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

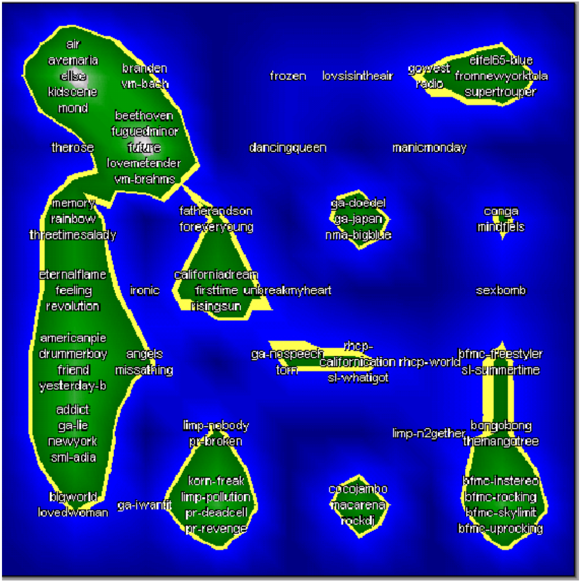
- Exploratory Analysis and Clustering
- Standard approaches, stability, affinity propagation

Part 3: Clustering

- Approaches
  - K-Means
  - EM
  - Selecting the number of clusters
- Clustering the EGEE jobs
  - Dealing with heterogeneous data
  - Assessing the results

Clustering

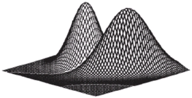
http://www.ofai.at/ elias.pampalk/music/



Clustering Questions

Hard or soft ?

- Hard: find a partition of the data
- Soft: estimate the distribution of the data as a mixture of components.



Parametric *vs* non Parametric ?

- Parametric: number K of clusters is known
- Non-Parametric: find K
  (wrapping a parametric clustering algorithm)

Caveat:

- Complexity
- Outliers
- Validation

Formal Background

Notations

$\mathcal{E}$	$\{\mathbf{x}_1, \ldots \mathbf{x}_N\}$ dataset	
N	number of data points	
K	number of clusters	given or optimized
C_k	k-th cluster	Hard clustering
$\tau(i)$	index of cluster containing $\mathbf{x}_i$	
f_k	k-th model	Soft clustering
$\gamma_k(i)$	$Pr(\mathbf{x}_i \vert f_k)$	

Solution

Hard Clustering	Partition $\Delta = (C_1, \ldots C_k)$
Soft Clustering	$\forall i \ \sum_k \gamma_k(i) = 1$

Formal Background, 2

Quality / Cost function

Measures how well the clusters characterize the data

- (log)likelihood — soft clustering
- dispersion — hard clustering

$$\sum_{k=1}^{K} \frac{1}{|C_k|^2} \sum_{\mathbf{x}_i, \mathbf{x}_j \ in \ C_k} d(\mathbf{x}_i, \mathbf{x}_j)^2$$

Tradeoff

Quality increases with $K \Rightarrow$ Regularization needed

to avoid one cluster per data point

Clustering vs Classification

Marina Meila
http://videolectures.net/

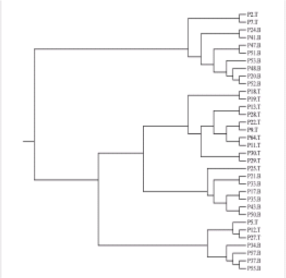
	Classification	Clustering
K	# classes (given)	# clusters (unknown)
Quality	Generalization error	many cost functions
Focus on	Test set	Training set
Goal	Prediction	Interpretation
Analysis	discriminant	exploratory
Field	mature	new

Non-Parametric Clustering

Hierarchical Clustering

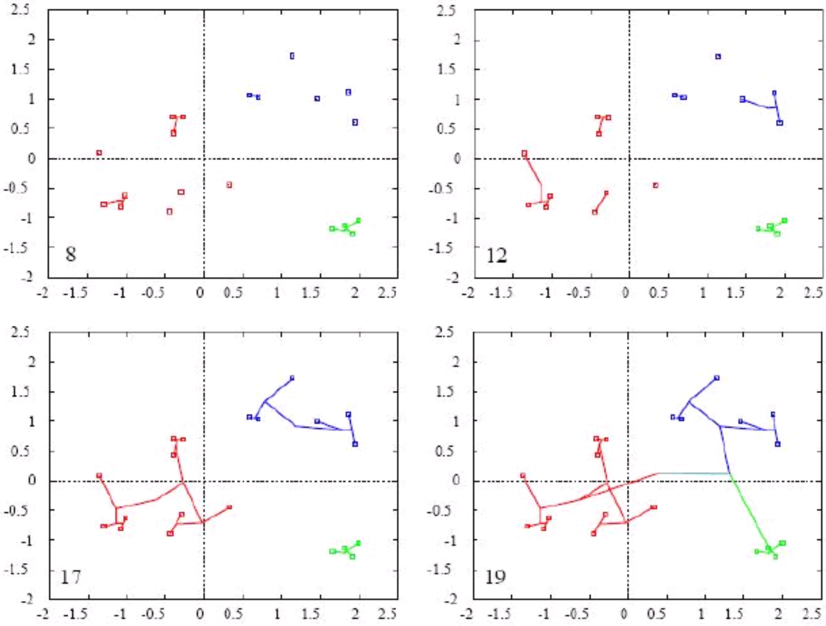
Principle

- agglomerative (join nearest clusters)
- divisive (split most dispersed cluster)

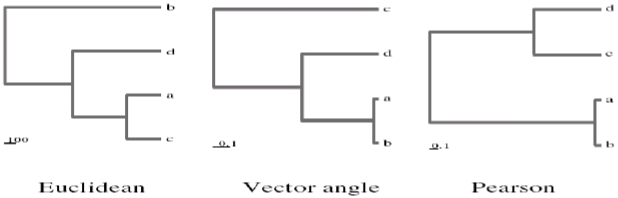


CONS: Complexity $\mathcal{O}(N^3)$

Hierarchical Clustering, example



Influence of distance/similarity



$$d(x, x') = \begin{cases} \sqrt{\sum_i (x_i - x_i')^2} & \text{Euclidean distance} \\ 1 - \frac{\sum_i x_i x_i'}{||x||.||x'||} & \text{Cosine angle} \\ 1 - \frac{\sum_i (x_i - \bar{x})(x_i' - \bar{x}')}{||x - \bar{x}||.||x' - \bar{x}'||} & \text{Pearson} \end{cases}$$

Parametric Clustering

K is known

Algorithms based on distances

- K-means
- graph / cut

Algorithms based on models

- Mixture of models: EM algorithm

K-Means

Algorithm

1. Init:
   Uniformly draw K points $\mathbf{x}_{i_j}$ in $\mathcal{E}$
   Set $C_j = \{\mathbf{x}_{i_j}\}$
2. Repeat
3. Draw without replacement $\mathbf{x}_i$ from $\mathcal{E}$
4. $\tau(i) = argmin_{k=1\ldots K}\{d(\mathbf{x}_i, C_k)\}$ find best cluster for $\mathbf{x}_i$
5. $C_{\tau(i)} = C_{\tau(i)} \bigcup \mathbf{x}_i$ add $\mathbf{x}_i$ to $C_{\tau(i)}$
6. Until all points have been drawn
7. If partition $C_1 \ldots C_K$ has changed Stabilize
   Define $\mathbf{x}_{i_k} =$ best point in C_k, $C_k = \{x_{i_k}\}$, goto 2.

Algorithm terminates

K-Means, Knobs

Knob 1 : define $d(\mathbf{x}_i, C_k)$ — favors

- ▶ $min\{d(\mathbf{x}_i, \mathbf{x}_j), \mathbf{x}_j \in C_k\}$ — long clusters
- * $average\{d(\mathbf{x}_i, \mathbf{x}_j), \mathbf{x}_j \in C_k\}$ — compact clusters
- ▶ $max\{d(\mathbf{x}_i, \mathbf{x}_j), \mathbf{x}_j \in C_k\}$ — spheric clusters

Knob 2 : define "best" in C_k

- ▶ Medoid — $argmin_i\{\sum_{\mathbf{x}_j \in C_k} d(\mathbf{x}_i, \mathbf{x}_j)\}$
- * Average (does not belong to $\mathcal{E}$) — $\frac{1}{|C_k|} \sum_{\mathbf{x}_j \in C_k} \mathbf{x}_j$

No single best choice

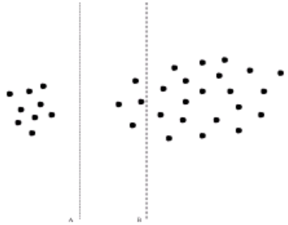


FIG. 1. Optimizing the diameter produces B while A is clearly more desirable.

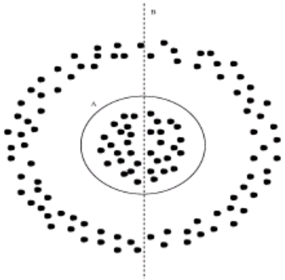


FIG. 2. The inferior clustering B is found by optimizing the 2-median measure.

K-Means, Discussion

PROS

- Complexity $\mathcal{O}(K \times N)$
- Can incorporate prior knowledge initialization

CONS

- Sensitive to initialization
- Sensitive to outliers
- Sensitive to irrelevant attributes

K-Means, Convergence

- For cost function

$$\mathcal{L}(\Delta) = \sum_k \sum_{i,j \;/\; \tau(i)=\tau(j)=k} d(\mathbf{x}_i, \mathbf{x}_j)$$

- for $d(\mathbf{x}_i, C_k) = \text{ average } \{d(\mathbf{x}_i, \mathbf{x}_j), \mathbf{x}_j \in C_k\}$
- for "best" in C_k = average of $\mathbf{x}_j \in C_k$

K-means converges toward a (local) minimum of $\mathcal{L}$.

K-Means, Practicalities

Initialization

- Uniform sampling
- Average of $\mathcal{E}$ + random perturbations
- Average of $\mathcal{E}$ + orthogonal perturbations
- Extreme points: select $\mathbf{x}_{i_1}$ uniformly in $\mathcal{E}$, then

$$\text{Select } x_{i_j} = argmax\{\sum_{k=1}^{j} d(\mathbf{x}_i, x_{i_k})\}$$

Pre-processing

- Mean-centering the dataset

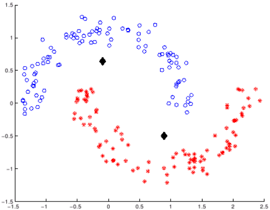
Model-based clustering

Mixture of components

- Density $f = \sum_{k=1}^{K} \pi_k f_k$
- f_k: the k-th component of the mixture
- $\gamma_k(i) = \frac{\pi_k f_k(x)}{f(x)}$
- induces $C_k = \{\mathbf{x}_j \ / \ k = argmax\{\gamma_k(j)\}\}$

Nature of components: prior knowledge

- Most often Gaussian: $f_k = (\mu_k, \Sigma_k)$
- Beware: clusters are not always Gaussian...



Model-based clustering, 2

Search space

- Solution : $(\pi_k, \mu_k, \Sigma_k)_{k=1}^{K} = \theta$

Criterion: log-likelihood of dataset

$$\ell(\theta) = \log(Pr(\mathcal{E})) = \sum_{i=1}^{N} \log Pr(\mathbf{x}_i) \propto \sum_{i=1}^{N} \sum_{k=1}^{K} \log(\pi_k f_k(\mathbf{x}_i))$$

to be maximized.

Model-based clustering with EM

Formalization

- Define $z_{i,k} = 1$ iff $\mathbf{x}_i$ belongs to C_k.
- $E[z_{i,k}] = \gamma_k(i)$ prob. $\mathbf{x}_i$ generated by $\pi_k f_k$
- Expectation of log likelihood

$$
\begin{aligned}
E[\ell(\theta)] &\propto \sum_{i=1}^N \sum_{k=1}^K \gamma_i(k) \log(\pi_k f_k(\mathbf{x}_i)) \\
&= \sum_{i=1}^N \sum_{k=1}^K \gamma_i(k) \log \pi_k + \sum_{i=1}^N \sum_{k=1}^K \gamma_i(k) \log f_k(\mathbf{x}_i)
\end{aligned}
$$

EM optimization

E step Given θ, compute

$$\gamma_k(i) = \frac{\pi_k f_k(\mathbf{x}_i)}{f(x)}$$

M step Given $\gamma_k(i)$, compute

$$\theta^* = (\pi_k, \mu_k, \Sigma_k)^* = argmin E[\ell(\theta)]$$

Maximization step

π_k: Fraction of points in C_k

$$\pi_k = \frac{1}{N} \sum_{i=1}^{N} \gamma_k(i)$$

μ_k: Mean of C_k

$$\mu_k = \frac{\sum_{i=1}^{N} \gamma_k(i) \mathbf{x}_i}{\sum_{i=1}^{N} \gamma_k(i)}$$

Σ_k: Covariance

$$\Sigma_k = \frac{\sum_{i=1}^{N} \gamma_k(i)(\mathbf{x}_i - \mu_k)(\mathbf{x}_i - \mu_k)'}{\sum_{i=1}^{N} \gamma_k(i)}$$

Choosing the number of clusters

K-means constructs a partition whatever the K value is.

Selection of K

- Bayesian approaches
  Tradeoff between accuracy / richness of the model
- Stability
  Varying the data should not change the result
- Gap statistics
  Compare with null hypothesis: all data in same cluster.

Bayesian approaches

Bayesian Information Criterion

$$BIC(\theta) = \ell(\theta) - \frac{\#\theta}{2} \log N$$

Select $K = \text{argmax } BIC(\theta)$
where $\#\theta$ = number of free parameters in θ:

- if all components have same scalar variance σ

$$\#\theta = K - 1 + 1 + Kd$$

- if each component has a scalar variance σ_k

$$\#\theta = K - 1 + K(d + 1)$$

- if each component has a full covariance matrix Σ_k

$$\#\theta = K - 1 + K(d + d(d - 1)/2)$$

Gap statistics

Principle: hypothesis testing

1. Consider hypothesis H_0: there is no cluster in the data. $\mathcal{E}$ is generated from a no-cluster distribution π.
2. Estimate the distribution $f_{0,K}$ of $\mathcal{L}(C_1, \ldots C_K)$ for data generated after π. Analytically if π is simple
   Use Monte-Carlo methods otherwise
3. Reject H_0 with confidence α if the probability of generating the true value $\mathcal{L}(C_1, \ldots C_K)$ under $f_{0,K}$ is less than α.

Beware: the test is done for all K values...

Gap statistics, 2

Algorithm

Assume $\mathcal{E}$ extracted from a no-cluster distribution,
e.g. a single Gaussian.

1. Sample $\mathcal{E}$ according to this distribution
2. Apply K-means on this sample
3. Measure the associated loss function

Repeat : compute the average $\bar{\mathcal{L}}_0(K)$ and variance $\sigma_0(K)$
Define the gap:

$$Gap(K) = \bar{\mathcal{L}}_0(K) - \mathcal{L}(C_1, \ldots C_K)$$

Rule Select min K s.t.

$$Gap(K) \geq Gap(K+1) - \sigma_0(K+1)$$

What is nice: also tells if there are no clusters in the data...

Stability

Principle

- Consider $\mathcal{E}'$ perturbed from $\mathcal{E}$
- Construct $C'_1, \ldots C'_K$ from $\mathcal{E}'$
- Evaluate the "distance" between $(C_1, \ldots C_K)$ and $(C'_1, \ldots C'_K)$
- If small distance (stability), K is OK

Distortion $D(\Delta)$

$$\begin{array}{llll} \text{Define} & S & S_{ij} = & < \mathbf{x}_i, \mathbf{x}_j > \\ & & (\lambda_i, v_i) & \text{i-th (eigenvalue, eigenvector) of } S \\ & X & X_{i,j} = & 1 \text{ iff } \mathbf{x}_i \in C_j \end{array}$$

$$D(\Delta) = \sum_i ||\mathbf{x}_i - \mu_{\tau(i)}||^2 = tr(S) - tr(X'SX)$$

Minimal distortion $D^* = tr(S) - \sum_{k=1}^{K-1} \lambda_k$

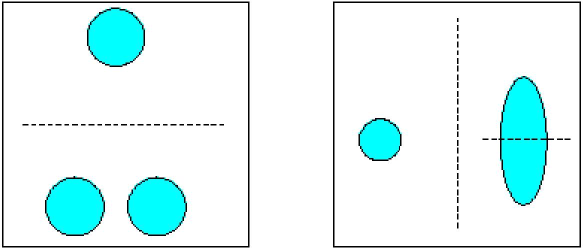
Stability, 2

Results

- Δ has low distortion $\Rightarrow (\mu_1, \ldots \mu_K)$ close to space $(v_1, \ldots v_K)$.
- Δ_1, and Δ_2 have low distortion $\Rightarrow$ "close"
- (and close to "optimal" clustering)

Meila ICML 06

Counter-example



From K-Means to K-Centers

Assumptions for K-Means

- A distance or dissimilarity
- Possibility to create artefacts — barycenters
- Not applicable in some domains — *average molecule?* *average sentence?*

K-Centers, position of the problem

- A combinatorial optimization problem.
  Find $\sigma : \{1, \ldots, N\} \mapsto \{1, \ldots, N\}$ minimizing:

$$E[\sigma] = \sum_{i=1}^{N} d(\mathbf{x}_i, \mathbf{x}_{\sigma(i)})$$

(What is missing here ?)

Affinity Propagation

Frey and Dueck 2007

Find σ maximizing:

$$E[\sigma] = \sum_{i=1}^{N} S(\mathbf{x}_i, \mathbf{x}_{\sigma(i)}) - \sum_{i=1}^{N} \chi_i[\sigma]$$

Where

$$S(\mathbf{x}_i, \mathbf{x}_j) = \begin{cases} -d(\mathbf{x}_i, \mathbf{x}_j) & \text{if } i \neq j \\ -s^* & \text{otherwise} \end{cases}$$

$$\chi_i[\sigma] = \begin{cases} \infty & \text{if } \sigma(\sigma(i)) \neq \sigma(i) \\ 0 & \text{otherwise} \end{cases}$$

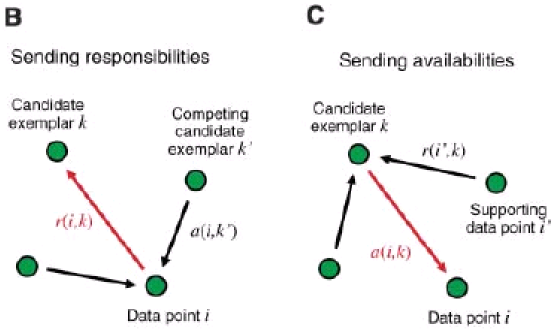
Remark: K is not fixed.

Instead, fix s^* usual: median $\{d(\mathbf{x}_i, \mathbf{x}_j)\}$

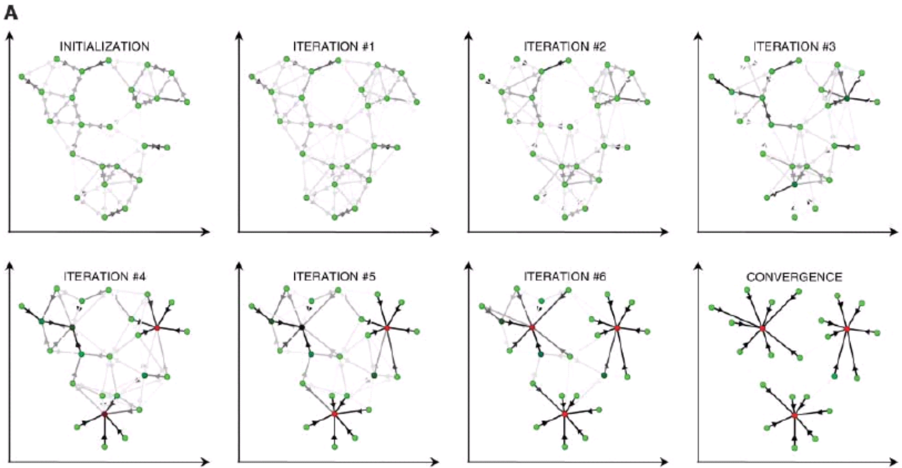
Affinity Propagation, Principle

Algorithm: Message propagation

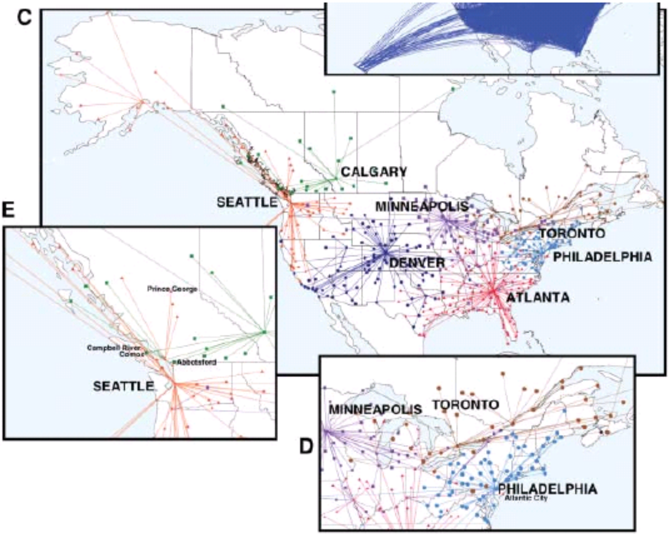
- Responsibility $r(i, k)$ could $\mathbf{x}_k$ be examplar for $\mathbf{x}_i$
- Availability $a(i, k)$.



Affinity Propagation, cont'd



Affinity Propagation, cont'd



Algorithm

Iterate

$$r(i,k) = S(i,k) - max_{k',k' \neq k}\{a(i,k') + S(i,k')\}$$
$$r(k,k) = S(k,k) - max_{k',k' \neq k}\{S(k,k')\}$$

$$a(i,k) = min\{0, r(k,k) + \sum_{i',i' \neq i,k} \max\{0, r(i',k)\}\}$$
$$a(k,k) = \sum_{i',i' \neq k} \max\{0, r(i',k)\}$$

Solution

$$\sigma(i) = argmax\{r(i,k) + a(i,k), k = 1 \dots N\}$$

Stop criterion

- After a maximal number of iterations
- After a maximal number of iterations with no change.