jour interdites car les
		aonnees sont des clicnes issus des systemes de production
Types de données stockées	Dynamiques : mises à jour fréquente	Statique, évolution par chargement
Gestion des redondances	Est évitée car elle pose des problèmes d'incohérence de	Redondance peut être nécessaire pour optimiser les
n se anna 1997 an 1997 Na shearann an 1997 an	données	performances → pas de problème de cohérence car la
		donnée de base est déjà une copie
Domaine couvert	Modèle le plus souvent propre à une application	Rôle transversal dans l'entreprise et organisé par sujet
Mode d'accès et conséquence	Par l'intermédiaire d'application ; le modèle de données	Directe ou légèrement masquée par un outil d'aide à la
sur le modèle de données	n'est visible que par l'utilisateur qui ne voit le système	décision→ le modèle doit être simple
	qu'au travers des applications qu'il utilise Ie modèle de données peut être complexe	
Type de requête	Simples car prévisibles → le modèle de données est	Complexe, surtout si l'utilisateur est autonome. Il est
	conçu pour éviter les requêtes trop complexes. La plupart	quasiment impossible de garantir que tous les accès
	des requêtes s'appuient sur un index, d'où des temps de	passeront par les index : le temps de reponse peut
	réponses proportionnels au volume stocké. Les	aepenare au volume stocke et pas seulement au volume
	performances sont stables car toutes les requêtes sont	associe au resultat de la requete
	predefinies	Long
Horizon temporel		LOIN Trade impréssionles
Nombre et type d'accès	Reguliers et previsibles	Tres integuners et imprevisioles
Volume	Rarement supérieure à la dizaine de gigas	Superieur car historisation



Source : Franco J.M (1997), le Data Warehouse et le Data Mining, Eyrolles, Paris, p. 100

Model-based vs Data-based







Supervised learning



• Finite amount of noisy observations.

• No a priori knowledge of the phenomenon.

Model learning



The Practice of Modelling



Comprehensible models

Decision trees

- Qualitative attributes
- Force the attributes to be treated separately
- classification surfaces parallel to the axes
- good for comprehension because they select and separate the variables









Decision trees

- Very used in practice. One of the favorite data mining methods
- Work with noisy data (statistical approaches) can learn logical model out of data expressed by and/or rules
- ID3, C4.5 ---> Quinlan
- Favoring little trees --> simple models

- At every stage the most discriminant attribute
- The tree is being constructed top-down adding a new attribute at each level
- The choice of the attribute is based on a statistical criteria called : "the information gain"
- Entropie = -pouilog2poui pnonlog2pnon
- Entropie = 0 if Poui/non = 1
- Entropie = 1 if Poui/non = 1/2

Information gain

- S = set of instances, A set of attributes and v set of values of attributes A
- Gain (S,A) = Entropie(S)- $\Sigma_v |S_v|/|S|^*$ Entropie(S_v)
- the best A is the one that maximises the Gain
- The algorithm runs in a recursive way
- The same mechanism is reapplied at each level

Example Decision Tree

فہ	ical a	Ical	1011S
catego	catego	contin	class

Tid	Refund	Marital Status	l axable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



(© 1999, Lhiv. of Minnesota High Performance Data Mining (Vipin Kumar and Mahesh Joshi) 36

BUT !!!!



Other comprehensible models

Fuzzy logic

Realize an I/O mapping with linguistic rules
If I eat "a lot" then I take weight "a lot"



The fuzzy










IF x is very small THEN y is small IF x is small THEN y is medium IF x is medium THEN y is medium



Non comprehensible models

- From more to less
 - linear discriminant
 - local approaches
 - fuzzy rules
 - Support Vector Machine
 - RBF
 - global approaches
 - NN
 - polynômes, wavelet,...
 - Support Vector Machine

The neural network





suggestion de décision



precise universal black-box semi-automatic

Nonlinear relationship



Observations



Global modeling



Prediction with global models



Advantages

- Exist without data
- Information compression
 - Mainly SVM: mathématiques, pratiques, logique et génériques.
- Detect a global structure in the data
- Allow to test the sensitivity of the variables
- Can easily incorporate prior knowledge

Drawbacks

- Make assumption of uniformity
- Have the bias of their structure
- Are hardly adapting
- Which one to choose.

BAGFS: ensemble method

Weak classifiers' ensembles

- Classifier capacity reduced in 2 ways :
 simplified internal architecture
 NOT all the available information
- Better generalisation, reducing overfitting
- Improving accuracy
- by decorrelating classifiers errors
- by increasing the variability in the learning space.

`Bagging' : resampling the learning set

- Bootstraps aggregating (Leo Breiman)
 - random and independant perturbation of the learning set.
 - vital element : instability of the inducer*.
 - e.g. C4.5, neural network but not kNN !
 - increase accuracy by reducing variance
- * inducer = base learning algorithm : c4.5, kNN, ...

Learning set resampling : `Arcing'

- Adaptive resampling or reweighting of the learning set (*Leo Breiman* terminology).
- Boosting (Freund & Schapire)
 - sequential reweighting based on the description accuracy.
 - e.g. AdaBoost.M1 for multi-class problems.
 - needs unstability so as bagging
 - better variability than bagging.
 - sensible to noisy databases.
 - better than *bagging* on non-noisy databases

Mutliple Feature Subsets :

Stephen D. Bay (1/2) problem ?

- kNN is stable vertically so Bagging doesn't work.
- horizontally : MFS combining random selections of features with or without replacement.

question ?

what about other inducers such C4.5 ??

Multiple Feature Subsets : Stephen D. Bay (2/2)

- **Hypo** : kNN uses its ' horizontal ' instability.
- Two parameters :
 - □ K=n/N, proportion of features in subsets.
 - R, number of subsets to combine.
- MFS is better than single kNN with FSS and BSS, feature selections techniques.
- Image: MFS is more stable than kNN on added irrelevant features.
- Image: MFS decreases variance <u>and</u> bias through randomness.

BAGFS : a multiple classifier system

- BAGFS = MFS inside each Bagging.
- BAGMFS = MFS & Bagging together.
- 3 parameters
 - **B**, number of bootstraps
 - □ **K**=n/N, proportion of features in subsets
 - R, number of feature subsets
- decision rule : majority vote

BAGFS architecture around C4.5



Experiments

- Testing parametrization
 - optimizing K between 0.1 and 1 by means of a nested 10-fold cross-validation
 - \square R= 7, B= 7 for two-level method : Bagfs 7x7
 - set of 50 classifiers otherwize : Bag 50, BagMfs
 50, MFS 50, Boosting 50

Experimental Results

	c45	bagmfs 50	bagfs 7x7	boosting 50	bag 50	mfs 50
hepatitis	77.6	82.7	84.1	82.1	81.0	83.2
glass	64.8	77.3	76.6	74.4	74.8	75.2
iris	92.7	93.4	93.2	92.4	92.3	93.5
ionosphere	90.9	93.7	93.5	93.2	92.8	93.6
liver disorders	64.1	73.5	70.5	72.3	72.8	65.6
new-thyroid	92.0	94.9	94.5	93.5	93.8	92.7
ringnorm	91.9	97.9	97.7	95.3	95.6	97.6
twonorm	85.4	96.9	96.7	96.4	96.6	96.6
satimage	86.8	91.4	91.3	90.0	90.8	92.1
waveform	76.2	84.6	83.9	84.0	83.2	83.9
breast-cancer-w	94.7	96.9	96.8	95.5	95.3	96.8
wine	85.7	92.3	90.8	91.3	91.3	89.6
segmentation	93.4	98.2	98.4	95.1	96.6	98.7
Image	96.5	97.3	97.8	96.7	97.6	97.6
car	92.1	93.2	92.5	92.1	93.2	92.2
diabetes	72.4	75.7	75.7	76.2	75.7	74.0
	84.8	90.0	89.6	88.8	89.0	88.9

• McNemar test of significance (95%) : Bagfs performs never signif. worse and even sign. better on at least 4 databases (see red databases).

BAGFS : discussions

- How adjusting the parameters B, K, R
 - internal cross validation ?
 - dimensionality and variability measures hypothesis

Interest of a second level ?

- About irrelevant and (un)informative features ?
- Does bagging + feature selections work better ?
- How proving the interest of MFS randomness ?
- How using bootstraps complementary ?
 - Can we ?
 - What to do ?
- How proving horizontal unstability of C4.5 ?
- Comparison with 1-level bagging and MFS
 - Same number of classifiers ?
 - Advantage of tuning parameters ?

Which best model ?? when they all can perfectly fit the data They all can perfectly fit the data but



they don't approach the data in the same way. This approach depends on their structure



This explains the importance of Cross-validation



Which one to choose

- Capital role of crossvalidation.
- Hard to run
- One possible response



Lazy methodsComing from fuzzy





Lazy Methods

- Accuracy entails to keep the data and don't use any intermediary model: the best model is the data
- Accuracy requires powerful local models with powerful cross-validation methods



lazy methods is a new trend which is a revival of an old trend

Made possible again due to the computer power

Lazy methods

- A lot of expressions for the same thing:
 - memory-based, instance-based, examplesbased, distance-based
 - nearest-neighbour
- lazy for regression, classification and time series prediction
- Iazy for quantitative and qualitative features

Local modeling



Prediction with local models



Local modeling procedure

The identification of a local model can be summarized in these steps:

- Compute the distance between the query and the training samples according to a predefined metric.
- Rank the neighbors on the basis of their distance to the query.
- Select a subset of the nearest neighbors according to the bandwidth which measures the size of the neighborhood.
- Fit a local model (e.g. constant, linear,...).

The work focused on the bandwidth selection problem.
Bias/variance trade-off: overfitting



too few neighbors \Rightarrow overfitting \Rightarrow large prediction error

Bias/variance trade off: underfitting



too many neighbors \Rightarrow underfitting \Rightarrow large prediction error

Validation croisée: Press

- Fait un leave-one-out sans le faire pour les modèles linéaires
- Un gain computationnel énorme
- Rend possible une des validations croisées les plus puissantes à un prix computationel infime.

Data-driven bandwidth selection



Advantages

- No assumption of uniformity
- Justified in real life
- Adaptive
- Simple

From local learning to Lazy Learning (LL)

- By speeding up the local learning procedure, we can delay the learning procedure to the moment when a prediction in a query point is required (query-by-query learning).
- This method is called lazy since the whole learning procedure is deferred until a prediction is required.
- Example of non lazy methods (eager) are neural networks where learning is performed in advance, the fitted model is stored and data are discarded.

Static benchmarks

- Datasets: 15 real and 8 artificial datasets from the ML repository.
- Methods: Lazy Learning, Local modeling, Feed Forward Neural Networks, Mixtures of Experts, Neuro Fuzzy, Regression Trees (Cubist).
- **Experimental methodology**: 10-fold cross-validation.
- **Results**: Mean absolute error, relative error, paired t-test.

Observed data

Artificial data

Dataset	No. examples	No. inputs
Housing	330	8
Сри	506	13
Prices	209	6
Mpg	159	16
Servo	392	7
Ozone	167	8
Bodyfat	252	13
Pool	253	3
Energy	2444	5
Breast	699	9
Abalone	4177	10
Sonar	208	60
Bupa	345	6
Iono	351	34
Pima	768	8

Dataset	No. examples	No. inputs
Kin_8nh	8192	8
Kin_8fm	8192	8
Kin_8nm	8192	8
Kin_32fh	8192	32
Kin_32nh	8192	32
Kin_32fm	8192	32
Kin_32	8192	32



Experimental results: paired comparison (I)

Each method compared with all the others (9*23 = 207 comparisons)

Method	No. times significantly worse
LL linear	74
LL constant	96
LL combination	23
Local modeling linear	58
Local modeling constant	81
Cubist	40
Feed Forward NN	53
Mixtures of experts	80
Local Model Network (fuzzy)	132
Local Model Network (k-mean)	145

The lower, the better !!

Experimental results: paired comparison (II)

Each method compared with all the others (9*23 = 207 comparisons)

Method	No. times significantly better
LL linear	80
LL constant	59
LL combination	129
Local modeling linear	89
Local modeling constant	74
Cubist	110
Feed Forward NN	116
Mixtures of experts	72
Local Model Network (fuzzy)	32
Local Model Network (k-mean)	21

The larger, the better !!

Lazy Learning for dynamic tasks

Iong horizon forecasting based on the iteration of a LL one-step-ahead predictor.

- Nonlinear control
 - Lazy Learning inverse/forward control.
 - Lazy Learning self-tuning control.
 - Lazy Learning optimal control.

Dynamic benchmarks

- Multi-step-ahead prediction:
 - Benchmarks: Mackey Glass and 2 Santa Fe time series
 - Referential methods: recurrent neural networks.
- Nonlinear identification and adaptive control:
 - Benchmarks: Narendra nonlinear plants and bioreactor.
 - Referential methods: neuro-fuzzy controller, neural controller, linear controller.

Santa Fe time series



Task: predict the continuation of the series for the next 100 steps.

Lazy Learning prediction



LL is able to predict the abrupt change around t =1060 !

Awards in international competitions

- Data analysis competition: awarded as a runnerup among 21 participants at the 1999 ColL International Competition on Protecting rivers and streams by monitoring chemical concentrations and algae communities.
- Time series competition: ranked second among 17 participants to the International Competition on Time Series organized by the International Workshop on Advanced Black-box techniques for nonlinear modeling in Leuven, Belgium