KD Ubiq Summer School 2008 Behavioural Modelling of a Grid System

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Overview of the Tutorial

Autonomic Computing

- ML & DM for Systems: Introduction, motivations, applications
- Zoom on an application: Performance management

Autonomic Grid

- ► EGEE: Enabling Grids for e-Science in Europe
- Data acquisition, Logging and Bookkeeping files
- (change of) Representation, Dimensionality reduction

Modelling Jobs

- Exploratory Analysis and Clustering
- Standard approaches, stability, affinity propagation

Part 2

Grid Systems

Presentation of EGEE, Enabling Grids for e-Science in Europe

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- Acquiring the data The grid observatory
- Preparation of the data
 - Functional dependencies
 - Dimensionality reduction
 - Propositionalization

Computing Systems: The landscape



parallel

- distributed
- homogeneous soft and hard
- resources
 - dedicated
 - static
 - controlled
- reduced software stack
- no built-in fault tolerance

heterogeneous soft and hard

- resources
 - shared
 - dynamic
 - aggregated
- middleware
- faults: the norm

Storage and Computation have to be distributed



EGEE: Enabling Grids for E-Science in Europe



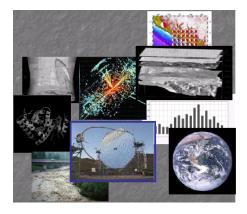
EGEE, 2

- \blacktriangleright Infrastructure project started in 2001 \rightarrow FP6 and FP7
- Large scale, production quality grid
- Core node: Lab. Accelerateur Linéaire, Université Paris-Sud
- ▶ 240 partners, 41,000 CPUs, all over the world
- 5 Peta bytes storage
- 24 \times 7, 20 K concurrent jobs
- Web: www.eu-egee.org

Storage as important as CPU

Applications

- High energy physics
- Life sciences
- Astrophysics
- Computational chemistry
- Earth sciences
- Financial simulation
- Fusion
- Multimedia
- Geophysics



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Autonomic Grid

Requisite: The Grid Observatory

- Cluster in the EGEE-III proposal 2008-2010
- Data collection and publication: filtering, clustering

Workload management

- Models of the grid dynamics
- Models of requirements and middleware reaction: time series and beyond
- Utility based-scheduling, local and global: MAB problem
- Policy evaluations: very large scale optimization

Fault detection and diagnosis

 Categorization of failure modes from the Logging and Bookkeeping: feature construction, clustering,

Abrupt changepoint detection

Autonomic Grid: The Grid Observatory

Data acquisition

- Data have not been stored with DM in mind never
- Data [partially] automatically generated here for EGEE services
 - redundant
 - little expert help

It's no longer: the expert feeds the machine with data. Rather, machines feed machines... J. Gama

Data preprocessing

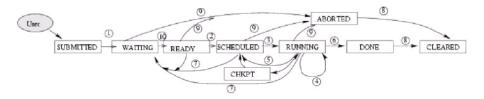
- ▶ 80% of the human cost
- Governs the quality of the output

The grid system and the data

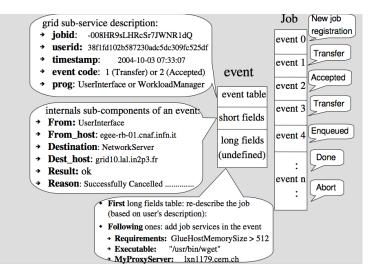
The Workload Management System

 User Interface
 User submits job description and requirements, and gets the results
 Resource Broker
 Job Submission Service
 Logging and Bookkeeping Service
 User submits job description Decides Computing Element
 Submits to CE and Checks
 Archive the data

Job Lifecycle



The data



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Data Tables

Events

jobid	event	i.	code	host	I	time_stamp		l	arrived		10	evel
BrI1BgbIqkwtszqGfmA		i		atlfarm008.mi.infn.it		2004-09-17			2004-09-17			8
BrI1BgbIqkwtszqGfmA	1	1	1	atlfarm008.mi.infn.it	L	2004-09-17	16:17:48	Ľ	2004-09-17	16:17:49	1	8
BrI1BgbIqkwtszqGfmA	2	1	2	lxb0728.cern.ch	L	2004-09-17	16:17:53	L	2004-09-17	16:17:53	1	8
BrI1BgbIqkwtszqGfmA	3	1	4	lxb0728.cern.ch	L	2004-09-17	16:18:00	L	2004-09-17	16:18:01	1	8
BrI1BgbIqkwtszqGfmA	4	1	1	atlfarm008.mi.infn.it	L	2004-09-17	16:18:00	L	2004-09-17	16:18:01	1	8
BrI1BgbIqkwtszqGfmA	5	L	5	lxb0728.cern.ch	I	2004-09-17	16:18:01	l	2004-09-17	16:18:01	1	8

Short Fields

1	0 1	JOBTYPE	SIMPLE
i i	0 i	NS	1xb0728.cern.ch:7772
i i	0 1	NSUBJOBS	0
i i	0 i	SEED	uLUOBArrdV98041PLThJ50
i i	o i	SEQCODE	UI=000001:NS=00000000000:WM=000000:BH=0000000000:JSS=000000:LM=000000:LBMS=000000:APP=000000
i i	0 1	SRC INSTANCE	
i	1 1	DESTINATION	NetworkServer
i	1	DEST_HOST	1xb0728.cern.ch
1	1	DEST_INSTANCE	1xb0728.cern.ch:7772
1	1	DEST_JOBID	
1	1	REASON	
1	1	RESULT	START
1	1	SEQCODE	UI=000002:NS=0000000000:WM=000000:BH=0000000000:JSS=000000:LM=000000:LRMS=000000:APP=000000
1	1	SRC_INSTANCE	1
1	2	FROM	UserInterface
1	2		1xb0728.cern.ch
1	2	FROM_INSTANCE	1
1		LOCAL_JOBID	1
1	2		UI=000003:NS=0000000001:WM=000000:BH=0000000000:JSS=000000:LM=0000000:LRMS=0000000:APP=0000000
1	2		7772
1	3		/var/edgwl/workload_manager/input.fl
1	3	REASON	1
1	3		l ox
1	3		UI=000003:NS=0000000003:WM=000000:BH=0000000000:JSS=000000:LM=000000:LRMS=000000:APP=000000
1	3	SRC_INSTANCE	

Data Tables

Long Fields (4Gb)

| iobid | event | name | value

| ---BrI1BgbIqkwtszqGfmA | 0 | JDL |[requirements = (((Member("VO-atlas-lcg-release -0.0.2", other.GlueHostApplicationSoftwareRunTimeEnvironment)) && Member("VO-atlas-release -8.0.5".other.GlueHostApplicationSoftwareRunTimeEnvironment)) && (other.GlueCEPolicyMaxCPUTime >= (Member("LCG -2_1_0",other.GlueHostApplicationSoftwareRunTimeEnvironment) ? (36000000 / 60) : 36000000) / other.GlueHostBenchmarkSI00)) && (other.GlueHostNetworkAdapterOutboundIP == true)) 総 (other.GlueHostMainMemoryRAMSize >= 512); RetryCount = 0; edg_jobid = "https://lxb0728.cern.ch:9000/---BrI1BgbIqkwtszqGfmA"; Arguments = "dc2.003048.evgen.H4_170_WW._00002.pool.root dc2.003048.simul.H4_170_WW._00208.pool.root.2 -6 6 50 350 208"; Environment = { "LEXOR WRAPPER LOG=lexor wrapper.log", "LEXOR STAGEOUT MAXATTEMPT=5", "LEXOR STAGEOUT INTERVAL=60", "LEXOR LCG_GFAL_INFOSYS=1xb2011.cern.ch:2170","LEXOR_T_RELEASE=8.0.5", "LEXOR_T_PACKAGE=8.0.5.6/JobTransforms","LEXOR_T_BASEDIR=JobTransforms-08-00-05-06", "LEXOR_TRANSFORMATION=share/ dc2.g4sim.trf"."LEXOR STAGEIN_LOG=dq_233387_stagein.log","LEXOR_STAGEIN_SCRIPT=dq_233387_stagein.sh", "LEXOR_STAGEOUT_LOG=dg_233387_stageout.log","LEXOR_STAGEOUT_SCRIPT=dg_233387_stageout.sh" }; MyProxyServer = "lxb0727.cern.ch"; JobType = "normal"; Executable = "lexor_wrap.sh"; StdOutput = "dc2.003048.simul.H4_170_WW._00208.job.log.2"; OutputSandbox = { "metadata.xml","lexor_wrapper.log","dq_233387_stagein.log","dq_233387_stageout.log", "dc2.003048.simul.H4_170_WW._00208.job.log.2" }; VirtualOrganisation = "atlas"; rank = (other.GlueCEStateEstimatedResponseTime > 999) ? -(other.GlueCEStateEstimatedResponseTime) : -(other.GlueCEStateRunningJobs); Type = "job"; StdError = "dc2.003048.simul.H4_170_WW._00208.job.log.2"; DefaultRank = -other.GlueCEStateEstimatedResponseTime; InputSandbox = { "/home/negri/windmill-0.9.15/lexor/inputsandbox/lexor_wrap.sh". "/home/negri/windmill-0.9.15/lexor/inputsandbox/dqlcg.pv", "/home/negri/windmill-0.9.15/lexor/inputsandbox/edgrmpi.sh", "/home/negri/windmill-0.9.15/lexor/inputsandbox/dgrep.pl", "/home/negri/windmill-0.9.15/lexor/inputsandbox/run_dqlcg.sh", "/tmp/lexor/negri/dq_233387_stagein.sh", "/tmp/lexor/negri/dq_233387_stageout.sh" }]

Preparation of the data

- 1. Functional dependencies
- 2. Dimensionality reduction
 - Principal Component Analysis
 - Random Projection
 - Non linear Dimensionality Reduction
- 3. Propositionalization

curse of dimensionality

Functional dependency

Definition

Given attributes X and X', X' depends on X on $\mathcal{E}(X' \prec X)$ iff

$$\exists f: dom(X') \mapsto dom(X) \ s.t. \ \forall i = 1 \dots N, X(\mathbf{x}_i) = f(X'(\mathbf{x}_i))$$

Examples

- X' = City code, X = City name
- X' = Machine name, X = IP
- X' =Job ID, X =User ID

Why removing FD ?

- Curse of dimensionality
- Biased distance

Functional dependency, 2

Trivial cases

#dom(X) = #dom(X') = N number of examples

Algorithm

Size:

$$(X' \prec X) \Rightarrow #dom(X) \leq #dom(X')$$

Sample Repeat Select $v \in dom(X')$ $\mathcal{E}_v = \text{select } \mathbf{x}_i \text{ where } X'(\mathbf{x}_i) = v$ Define $X(\mathcal{E}_v) = \{w \in dom(X), \exists x \in \mathcal{E}_v \mid X(x) = w\}$ If $(\#X(\mathcal{E}_v) > 1)$ return false Until stop return true

Dimensionality Reduction - Intuition

Degrees of freedom

- Image: 4096 pixels; but not independent
- Robotics: (# camera pixels + # infra-red) × time; but not independent

Goal

Find the (low-dimensional) structure of the data:

- Images
- Robotics
- Genes

Dimensionality Reduction

In high dimensions

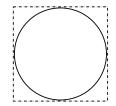
- Everybody lives in the corners of the space Volume of Sphere $V_n = \frac{2\pi r^2}{n} V_{n-2}$
- All points are far from each other

Approaches

- Linear dimensionality reduction
 - Principal Component Analysis
 - Random Projection
- Non-linear dimensionality reduction

Criteria

- Complexity/Size
- Prior knowledge



e.g., relevant distance

Linear Dimensionality Reduction

Training set

unsupervised

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$$\mathcal{E} = \{(\mathbf{x}_k), \mathbf{x}_k \in \mathbb{R}^D, k = 1 \dots N\}$$

Projection from \mathbb{R}^D onto \mathbb{R}^d

$$\begin{split} \mathbf{x} \in \mathbb{R}^D \to & h(\mathbf{x}) \in \mathbb{R}^d, \ d << D \\ & h(\mathbf{x}) = A \mathbf{x} \end{split}$$
s.t. minimize
$$\sum_{k=1}^N ||\mathbf{x}_k - h(\mathbf{x}_k)||^2$$

Principal Component Analysis

Covariance matrix S Mean $\mu_i = \frac{1}{N} \sum_{k=1}^{N} X_i(\mathbf{x}_k)$

$$S_{ij} = rac{1}{N}\sum_{k=1}^{N}(X_i(\mathbf{x}_k) - \mu_i)(X_j(\mathbf{x}_k) - \mu_j)$$

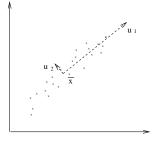
symmetric \Rightarrow can be diagonalized

$$S = U\Delta U' \quad \Delta = Diag(\lambda_1, \dots \lambda_D)$$

Thm: Optimal projection in dimension dprojection on the first d eigenvectors of S

Let u_i the eigenvector associated to eigenvalue λ_i $\lambda_i > \lambda_{i+1}$

$$h: \mathbb{R}^D \mapsto \mathbb{R}^d, h(\mathbf{x}) = <\mathbf{x}, u_1 > u_1 + \ldots + <\mathbf{x}, u_d > u_d$$



Sketch of the proof

1. Maximize the variance of
$$h(\mathbf{x}) = A\mathbf{x}$$

$$\sum_{k} ||\mathbf{x}_{k} - h(\mathbf{x}_{k})||^{2} = \sum_{k} ||\mathbf{x}_{k}||^{2} - \sum_{k} ||h(\mathbf{x}_{k})||^{2}$$

Minimize
$$\sum_{k} ||\mathbf{x}_{k} - h(\mathbf{x}_{k})||^{2} \Rightarrow \text{Maximize } \sum_{k} ||h(\mathbf{x}_{k})||^{2}$$

$$Var(h(\mathbf{x})) = \frac{1}{N} \left(\sum_{k} ||h(\mathbf{x}_{k})||^{2} - ||\sum_{k} h(\mathbf{x}_{k})||^{2} \right)$$

As

$$||\sum_{k} h(\mathbf{x}_{k})||^{2} = ||A\sum_{k} \mathbf{x}_{k}||^{2} = N^{2}||A\mu||^{2}$$

where $\mu = (\mu_1, \dots, \mu_D)$. Assuming that \mathbf{x}_k are centered $(\mu_i = 0)$ gives the result.

Sketch of the proof, 2

2. Projection on eigenvectors u_i of SAssume $h(\mathbf{x}) = A\mathbf{x} = \sum_{i=1}^{d} \langle \mathbf{x}, v_i \rangle v_i$ and show $v_i = u_i$. $Var(AX) = (AX)(AX)' = A(XX')A' = ASA' = A(U\Delta U')A'$ Consider d = 1, $v_1 = \sum w_i u_i$ $\sum w_i^2 = 1$ $remind \lambda_i > \lambda_{i+1}$

$$Var(AX) = \sum \lambda_i w_i^2$$

maximized for $w_1 = 1, w_2 = \ldots = w_N = 0$ that is, $v_1 = u_i$.

Principal Component Analysis, Practicalities Data preparation

Mean centering the dataset

$$\mu_i = \frac{1}{N} \sum_{k=1}^N X_i(\mathbf{x}_k)$$

$$\sigma_i = \sqrt{\frac{1}{N} \sum_{k=1}^N X_i(\mathbf{x}_k)^2 - \mu_i^2}$$

$$z_k = (\frac{1}{\sigma_i} (X_i(\mathbf{x}_k) - \mu_i))_{i=1}^D$$

Matrix operations

Computing the covariance matrix

$$S_{ij} = \frac{1}{N} \sum_{k=1}^{N} X_i(z_k) X_j(z_k)$$

► Diagonalizing S = U'∆U might be not affordable... Complexity $\mathcal{O}(D^3)$

Random projection

Random matrix

define

$$egin{aligned} A: \mathbb{R}^D &\mapsto \mathbb{R}^d \quad A[d,D] \quad A_{i,j} \sim \mathcal{N}(0,1) \ & h(\mathbf{x}) = rac{1}{\sqrt{d}} A \mathbf{x} \end{aligned}$$

Property: h preserves the norm in expectation

$$E[||h({\bf x})||^2] = ||{\bf x}||^2$$
 With high probability
$$1 - 2exp\{-(\varepsilon^2 - \varepsilon^3)\frac{d}{4}\}$$

$$|\mathbf{1} - \varepsilon)||\mathbf{x}||^2 \le ||\mathbf{h}(\mathbf{x})||^2 \le (1 + \varepsilon)||\mathbf{x}||^2$$

Random projection

Proof

$$h(\mathbf{x}) = \frac{1}{\sqrt{d}} A \mathbf{x}$$

$$E(||h(\mathbf{x})||^2) = \frac{1}{d} E \left[\sum_{i=1}^d \left(\sum_{j=1}^D A_{i,j} X_j(\mathbf{x}) \right)^2 \right]$$

$$= \frac{1}{d} \sum_{i=1}^d E \left[\left(\sum_{j=1}^D A_{i,j} X_j(\mathbf{x}) \right)^2 \right]$$

$$= \frac{1}{d} \sum_{i=1}^d \sum_{j=1}^D E[A_{i,j}^2] E[X_j(\mathbf{x})^2]$$

$$= \frac{1}{d} \sum_{i=1}^d \sum_{j=1}^D \frac{||\mathbf{x}||^2}{D}$$

$$= ||\mathbf{x}||^2$$

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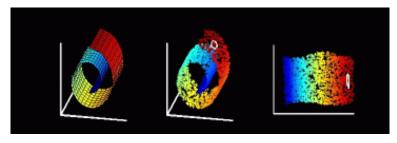
Random projection, 2

Johnson Lindenstrauss Lemma For $d > \frac{9 \ln N}{\varepsilon^2 - \varepsilon^3}$, with high probability $(1 - \varepsilon)||\mathbf{x}_i - \mathbf{x}_j||^2 \le ||h(\mathbf{x}_i) - h(\mathbf{x}_j)||^2 \le (1 + \varepsilon)||\mathbf{x}_i - \mathbf{x}_j||^2$

More:

http://www.cs.yale.edu/clique/resources/RandomProjectionMethod.pdf

Non-Linear Dimensionality Reduction



Conjecture

Examples live in a manifold of dimension $d \ll D$

Goal: consistent projection of the dataset onto \mathbb{R}^d Consistency:

- Preserve the structure of the data
- e.g. preserve the distances between points

Multi-Dimensional Scaling

Position of the problem

- Given $\{\mathbf{x}_1, \ldots, \mathbf{x}_N, \mathbf{x}_i \in \mathbb{R}^D\}$
- Given $sim(\mathbf{x}_i, \mathbf{x}_j) \in \mathbb{R}^+$
- Find projection Φ onto \mathbb{R}^d

$$\begin{array}{ll} x \in \mathbb{R}^D \to & \Phi(x) \in \mathbb{R}^d \\ sim(\mathbf{x}_i, \mathbf{x}_j) \sim & sim(\Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j)) \end{array}$$

Optimisation

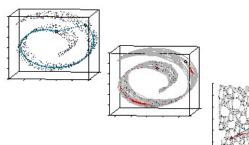
Define X, $X_{i,j} = sim(\mathbf{x}_i, \mathbf{x}_j)$; X^{Φ} , $X_{i,j}^{\Phi} = sim(\Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j))$ Find Φ minimizing ||X - X'||Rq : Linear Φ = Principal Component Analysis But linear MDS does not work: preserves all distances, while only *local* distances are meaningful

Non-linear projections

Approaches

- Reconstruct global structures from local ones and find global projection
- Only consider local structures

Intuition: locally, points live in \mathbb{R}^d



Isomap

LLE

Isomap

Tenenbaum, da Silva, Langford 2000 http://isomap.stanford.edu

Estimate $d(x_i, x_j)$

- ▶ Known if **x**_i and **x**_j are close
- Otherwise, compute the shortest path between x_i and x_j geodesic distance (dynamic programming)

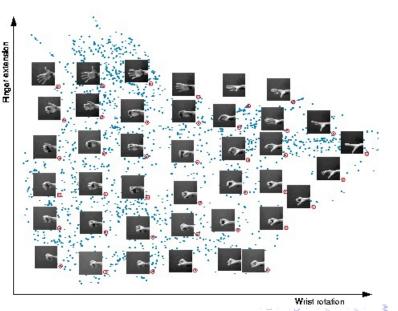
Requisite

If data points sampled in a convex subset of \mathbb{R}^d , then geodesic distance \sim Euclidean distance on \mathbb{R}^d .

General case

- Given $d(\mathbf{x}_i, \mathbf{x}_j)$, estimate $< \mathbf{x}_i, \mathbf{x}_j >$
- Project points in \mathbb{R}^d

Isomap, 2



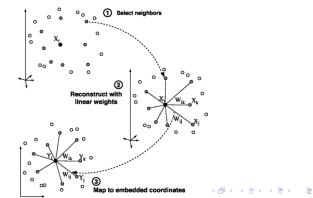
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Locally Linear Embedding

Roweiss and Saul, 2000 http://www.cs.toronto.edu/~roweis/lle/

Principle

 Find local description for each point: depending on its neighbors



Local Linear Embedding, 2

Find neighbors

For each \mathbf{x}_i , find its nearest neighbors $\mathcal{N}(i)$ Parameter: number of neighbors

Change of representation

Goal Characterize \mathbf{x}_i wrt its neighbors:

$$\mathbf{x}_i = \sum_{j \in \mathcal{N}(i)} w_{i,j} \mathbf{x}_j \quad ext{ with } \sum_{j \in \mathcal{N}(i)} w_{ij} = 1$$

Property: invariance by translation, rotation, homothety How Compute the local covariance matrix:

$$C_{j,k} = < x_j - x_i, x_k - x_i >$$

Find vector w_i s.t. $Cw_i = 1$

Local Linear Embedding, 3

Algorithm Local description: Matrix W such that

$$\sum_{j} w_{i,j} = 1$$

$$W = \operatorname{argmin} \{\sum_{i=1}^{N} ||\mathbf{x}_i - \sum_j w_{i,j} \mathbf{x}_j||^2\}$$

Projection: Find $\{z_1, \ldots, z_n\}$ in \mathbb{R}^d minimizing

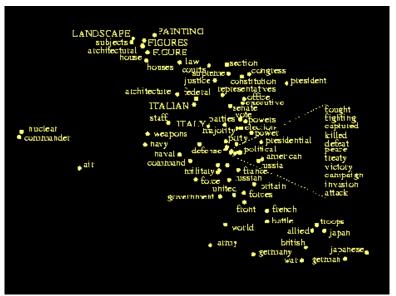
$$\sum_{i=1}^{N} ||z_i - \sum_j w_{i,j} z_j||^2$$

Minimize ((I - W)Z)'((I - W)Z) = Z'(I - W)'(I - W)Z

Solutions: vectors z_i are eigenvectors of (I - W)'(I - W)

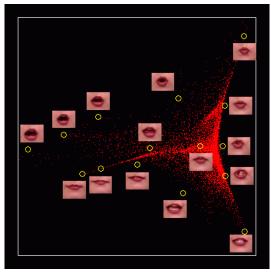
► Keeping the *d* eigenvectors with lowest eigenvalues > 0

Example, Texts



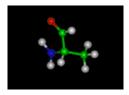
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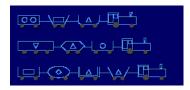
Example, Images



LLE

Relational domains





Relational learning

 PROS
 Inductive Logic Programming

 Use domain knowledge
 Data Mining

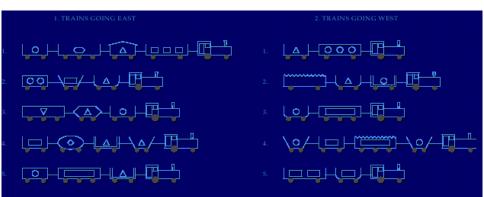
 CONS
 Data Mining

 Covering test ≡ subgraph matching
 exponential complexity

Getting back to propositional representation: propositionalization

West - East trains

Michalski 1983



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Linus (ancestor)

Lavrac et al, 94

$$\begin{array}{lll} \textit{West}(a) \leftarrow & \textit{Engine}(a,b), \textit{first_wagon}(a,c), \textit{roof}(c), \textit{load}(c,\textit{square},3)...\\ \textit{West}(a') \leftarrow & \textit{Engine}(a',b'), \textit{first_wagon}(a',c'), \textit{load}(c',\textit{circle},1)... \end{array}$$

West	Engine(X)	First Wagon(X,Y)	Roof(Y)	$Load_1(Y)$	$Load_2(Y)$
а	b	С	yes	square	3
a'	b'	c'	no	circle	1

Each column: a role predicate, where the predicate is determinate linked to former predicates (left columns) with a single instantiation in every example

Stochastic propositionalization

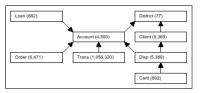
Kramer, 98

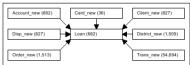
Construct random formulas \equiv boolean features

SINUS - RDS

http://www.cs.bris.ac.uk/home/rawles/sinus http://labe.felk.cvut.cz/~zelezny/rsd

- Use modes (user-declared) modeb(2,hasCar(+train,-car))
- Thresholds on number of variables, depth of predicates...
- Pre-processing (feature selection)





DB Schema

Propositionalization

RELAGGS

Database aggregates

- average, min, max, of numerical attributes
- number of values of categorical attributes

Going ubiquitous in Data Preparation

Principles: same as usual

- Act locally
- Think globally

The local level

- An ideal feature \equiv a good hypothesis
- What is a promising hypothesis ?
 - Behaves well on (part of) the data

Is not trivial

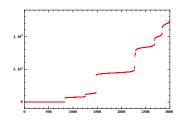
Going ubiquitous in Data Preparation, 2

What is a good behaviour?

- Showing regularities
- Locally constant

How to test triviality?

- Syntactical analysis:
 xy yx = 0
- Statistical triviality:
 - Test on random data
 - Test on permutations of the data



Going ubiquitous in Data Preparation, 3

Internally: an optimization problem

- Define bins
- Compute histogram, associated quantity of information

Compare histograms on real data / on random data

Externally: an optimization problem

- Upon receiving a new feature
- Check whether this is relevant to your data
- Check whether this brings new information