Addendum to the proof
of log n approximation ratio
for the greedy set cover algorithm

- (From Vazirani's very nice book "Approximation algorithms")
- Let $x_1, x_2, ..., x_n$ be the order in which the elements are covered (break ties arbitrarily)
- Lemma: $c(x_i) <= C^*/(n-i+1)$
- Proof. Suppose we are selecting a set that will cover x_i.
  The remaining elements can be covered with C^* sets.
  Thus there largest set in C^*, the optimal solution, will cover at least $(n-i+1)/C^*$ elements.
  I.e., The cost per element is at most $C^*/(n-i+1)$

Thus

- Theorem. The approximation cost is at most $H(n)$
- Proof. The cost is at most the sum of the costs $c(x_i)$

$$\sum_{i=1}^{n} c(x_i) \leq \frac{C^*}{n-i+1} \leq C^* \sum_{i=1}^{n} \frac{1}{n} \leq C^* H(n)$$

- Proving the bound $H(s)$ is more tedious.

Finding
fragments of orders, partial orders, and total orders from 0-1 data

Themes of the chapter

- Given a 0/1 a matrix
- Rows: observations, columns variables
- Can one find ordering information for the observations?
- Without additional assumptions, no; with some assumptions, yes

- Paleontological application:
  - find orders for subsets of fossil sites
  - a good ordering for (a subset of) the rows is one where the 1s are consecutive

- Also other applications

Themes of the chapter

- Finding small total orders (fragments) from 0-1 data
  - Local models/patterns

- Finding partial orders from 0-1 data
  - A global model

- Find total orders for 0-1 data
  - A global model

Finding small total orders (fragments) from 0-1 data

- Model: a subset of observations and a total order on the subset

- Task: find **all** such models fulfilling certain criteria

- Algorithm: a pattern discovery algorithm (levelwise search)

Finding partial orders from 0-1 data

- Model: a partial order over all observations

- Loglikelihood: proportional to the number of cases the observed occurrence patterns violate the continuity of species

- Prior: prefer partial orders that are as specific as possible

- Task: find **a** model with high likelihood * prior

- Algorithm: Find fragments and use heuristic search to build a good partial order

Find total orders for 0-1 data

- Model: a total order

- Loglikelihood: how many cases the observed occurrence patterns violate the continuity of species

- Task: find **the** best total order for the observations

- Algorithm: spectral method

Type of data

- 0-1 data, large number of variables
- Examples:
  - Occurrences of words in documents
  - Occurrences of species in paleontological sites
  - Occurrence of a particular motif in a promoter region of a gene
- Typically the data is sparse: only a few 1s
- Asymmetry between 0s and 1s
  - A "1" means that there really was something
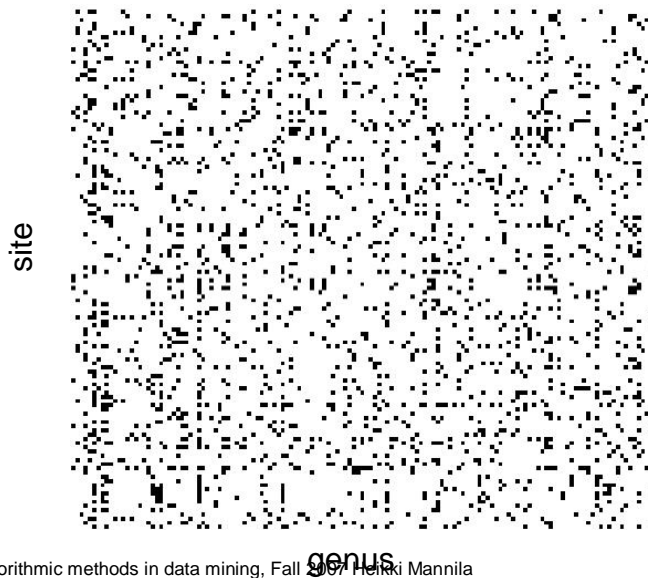 - A "0" has less information (in a way)

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Example

- Paleontological data from the NOW (Neogene Mammal Database)
- Fossil **sites** (one location, one layer)
- Each site contains fossils that are about the same age (+- 1 Ma)
- Variables: species/genera
- A "1" is reasonably certain
- A "0" might be due to several reasons
  - The species was not extant at that time
  - The remains did not fossilize
  - The tooth was overlooked
  - …

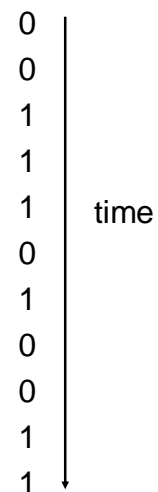Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Site-genus -matrix

site

genus

Background knowledge

- Species do not vanish and return

- An ordering of the sites with a "0" between "1"s is improbable

0
0
1
1
1
0
1
0
0
1
1

time

Example: seriation in paleontological data

- Given data about the occurrences of genera in fossil sites

- Want to find an ordering in which occurrences of a genus are consecutive

- **Lazarus count**: how many 0s are between 1s

Genus

Site

```
1 1 1 0 0 0 0 0 0 0
0 0 0 0 1 1 1 1 0 1
0 0 0 1 1 1 1 0 1 0
1 1 0 1 0 1 0 0 0 0
1 1 1 1 0 0 0 0 0 0
0 0 0 0 0 1 1 1 1 0
0 0 0 0 0 0 1 1 1 1
0 1 1 1 1 1 1 0 0 0
0 1 0 1 1 0 0 0 0 0
0 0 1 1 1 1 1 1 0 0
```

A better ordering

A smaller Lazarus count

```
1 1 1 0 0 0 0 0 0 0
1 1 1 1 0 0 0 0 0 0
1 1 0 1 0 1 0 0 0 0
0 1 0 1 1 0 0 0 0 0
0 1 1 1 1 1 1 0 0 0
0 0 1 1 1 1 1 1 0 0
0 0 0 1 1 1 1 0 1 0
0 0 0 0 1 1 1 1 0 1
0 0 0 0 0 1 1 1 1 0
0 0 0 0 0 0 1 1 1 1
```

Find small total orders (fragments) from 0-1 occurrence data

- Fragment: a total ordering of **a subset** of observations
- E.g., c<a<d<f

- Intuitive interpretation:

- For most variables the sequence of observations has no pattern of the form …1…0…1…

	1	1	1	0	0	0	0	0	0	1
	0	1	1	1	0	0	1	0	1	0
	1	1	0	0	0	1	0	0	1	0
c	0	1	0	1	1	0	0	0	0	
a	0	1	1	1	1	1	1	0	0	0
d	0	0	1	1	1	1	1	1	0	0
f	0	0	0	1	1	1	1	0	1	0
	0	0	0	0	1	1	1	0	1	
	0	1	0	1	0	1	1	1	1	0
	1	0	1	0	0	0	1	1	1	1

Fragments of order

- 0/1 data set
- Fragment of order *f* is a sequence of observations
  $$t_1 < t_2 < t_3 < … < t_k$$

- An variable *A* **disagrees** with fragment *f*, if for some *i<j<h* we have $t_i(A)=t_h(A)=1$, but $t_j(A)=0$.
- Otherwise t **agrees** with f:
- Then the column for *A* has the form

      0 0 …0 0 1 1 … 1 1 0 0 … 0 0

  for the observations in *f*

Example

A	1	0	0	1
B	1	1	1	0
C	0	0	0	1
D	1	0	1	0
E	1	0	1	1
F	1	1	1	1

a<b<c<d:

	dis	ag	dis	dis
	1101	0100	0101	1010

b<d<f<a:

	ag	dis	ag	ag
	1111	1010	1110	0011

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

What is a good fragment of order?

- A sequence f of rows, say, u<v<w<t

- Da(f): the number of variables disagreeing with the ordering

- Fr(f): the number of variables having at least 2 ones in the rows of f

- A good fragment has high Fr(f) and low Da(f)

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Problem statement

- Given thresholds σ and γ
- Find all fragments of order f such that in the data

  $Fr(f) > \sigma$

  $Da(f) < \gamma$
- and all subfragments of f satisfy these
- and the fragment has smaller Da value than its peers
  - Any other fragments from the same set of objects

Algorithm

- How to find fragments with the specific properties?
- Start from fragments of length 2
  - No disagreements are possible
  - Only the bound $Fr(f) > \sigma$ needs to be tested

- Iteration:
  - Assume fragments of length k-1 are known
  - Then we can build candidate fragments of length k
  - Continue until no new patterns are found

- A complete algorithm: all fragments will be found

Monotonicity property

- Fragment $t_1 < t_2 < t_3 < \ldots < t_k$ can satisfy the requirements only if all subfragments of length k-1 satisfy them

- All these have to be in the collection of fragments of size k-1

- The levelwise algorithm

Algorithm

- Find F2, fragments of size 2
- C = all triples A<B<C such that A<B, A<C, and B<C are in F2
- k ß 3

- While C is not empty
    compute Da(f) for all f in C
    Fk ß {f in C | Fr(f) > σ and Da(f) < γ }
    k ß k+1
    C ß all fragments of length k such that all the subfragments of
        length k-1 are in Fk

Complexity of the algorithm

- Potentially exponential in the number of variables

- |F+C| = the size of the answer + all the candidates

- Proportional to
    |F+C| n m
  for a matrix with n rows and m columns

- Too low values of σ or too high values of γ will lead to huge outputs
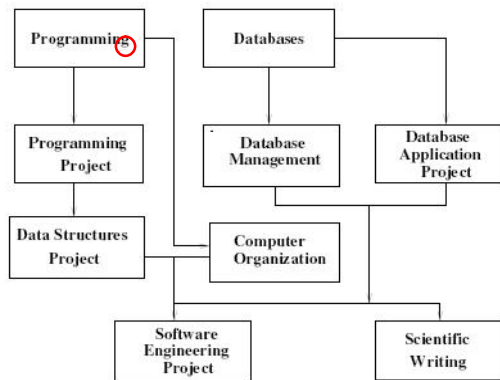
Experimental results

- Data about students and courses
- Columns: students
- Rows: courses
- $D(s,c)=1$ if student s has taken course c
- Here we know the true ordering
    - Or actually two: official ordering
    - Real order in which the student took the courses

Part of the recommendations

Discovered fragment f
Fr(f)=1361, Da(f)=3.2%

```
Programming          Databases

Programming          Database        Database
Project              Management      Application
                                     Project

Data Structures      Computer
Project              Organization

        Software                Scientific
        Engineering             Writing
        Project
```

⟨Programming,
Computer Organization,
Programming Project,
Data Structures Project,
Scientific Writing⟩

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Results

σ (in %)	τ (in %)	$Max\ l$	$|\mathcal{T}|$	α (in %)	β (in %)
20	0	3	2	96.3	99.5
20	2.5	5	578	48.6	70.5
20	5	6	1528	40.0	66.0
15	0	3	28	89.9	98.6
15	2.5	6	1934	46.8	78.2
15	5	7	5158	38.9	72.3

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Results (paleontological data)

- Fragments for sites

- Or transpose the matrix: fragments for species

- Sequences of sites such that there are very few Lazarus events
- Provide ways of looking at projections of the data

- Can be used to find partial orders

Example: words in documents

- Represent collections of documents as term vectors
- Which words occur (1) in the document or not (0)
- Very large dimensionality, lots of observations

Example from Citeseer (in 2005)

"database system"	"query"	"selectivity estimation"	Hits
1	1	1	49
1	1	0	1930
0	1	1	221
1	0	1	4

What does this tell us about these terms?
Databases and *selectivity estimation* together
do not occur without *queries*

Databases < queries < selectivity estimation

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Old (2005) example from Google Scholar

- prior   distribution   – MCMC
    151,000 documents

- prior   distribution   MCMC
    2950 documents

- – prior   distribution   MCMC
    1050 documents

- prior   – distribution   MCMC
    165 documents

prior < distribution < MCMC

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Example from Google Scholar, Nov. 24, 2007

- prior   distribution – MCMC
    2,220,000 documents

- prior   distribution   MCMC
    16,300 documents

- – prior   distribution   MCMC
    6,030 documents

- prior   – distribution   MCMC
    1,230 documents

> prior < distribution < MCMC

An aside: have the ratios of the frequencies changed?

Query	2005	2007	Ratio
p d m	2950	16300	5.5
p d –m	151000	2220000	14.7
–p d m	1050	6030	5.7
p –d m	165	1230	7.5

Next theme

- Find small total orders from 0-1 data

- Finding partial orders from 0-1 data

- Find total orders for 0-1 data

Finding partial orders from 0-1 data

- Model: a partial order over all observations

- Loglikelihood: proportional to the number of cases the observed occurrence patterns violate the continuity of species

- Prior: prefer partial orders that are as specific as possible

- Task: find a model with high likelihood * prior

- Algorithm: Find fragments and use heuristic search to build a good partial order

Why partial orders?

- Determining the ages of sites is difficult
- Radioisotope methods apply only to few sites
- In paleontology the so-called MN system: 18 classes for the last 25 Ma
- Classes are assigned by ad hoc methods

- Searching for a total order might not be a good idea
- The MN system is a partial order

Finding partial orders from data

- How to find a partial order that fits well with the data?
- What does this mean?

What is a good partial order?

- The Lazarus count of a species with respect to a partial order P:
  - For how many sites the species was extinct at the site, but extant before and after it (as determined by P)
  - The same definition as for total orders
- A good partial order has small Lazarus count

- Can be formulated as a likelihood (a Lazarus event is a false positive)

1	1	0	0
2	1	1	0
3	0	0	1
4	1	1	1
5	1	1	1

Laz	No Laz	No Laz

What is a good partial order?

- Find a partial order that has a low Lazarus count
- The trivial partial order has Lazarus count 0
- Want to find a partial order that is specific (close to a total order) and agrees with the data
- Measures of specificity:
  - the number of linear extensions of P (hard to compute)
  - number of edges in P
- Find a partial order that has high
    specificity * likelihood

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Algorithm for finding partial orders

- Compute fragments from the unordered data

- E.g., a < d < b < e < f and b < e < c and b < a < c < f and …

- Form a precedence matrix: in what fraction of the fragments does a precede b

- Form a partial order that approximates the precedence matrix (heuristic search)

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Fragments and reverse fragments

- The fragment generation will produce for each fragment f also its reverse f^R

- The pairwise precedence matrix would be useless

- Divide the fragments into two classes (graph cutting)
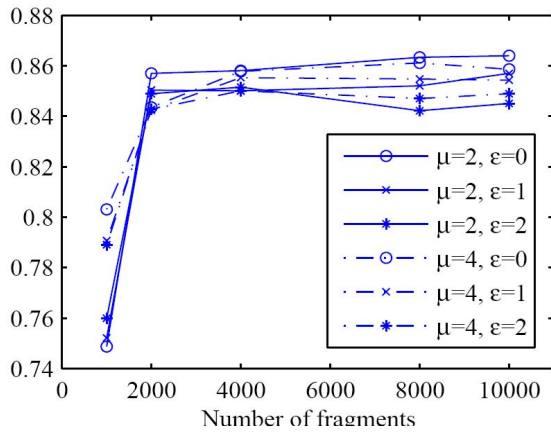- Discard one class
- Build the precedence matrix

From precedence matrix to partial order

- Heuristic search
- Add edges to the partial order so that the match with the precedence matrix improves
- Keep track of transitivity

- Difficult (and interesting) algorithmic problem
- Empirical results look good
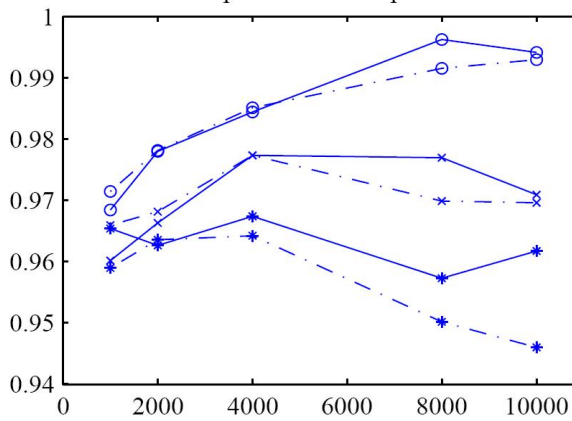
- Very recent theoretical results

The fraction of pairs ordered in the same way by P and P_{MN}

Legend:
- $\mu=2, \varepsilon=0$
- $\mu=2, \varepsilon=1$
- $\mu=2, \varepsilon=2$
- $\mu=4, \varepsilon=0$
- $\mu=4, \varepsilon=1$
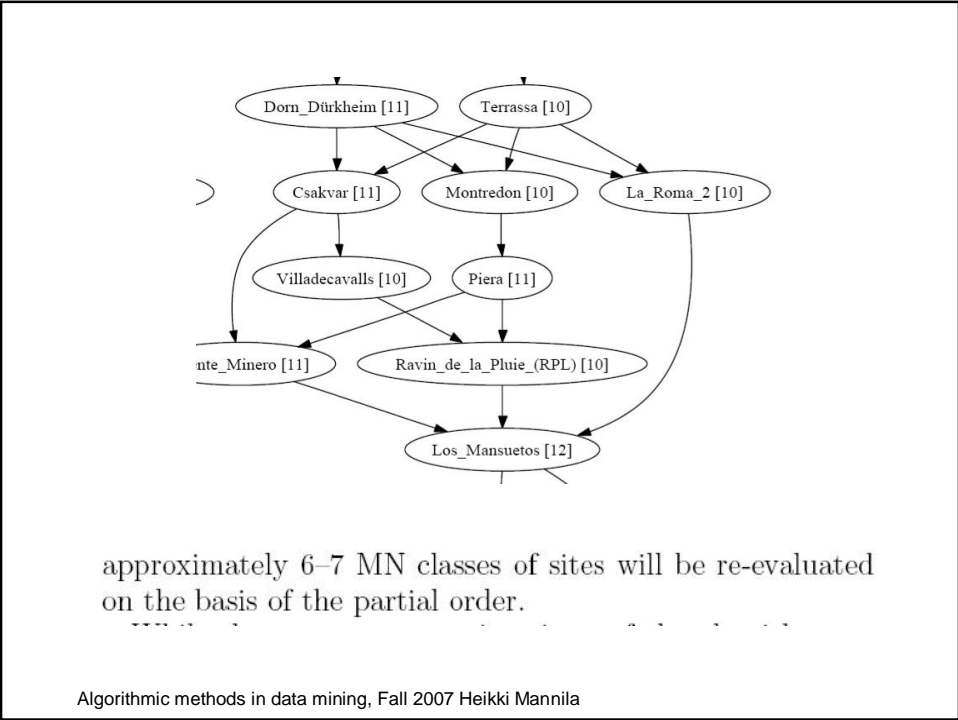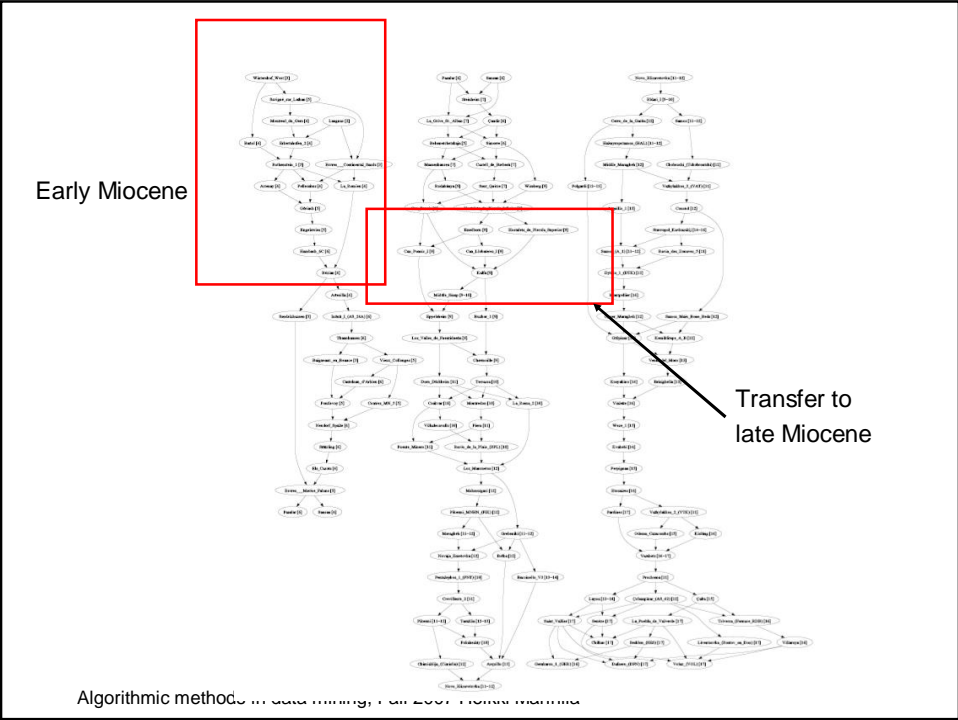- $\mu=4, \varepsilon=2$

Number of fragments

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

The completeness of the partial order

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Early Miocene

Transfer to
late Miocene

approximately 6–7 MN classes of sites will be re-evaluated
on the basis of the partial order.

Themes of the talk

- Find small total orders from 0-1 data

- Finding partial orders from 0-1 data

- Find total orders for 0-1 data

Finding good total orders for a matrix

- Given a site-genus matrix
- What is a good total ordering for the rows?
- One in which there are as few Lazarus events as possible
- Model class: total orders
- Loglikelihood proportional to the number of Lazarus events

How to find such an ordering of the rows?

- If there is an ordering that has no Lazarus events, it can be found in linear time (Booth & Lueker)
  - consecutive ones property

- But normally there are (lots of) Lazarus events

Finding good total orders for a matrix

- The problem of finding the best ordering of the matrix is NP-hard

- Finding whether there is a submatrix of size k that has no Lazarus events is NP-hard
- The fragment method finds such submatrices

- Local search, traveling salesperson approaches

- Spectral methods

Spectral ordering for finding good total orders for a matrix

- Spectral ordering

- Compute a similarity measure *s(i,j)* between sites (e.g., dot product)

- Laplacian L(i,j)

$$L(i,j) = \begin{cases} -s(i,j), & i \neq j \\ \sum_k s(i,k), & i = j \end{cases}$$

- The eigenvector *v* corresponding to the second smallest eigenvalue of L satisfies

$$\sum_i v_i = 0, \quad \sum_i v_i^2 = 1, \text{ and } \sum_i s(i,j)(v_i - v_j)^2 = 1 \text{ is minimized.}$$

- Maps the points to 1-d, keeping similar points close to each other
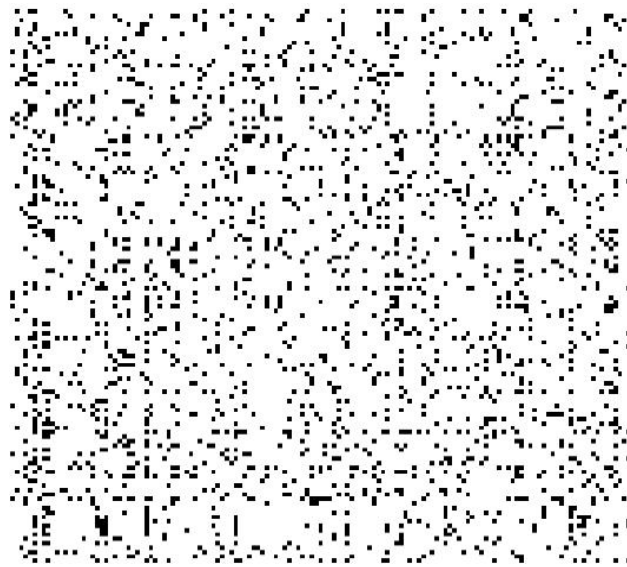- The values v_i can be used to order the points

Empirical observation

- The eigenvector seems to minimize also Lazarus events

- Even better than some combinatorial algorithms

- Why?

- No really good intuitive theoretical understanding
  - Related to mixing time of Markov chains etc.

Site-genus -matrix

After spectral ordering

Fortelius, Jernvall, Gionis, Mannila, Paleobiology 32 (2006)

gl	sl	gn	sn	c	Nh	ch	NMN	cMN
10	10	139	124	0.97	21	0.98	119	0.96
10	5	139	259	0.96	35	0.97	230	0.95
5	10	198	136	0.97	22	0.99	125	0.97
5	5	201	273	0.96	35	0.98	240	0.96
2	10	281	147	0.97	22	0.99	132	0.97
2	2	285	512	0.94	46	0.97	444	0.94

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

gl	sl	Ls	LMN	Lage	Lazs	LazMN	Lazage
10	10	-4881	-5153	-4998	3792	4174	3974
10	5	-9038	-9573	-9416	9728	10906	10563
5	10	-6008	-6455	-6275	5220	5901	5622
5	5	-10723	-11340	-11132	13003	14638	14147
2	10	-6904	-7429	-7234	6398	7314	6969
2	2	-16660	-17610	-17323	30568	34886	33621

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Questions

- Computational
  - Why does it work so well?
  - How well does it actually work (what is the smallest number of Lazarus events for this data?)
  - How to interpret the coefficients?

- Paleontological
  - Fully based on the occurrence matrix (excellent and bad)
  - Site-species data is only one type of data; how to use other types of data for the ordering?
  - …

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Rough estimates of the sizes of the model classes

- N observations
- Fragments of size at most k

  - N^k individual fragments

  - 2^{N^k} sets of fragments

- Partial orders $\quad 2^{O(N^2)}$

- Total orders $\quad N!$

Algorithmic methods in data mining, Fall 2007 Heikki Mannila

Concluding remarks

- General task: finding order from unordered data
- Here using species continuity as the additional information
- Other applications are possible

- Model classes
  - Fragments
  - Partial orders
  - Total orders

Lots of open questions

- The unreasonable effectiveness of spectral methods on discrete optimization task

- Approximation guarantees

- Fragments from other applications

- MDL description of sequences via partial orders

- Etc.

References

- A. Gionis, T. Kujala and H. Mannila: Fragments of order. *ACM SIGKDD 2003*, p. 129-136.
- A. Ukkonen, M. Fortelius, H. Mannila: Finding partial orders from unordered 0-1 data. *ACM SIGKDD 2005*, p. 285-293.
- M. Fortelius, A. Gionis, J. Jernvall, H. Mannila, Spectral Ordering and Biochronology of European Fossil Mammals. *Paleobiology* 32, 2, 206-214 (2006).
- K. Puolamäki, M. Fortelius, H. Mannila: Seriation in Paleontological Data Using Markov Chain Monte Carlo Methods. *PLoS Comput Biol* 2(2): e6
- A. Gionis, H. Mannila, K. Puolamaki, and A. Ukkonen, Algorithms for Discovering Bucket Orders from Data, 12th International Conference on Knowledge Discovery and Data Mining (KDD) 2006, p. 561-566.

Algorithmic methods in data mining, Fall 2007 Heikki Mannila