From-Below Approximations in Boolean Matrix Factorization: Geometry and New Algorithm II

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List of Algorithms for Boolean Matrix Factorization (BMF)

- Algorithm 1
- GreConD
- ASSO
- Tiling (LTM algorithm)
- PaNDa
- Hyper (Hyper+)

ASSO Algorithm in Short

- Author: Pauli Miettinen from Max-Planck-Institut für Informatik, originally from Finland.
- First introduced in: The Discrete Basis Problem (2006), MSC thesis as Association algorithm.
- Probably currently the most discussed BMF algorithm in the data mining literature.

ASSO Algorithm Pseudocode

Input: A matrix $\mathcal{C} \in \{0,1\}^{n \times m}$ for data, a positive integer k, a threshold value $\tau \in [0,1]$, and real-valued weights w^+ and w^-.

for $i = 1, \ldots, m$ **do**

  `Construct matrix` $\mathcal{A}$ `row by row`

  $a_i \leftarrow (1(c(i \Rightarrow j, \mathcal{C}) \geq \tau))_{j=1}^{m}$

end

$\mathcal{B}$ `and` $\mathcal{S}$ `are empty matrices`

$\mathcal{B} \leftarrow []$, $\mathcal{S} \leftarrow []$

`Select the` k `basis vectors from` $\mathcal{A}$

for $l = 1, \ldots, k$ **do**

  $(a_i, s) \leftarrow \max_{a_i, s \in \{0,1\}^{n \times 1}} \mathit{cover}(\begin{bmatrix} \mathcal{B} \\ a_i \end{bmatrix}, [\mathcal{S}\ s], \mathcal{C}, w^+, w^-)$

  $\mathcal{B} \leftarrow \begin{bmatrix} \mathcal{B} \\ a_i \end{bmatrix}$, $\mathcal{S} \leftarrow [\mathcal{S}\ s]$

end

return $\mathcal{B}$ a $\mathcal{S}$

ASSO Continuation

- $cover(\mathcal{B}, \mathcal{S}, \mathcal{C}, w^+, w^-)$ is equal to:

$$w^+ \left|\{(i,j) : c_{ij} = 1, (\mathcal{S} \circ \mathcal{B})_{ij} = 1\}\right| - w^- \left|\{(i,j) : c_{ij} = 0, (\mathcal{S} \circ \mathcal{B})_{ij} = 1\}\right|.$$

- Unfortunately it is more complicated.
- Vector s is compute from a_i in greedy manner: $cover$ function is compute separately for each row of input matrix C, $s_j = 1$ if value of $cover > 0$ for row C_j.
- Take to account covered part (not mentioned in pseudocode).
- $cover$ function does not count covered part.

Example (ASSO Algorithm, Miettinen's implementation - First Factor)

$k = 3, \tau = 0.9, w^+ = 1, w^- = 1$

$$C = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \end{pmatrix}, covered = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$cover$ for the first row: -2 + 4 + 2 + 0 = 6
$cover$ for the second row: 0 + 2 + 2 + 2 = 6
$cover$ for the third row: 1 + 1 + 1 + 1 = 4
$cover$ for the fourth row: -1 + 3 + 3 + 1 = **7**

$$\begin{pmatrix} 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} \circ \begin{pmatrix} 0 & 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix}$$

Example (ASSO Algorithm, Miettinen's implementation - Second Factor)

$k = 3, \tau = 0.9, w^+ = 1, w^- = 1$

$$C = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \end{pmatrix}, covered = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix}$$

$cover$ for the first row: -2 + 1 - 1 - 1 = 1
$cover$ for the second row: 0 + 0 + 0 + 0 = 0
$cover$ for the third row: 1 + 0 + 0 + 0 = **1**
$cover$ for the fourth row: -1 + 0 + 0 + 0 = 0

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{pmatrix} \circ \begin{pmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix}$$

Example (ASSO Algorithm, Miettinen's implementation - Third Factor)

$k = 3, \tau = 0.9, w^{+} = 1, w^{-} = 1$

$$C = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \end{pmatrix}, covered = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix}$$

$cover$ for the first row: -3 + 1 + 0 - 1 = **1**
$cover$ for the second row: -1 + 0 + 0 + 0 = 0
$cover$ for the third row: 0 + 0 + 0 + 0 = 0
$cover$ for the fourth row: -2 + 0 + 0 + 0 = 0

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \circ \begin{pmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix}$$

ASSO Algorithm Remark

There exist several variants of ASSO:

- ASSO + transpose
- ASSO + clustering
- ASSO + exhaustive search
- ASSO + iterative search

- One specific feature: **There is no way how to remove E_o!**
- Empirical time complexity: 4-5x slower than GreConD.

Tiling Algorithm in Short

- First introduced in: Tiling Databases (2004).
- Originally called LTM algorithm.
- Base on idea from CHARM, LPMiner and BAMBOO algorithm.
- Introduced notion of tile $\tau(I,D) = \{(tid,i) \in cover(I,D), i \in I\}$.
- Tiles can be seen as rectangles in binary data.

Tiling Algorithm Pseudocode

Input: Binary database D, minimal size of tile δ, itemset I initially called with $I = \emptyset$.

$T \leftarrow \emptyset$
$D \leftarrow \text{PRUNE}(D, \delta, I)$
forall the i *occurring in* D **do**
  if $|cover(\{i\})| \cdot (|I| + 1) \geq \delta$ **then**
    $T \leftarrow T \cup \tau(I \cup \{i\})$
  end
  $D^i \leftarrow \emptyset$
  forall the j *occurring in* D *such that* $j > i$ **do**
    $C \leftarrow cover(\{i\}) \cap cover(\{j\})$
    Add (j, C) to D^i
    Recursively compute for $I \cup \{i\}$
  end
end

PRUNE Procedure Pseudocode

Input: D, δ, I.

repeat
  forall the i *occurring in* D **do**
    if $UB_{I \cup \{i\}} < \delta$ **then**
      Remove i from D
    end
    forall the $tid \in cover(\{i\})$ **do**
      if $size(tid) < ML_{I \cup \{i\}}$ **then**
        Remove tid from $cover(\{i\})$
      end
    end
  end
until *nothing change*

Explain Prune Procedure

$UB_{I\cup\{i\}} = max\{(|I| + l) \cdot supp_{\geq l}(i, D^I) \mid l \in \{1, 2, \dots\}\}$

- If $UB_{I\cup\{i\}} < \delta$ then remove item (column) i from D.
- Upper bound of the largest possible tile containing $I \cup \{i\}$.

$ML_{I\cup\{i\}} = min\{l \mid l \cdot supp_{\geq l}(i, D^I) \geq \delta\}$

- If $size(tid) < ML_{I\cup\{i\}}$ then remove transaction (row) tid from D.
- Minimal size of transaction containing i, that can still generate a tile with area at least δ.

Tiling Algorithm

- Produces all tiles with support $> \delta$.
- Easily can be change to find top-k largest tiles.
- Can be modified to solve (approximately) Minimum tiling problem (completely cover input database with the smallest number of tiles).
- We must modify algorithm cost function - it must take into account already covered area.
- In each step is extracted tile with the highest still uncovered part.
- Step $=$ run whole Tiling algorithm!

Tiling Algorithm Remarks

- Modification of Tiling algorithm for BMF, is very slow!
- Produce the same results as Algorithm 1 (in special settings, fix order of tiles).
- In normal case there is more tiles with the same uncovered part - leads to the clash of decision function for selecting tiles.

PaNDa Algorithm in Short

- First introduced in: Mining Top-K Patterns from Binary Datasets in Presence of Noise.
- Basic idea: Select noise-free pattern and extend this pattern with some noise.
- Notion of pattern $P = \langle P_T, P_I \rangle$ in binary database, where $P_T \in \{0,1\}^n, P_I \in \{0,1\}^m$.
- Pattern can be seen as rectangle in binary database.
- Compute the set of patterns Π with the smallest cost.
- Cost function of PaNDa algorithm for set of patterns Π and database $\mathcal{D}$:

$$\gamma(\Pi, \mathcal{D}) = \sum_{P \in \Pi} \gamma_P(P_T, P_I) + \gamma_N(N)$$

where $\gamma_P(P_T, P_I) = |P_T| + |P_I|$ and $\gamma_N(N) = |N|$.

PaNDa Algorithm Pseudocode

Input: $\mathcal{D}$ binary database, k number of extracted patterns

$\Pi \leftarrow \emptyset$
$\mathcal{D}_{\mathcal{R}} \leftarrow \mathcal{D}$
for $i = 1 \ldots k$ **do**
  $C, E \leftarrow$ FIND-CORE($\mathcal{D}_{\mathcal{R}}, \Pi, \mathcal{D}$)
  $C^+ \leftarrow$ EXTEND-CORE($C, E, \Pi, \mathcal{D}$)
  if $\gamma(\Pi, \mathcal{D}) \leq \gamma(\Pi \cup C^+, \mathcal{D})$ **then**
    break
  end
  $\Pi \leftarrow \Pi \cup C^+$
  $\mathcal{D}_{\mathcal{R}}(i, j) \leftarrow 0 \; \forall i, j$ s.t. $C^+_T(i) = 1 \wedge C^+_I(i) = 1$
end
return Π

Core Pattern Discovery, FIND-CORE Procedure

Input: $\mathcal{D}_{\mathcal{R}}, \Pi, \mathcal{D}$

$E \leftarrow \emptyset$
$S = \{s_1, \ldots, s_m\} \leftarrow$ SORT-ITEMS-IN-DB($\mathcal{D}_{\mathcal{R}}$)
$C \leftarrow \langle C_T = 0^n, C_I = 0^m \rangle$
$C_I(s_1) \leftarrow 1$
$C_T(i) \leftarrow 1 \ \forall i$ s.t. $\mathcal{D}_{\mathcal{R}}(i, s_1) = 1$
for $h = 2, \ldots, m$ **do**
    $C^* \leftarrow C$
    $C^*_I(s_h) \leftarrow 1$
    $C^*_T(i) \leftarrow 0 \ \forall i$ s.t. $\mathcal{D}_{\mathcal{R}}(i, s_h) = 0$
    if $\gamma(\Pi \cup C^*, \mathcal{D}) \leq \gamma(\Pi \cup C, \mathcal{D})$ **then**
        $C \leftarrow C^*$
    else
        E.append(s_h)
    end
end
return C, E

Extension of Core Pattern, EXTEND-CORE Procedure

Input: $C, E, \Pi, \mathcal{D}$

```
while E ≠ ∅ do
    e ← E.pop()
    C* ← C
    C*_I(e) ← 1
    if γ(Π ∪ C*, D) ≤ γ(Π ∪ C, D) then
        C ← C*
    end
    for i = 1, ..., n s.t. C*_T(i) = 0 do
        C* ← C
        C*_T(i) ← 1
        if γ(Π ∪ C*, D) ≤ γ(Π ∪ C, D) then
            C ← C*
        end
    end
end
return C
```

PaNDa Remarks

- Sorting items in database:
  - Frequency (best results)
  - Correlation
  - Prefix-tree
  - Couples frequency
- Empirical time complexity: 5x slower than GreConD.

Hyper Algorithm

- First introduced in: Summarizing Transactional Databases with Overlapped Hyperrectangles (2011).
- Notion of hyperrectangle $H = T \times I = \{(i,j) : i \in T, j \in I\}$.
- T is subset of all transactions and I is subset of all items.
- Hyperrectangle can be seen as rectangle in binary database.
- Price of hyperrectangle H_i:

$$\gamma(H_i) = \frac{|T_i| + |I_i|}{|T_i \times I_i \setminus R|}$$

where R is already covered part of input database.

HYPER Algorithm Pseudocode

Input: DB binary database, C_α set of frequent itemsets with minimal support α union with singleton sets of itemsets (sets with only one item)

```
R ← ∅
CBD ← ∅
while R ≠ DB do
    forall the H_i ∈ C_α do
        X_i ← FIND-HYPER(H_i, R)
    end
    H' ← min_{X_i} γ(X_i)
    R ← R ∪ H'
end
return CDB
```

Procedure for Finding Sub-hyperrectangle with Cheapest Price

Input: Hyperrectangle H, already covered part of input database R

forall the $S = \{t_j\} \times I_i \subseteq H$ **do**
    calculate the number of uncovered DB elements in S, $|S \setminus R|$
end
sort S according to $|S \setminus R|$ and put in U
$H' \leftarrow$ first hyperrectangle S popped from U
while $U \neq \emptyset$ **do**
    pop single transaction hyperrectangle S prom U
    if $\gamma(H' \cup S) > \gamma(H')$ **then**
        break
    else
        $H' \leftarrow H' \cup S$
    end
end
return H'

Example (HYPER Finding Sub-hyperrectangle with Cheapest Price)

$$H = \begin{array}{c|cccc} & i_2 & i_4 & i_5 & i_7 \\ t_1 & 1 & 1 & 1 & 1 \\ t_3 & 1 & 1 & 1 & 1 \\ t_4 & 1 & 1 & 1 & 1 \\ t_6 & 1 & 1 & 1 & 1 \\ t_8 & 1 & 1 & 1 & 1 \\ t_9 & 1 & 1 & 1 & 1 \end{array}, \quad R = \begin{array}{c|cccc} & i_2 & i_4 & i_5 & i_7 \\ t_1 & 0 & 1 & 0 & 1 \\ t_3 & 1 & 0 & 1 & 1 \\ t_4 & 0 & 0 & 0 & 0 \\ t_6 & 0 & 1 & 0 & 1 \\ t_8 & 0 & 0 & 0 & 0 \\ t_9 & 1 & 0 & 1 & 1 \end{array}$$

Sort transaction according to size of their uncovered part: $t_4, t_8, t_1, t_6, t_3, t_9$.

$H' = t_4 \times I, \gamma(H') = \frac{4+1}{4} = 1.25$
add $t_8 \times I$ to $H', \gamma(H') = \frac{4+2}{4+4} = 0.75$ decrease
add $t_1 \times I$ to $H', \gamma(H') = \frac{4+3}{4+4+4-2} = 0.70$ decrease
add $t_6 \times I$ to $H', \gamma(H') = \frac{4+4}{4+4+4+4-2-2} = 0.67$ decrease
add $t_3 \times I$ to $H', \gamma(H') = \frac{4+5}{4+4+4+4+4-2-2-3} = 0.69$ increase - stop

Final hyperrectangle $H' = t_4, t_8, t_1, t_6 \times I$.

Hyper Algorithm Remark

- In basic setting C_α is from Apriori algorithm.
- Variants of Hyper algorithm:
  - Maximal frequent itemset.
  - Frequent closed itemset (best results).
- Prune technique can accelerate HYPER algorithm.
- Empirical time complexity: it depends on size C_α for “reasonable” size is 4-5x slower than GreConD.
- Exact factorization (there is no E_o error BMF).
- Hyper+ approximate factorization (merges hyperrectangles, the merged ones contain 0s).
- Hyper+ is post-processing algorithm.

HYPER+ Algorithm Pseudocode

Input: Binary database DB, set of hyperrectangles CBD, final number of hyperrectangles β

$SCDB \leftarrow CBD$

while $\frac{|SCDB^C| \setminus |DB|}{|DB|} \leq \beta$ **do**

find $H_i, H_j \in SCDB$ whose merge is within the false positive budget

$$\frac{|(SCDB \setminus \{H_i, H_j\} \cup \{H_i \oplus H_j\})^C \setminus DB|}{|DB|} \leq \beta$$

and produce the maximum saving-false positive ratio

$$\frac{|T_i| + |T_j| + |I_i| + |I_j| - |T_i \cup T_j| - |I_i \cup I_j|}{|(H_i \oplus H_j) \setminus SCDB^C|}$$

$SCBD \leftarrow SCBD \setminus \{H_i, H_j\}$

$SCBD \leftarrow SCBD \cup \{H_i \oplus H_j\}$

end

return $SCDB$

Noise in Binary Data

- Big topic in Data Minig in general.
- Current consideration regarding noise in binary data seem not mature (ad hoc).
- For example: in work about ASSO algorithm - 40% of noise (means practically new data).
- It is reasonable to take it as some kind of error.

Experiments Scenario

- We use various random and real datasets.
- We compare GreEss (pessimistic estimate), GreConD, ASSO (basic), Tiling, PaNDa, and Hyper (frequent closed itemsets) algorithm.
- Error:

$$
\begin{aligned}
E(I, A \circ B) &= E_u(I, A \circ B) + E_o(I, A \circ B), \text{where} \\
E_u(I, A \circ B) &= |\{\langle i, j \rangle \,;\, I_{ij} = 1, (A \circ B)_{ij} = 0\}|, \\
E_o(I, A \circ B) &= |\{\langle i, j \rangle \,;\, I_{ij} = 0, (A \circ B)_{ij} = 1\}|.
\end{aligned}
$$

- We are interested in from-below approximation of binary data.
- For each algorithm we compute coverage quality for each obtained factor.
- Coverage quality:

$$c = 1 - \frac{E_u(I, A \circ B)}{||I||}$$

Synthetic Data - Randomly Generated Matrices

- It is senseless compute Boolean matrix factorization on fully random data (there are no rational factors).
- We compute random binary matrices $n \times k$ and $k \times m$.
- Boolean product of these matrices represent our synthetic data with size $n \times m$.
- Such matrix is decomposable with (at most) k factors.

Synthetic Data

dataset	size	basis	dens A	dens B
Set 1	300×100	20	0.10	0.10
Set 2	500×250	20	0.05	0.05
Set 3	500×250	20	0.10	0.05
Set 4	500×250	30	0.12	0.12
Set 5	1000×500	50	0.10	0.10
Set 6	10000×1000	50	0.10	0.10

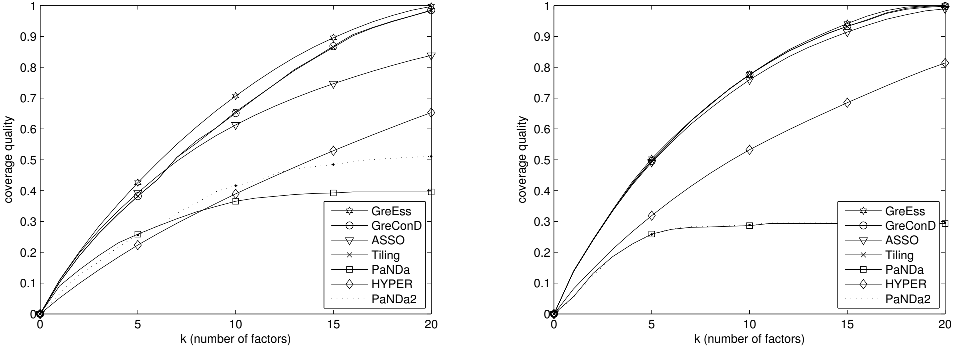
Table: Synthetic datasets $I = A \circ B$

Statistics on Synthetic Data

dataset	avg $\|\|I\|\|$	avg $\|\|\mathcal{E}(I)\|\|$	avg $\|\|\mathcal{E}(I)\|\|/\|\|I\|\|$
Set 1	5039	2764	0.549
Set 2	11966	6412	0.536
Set 3	22841	5207	0.228
Set 4	44027	8894	0.202
Set 5	195990	34005	0.174
Set 6	3907433	47359	0.012

Table: Essential part of I (synthetic data)

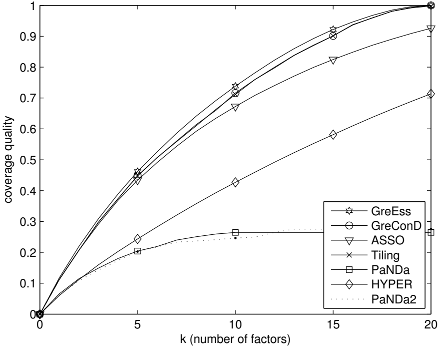
Results for Synthetic Data I.



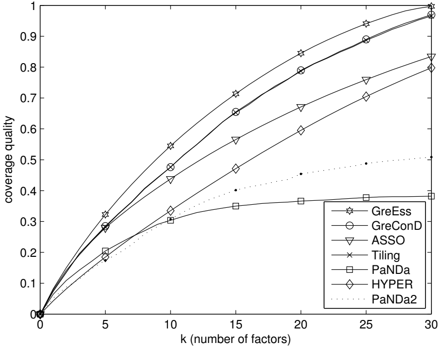
(a) Set 1 (b) Set 2

Figure: Coverage by the first k factors (synthetic data)

Results for Synthetic Data II.



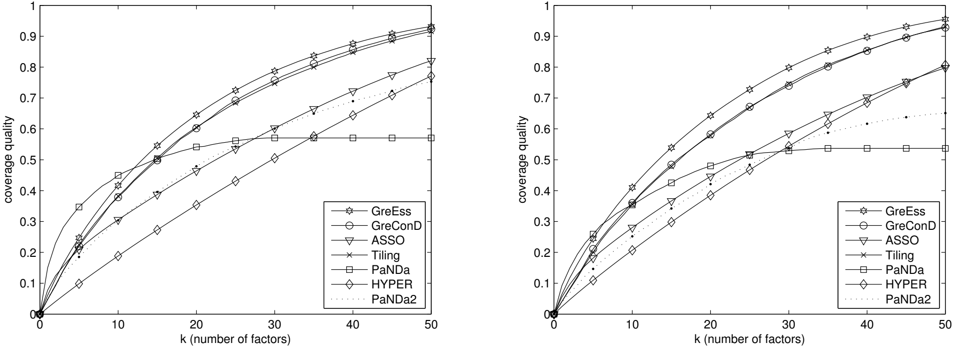
(a) Set 3



(b) Set 4

Figure: Coverage by the first k factors (synthetic data)

Results for Synthetic Data III.



(a) Set 5 (b) Set 6

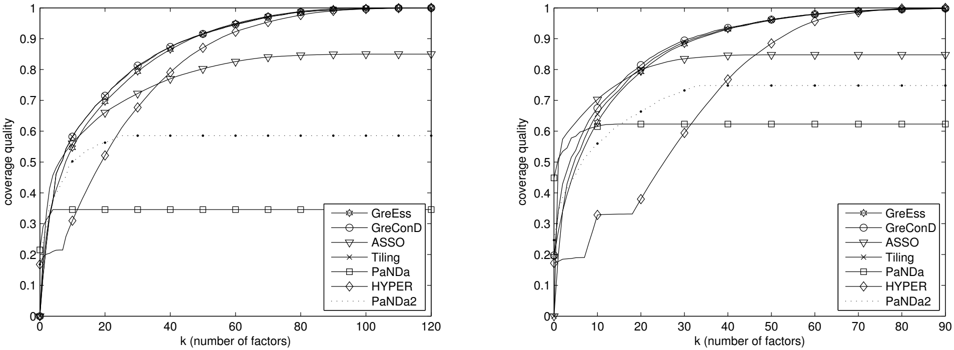
Figure: Coverage by the first k factors (synthetic data)

Real Datasets

dataset	size	$\|\|I\|\|$	$\|\|\mathcal{E}(I)\|\|$	$\|\|\mathcal{E}(I)\|\|/\|\|I\|\|$
Mushroom	8124×119	186852	82965	0.444
DBLP	19×6980	40637	1601	0.039
Paleo	501×139	3537	1906	0.539
Chess	3196×76	118252	71296	0.603
DNA	4590×392	26527	1685	0.064

Table: Essential part of I (real data)

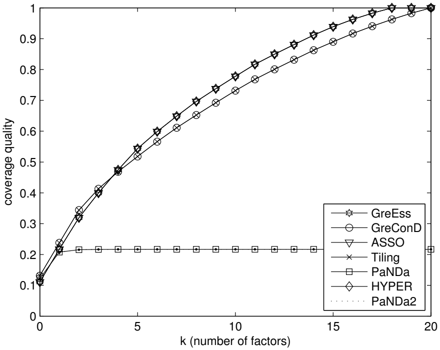
Results for Real Datasets I.



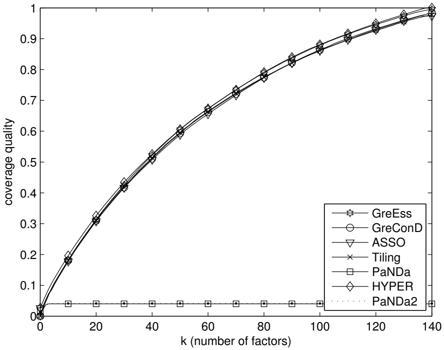
(a) Mushroom (b) Chess

Figure: Coverage by the first k factors (real data)

Results for Real Datasets II.



(a) DBLP



(b) Paleo

Figure: Coverage by the first k factors (real data)

Results for Real Datasets III.

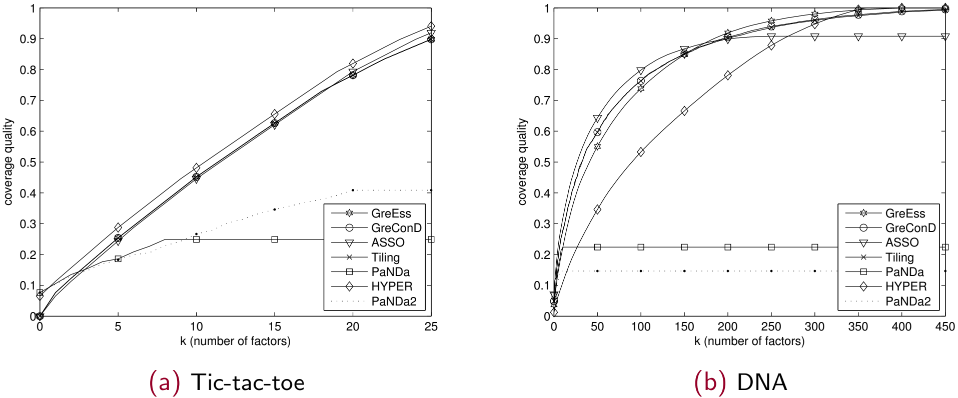


Figure: Coverage by the first k factors (real data)

dataset	coverage ($100c\%$)	Tiling	number of factors required for the prescribed coverage ASSO	GreConD	PaNDa	PaNDa2	Hyper	GreEss
Mushroom	25%	3	2	3	1	2	8	2
	50%	7	6	7	NA	10	19	8
	75%	24	36	24	NA	NA	37	26
	100%	119	NA	120	NA	NA	122	105
DBLP	25%	2	2	2	NA	NA	2	2
	50%	5	5	5	NA	NA	5	5
	75%	10	10	11	NA	NA	10	10
	100%	21	19	20	NA	NA	19	19
Paleo	25%	16	16	16	NA	NA	14	15
	50%	39	40	39	NA	NA	38	38
	75%	75	76	76	NA	NA	73	73
	100%	151	NA	152	NA	NA	139	145
Chess	25%	2	1	1	1	1	9	1
	50%	5	2	4	NA	7	26	6
	75%	16	15	15	NA	NA	39	17
	100%	124	NA	124	NA	NA	90	113
DNA	25%	8	6	8	NA	NA	24	13
	50%	32	27	33	NA	NA	67	41
	75%	94	80	96	NA	NA	155	105
	100%	489	NA	496	NA	NA	392	408
Tic-tac-toe	25%	5	6	5	NA	10	5	5
	50%	12	12	12	NA	NA	11	12
	75%	19	19	19	NA	NA	18	19
	100%	31	29	32	NA	NA	29	32

Conclusion

- GreEss algorithm outperform existing algorithms in both number of factors and coverage quality.
- Empirical time complexity: GreEss is 2x slower than GreConD algorithm.
- Extracted factors seem to be more reasonable than factors from different algorithms (more detailed study is needed for support this claim).