#### Data Mining and Matrices 08 – Boolean Matrix Factorization

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# Outline



#### 2 What is BMF

- 3 BMF vs. other three-letter abbreviations
- 4 Binary matrices, tiles, graphs, and sets
- 5 Computational Complexity
- 6 Algorithms
- 7 Wrap-Up

#### An example

- Let us consider a data set of people and their traits
  - People: Alice, Bob, and Charles
  - Traits: Long-haired, well-known, and male



## An example



- We can write this data as a binary matrix
- The data obviously has two groups of people and two groups of traits
  - and
    and
    and



- are long-haired and well-known
- and 🔣 are well-known males
- Can we find these groups automatically (using matrix factorization)?

## SVD?

• Could we find the groups using SVD?



#### • SVD cannot find the groups.

## SVD?

• Could we find the groups using SVD?



#### • SVD cannot find the groups.

# SDD?

• The groups are essentially "bumps", so perhaps SDD?



#### • SDD cannot find the groups, either

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#### NMF?

• The data is non-negative, so what about NMF?



• Already closer, but is the middle element in the group or out of the group?

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# Clustering?

 So NMF's problem was that the results were not precise yes/no. Clustering can do that...





The data Cluster assignment matrix

• Precise, yes, but arbitrarily assigns 3 and "well-known" to one of the groups



## Boolean matrix factorization

• What we want looks like this:



- The problem: the sum of these two components is not the data
  - ► The center element will have value 2
- Solution: don't care about multiplicity, but let 1 + 1 = 1

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# Boolean matrix product

#### Boolean matrix product

The **Boolean product** of binary matrices  $\mathbf{A} \in \{0, 1\}^{m \times k}$  and  $\mathbf{B} \in \{0, 1\}^{k \times n}$ , denoted  $\mathbf{A} \boxtimes \mathbf{B}$ , is such that

$$(\mathsf{A} oxtimes \mathsf{B})_{ij} = igvee_{\ell=1}^k \mathsf{A}_{i\ell} \mathsf{B}_{\ell j} \; .$$

- The matrix product over the Boolean semi-ring  $(\{0,1\},\wedge,\vee)$ 
  - Equivalently, normal matrix product with addition defined as 1 + 1 = 1
  - Binary matrices equipped with such algebra are called Boolean matrices
- The Boolean product is only defined for binary matrices
- $\mathbf{A} \boxtimes \mathbf{B}$  is binary for all  $\mathbf{A}$  and  $\mathbf{B}$

# Definition of the BMF

#### Boolean Matrix Factorization (BMF)

The (exact) Boolean matrix factorization of a binary matrix  $\mathbf{A} \in \{0,1\}^{m \times n}$  expresses it as a Boolean product of two factor matrices,  $\mathbf{B} \in \{0,1\}^{m \times k}$  and  $\mathbf{C} \in \{0,1\}^{k \times n}$ . That is  $\mathbf{A} = \mathbf{B} \boxtimes \mathbf{C}$ .

- Typically (in data mining), k is given, and we try to find **B** and **C** to get as close to **A** as possible
- Normally the optimization function is the squared Frobenius norm of the residual,  $\|\mathbf{A} (\mathbf{B} \boxtimes \mathbf{C})\|_F^2$ 
  - Equivalently,  $|\mathbf{A} \oplus (\mathbf{B} \boxtimes \mathbf{C})|$  where
    - \* |A| is the sum of values of A (number of 1s for binary matrices)
    - $\star$   $\oplus$  is the element-wise exclusive-or (1+1=0)
  - ► The alternative definition is more "combinatorial" in flavour

## The Boolean rank

- The Boolean rank of a binary matrix  $\mathbf{A} \in \{0,1\}^{m \times n}$ , rank<sub>B</sub>( $\mathbf{A}$ ) is the smallest integer k such that there exists  $\mathbf{B} \in \{0,1\}^{m \times k}$  and  $\mathbf{C} \in \{0,1\}^{k \times n}$  for which  $\mathbf{A} = \mathbf{B} \boxtimes \mathbf{C}$ 
  - Equivalently, the smallest k such that **A** is the element-wise or of k rank-1 binary matrices
- Exactly like normal or nonnegative rank, but over Boolean algebra
- Recall that for the non-negative rank  $\mathsf{rank}_+(\mathsf{A}) \ge \mathsf{rank}(\mathsf{A})$  for all  $\mathsf{A}$
- For Boolean and non-negative ranks we have rank<sub>+</sub>(A) ≥ rank<sub>B</sub>(A) for all binary A
  - Essentially because both are anti-negative but BMF can have overlapping components without cost
- Between normal and Boolean rank things are less clear
  - There exists binary matrices for which rank( $\mathbf{A}$ )  $\approx \frac{1}{2}$  rank<sub>B</sub>( $\mathbf{A}$ )
  - There exists binary matrices for which rank<sub>B</sub>( $\mathbf{A}$ ) =  $O(\log(rank(\mathbf{A})))$
  - The logarithmic ratio is essentially the best possible
    - \* There are at most  $2^{\operatorname{rank}_B(\mathbf{A})}$  distinct rows/columns in  $\mathbf{A}$

### Another example

- $\bullet$  Consider the complement of the identity matrix  $\bar{\mathbf{I}}$ 
  - It has full normal rank, but what about the Boolean rank?



- The factorization is symmetric on diagonal so we draw two factors at a time
- The Boolean rank of the data is  $12 = 2 \log_2(64)$

## Another example

- $\bullet$  Consider the complement of the identity matrix  $\overline{\mathbf{I}}$ 
  - It has full normal rank, but what about the Boolean rank?







Boolean rank-12

- The factorization is symmetric on diagonal so we draw two factors at a time
- The Boolean rank of the data is  $12 = 2 \log_2(64)$
- Let's draw the components in reverse order to see the structure

## Another example

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# BMF vs. SVD

- Truncated SVD gives Frobenius-optimal rank-k approximations of the matrix
- But we've already seen that matrices can have smaller Boolean than real rank ⇒ BMF can give exact decompositions where SVD cannot
  - Contradiction?
- The answer lies in different algebras: SVD is optimal if you're using the normal algebra
  - ▶ BMF can utilize its different addition in some cases very effectively
- In practice, however, SVD usually gives the smallest reconstruction error
  - Even when it's not exactly correct, it's very close
- But reconstruction error isn't all that matters
  - BMF can be more interpretable and more sparse
  - BMF finds different structure than SVD

# BMF vs. SDD

- Rank-1 binary matrices are sort-of bumps
  - The SDD algorithm can be used to find them
  - But SDD doesn't know about the binary structure of the data
  - And overlapping bumps will cause problems to SDD
- The structure SDD finds is somewhat similar to what BMF finds (from binary matrices)
  - But again, overlapping bumps are handled differently



# BMF vs. NMF

- Both BMF and NMF work on anti-negative semi-rings
  - There is no inverse to addition
  - "Parts-of-whole"
- BMF and NMF can be very close to each other
  - Especially after NMF is rounded to binary factor matrices
- But NMF has to scale down overlapping components



# BMF vs. clustering

- BMF is a relaxed version of clustering in the hypercube  $\{0,1\}^n$ 
  - ► The left factor matrix **B** is sort-of cluster assignment matrix, but the "clusters" don't have to partition the rows
  - The right factor matrix **C** gives the centroids in  $\{0,1\}^n$
- If we restrict **B** to a cluster assignment matrix (each row has exactly one 1) we get a clustering problem
  - Computationally much easier than BMF
  - Simple local search works well
- But clustering also loses the power of overlapping components

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## Frequent itemset mining

- In **frequent itemset mining**, we are given a transaction-item data (who bought what) and we try to find items that are typically bought together
  - A frequent itemset is a set of items that appears in many-enough transactions
- The transaction data can be written as a binary matrix
  - Columns for items, rows for transactions
- Itemsets are subsets of columns
  - Itemset = binary *n*-dimensional vector **v** with **v**<sub>i</sub> = 1 if item *i* is in the set
- An itemset is frequent if sufficiently many rows have 1s on all columns corresponding to the itemset
  - ▶ Let  $\mathbf{u} \in \{0,1\}^m$  be such that  $\mathbf{u}_j = 1$  iff the itemset is present in transaction j
  - Then uv<sup>T</sup> is a binary rank-1 matrix corresponding to a monochromatic (all-1s) submatrix of the data

## Tiling databases

- When tiling databases we try to find tiles that cover (most) of the 1s of the data
  - A tile is a monochromatic submatrix of the data (rank-1 binary matrix)
  - A tiling is collection of these tiles such that all (most) 1s of the data belong to at least one of the tiles
- In minimum tiling, the goal is to find the least number of tiles such that all 1s in the data belong to at least one tile
- In maximum *k*-tiling the goal is to find *k* tiles such that as many 1s of the data as possible belong to at least one tile
- In terms of BMF:
  - Tiling with k tiles = rank-k BMF (Boolean sum of k tiles)
  - Tiling can never represent a 0 in the data as a 1
  - Minimum tiling = Boolean rank
  - Maximum k-tiling = best rank-k factorization that never covers a 0

Binary matrices and bipartite graphs



- There is a bijection between  $\{0,1\}^{m \times n}$  and (unweighted, undirected) bipartite graphs of m + n vertices
  - ► Every A ∈ {0,1}<sup>m×n</sup> is a bi-adjacency matrix of some bipartite graph G = (V ∪ U, E)
  - ▶ V has m vertices, U has n vertices and  $(v_i, u_j) \in E$  iff  $A_{ij} = 1$

# BMF and (quasi-)biclique covers



- A **biclique** is a complete bipartite graph
  - Each left-hand-side verted is connected to each right-hand-side vertex
- Each rank-1 binary matrix defines a biclique (subgraph)
  - ▶ If  $\mathbf{v} \in \{0, 1\}^m$  and  $\mathbf{u} \in \{0, 1\}^n$ , then  $\mathbf{v}\mathbf{u}^T$  is a biclique between  $v_i \in V$  and  $u_i \in U$  for which  $\mathbf{v}_i = \mathbf{u}_i = 1$
- Exact BMF corresponds to covering each edge of the graph with at least one biclique
  - In approximate BMF, quasi-bicliques cover most edges

#### Binary matrices and sets



- There is a bijection between  $\{0,1\}^{m \times n}$  and sets systems of m sets over n-element universes,  $(U, \mathcal{S} \in 2^U), |\mathcal{S}| = m, |U| = n$ 
  - Up to labeling of elements in U
  - The columns of  $\mathbf{A} \in \{0,1\}^{m \times n}$  correspond to the elements of U
  - ► The rows of A correspond to the sets in S
  - ▶ If  $S_i \in S$ , then  $u_j \in S_i$  iff  $A_{ij} = 1$

### BMF and the Set Basis problem



- In the Set Basis problem, we are given a set system (U, S), and our task is to find collection  $C \subseteq 2^U$  such that we can cover each set  $S \in S$  with a union of some sets of C
  - For each  $S \in S$ , there is  $C_S \subseteq C$  such that  $S = \bigcup_{C \in C_S} C$
- A set basis corresponds to exact BMF
  - The size of the smallest set basis is the Boolean rank
- N.B.: this is the same problem as covering with bicliques

# Binary matrices in data mining

- A common use for binary matrices is to represent presence/absence data
  - Animals in spatial areas
  - Items in transactions
- Another common use are binary relations
  - "has seen" between users and movies
  - "links to" between anchor texts and web pages
- Also any directed graphs are typical
- A common problem is that presence/absence data doesn't necessarily tell about absence
  - We know that 1s are probably "true" 1s, but 0s might either be "true" 0s or missing values
    - If a species is not in some area, is it because we haven't seen it or because it's not there?

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## The Basis Usage problem

- Alternating projections -style algorithms are very common tool for finding matrix factorizations
  - E.g. the alternating least squares algorithm
- As a subproblem they require you to solve the following problem: Given matrices  ${\bf Y}$  and  ${\bf A},$  find matrix  ${\bf X}$  such that  $\|{\bf Y}-{\bf A}{\bf X}\|$  is minimized
  - ► Each column of X is independent: Given vector y and matrix A, find a vector x that minimizes ||y Ax||
    - \* Linear regression if no constraints on x and Euclidean norm is used
- The Basis Usage problem is the Boolean variant of this problem:

#### Basis Usage problem

Given binary matrices **A** and **B**, find binary matrix **C** that minimizes  $\|\mathbf{A} - (\mathbf{B} \boxtimes \mathbf{C})\|_F^2$ .

• How hard can it be?

# The problem of selecting the best components

• Consider the problem of selecting the best *k* rank-1 binary matrices from a given set

#### BMF component selection

Given a binary matrix  $\mathbf{A}$ , set of *n* rank-1 binary matrices  $S = {\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_n : \operatorname{rank}(\mathbf{S}_i) = 1}$ , and integer *k*, find  $C \subset S$  of size *k* such that  $\|\mathbf{A} - \bigvee_{\mathbf{S} \in C} \mathbf{S}\|_F^2$  is minimized.

- If matrices S<sub>i</sub> are *tiles* of A, this problem is equivalent to the Max-k cover problem
  - **S** is a tile of **A** if for all i, j: when  $\mathbf{A}_{ij} = 0$  then  $\mathbf{S}_{ij} = 0$
  - ▶ The Max *k*-cover problem: given a set system (U, S), find *partial cover*  $C \subset S$  of size k (|C| = k) such that  $|\bigcup C| = |\bigcup_{C \in C} C|$  is maximized
  - Equivalence: U has an element for each A<sub>ij</sub> = 1, S ∈ S are equivalent to S ∈ S, and UC is equivalent to V<sub>S∈C</sub> S
- But when the matrices **S**<sub>i</sub> can cover 1s in **A**, the problem is much harder

## The Positive-Negative Partial Set Cover problem

- When the matrices **S**<sub>i</sub> can cover 1s in **A**, Max k-cover is not sufficient
  - We need to model the error we make when not covering 1s (as in the Max k-cover)
  - And we need to model the error we make when covering 0s

#### Positive-Negative Partial Set Cover problem $(\pm PSC)$

Given a set system  $(P \cup N, S \in 2^{P \cup N})$  and integer k, find a partial cover  $C \subset S$  of size k such that C minimizes  $|P \setminus (\bigcup C)| + |N \cap (\bigcup C)|$ .

- $\pm \text{PSC}$  minimizes the number of uncovered positive elements plus the number of covered elements
- Equivalence to component selection:
  - Element  $\mathbf{A}_{ij} \in P$  if  $\mathbf{A}_{ij} = 1$ , else  $\mathbf{A}_{ij} = N$
  - Each matrix  $S_i \in S$  corresponds to a set  $S_i$  in S  $(A_{ij} \in S_{ell})$  iff  $(S_{ell})_{ij} = 1$
  - $\bigcup C$  is equivalent to  $\bigvee_{\mathbf{S}\in C} \mathbf{S}$
  - ►  $\|\mathbf{A} \bigvee \mathbf{S}\|_{F}^{2} = |\mathbf{A} \oplus (\bigvee \mathbf{S})|$  (for binary **A** and **S**)

Miettinen On the Positive-Negative Partial Set Cover Problem. Inf. Proc. Lett. 108(4), 2008

### Back to the Basis Usage

- But what has the Basis Usage problem to do with  $\pm PSC?$ 
  - They're also almost equivalent problems
- To see the equivalence, consider the one-column problem: given a and B, find c such that  $\|\mathbf{a} \mathbf{Bc}\|_F^2$  is minimized
  - $\mathbf{a}_i \in P$  if  $\mathbf{a}_i = 1$ , o/w  $\mathbf{a}_i \in N$
  - ▶ Sets in S are defined by the columns of **B**:  $\mathbf{a}_i \in S_j$  if  $\mathbf{B}_{ij} = 1$
  - If set  $S_j$  is selected to C, then  $\mathbf{c}_j = 1$  (o/w  $\mathbf{c}_j = 0$ )
  - And  $|P \setminus (\bigcup C)| + |N \cap (\bigcup C)| = |\mathbf{A} \oplus (\mathbf{Bc})| = \|\mathbf{A} \mathbf{Bc}\|_F^2$
- So while Basis Usage and Component selection look different, they actually are essentially the same problem
  - Unfortunately this is also a hard problem, making algorithm development complicated

#### Example of $\pm \mathsf{PSC}$ and Basis Usage

defines the sets



## Computational complexity

- Computing the Boolean rank is as hard as solving the Set Basis problem, i.e. NP-hard
  - Approximating the Boolean rank is as hard as approximating the minimum chromatic number of a graph, i.e. very hard
  - Compare to normal rank, which is easy save for precision issues
- Finding the least-error approximate BMF is NP-hard
  - And we cannot get any multiplicative approximation factors, as recognizing the case with zero error is also NP-hard
  - The problem is also hard to approximate within additive error
- Solving the  $\pm$ PSC problem is NP-hard and it is NP-hard to approximate within a superpolylogarithmic factor
  - Therefore, the Basis Usage and Component Selection problems are also NP-hard even to approximate

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### Two simple ideas

- Idea 1: Alternating updates
  - ► Start with random **B**, find new **C**, update **B**, etc. until convergence
  - Guaranteed to converge in nm steps for  $m \times n$  matrices
  - Problem: requires solving the BU problem
    - \* But it can be approximated
  - Problem: Converges too fast
    - ★ The optimization landscape is bumpy (many local optima)
- Idea 2: Find many dense submatrices (quasi-bicliques) and select from them
  - Existing algorithms find the dense submatrices
  - Finding the dense submatrices is slow
  - Problem: requires solving the BU problem

# Expanding tiles: the Panda algorithm

- The Panda algorithm starts by finding large tiles of the matrix
- These are taken one-by-one (from the largest) as a *core* of the next factor
  - The core is expanded by adding to it rows and columns that make it non-monochromatic (add noise)
  - After the extension phase ends, the rows and columns in the expanded core define new component that is added to the factorization
  - The next selected core is the tile that has the largest area outside the already-covered area
- Problem: when to stop the extension of the core
  - Panda adds noisy rows and columns to the core as long as that minimizes the noise plus the number of selected rows and columns (poor man's MDL)

### Using association accuracy: the Asso algorithm

- The Asso algorithm uses the correlations between rows to define *candidate factors*, from which it selects the final (column) factors
  - Assume two rows of A share the same factor
  - Then both of these rows have 1s in the same subset of columns (assuming no noise)
  - Therefore the probability of seeing 1 in the other row on a column we've observed 1 on the other row is high
- Asso computes the empirical probabilities of seeing 1 in row *i* if it's seen in row *j* into *m* × *m* matrix
  - This matrix is rounded to binary
  - A greedy search selects a column of this matrix and its corresponding row factor to create the next component
- Problem: requires solving the BU problem
  - Greedy heuristic works well in practice
- Problem: introduces a parameter to round the probabilities
- Problem: noisy or badly overlapping factors do not appear on the rounded matrix

# Selecting the parameters: The MDL principle

- Typical matrix factorization methods require the user to pre-specify the rank
  - ► Also SVD is usually computed only up to some top-k factors
- With BMF, the minimum description length (MDL) principle gives a powerful way to automatically select the rank
- Intuition: data consists of structure and noise
  - Structure can be explained well using the factors
  - Noise cannot be explained well using the factors
- Goal: find the size of the factorization that explains all the structure but doesn't explain the noise
- Idea: Quantify how well we explain the data by how well we can compress it
  - If a component explains many 1s of the data, it's easier to compress the factors than each of the 1s

#### The MDL principle

The best rank is the one that lets us to express the data with the least number of bits

# MDL for BMF: Specifics

- We compress our data by compressing the factor matrices and the residual matrix
  - $\blacktriangleright\,$  The residual is the exclusive or of the data and the factorization,  $R=A\oplus(B\boxtimes C)$
  - The residual is needed because the compression must be lossless
- In MDL parlance, **B** and **C** constitute the **hypothesis** and **R** explains the data given the hypothesis
  - ► Two-part MDL: minimize L(H) + L(D | H), where L() is the encoding length
- Question: how do we encode the matrices?
  - One idea: consider each column of **B** separately
  - Encode the number of 1s in the column, call it b (log<sub>2</sub>(m) bits when m is already known)
  - Enumerate every *m*-bit binary vector with *b* 1s in lexicographical order and send the number
    - ★ There are  $\binom{m}{b}$  such vectors, so we can encode the number with  $\log_2\binom{m}{b}$  bits
    - ★ We don't really need to do the enumeration, just to know how many (fractional) bits it would take

### MDL for BMF: An Example

- MDL can be used to find all parameters for the algorithm, not just one
- To use MDL, run the algorithm with different values of k and select the one that gives the smallest description length
  - Usually approximately convex, so no need to try all values of k



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#### Lessons learned

- BMF finds binary factors for binary data yielding binary approximation  $\rightarrow$  easier interpretation, different structure than normal algebra
- Many problems associated with BMF are hard even to approximate
  - ▶ Boolean rank, minimum-error BMF, Basis Usage, ...
- $\bullet~$  BMF has very combinatorial flavour  $\rightarrow~$  algorithms are less like other matrix factorization algorithms
- MDL can be used to automatically find the rank of the factorization

# Suggested reading

- Slides at http://www.mpi-inf.mpg.de/~pmiettin/bmf\_ tutorial/material.html
- Miettinen et al. *The Discrete Basis Problem*, IEEE Trans. Knowl. Data Eng. 20(10), 2008.
  - Explains the Asso algorithm and the use of BMF (called DBP in the paper) in data mining
- Lucchese et al. *Mining Top-k Patterns from Binary Datasets in presence of Noise.* SDM '10
  - Explains the Panda algorithm
- Miettinen & Vreeken MDL4BMF: Minimum Description Length for Boolean Matrix Factorization
  - Explains the use of MDL with BMF