BINARY MATRIX FACTORISATIONS

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In the sleepy days when the provinces of France were still quietly provincial, matrices with Boolean entries were a favored occupation of aging professors at the universities of Bordeaux and Clermont-Ferrand. But one day…

Gian-Carlo Rota
Foreword to *Boolean matrix theory and applications* by K. H. Kim, 1982

PART I
DEFINITIONS AND THEORY

CONTENTS

MOTIVATING EXAMPLE

Images by John Tenniel, openclipart.org, and Wikipedia

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TABLE OF FEATURES

long-haired	✔	✔	✘
well-known	✔	✔	✔
male	✘	✔	✔

BINARY MATRIX

long-haired	1	1	0
well-known	1	1	1
male	0	1	1

BOOLEAN MATRIX FACTORISATION

Alice & Bob: long-haired and well-known

Bob & Charles: well-known males

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

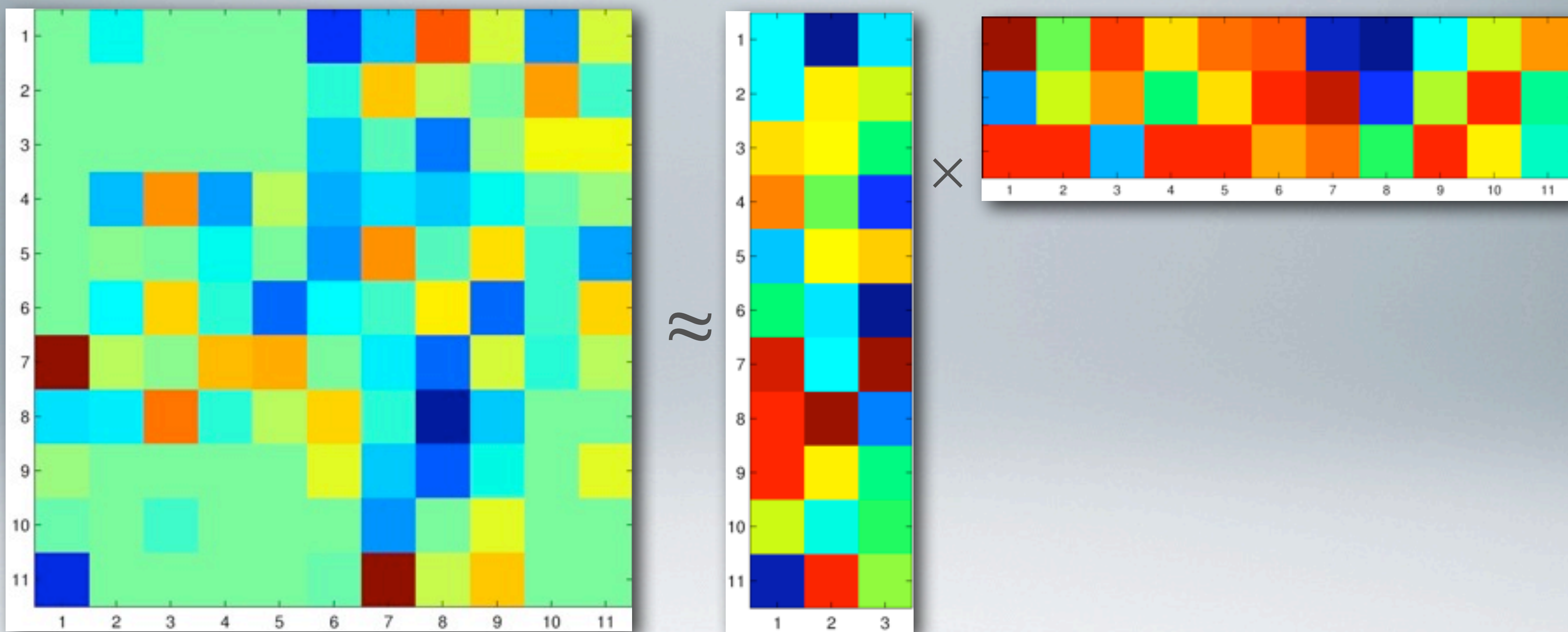
				A	B	C
long-haired	1	0		1	1	0
well-known	1	1	∘	0	1	1
male	0	1				

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

MODULO-2 EXAMPLE

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

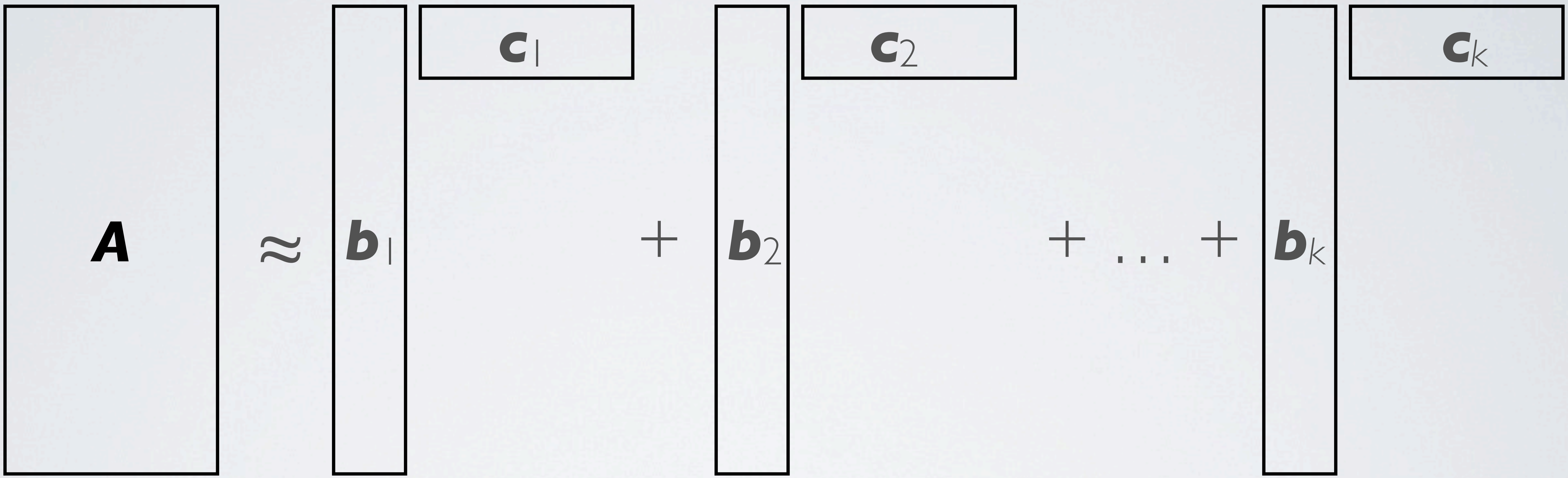
MATRIX FACTORISATIONS



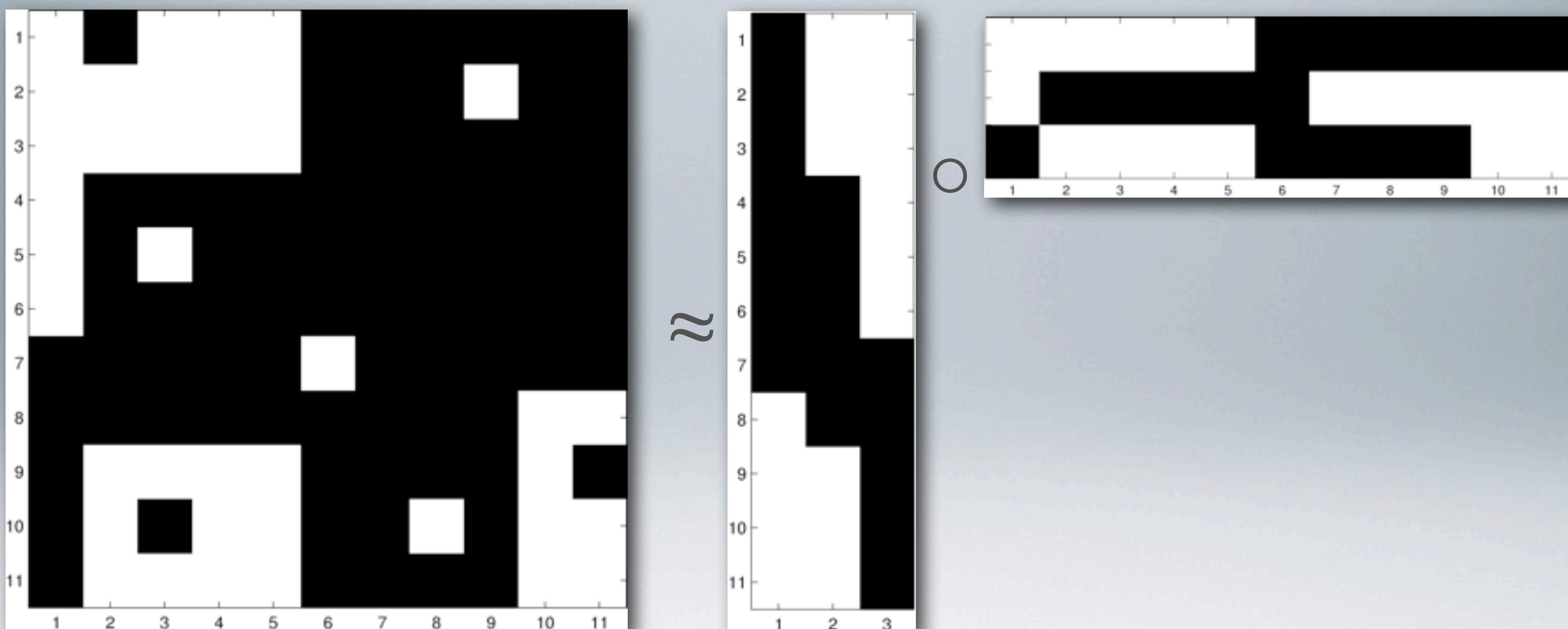
DEFINITION

- A **factorisation** of matrix $\boldsymbol{A}$ represents it as a product of two (or more) **factor matrices**: $\boldsymbol{A} = \boldsymbol{BC}$
  - $\boldsymbol{A}$ is n-by-m, $\boldsymbol{B}$ is n-by-k, and $\boldsymbol{C}$ is k-by-m
    - k is the **size** (or **rank**) of the factorisation
- Factorisation can be **exact** ($\boldsymbol{A} = \boldsymbol{BC}$) or **approximate** ($\boldsymbol{A} \approx \boldsymbol{BC}$)

K RANK-1 FACTORISATIONS



BINARY MATRIX FACTORISATIONS



BINARY MATRIX FACTORISATIONS

- All involved matrices (***A***, ***B***, and ***C***) are binary (0/1)
- Loss function is sum of absolute differences

$$|\mathbf{A} - \mathbf{B}\times\mathbf{C}| = \sum_{ij} |a_{ij} - (\mathbf{B}\times\mathbf{C})_{ij}|$$

  - Or squared Frobenius
- The **algebra** is different for different factorisations
  - We consider normal, modulo-2, and Boolean algebras

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NORMAL ALGEBRA

Binary matrix factorisation under $\mathbb{R}$ (RMF).
Given an *n*-by-*m* binary matrix $\boldsymbol{A}$ and integer *k*, find *n*-by-*k* and *k*-by-*m* binary matrices $\boldsymbol{B}$ and $\boldsymbol{C}$ such that $|\boldsymbol{A} - \boldsymbol{B}\times\boldsymbol{C}|$ is minimised.

- Algebra is normal ($1+1 = 2$)
  $\Rightarrow \boldsymbol{B}\times\boldsymbol{C}$ is not necessarily binary

BOOLEAN ALGEBRA

Boolean matrix factorisation (**BMF**).
Given an *n*-by-*m* binary matrix $\boldsymbol{A}$ and integer *k*, find *n*-by-*k* and *k*-by-*m* binary matrices $\boldsymbol{B}$ and $\boldsymbol{C}$ such that $|\boldsymbol{A} - \boldsymbol{B} \circ \boldsymbol{C}|$ is minimised.

- Algebra is Boolean ($1+1 = 1$)
  $\Rightarrow \boldsymbol{B} \circ \boldsymbol{C}$ is always binary

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MODULO-2 ALGEBRA

Binary matrix factorisation under modulo-2 algebra (**XMF**).
Given an *n*-by-*m* binary matrix ***A*** and integer *k*, find *n*-by-*k* and *k*-by-*m* binary matrices ***B*** and ***C*** such that $|\boldsymbol{A} - \boldsymbol{B} \otimes \boldsymbol{C}|$ is minimised.

- Algebra is modulo-2 ($1+1 = 0$)
  $\Rightarrow \boldsymbol{B} \otimes \boldsymbol{C}$ is always binary

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OTHER OPTIONS

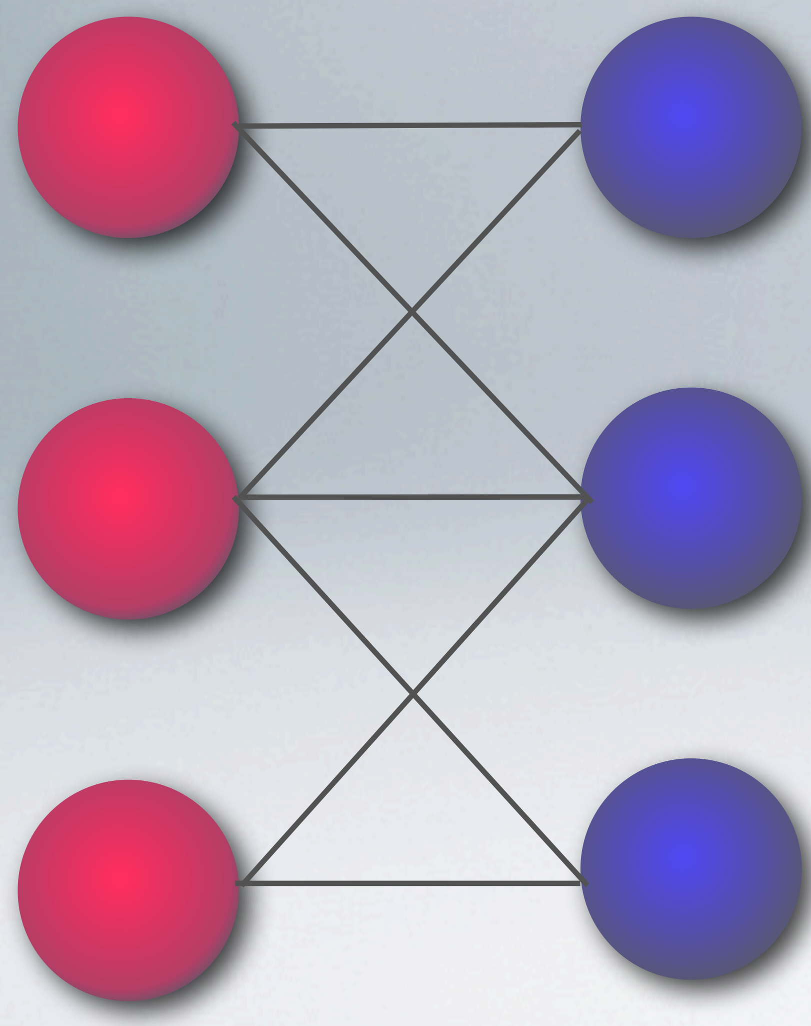
- Other definitions of underlying algebra are possible
- Example: define addition to be logical implication
    - Non-commutative
        - $\boldsymbol{A} + \boldsymbol{B} \neq \boldsymbol{B} + \boldsymbol{A}$
        - $(\boldsymbol{AB})^{\top} \neq \boldsymbol{B}^{\top}\boldsymbol{A}^{\top}$

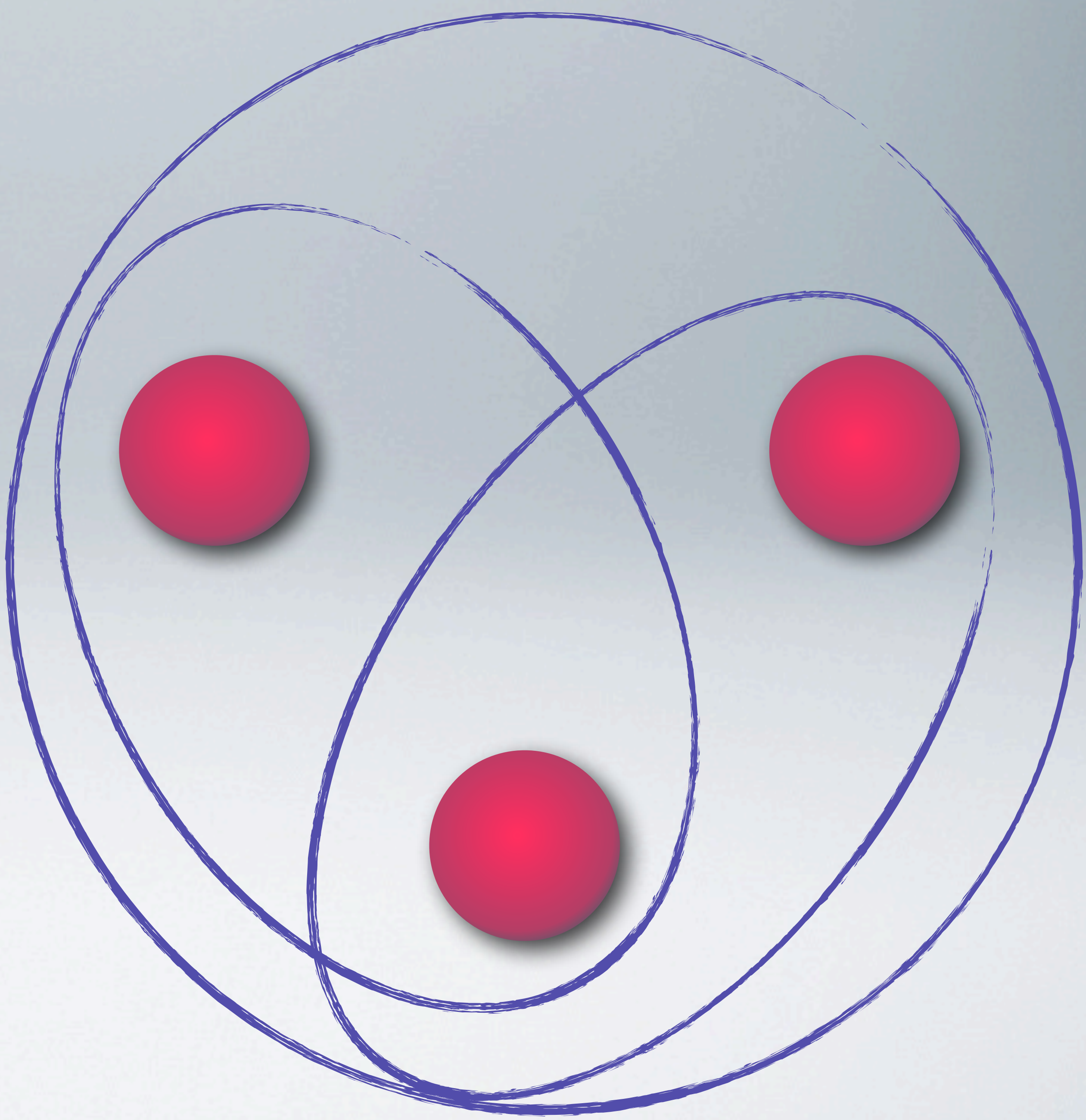
	0	1
0	1	1
1	0	1

COMPARISON

	RMF	BMF	XMF
Addition	1+1=2	1+1=1	1+1=0
Algebra	semi-ring	semi-ring	field
Closed?	not closed	closed	closed

DIFFERENT VIEWS OF BINARY DATA



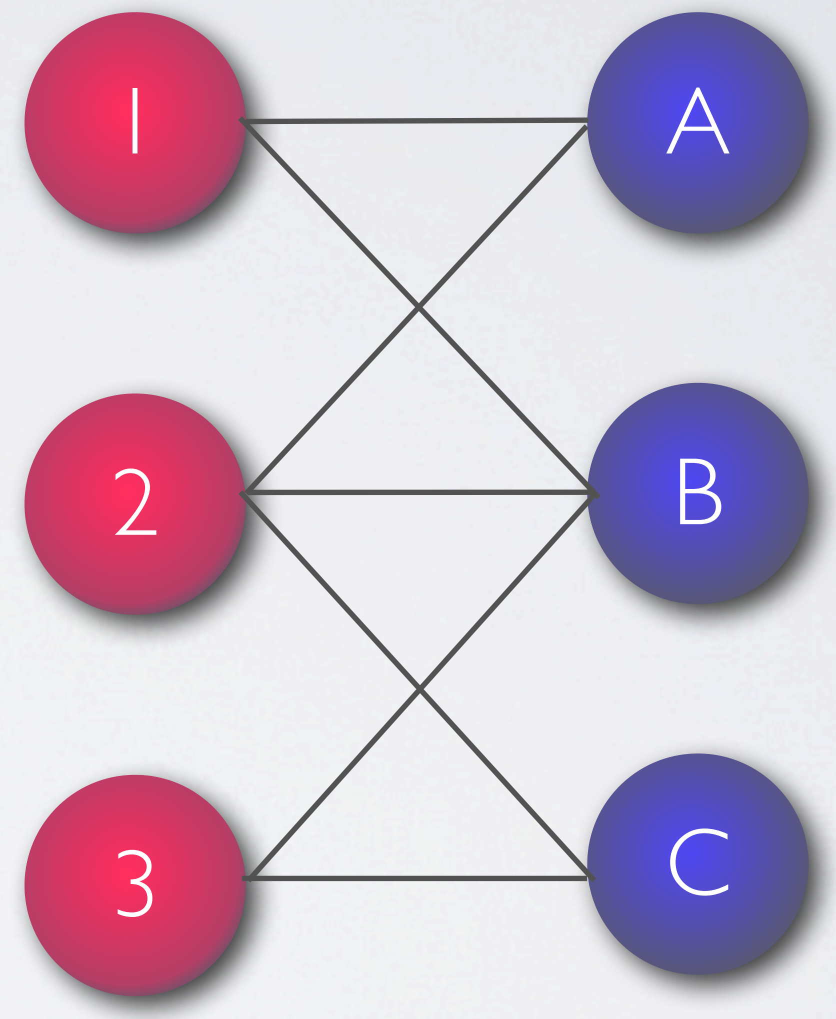


BIPARTITE GRAPHS

A

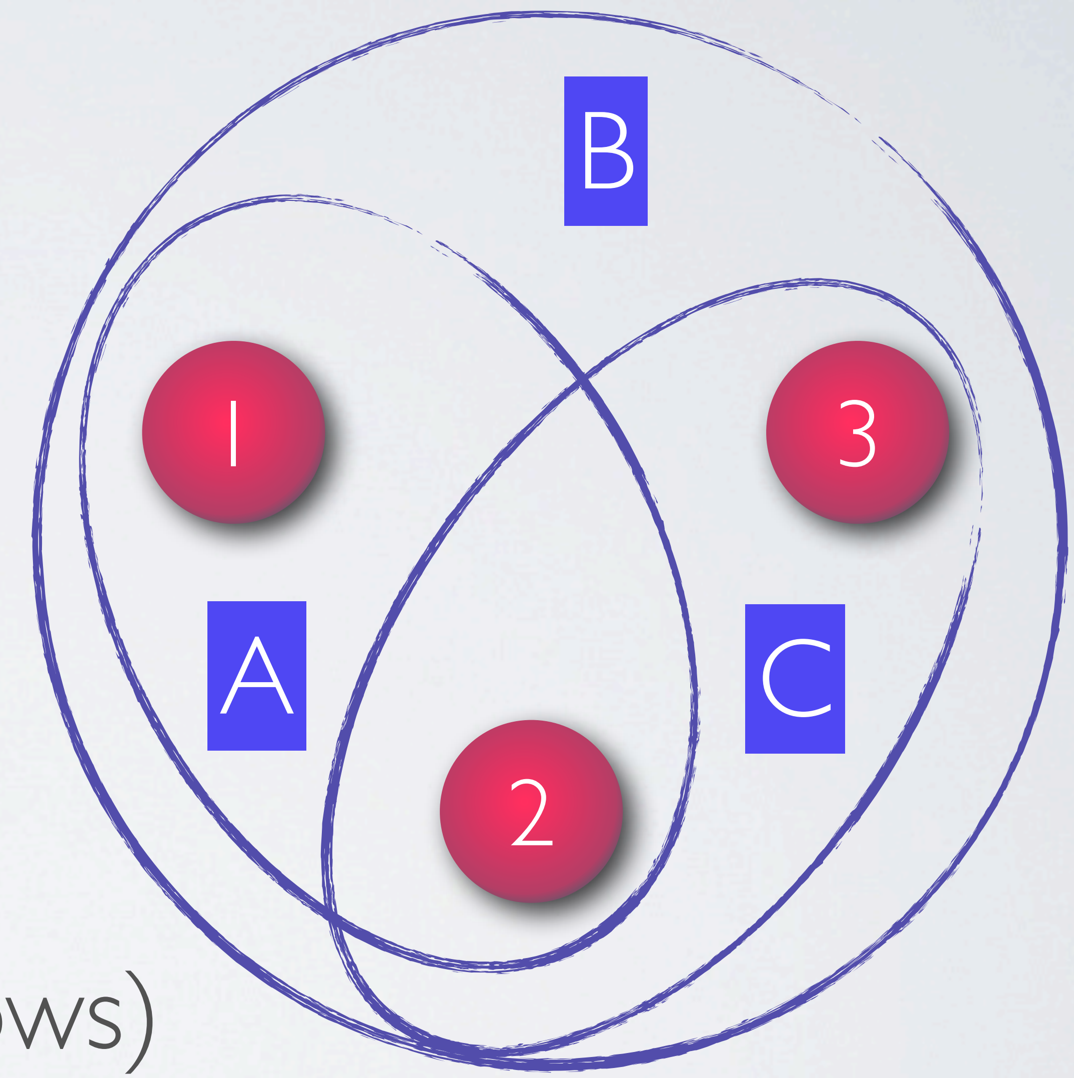
	A	B	C
1	1	1	0
2	1	1	1
3	0	1	1

$G(\boldsymbol{A})$



SETS AND COLLECTIONS

	A	B	C
1	1	1	0
2	1	1	1
3	0	1	1



$U(\boldsymbol{A})$ is an induced universe (rows)
$C(\boldsymbol{A})$ is an induced collection of sets (columns)

TILING & CLUSTERING AS MATRIX FACTORISATIONS

Image by Wikipedia user PJM

K-MEANS AS MATRIX FACTORISATION

- Given *m* data points (in $\mathbf{R}^n$), partition them in *k* clusters such that

  $$\sum_{i=1}^{k} \sum_{x_j \in C_i} \|\mathbf{x}_j - \boldsymbol{\mu}_i\|_2^2$$

  is minimised

- Equivalently, minimise $\|\boldsymbol{X} - \boldsymbol{MC}\|^2$, where
  - ***X*** is the data (*n*-by-*m*), ***M*** (*n*-by-*k*) has the centroids as its columns, and **C** (*k*-by-*m*) is a **cluster assignment matrix**
    - Each column of **C** has exactly one 1, and rest is 0s

TILING AS MATRIX FACTORISATION

- Maximum *k*-tiling: find at most *k* **tiles** such that the tiling has maximum area [1]
  - Data is binary matrix, tiles are submatrices full of 1s
  - Area of a tiling is the number of 1s in the data that belong to at least one tile
- We turn this to *minimum-error tiling*
  - Minimise the number of 1s in the data that do not belong to any tile

[1] F. Geerts et al., Tiling databases, in: DS '04, 77–122.

TILING AS MATRIX FACTORISATION

- We want to find factor matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ such that $(\boldsymbol{AB})_{ij} = 1$ iff element (i, j) belongs to at least one tile
  - Minimise $|\boldsymbol{X} - \boldsymbol{AB}|$
- Single tile is an outer product of two binary vectors: $\boldsymbol{ab}^T$
  - $b_j = 1$ if an item j belongs to the tile; $a_i = 1$ if a transaction i belongs to the tile
- But how to combine the tiles?

COMBINING THE TILES

- The problem: $\sum_{i=1}^{k} \mathbf{a}_i \mathbf{b}_i^T$ is not necessarily binary
  - RMF: $|\boldsymbol{X} - \boldsymbol{AB}|$ will add an error every time $x_{ij} = 1$ belongs to more than one tile
  - BMF: don't count multiplicity (1+1 = 1)
  - XMF: consider parity (1+1 = 0)

RNF, BMF, AND XMF AS TILING

- Unlike tiling, all methods allow holes in the tiles
- BMF is otherwise like tiling
- RMF penalises for overlapping tiles
- XMF removes the overlapping part of pairs of tiles
  - For nested tiles, this would be removing exceptional areas

MATRIX RANKS

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

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

DEFINITIONS

Normal matrix rank.
The **rank** of a matrix $\boldsymbol{A}$, $\text{rank}_R(\boldsymbol{A})$, is the least integer k such that $\boldsymbol{A}$ can be expressed exactly with a decomposition of size k.

Boolean matrix rank.
The **Boolean rank** of a binary matrix $\boldsymbol{A}$, $\text{rank}_B(\boldsymbol{A})$, is the least integer k such that $\boldsymbol{A}$ can be expressed exactly with a Boolean decomposition of size k.

DEFINITIONS

Boolean matrix rank.
The **Boolean rank** of a binary matrix $\boldsymbol{A}$, $\mathrm{rank}_B(\boldsymbol{A})$, is the least integer k such that $\boldsymbol{A}$ can be expressed exactly with a Boolean decomposition of size k.

Modulo-2 matrix rank.
The **modulo-2 rank** of a binary matrix $\boldsymbol{A}$, $\mathrm{rank}_X(\boldsymbol{A})$, is the least integer k such that $\boldsymbol{A}$ can be expressed exactly with a modulo-2 decomposition of size k.

DEFINITIONS

Modulo-2 matrix rank.
The **modulo-2 rank** of a binary matrix ***A***, $\text{rank}_X(\boldsymbol{A})$, is the least integer *k* such that ***A*** can be expressed exactly with a modulo-2 decomposition of size *k*.

Binary matrix rank over normal algebra.
The **binary rank** of a binary matrix ***A***, $\text{rank}_N(\boldsymbol{A})$, is the least integer *k* such that ***A*** can be expressed exactly with a binary decomposition (with normal algebra) of size *k*.

EXAMPLE OF BOOLEAN RANK

$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \qquad \text{rank}_B(\boldsymbol{A}) = 2$$

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

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EXAMPLE OF XOR RANK

$\mathrm{rank}_X(\boldsymbol{A}) = 3$

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

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

EXAMPLE OF BINARY RANK

$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \qquad \text{rank}_N(\boldsymbol{A}) = 2$$

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

COMPARISON OF RANKS

- How do these ranks compare?
  - Is one always the smallest?
  - Is one always the largest?
  - How big the differences can be?
  - How about the normal rank?

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BOOLEAN VS NORMAL

- Incommensurable [1]
  - For some ***A***, $\text{rank}_R(\boldsymbol{A}) < \text{rank}_B(\boldsymbol{A})$
  - For some ***A***, $\text{rank}_R(\boldsymbol{A}) > \text{rank}_B(\boldsymbol{A})$
- Extrema:
  - Exists *n*-by-*n* matrix ***A***: $\text{rank}_B(\boldsymbol{A}) = \log_2(\text{rank}_R(\boldsymbol{A}))$ [1]
  - Exists *n*-by-*n* matrix ***A***, when $n \to \infty$: $\text{rank}_R(\boldsymbol{A}) = \text{rank}_B(\boldsymbol{A}) / 2$ [2]

As good as it gets

?

[1] S.D. Monson et al., A Survey of Clique and Biclique Coverings and Factorizations of (0,1)-Matrices, *Bull. ICA*. 14 (1995), 17–86.
[2] P. Kaski, personal communication.

BINARY VS THE OTHERS

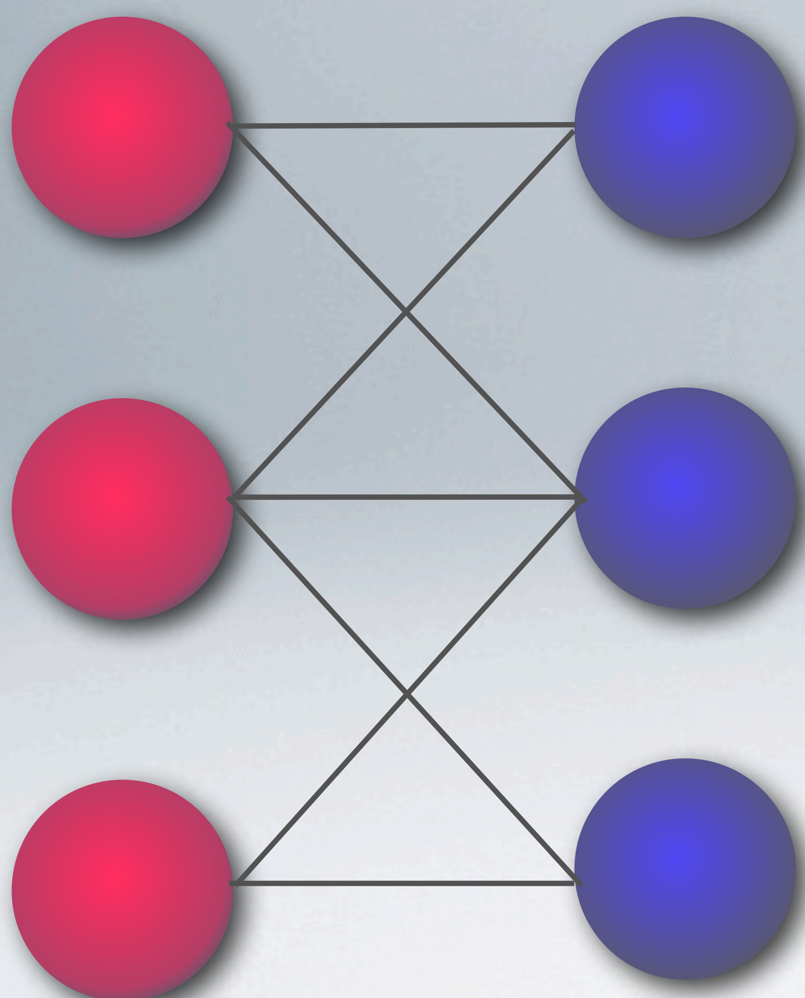
- Binary rank is always the biggest
  - $\text{rank}_N(\boldsymbol{A}) \geq \text{rank}_B(\boldsymbol{A})$ for all $\boldsymbol{A}$ [1]
  - $\text{rank}_N(\boldsymbol{A}) \geq \text{rank}_X(\boldsymbol{A})$ for all $\boldsymbol{A}$
    - All use binary numbers and binary doesn't allow overlap
  - $\text{rank}_N(\boldsymbol{A}) \geq \text{rank}_R(\boldsymbol{A})$ for all $\boldsymbol{A}$ [1]
    - Both use the same arithmetic

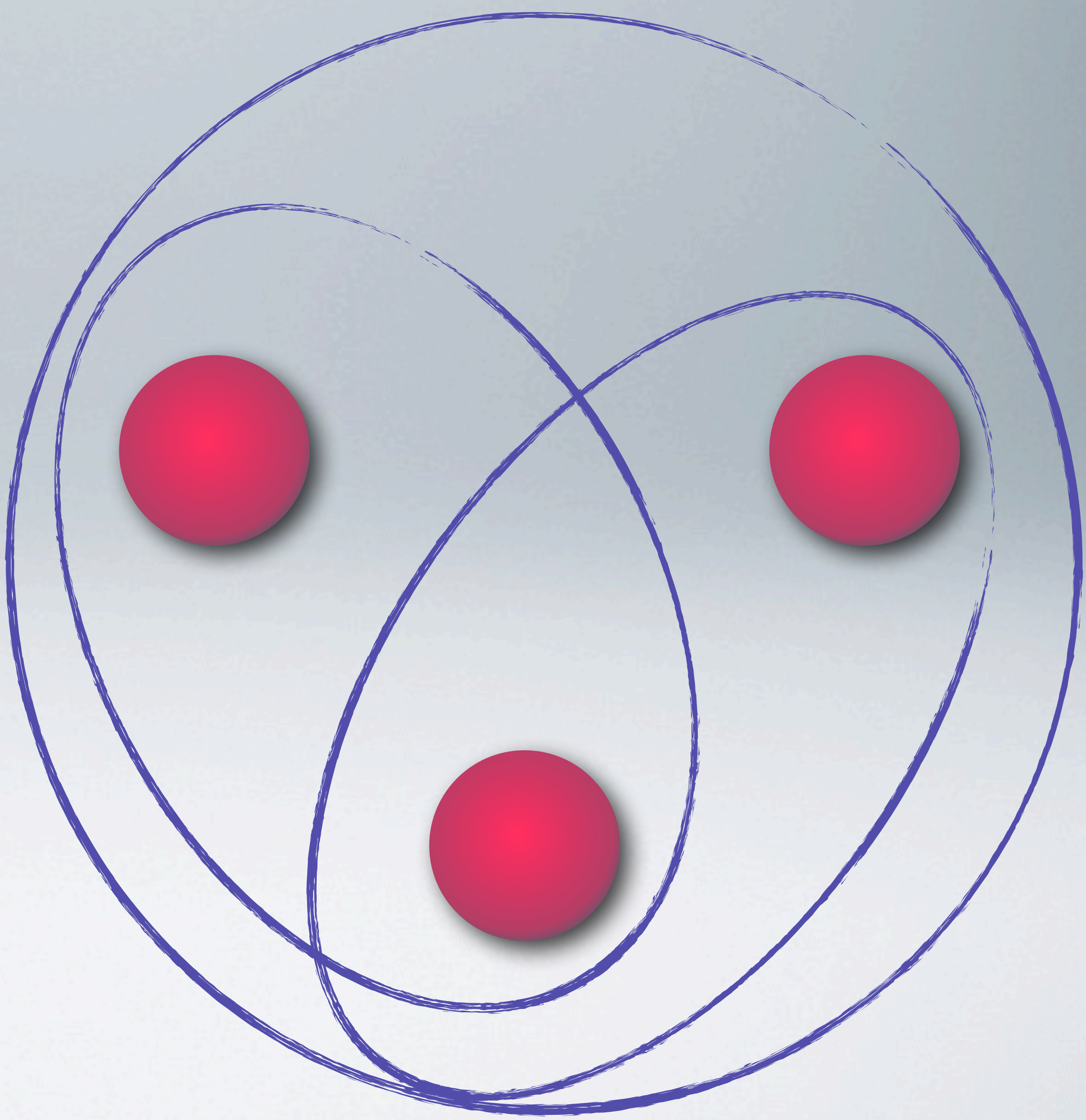
[1] D.A. Gregory, N.J. Pullman, Semiring rank: Boolean rank and nonnegative rank factorizations, *J. Combin. Inform. System Sci.* 8 (1983) 223–233.

SUMMARY

	Normal	Boolean	XOR	Binary
Normal	$=$	$\gtreqless$	$\gtreqless$	$\leq$
Boolean	$\gtreqless$	$=$	$\gtreqless$	$\leq$
XOR	$\gtreqless$	$\gtreqless$	$=$	$\leq$
Binary	$\geq$	$\geq$	$\geq$	$=$

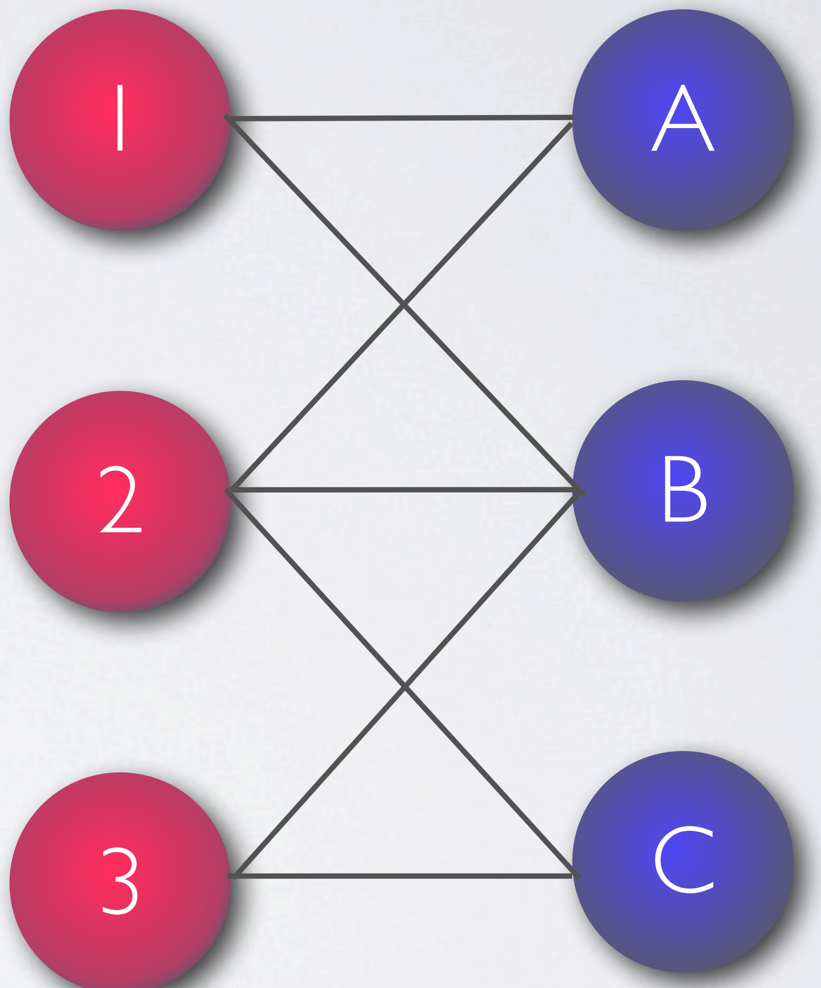
DIFFERENT VIEWS TO THE BOOLEAN RANK



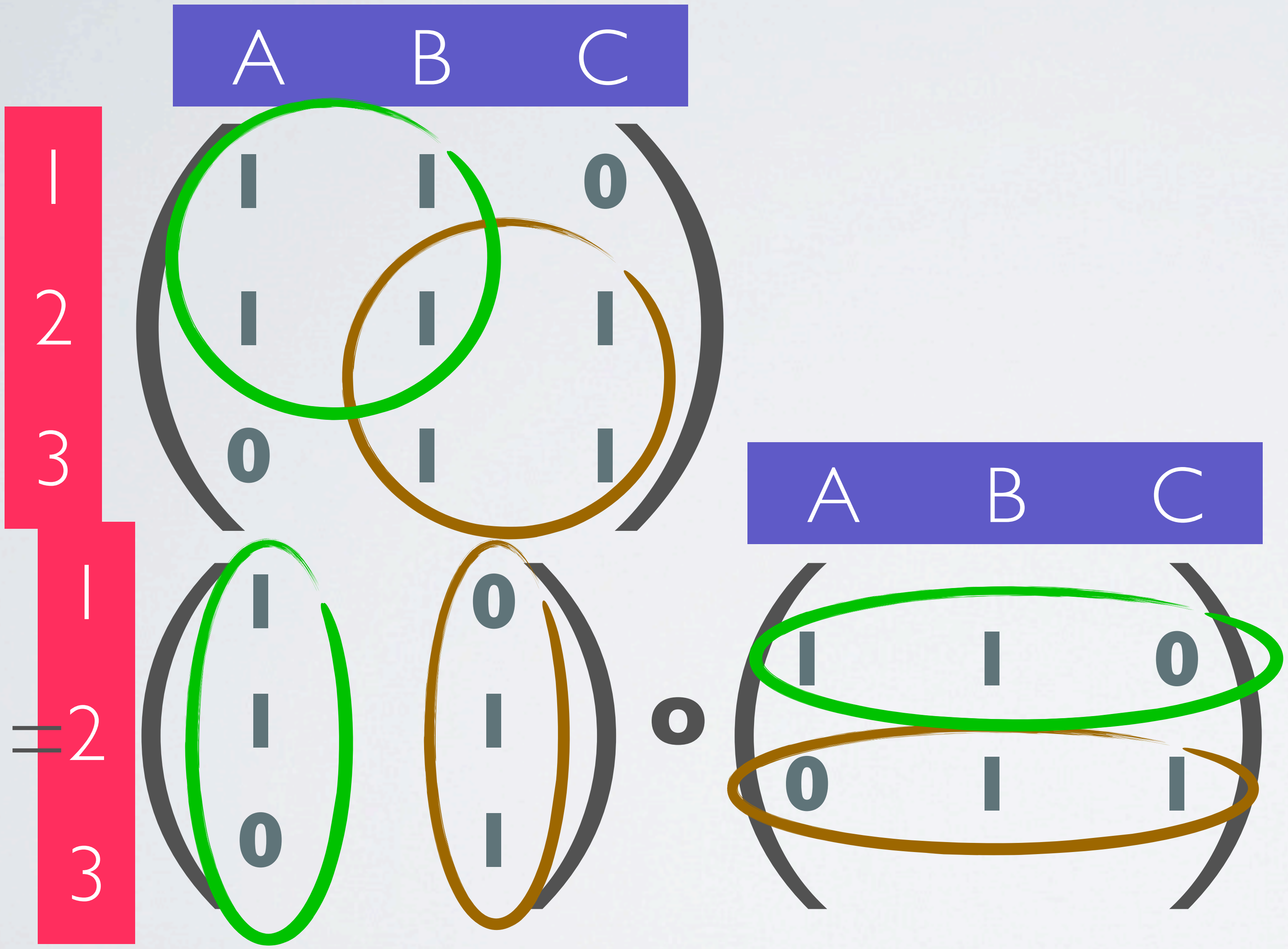


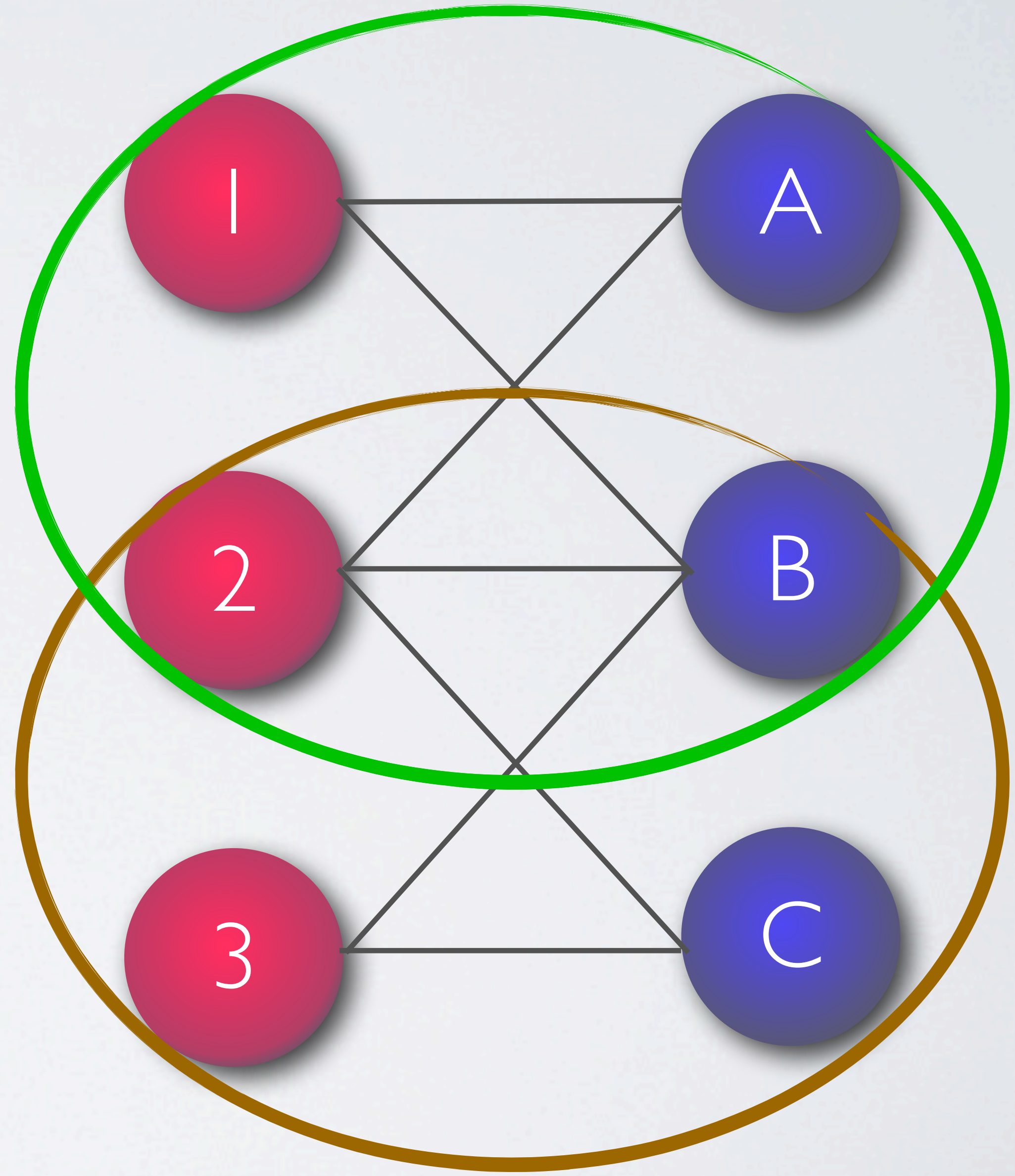
BOOLEAN RANK AND BICLIQUES

- The Boolean rank of a matrix ***A*** is **the least number of complete bipartite subgraphs needed to cover every edge** of the induced bipartite graph *G*(***A***)



BOOLEAN RANK AND BICLIQUES

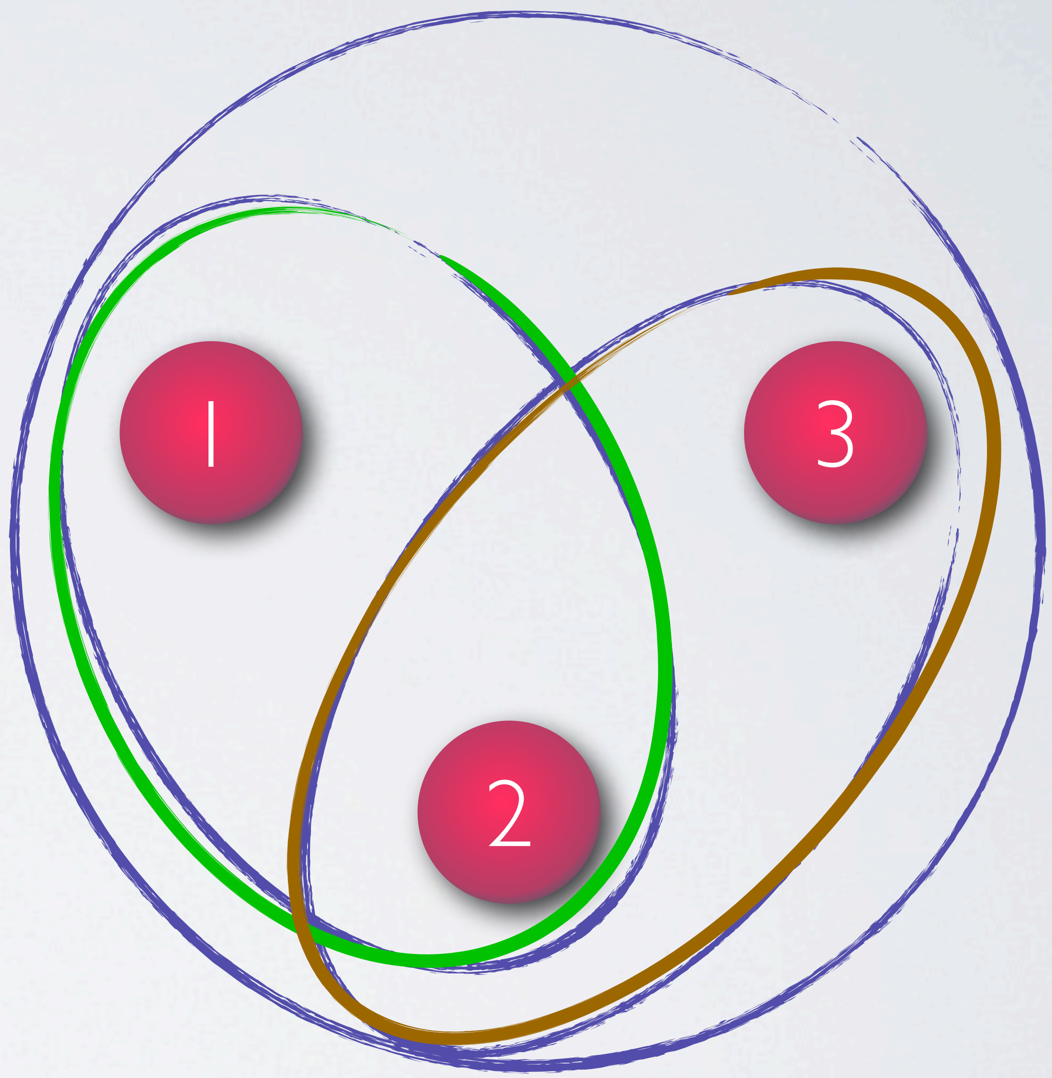




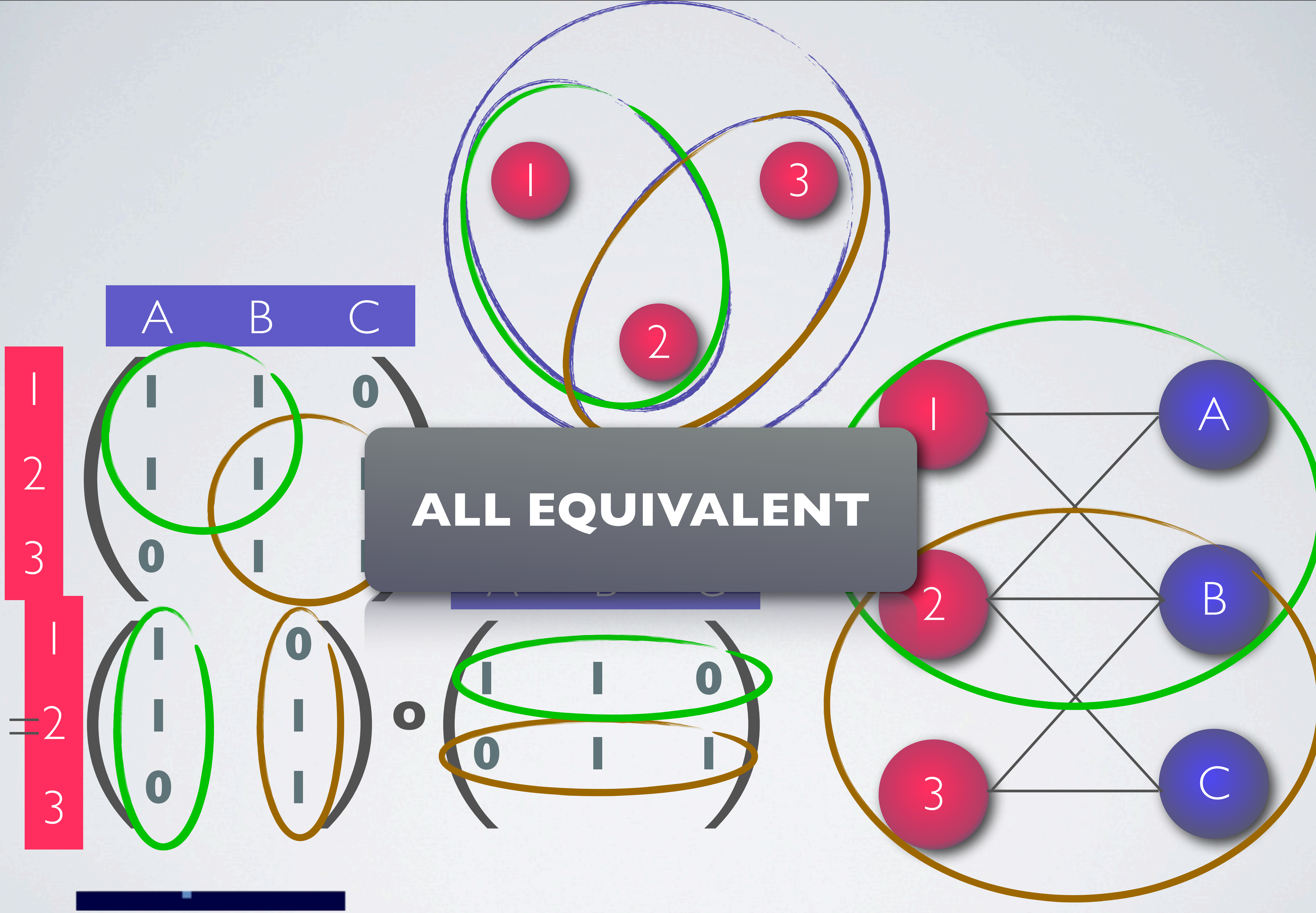
BOOLEAN RANK AND SETS

- The Boolean rank of a matrix ***A*** is **the least number of subsets of** *U*(***A***) **needed to cover every set** of the induced collection *C*(***A***)
  - For every *C* in *C*(***A***), if $\mathcal{S}$ is the collection of subsets, have subcollection $\mathcal{S}_C$ such that

$$\bigcup_{S \in \mathcal{S}_C} S = C$$



ALL EQUIVALENT



XOR AND BINARY

- XOR rank
  - Replace set union with symmetric difference and covering with parity
- Binary rank
  - Non-overlapping subsets / bicliques are sufficient, not necessary
    - Clustering

XOR RANK EXAMPLE

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

BINARY RANK EXAMPLE

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

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

A NOTE ON INVERSES

$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

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

A NOTE ON INVERSES

- Every full-XOR-rank matrix has an inverse
  - Can be found e.g. using Gauss–Jordan elimination
- Only permutation matrices have an inverse in Boolean algebra [1]
- Only permutation matrices have **binary** inverses under normal algebra

[1] K.H. Kim, *Boolean matrix theory and applications*, Marcel Dekker, 1982, p. 105.

COMPUTATIONAL COMPLEXITY

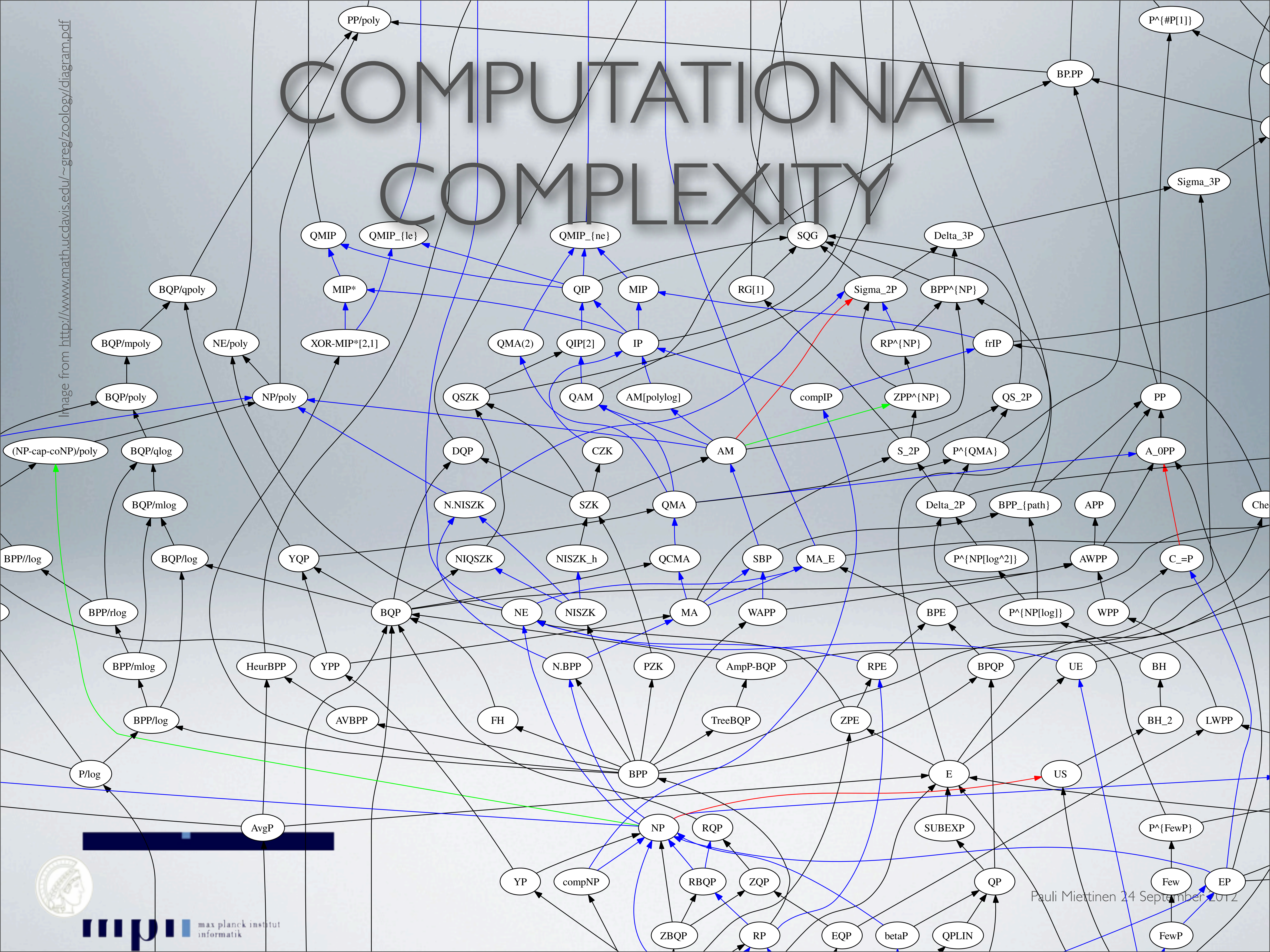


Image from http://www.math.ucdavis.edu/~greg/zoology/diagram.pdf

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FINDING THE RANKS

- XOR rank: polynomial time
  - Standard Gaussian elimination over modulo-2 arithmetic
- Boolean rank: NP-hard [1]
  - As hard to approximate as the clique ($\Omega(n^{1-\varepsilon})$ for all $\varepsilon > 0$) [2]
- Binary rank: Unknown
  - Restriction to non-overlapping factors is NP-hard (clustering) [3]

[1] D.S. Nau et al., A Mathematical Analysis of Human Leukocyte Antigen Serology, *Math. Biosci*. 40 (1978) 243–270.
[2] H.U. Simon, On approximate solutions for combinatorial optimization problems, *SIAM J. Discrete Math*. 3 (1990) 294–310.
[3] M. et al., The Discrete Basis Problem, *IEEE Trans. Knowl. Data En.* 20 (2008) 1348–1362.

BOOLEAN RANK AND TILING

- The Boolean rank of a matrix also tells us the minimum number of tiles needed to completely cover the matrix
- Minimum number of tiles can be approximated within $O(\log nm)$ [1, Thm. 2]
  - This requires an oracle that gives the largest-area tile [1]
- Without the oracle, the reduction requires exponential time
  - Except for certain sparse matrices…

[1] F. Geerts et al., Tiling databases, in: DS '04, 77–122.

MINIMUM-ERROR BMF

- NP-hard to approximate within any polynomially computable function [1]
  - Because it's NP-hard to recognise the zero-error case
- NP-hard to approximate within additive factor of $\max\{\sqrt[4]{n}, \sqrt[4]{m}\}$ [1]

[1] M., *Matrix Decomposition Methods for Data Mining: Computational Complexity and Algorithms*, PhD thesis, U. Helsinki, 2009.

MINIMUM-ERROR PROJECTIONS

- **Problem**: Given the data matrix $\boldsymbol{A}$ and one factor matrix ($\boldsymbol{B}$), find the other factor matrix ($\boldsymbol{C}$) that minimises the error
  - Per column: given a column vector $\boldsymbol{a}$ and a matrix $\boldsymbol{B}$, find a column vector $\boldsymbol{c}$ such that $\boldsymbol{a} \approx \boldsymbol{Bc}$
- ''Binary programming''
- Needed for alternating projections type algorithms (ALS)

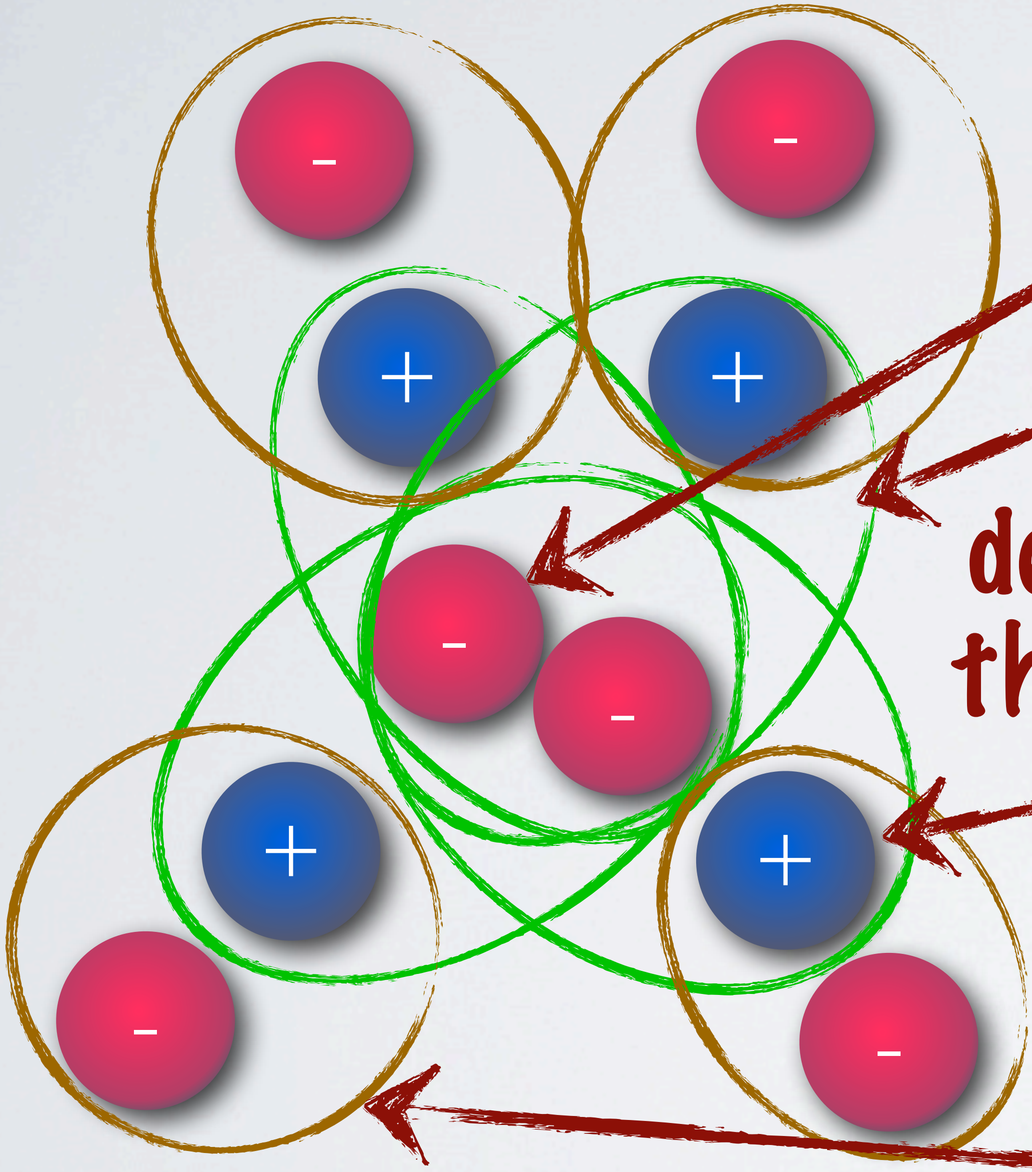
BOOLEAN PROJECTION, OR ±PSC

- The minimum-error projection under Boolean algebra is equivalent to the following problem

Positive-Negative Partial Set Cover (**±PSC**). Given a triple $(P, N, \mathcal{Q})$, where P and N are disjoint sets and $\mathcal{Q} \subseteq 2^{P \cup N}$, find a subcollection $\mathcal{D} \subseteq \mathcal{Q}$ that minimises $|P \setminus (\cup \mathcal{D})| + |N \cap (\cup \mathcal{D})|$.

EXAMPLE

defines the sets



defines the sign

a

0
0
1
1
1
1
0
0
0
0

B

1	1	1	1	0	0	0	0
1	1	1	1	0	0	0	0
1	0	0	0	1	0	0	0
0	1	0	0	0	1	0	0
0	0	1	0	0	0	1	0
0	0	0	1	0	0	0	1
0	0	0	0	1	0	0	0
0	0	0	0	0	1	0	0
0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	1

COMPLEXITY OF ±PSC

- NP-hard to approximate within $\Omega(2^{\log^{1-\varepsilon}|P|})$ for any $\boldsymbol{\varepsilon} > 0$ [1]
- There exists a polynomial-time approximation algorithm that achieves $2\sqrt{[(|Q|+|P|) \log |P|]}$ approximation ratio [1,2]
⇒ In Boolean case, even simple projections are hard

[1] P. Miettinen, On the positive-negative partial set cover problem, *Inform. Process. Lett.* 108 (2008) 219–221.
[2] D. Peleg, Approximation algorithms for the Label-Cover$_{MAX}$ and Red-Blue Set Cover problems, *J. Discrete Alg.* 5 (2007) 55–64.

THE BINARY CASE

- The zero-error case is NP-hard
  - Simple reduction from Exact Cover by 3-sets (X3C)
- A variant is the Closest Vector problem (CVP), where columns of ***B*** have to be linearly independent and the vectors take integer values
  - CVP is NP-hard to approximate within $n^{1/\log\log n}$ [1]

[1] I. Dinur et al., Approximating CVP to Within Almost-Polynomial Factors is NP-Hard, *Combinatorica*. 23 (2003) 205–243.

THE MODULO-2 CASE

- The problem of finding binary vector $\boldsymbol{x}$ such that, for given $\boldsymbol{a}$ and $\boldsymbol{B}$, the Hamming distance between $\boldsymbol{a}$ and $\boldsymbol{B} \otimes \boldsymbol{x}$ is minimised, is known as the Closest Codeword problem
  - NP-hard to approximate to within any constant factor [1]
    - And quasi-NP-hard to approximate within $2^{\log^{\varepsilon} n}$ for $0 < \varepsilon < 1/2$
  - Admits polynomial-time $n/\log(n)$ factorisation [2]

[1] S. Arora et al., The Hardness of Approximate Optima in Lattices, Codes, and Systems of Linear Equations, in: FOCS '93, 724–733.
[2] N. Alon et al., Deterministic Approximation Algorithms for the Nearest Codeword Problem, in: APPROX RANDOM '09, 339–351.

SUMMARY

	RMF	BMF	XMF
Rank	?	NP-hard even to approximate	Polynomial
Min. error decomp.	?	NP-hard even to approximate	?
Closest projection	NP-hard	NP-hard to approx. $\Omega(2^{\log^{1-\varepsilon}\lvert P\rvert})$	NP-hard to approx. w/ constant factor
Projection approx.	?	$2\sqrt{[(\lvert Q\rvert+\lvert P\rvert) \times \log \lvert P\rvert]}$	$O(n/\log(n))$

OPEN PROBLEMS

?

RANKS

- **P1.1** What is the largest possible ratio $\text{rank}_B(\boldsymbol{A})/\text{rank}_R(\boldsymbol{A})$
  - Best known is 2
- **P1.2** What are the extrema of the XOR rank w.r.t. the other ranks?
  - It's incommensurable to normal and Boolean rank

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COMPLEXITY

- **P1.3** Is binary rank NP-hard to compute?
- **P1.4** Is RMF NP-hard?
  - Probably, given that NMF is [1]
- **P1.5** Is XMF NP-hard?
- **P1.6** What's the approximability of binary projections?
- **P1.7** What's the approximability of maximum similarity problems?

[1] S.A. Vavasis, On the Complexity of Nonnegative Matrix Factorization, *SIAM J. Optim.* 20 (2010) 1364–1377.

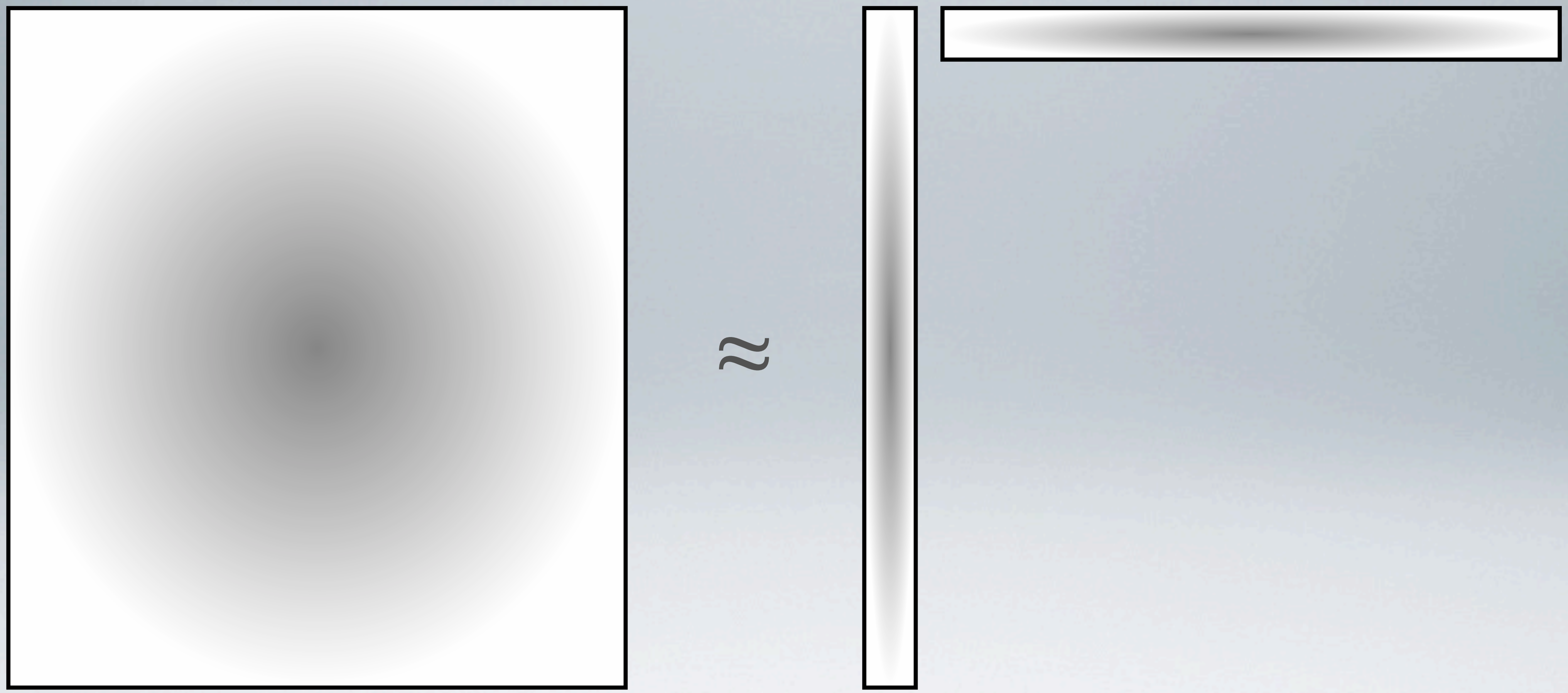
MISCELLANEOUS

- **P1.8** Are there meaningful (in data mining) definitions of the addition (or multiplication) not covered here?

PART II
ALGORITHMS AND EXTENSIONS

CONTENTS

RANK-1 DECOMPOSITIONS



RANK-1 DECOMPOSITIONS

- In rank-1 decompositions, addition doesn't matter
  - We can also use squared Frobenius for distance
- One could hope to use rank-1 approximations as building blocks for higher-rank decompositions
  - Problem: good rank-1 decomposition does not need to be a part of any good rank-2 decompositions

EXAMPLE

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

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

PROXIMUS

- The PROXIMUS algorithm [1] finds the binary rank-1 factorisation using iterative updates
  - To find ***b*** and ***c*** such that $\boldsymbol{A} \approx \boldsymbol{b}\boldsymbol{c}^T$, fix ***c*** and set

$$\mathbf{b}_i = \begin{cases} 1, & \text{if } 2(\boldsymbol{A}\mathbf{c})_i \geqslant \|\mathbf{c}\|_2^2 \\ 0, & \text{otherwise} \end{cases}$$

    and similarly for ***b*** fixed
- Proper initialisation is important

[1] M. Koyutürk, A. Grama, PROXIMUS: a framework for analyzing very high dimensional discrete-attributed datasets, in: KDD '03, 147–156.

IP, LP, AND MAX FLOW ALGORITHMS

- Minimum-error rank-1 binary factorisation can be presented as an integer programming
- Can be relaxed to a linear program that gives an upper bound for the error
  - This LP is totally unimodular ⇒ solution is binary
  - The solution is a 2-approximation
- A regularised version can be approximated with a max flow algorithm

B.-H. Shen et al., Mining Discrete Patterns via Binary Matrix Factorization, in: KDD '09, 757–765.

NORMAL ALGEBRA

$$\min \quad J(B, C) = \sum_{i,j} (\mathbf{A}_{ij} - (\mathbf{BC})_{ij})^2$$

$$\text{s.t.} \quad \mathbf{B}_{ij}^2 - \mathbf{B}_{ij} = 0$$

$$\mathbf{C}_{ij}^2 - \mathbf{C}_{ij} = 0$$

$$\sum_{i,j} \left(\mathbf{A}_{ij} - \left(\theta(\mathbf{B} - b)\theta(\mathbf{C} - c)\right)_{ij}\right)^2$$

PROXIMUS

- PROXIMUS uses rank-1 factorisations to make a hierarchical factorisation of the full data
  - Matrix rows are divided into two sets based on the column factor
  - Rank-1 decomposition is applied to those two sets separately (or recursion is stopped)
- Ensures that columns of ***B*** don't overlap ⇒ representation is binary

M. Koyutürk, A. Grama, PROXIMUS: a framework for analyzing very high dimensional discrete-attributed datasets, in: KDD '03, 147–156.

RMF AND NMF

Boundedness [1]. If $\boldsymbol{X}$ is a matrix taking values from [0,1] and if $\boldsymbol{X}$ admits a rank-k factorisation to nonnegative matrices, then there exists a nonnegative rank-k factorisation such that no value in the factor matrices is larger than 1.

[1] Z.-Y. Zhang et al., Binary matrix factorization for analyzing gene expression data, *Data Min. Knowl. Discov.* 20 (2010) 28–52.

NON-LINEAR PROGRAMMING

$$\begin{aligned} \min \quad & J(B, C) = \sum_{i,j} (\mathbf{A}_{ij} - (\mathbf{BC})_{ij})^2 \\ \text{s.t.} \quad & \mathbf{B}_{ij}^2 - \mathbf{B}_{ij} = 0 \\ & \mathbf{C}_{ij}^2 - \mathbf{C}_{ij} = 0 \end{aligned}$$

Solved by minimising (alternatively for ***B*** and ***C***):

$$\sum_{i,j} (\mathbf{A}_{ij} - (\mathbf{BC})_{ij})^2 + \frac{1}{2}\lambda\big((\mathbf{B}_{ij}^2 - \mathbf{B}_{ij}) + (\mathbf{C}_{ij}^2 - \mathbf{C}_{ij})\big)$$

Z.-Y. Zhang et al., Binary matrix factorization for analyzing gene expression data, *Data Min. Knowl. Discov.* 20 (2010) 28–52.

THRESHOLD METHOD

- Change the objective to $\sum_{i,j}\left(\mathbf{A}_{ij} - \left(\theta(\mathbf{B} - b)\theta(\mathbf{C} - c)\right)_{ij}\right)^2$
  - $\theta(\boldsymbol{X})$ is the (element-wise) Heaviside function
- Can be optimised using gradient descent after the Heaviside is replaced with $\phi(x) = 1/\left(1 + e^{-\lambda x}\right)$

Z.-Y. Zhang et al., Binary matrix factorization for analyzing gene expression data, *Data Min. Knowl. Discov.* 20 (2010) 28–52.

BOOLEAN ALGEBRA

Images by Wikipedia users Arab Ace and Sheilalau

THE BOOLEAN PROJECTION

- Peleg's algorithm approximates within $2\sqrt{[(k+a(\log a)]}$ [1]
  - a is the maximum number of 1s in ***A***'s columns
- Optimal solution
  - Either an $O(2^k knm)$ exhaustive search [1], or an integer program [2]
- Greedy algorithm: select each column of ***B*** if it improves the residual error [1]

[1] M., *Matrix Decomposition Methods for Data Mining: Computational Complexity and Algorithms*, PhD thesis, U. Helsinki, 2009.
[2] H. Lu et al., Optimal Boolean Matrix Decomposition: Application to Role Engineering, in: ICDE '08, 297–306.

THE ASSO ALGORITHM

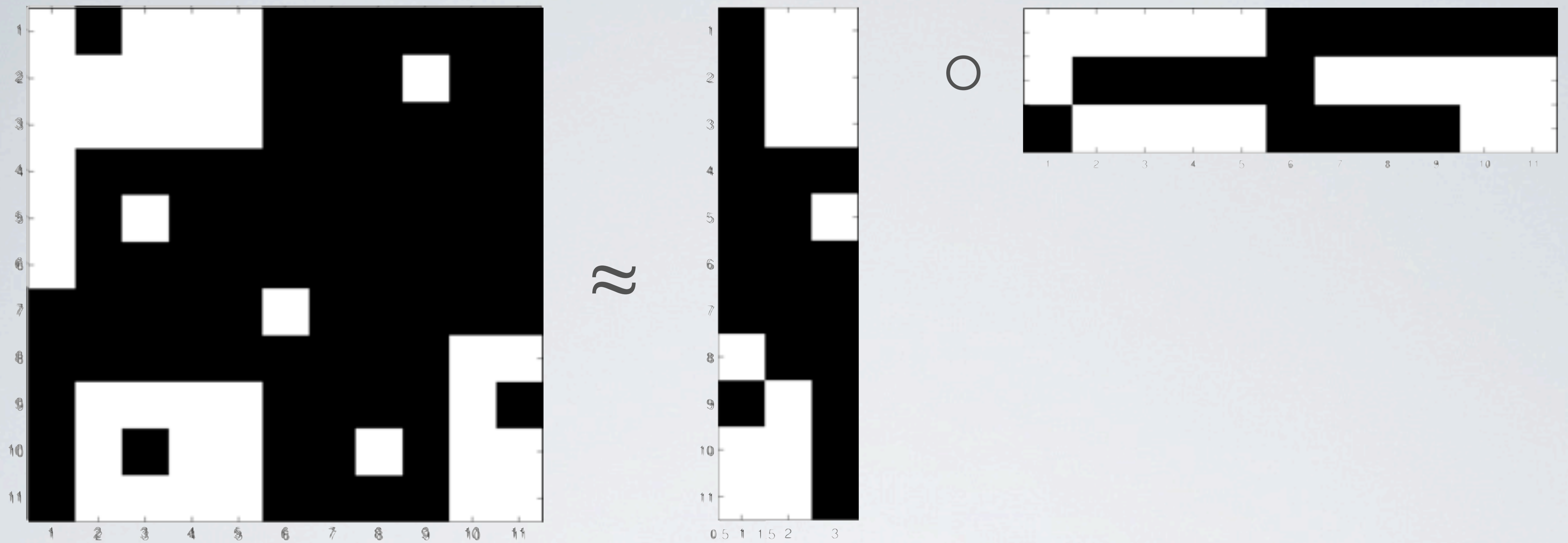
- Heuristic – too many hardness results to hope for good provable results in any case
- **Intuition**: If two columns share a factor, they have 1s in same rows
  - Noise makes detecting this harder
  - Pairwise row association rules reveal (some of) the factors

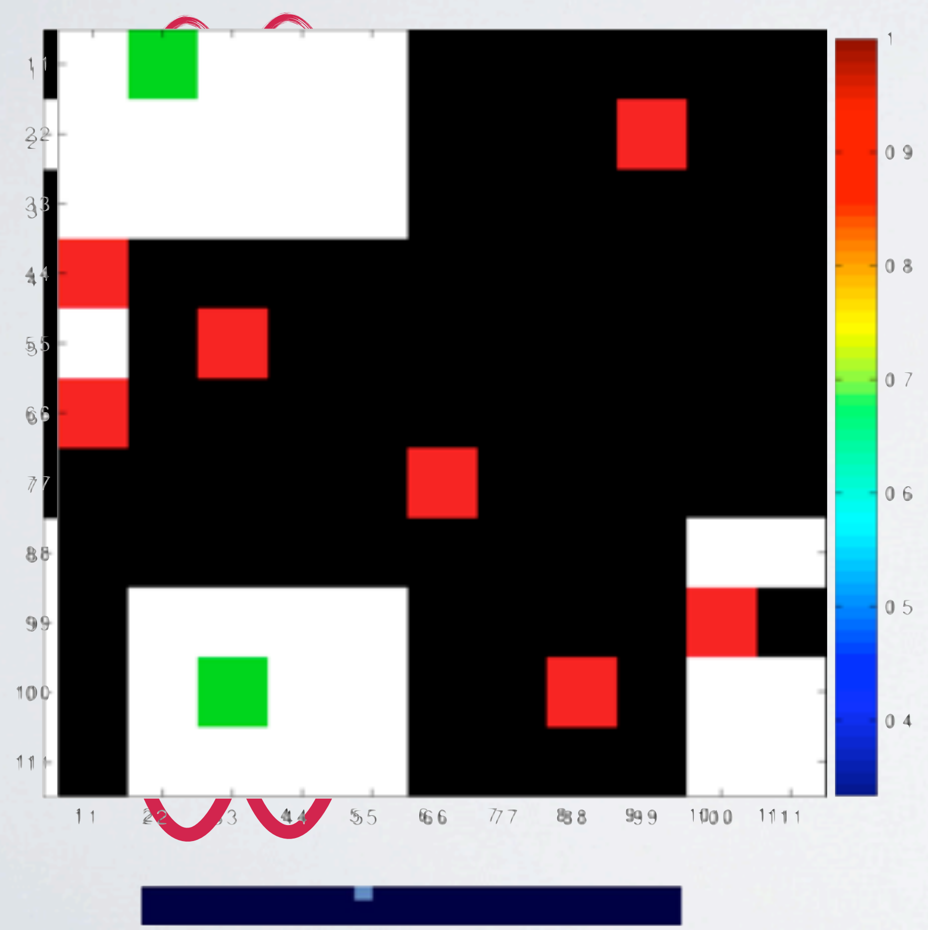
M. et al., The Discrete Basis Problem, *IEEE Trans. Knowl. Data En.* 20 (2008) 1348–1362.

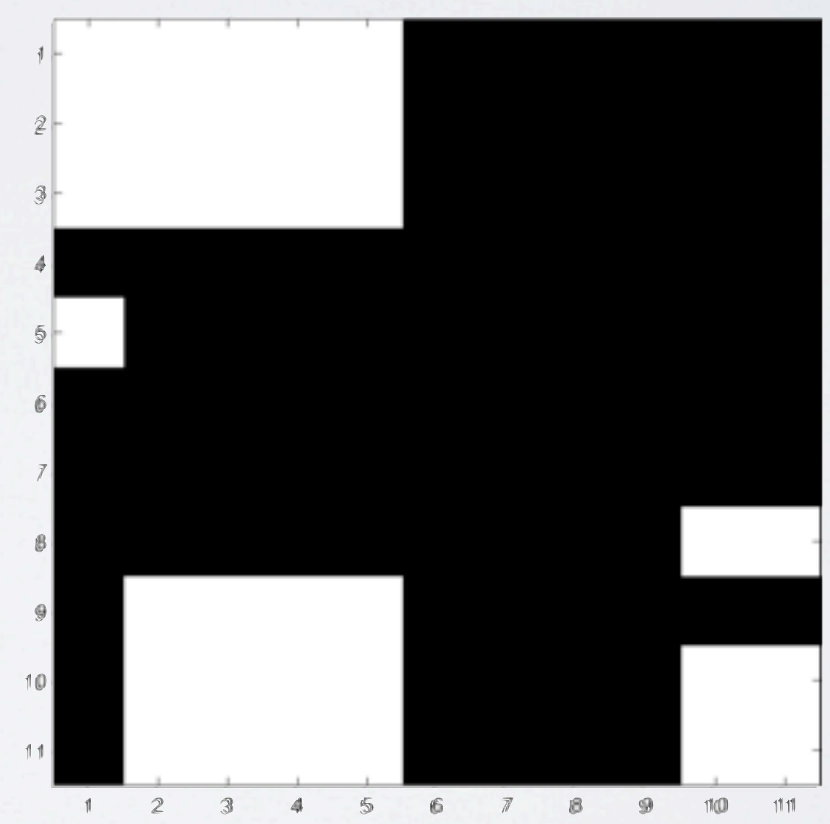
THE ASSO ALGORITHM

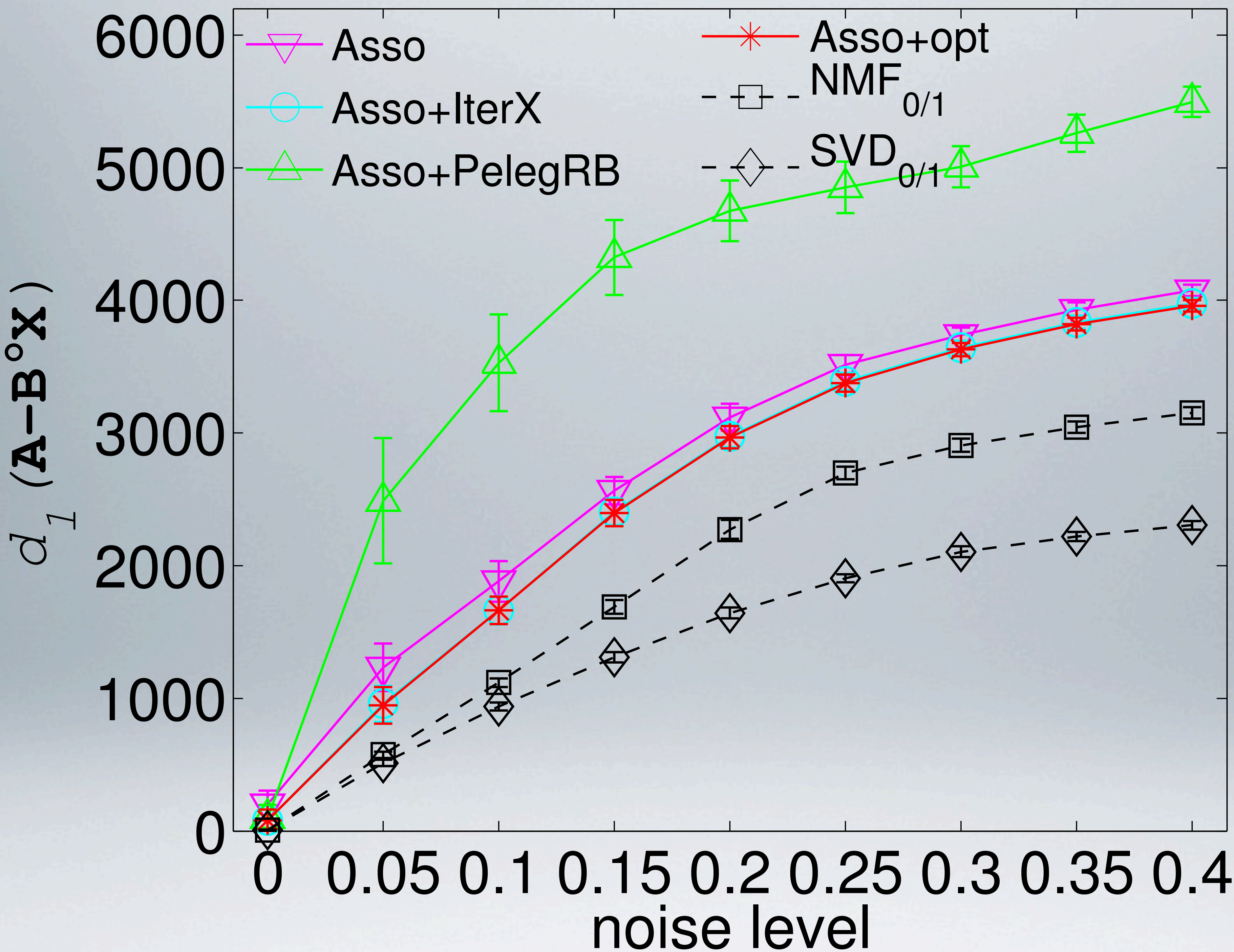
1. Compute pairwise association accuracies between rows of **A**
2. Round these (from a user-defined point *t*) to get a binary *n*-by-*n* matrix of candidate columns
3. Select greedily the candidate column that covers most of the not-yet covered 1s of **A**
4. Mark the 1s covered by the selected vector and return to 3 or quit if enough factors have been selected

M. et al., The Discrete Basis Problem, *IEEE Trans. Knowl. Data En.* 20 (2008) 1348–1362.









M., *Matrix Decomposition Methods for Data Mining: Computational Complexity and Algorithms*, PhD thesis, U. Helsinki, 2009, p. 72.

THE PANDA ALGORITHM

- **Intuition**: every good factor has a noise-free core
- Two-phase algorithm:
    1. Find error-free core pattern (maximum area itemset/tile)
    2. Extend the core with noisy rows/columns
- The core patterns are found using a greedy method
    - The 1s already belonging to some factor/tile are removed from the residual data where the cores are mined

C. Lucchese et al., Mining Top-K Patterns from Binary Datasets in presence of Noise, in: SDM '10, 165–176.

EXTENDING CORES IN PANDA

- The cores are extended in a greedy manner
  - A new column is added to a row factor in ***c***
  - All rows not yet in the corresponding column factor ***b*** are tried
- As extending a core always covers some 0s, the quality is decided by trying to minimise the number of 1s in factors ***b*** and ***c*** plus the noise

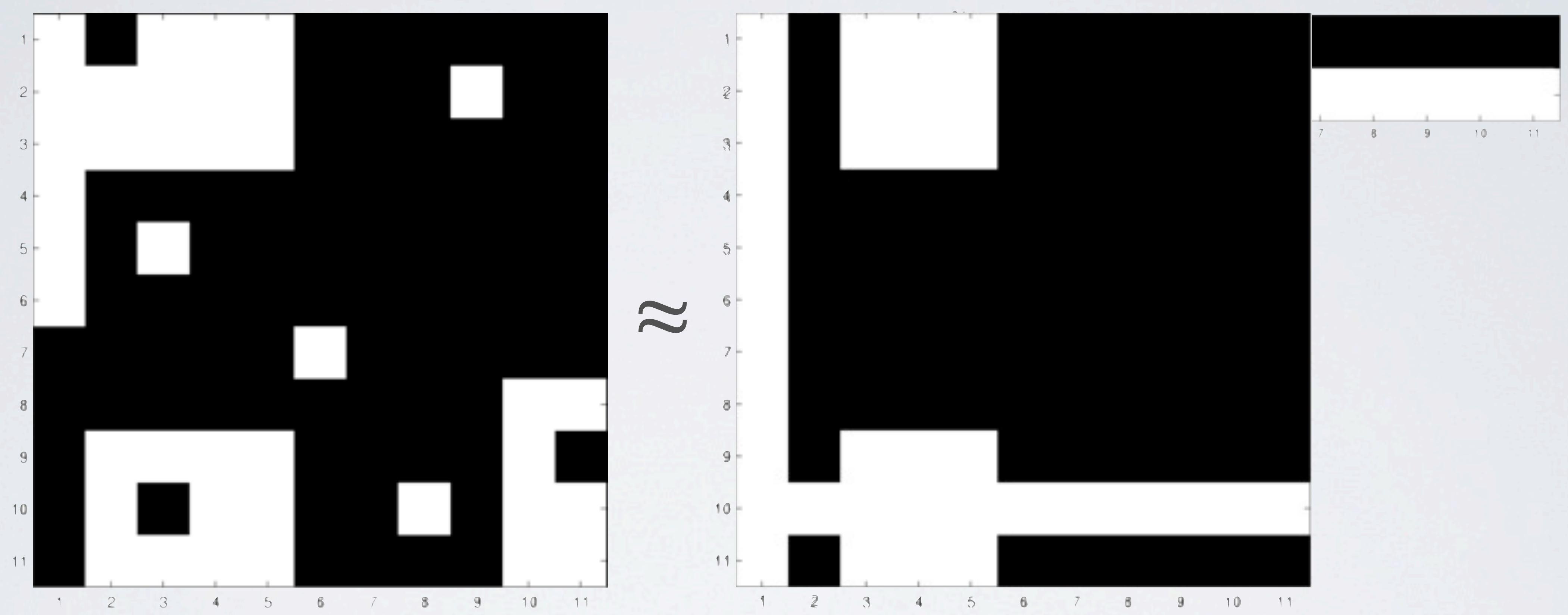
C. Lucchese et al., Mining Top-K Patterns from Binary Datasets in presence of Noise, in: SDM '10, 165–176.

NOTES ON PANDA

- Can automatically choose the rank of the decomposition
  - Parameter-free
- Uses sorting to speed up the computation
  - Consider the most promising candidates first
- Can be randomised

C. Lucchese et al., Mining Top-K Patterns from Binary Datasets in presence of Noise, in: SDM '10, 165–176.

EXAMPLE



MODULO-2 ALGEBRA

X

NO SPECIAL ALGORITHMS

- That I'm aware of, at least
- One could truncate any rank-*k* decomposition
  - No guarantees on quality, might cause more error than the trivial decomposition
  - No Eckart–Young theorem

SELECTING THE RANK

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

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

PRINCIPLES OF GOOD *K*

- **Goal:** Separate noise from structure
- We assume data has correct type of structure
  - There are k factors explaining the structure
  - Rest of the data does not follow the structure (noise)
- But how to decide where structure ends and noise starts?

WHAT HAS BEEN DONE BEFORE?

- Model order selection for matrix factorisations is studied before (mostly with SVD/PCA)
- Methods such as Guttman–Kaiser criterion [see 1] or Cattell's scree test [2] are not very good
  - Poor performance and need for subjective decisions

[1] K.A. Yeomans, P.A. Golder, The Guttman–Kaiser criterion as a predictor of the number of common factors, *The Statistician* 31 (1982) 221–229.
[2] R.B. Cattell, The Scree Test For The Number Of Factors, *Multivar. Behav. Res.* 1 (1966) 245–276.

CROSS VALIDATION

- Idea: hold part of the data, learn a model on the remaining, and fit the model to the withheld data
- Problems with matrix factorisations:
    - If we hold out only rows (or columns), no cost for fitting higher-order factorisations
    - If we hold out both, fitting the model becomes hard
    - Bi-cross-validation [1] does that, but requires singular data matrix and optimal projections

[1] A.B. Owen, P.O. Perry, Bi-cross-validation of the SVD and the nonnegative matrix factorization, *Ann. Appl. Stat.* 3 (2009) 564–594.

MINIMUM TRANSFER COST PRINCIPLE

- A variation of cross validation
- The withheld rows are mapped to their closest pairs in training data
    - For evaluation, the rows are represented using the representation of their pairs in training data
      ⇒ Penalises for over-fitting

M. Frank et al., The Minimum Transfer Cost Principle for Model-Order Selection, in: ECML PKDD '11, 423–438.

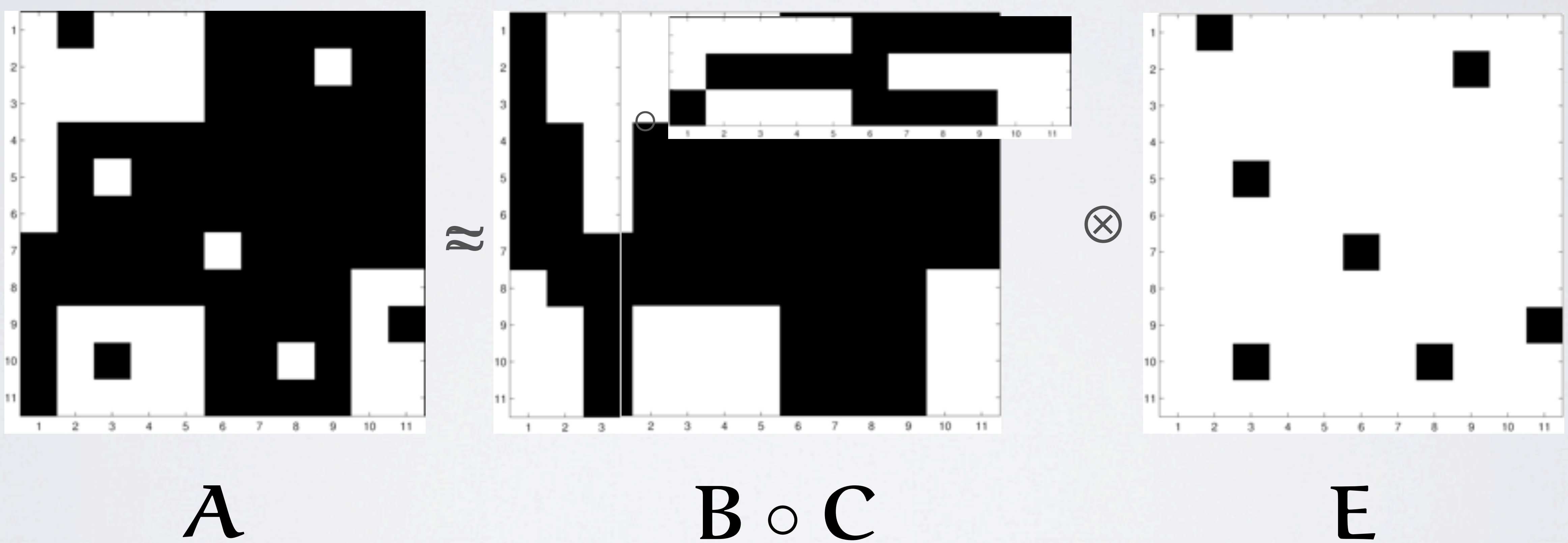
MINIMUM DESCRIPTION LENGTH PRINCIPLE

- The best model (order) is the one that allows you to explain your data with least number of bits
  - Two-part (crude) MDL: the cost of model $L(\mathcal{H})$ plus the cost of data given the model $L(D \mid \mathcal{H})$
- Problem: how to do the encoding
  - Has been done for BMF [1], similar encodings work for other binary factorisations

[1] M., J. Vreeken, Model Order Selection for Boolean Matrix Factorization, in: KDD '11, 51–59.

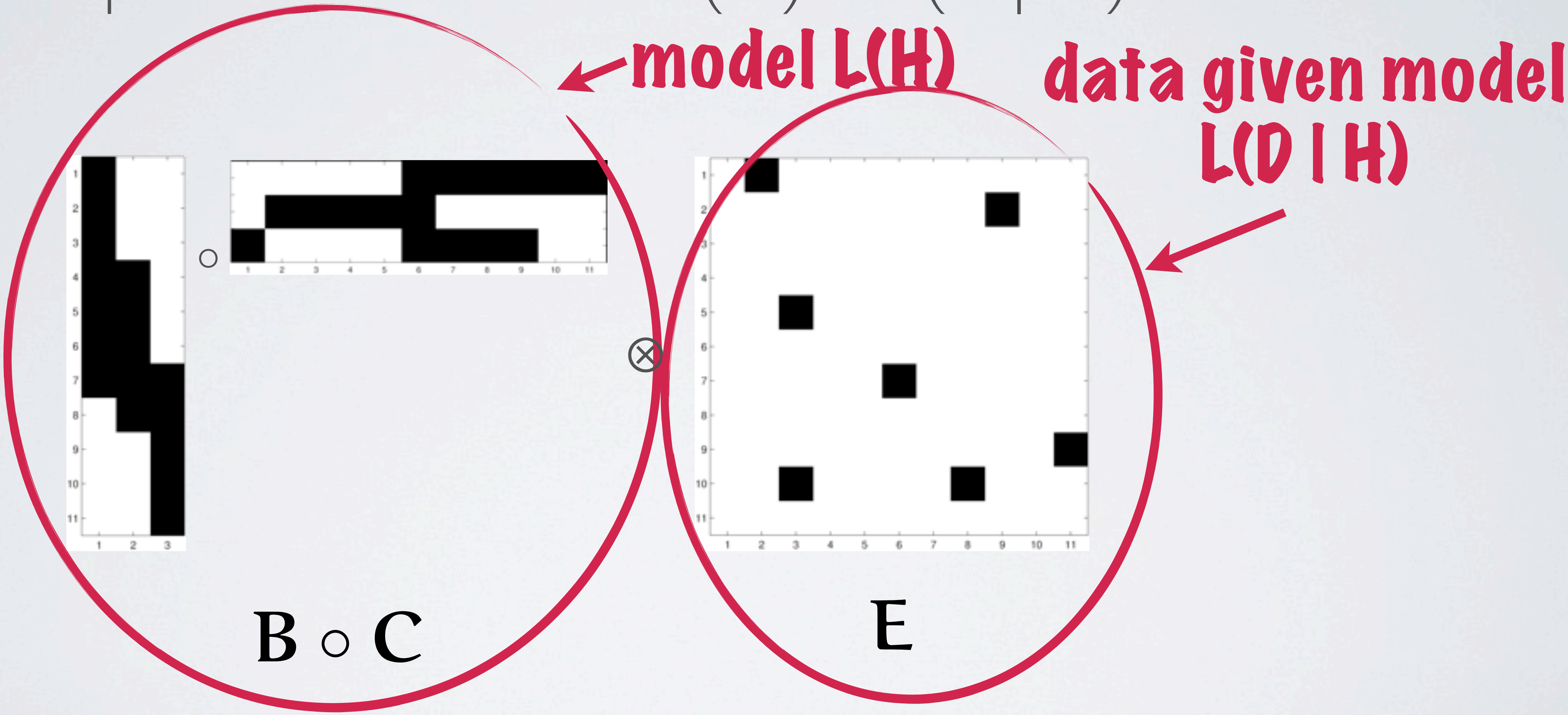
FITTING BMF TO MDL

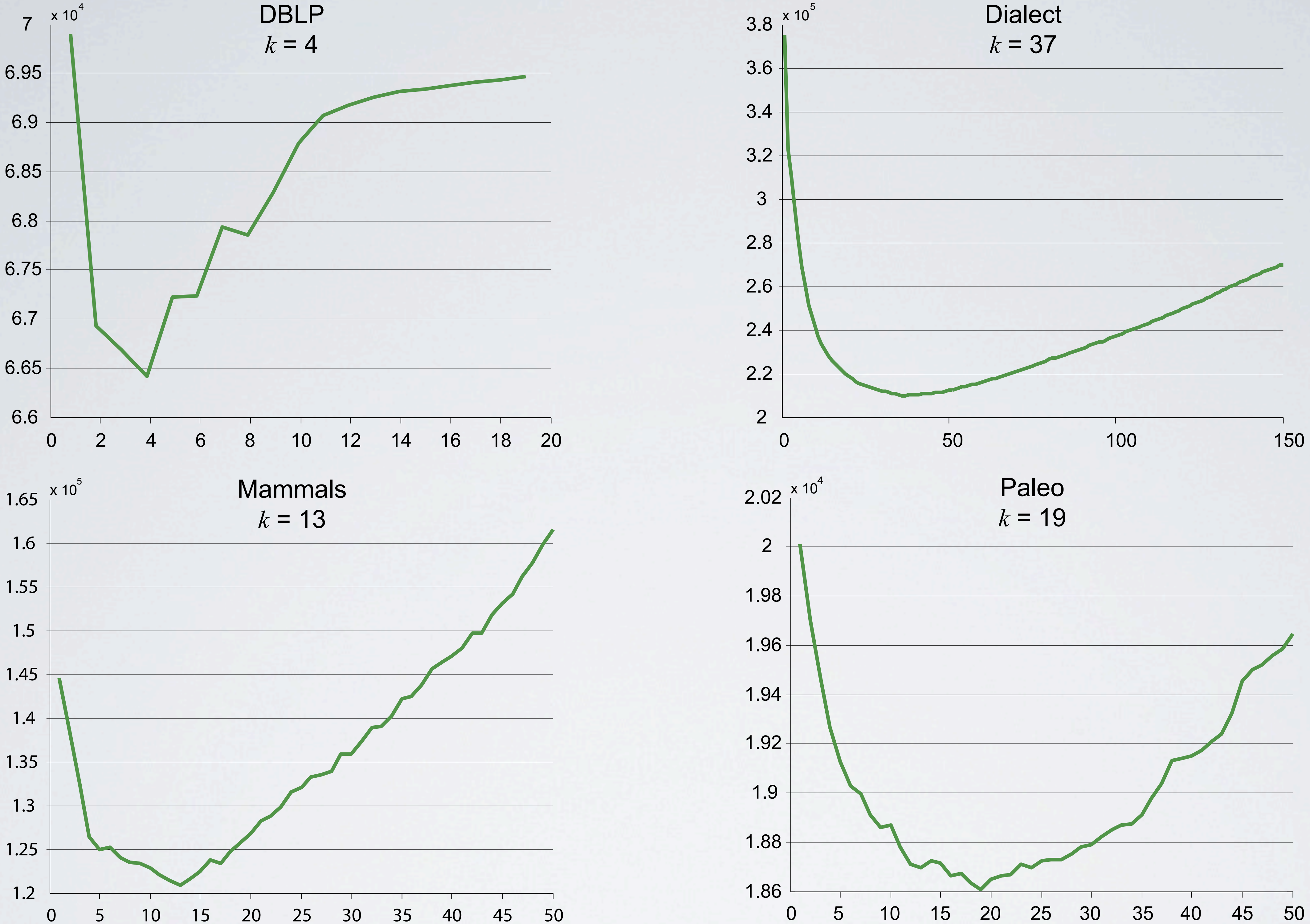
- MDL requires exact representation



FITTING BMF TO MDL

- Two-part MDL: minimise $L(\mathcal{H}) + L(D \mid \mathcal{H})$





EXAMPLE: ASSO & MDL

M., J. Vreeken, Model Order Selection for Boolean Matrix Factorization, in: KDD '11, 51–59.

SPARSE MATRICES

MOTIVATION

- Many real-world binary matrices are sparse
- Representing sparse matrices with sparse factors is desirable
  - Saves space, improves usability, …
- Sparse matrices should be computationally easier

SPARSE FACTORISATIONS

- Any binary matrix ***A*** that admits rank-*k* BMF has factorisation to matrices ***B*** and ***C*** such that the total number of 1s in ***B*** and ***C*** is at most twice that of ***A*** [1]
  - Can be extended to approximate factorisations
  - Tight result (consider a case when ***A*** has exactly one 1)
  - Holds also for exact RMF factorisations

[1] M., Sparse Boolean Matrix Factorizations, in: ICDM '10, 935–940.

APPROXIMATING THE BOOLEAN RANK

- Recall: we have log(*n*) approximation given an oracle
- We say *n*-by-*m* binary matrix ***A*** is log(*n*) uniformly sparse if each column of A has at most log(*n*) 1s

Theorem [1]**.** The Boolean rank of a log(*n*) uniformly sparse binary matrix A can be approximated within log(*n*).

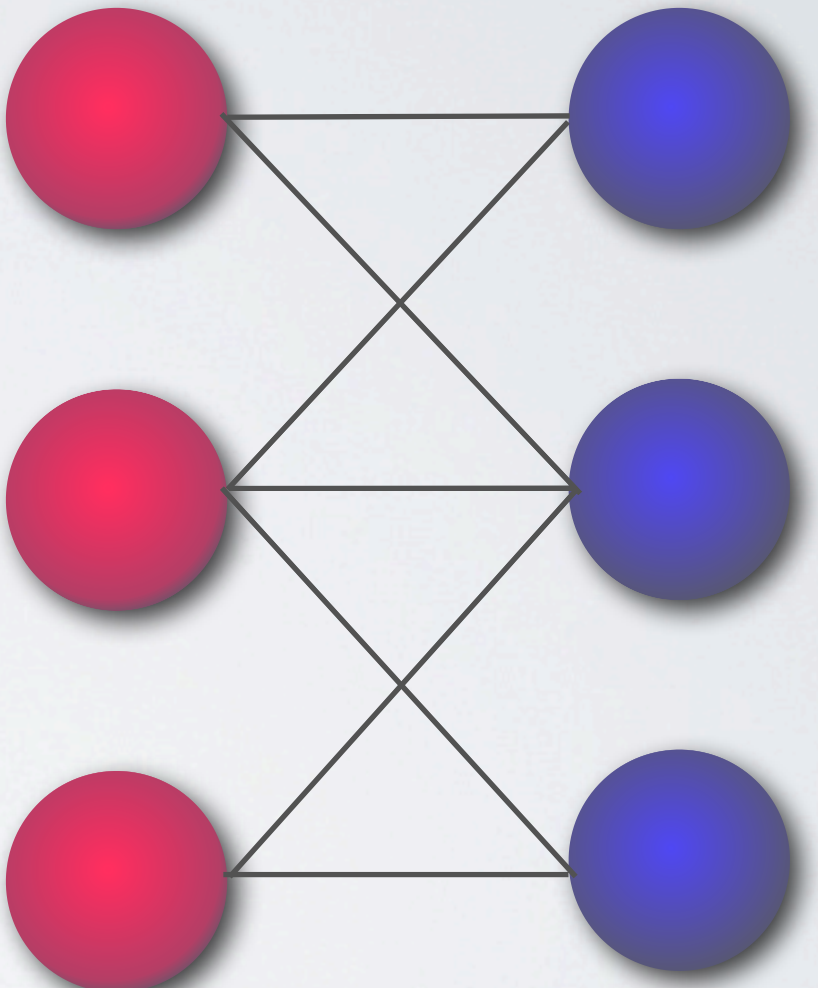
[1] M., Sparse Boolean Matrix Factorizations, in: ICDM '10, 935–940.

PROOF

- Each RHS node has ≤ log(n) neighbours
  ⇒ Optimum solution needs

  ≥ n/log(n) bicliques

- If we use n bicliques we get
  n/OPT ≤ n/(n/log(n))
  = log(n) □



EXTENSIONS

- We can approximate the Maximum k-tiling for $\log(n)$ uniformly sparse matrices within $e/(e-1)$
- If we have at most $\log(n)$ columns that have more than $\log(n)$ 1s, we can still approximate the rank within $\log^2(n)$
  - Both results require more complex reduction to the Set Cover problem [1]
  - Will also work on dense matrices, but will take exponential time

[1] R. Bělohlávek, V. Vychodil, Discovery of optimal factors in binary data via a novel method of matrix decomposition, *J. Comput. Syst. Sci.* 76 (2010) 3–20.

OPEN PROBLEMS

?

ALGORITHMS

- **P2.1** Are there good algorithms for XMF?
- **P2.2** Can we use the sparsity to really help us?

MODEL ORDER SELECTION

- **P2.3** How hard is it to minimise the MDL score directly?
  - Depends on the encoding, obviously
- **P2.4** Can we use binary methods to predict missing values and would these be better than continuous methods?


PP/poly
P^{#P[1]}
BP.PP
MP
PH
SF_4
Sigma_3P
AmpMP
1
2
3
The End
SUBEXP
P^{FewP}
QP
Few
EP
EQP
betaP
QPLIN
FewP
BPP

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Image by Lars Aronsson, Wikipedia

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