Symmetric Nonnegative Trifactorization

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Algebraic Graph Theory Seminar

Decompositions

Singular Value Decomposition	Nonnegative Matrix Factorization
$A \in \mathbb{R}^{n\times m}(\mathbb{C}^{n\times m})$	$A \in \mathbb{R}_+^{n\times m}$
$A = U\Sigma V^\top = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$	$A = WH^\top = \sum_{i=1}^{t} \mathbf{w}_i \mathbf{h}_i^\top$
U, V are orthogonal	$W \in \mathbb{R}_+^{n\times t}$, $H \in \mathbb{R}_+^{m\times t}$
Spectral Decomposition	SN-Trifactorization
$A \in \mathbb{R}^{n\times n}$, $A = A^\top$	$A \in \mathbb{R_+}^{n\times n}$, $A = A^\top$
$A = UDU^\top$	$A = BCB^\top$
U orthogonal, D diagonal	$B \in \mathbb{R}_+^{n\times k}$, $C \in \mathcal{S}_k^+$
Cholesky Decomposition	Completely Positive Factorization
$A \in \mathbb{R}^{n\times n}$	$A \in \mathbb{R_+}^{n\times n}$
positive definite	completely positive
$A = LL^\top$	$A = BB^\top$
L lower triangular	$B \in \mathbb{R}_+^{n\times k}$

$\mathbb{R}_+$ - nonnegative real numbers,

$\mathcal{S}_k^+$ -$k \times k$ symmetric nonnegative matrices

Boolean Rank

The *pattern matrix* of $A \in \mathbb{R}_+^{n\times m}$ is defined by

$$\mathrm{sign}(A)_{ij} = \begin{cases} 1; & \text{if } a_{ij} > 0, \\ 0; & \text{if } a_{ij} = 0. \end{cases}$$

Factorization:

$$\mathrm{sign}(A) = W_{0,1} H_{0,1}^\top$$

- $W_{0,1} \in \{0,1\}^{n\times t}$, $H \in \{0,1\}^{m\times t}$
- Boolean arithmetic $(1+1=1)$

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

The Boolean rank of A, denoted by $\mathrm{rk}_{0,1}(A)$, is the minimal t for which such factorization exists.

Exact NMF

$A \in \mathbb{R}_{+}^{n \times m}$

$$A = WH^{\top} = \sum_{i=1}^{t} \mathbf{w}_i \mathbf{h}_i^{\top}$$

- $W \in \mathbb{R}_{+}^{n \times t}$, $H \in \mathbb{R}_{+}^{m \times t}$

$\mathrm{rk}_{+}(A)$ is a minimal t for which such decomposition exists.

$$\mathrm{rk}_{+}(A) \geq \mathrm{rk}_{0,1}(A)$$

Approximate NMF

$$\min\{\|A - WH^\top\|_F\,;\, W \in \mathbb{R}_+^{n\times t}, H \in \mathbb{R}_+^{m\times t}\}$$

- Introduced by Paatero and Tapper in 1994.
- Popularised by Lee and Seung in 1999.
- Central in applications to analyse nonnegative data.

Nonnegativity, Symmetry and Rank

- $\mathbb{R}_+$ - the set of nonnegative real numbers
- $\mathcal{S}_n^+ = \{A \in \mathbb{R}_+^{n\times n}; A = A^T\}$

SN-Trifactorization of $A \in \mathcal{S}_n^+$:

$$A = BCB^\top,\ B \in \mathbb{R}_+^{n\times k}, C \in \mathcal{S}_k^+$$

Minimal possible k in such factorization is called the *SNT-rank* of A, and denoted by $\mathrm{st}_+(A)$.

$$\begin{pmatrix} 0 & 2 & 0 & 6 \\ 2 & 0 & 1 & 2 \\ 0 & 1 & 0 & 3 \\ 6 & 2 & 3 & 12 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 1 \\ 1 & 0 \\ 2 & 3 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 2 & 0 & 1 & 2 \\ 0 & 1 & 0 & 3 \end{pmatrix}$$

Approximate SN-Trifactorization

tri-symNMF is an approximate version of SN-Trifactorization:

$$A \in \mathcal{S}_n^+,\ A \approx BCB^\top,\ B \in \mathbb{R}_+^{n\times k}, C \in \mathcal{S}_k^+$$

- the columns of B identify communities (highly correlated items in the data set)
- communities interact via C (the entries of C represent the strength of connection between communities)

$\mathrm{st}_+(A)$ vs $\mathrm{rk}(A)$

- $\mathrm{rk}(A) \leq \mathrm{st}_+(A) \leq n$
- If $\mathrm{rk}(A) = 2$ then $\mathrm{st}_+(A) = 2$.
- $\mathrm{rk}(A) = 3$, $\mathrm{st}_+(A)$ cannot be bounded by a constant independent of n.

$\mathrm{st}_+(A)$ vs $\mathrm{rk}_+(A)$

$$\mathrm{rk}_+(A) \leq \mathrm{st}_+(A) \leq 2\,\mathrm{rk}_+(A)$$

Separable NMF: The columns of the first factor in $A = WH^\top$ are chosen from the columns of A.

$$P^\top AP = \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} \begin{pmatrix} I_k & Q \end{pmatrix},$$

P is a permutation matrix, $Q \in \mathbb{R}_+^{k \times (n-k)}$. Then: $\mathrm{st}_+(A) \leq k$.

$\mathrm{rk}_+(A) \neq \mathrm{st}_+(A)$

$$A = \begin{pmatrix} 1 & 1 & 2 & 2 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 2 & 2 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 2 \end{pmatrix}$$

$$= \begin{pmatrix} x+1 & y & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ x & y+1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & u \\ 1 & 0 & v \\ u & v & w \end{pmatrix} \begin{pmatrix} x+1 & 1 & 0 & x \\ y & 0 & 1 & y+1 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 2u(x+1)+2y(v+x+1)+w & u+y & v+x+1 & * \\ u+y & 0 & 1 & * \\ v+x+1 & 1 & 0 & * \\ * & * & * & * \end{pmatrix}$$

$$u = 1-y,\ v = 1-x \Rightarrow w = 2(1-x)(1-y) - 3 < 0$$

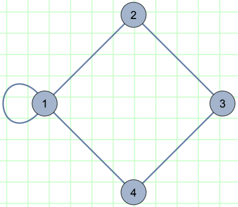
Minimal SNT-rank of graphs

$A \in \mathcal{S}_n^+$.

- The pattern graph $G(A) = (V(G), E(G))$ of A:
  - $V(G) = \{1, \ldots, n\}$,
  - $\{i, j\} \in E(G)$ iff $a_{ij} > 0$.

$G(A)$ is a simple graph with loops.

$$\mathrm{sign}(A) = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}, \quad G(A):$$



$\mathcal{S}^+(G)$: set of all matrices in $\mathcal{S}_n^+$ with the pattern graph G

$\mathrm{st}_+(G) = \min\{\mathrm{st}_+(A); A \in \mathcal{S}^+(G)\}$

Set-join

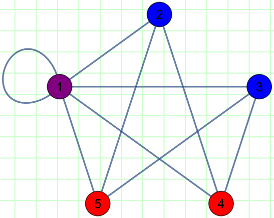
$\mathcal{S}$ a finite set, $\mathcal{K}, \mathcal{L} \subseteq \mathcal{S}$

The set-join of $\mathcal{K}$ and $\mathcal{L}$ on $\mathcal{S}$, denoted by $\mathcal{K} \vee_{\mathcal{S}} \mathcal{L}$ is the graph with

- $V(\mathcal{K} \vee_{\mathcal{S}} \mathcal{L}) = \mathcal{S}$,
- $E(\mathcal{K} \vee_{\mathcal{S}} \mathcal{L}) = \{\{i,j\}; i \in \mathcal{K}, j \in \mathcal{L}\}$

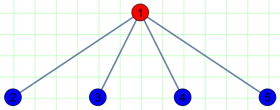
$\mathcal{S} = \{1,2,3,4,5\}$, $\mathcal{K} = \{1,2,3\}$, $\mathcal{L} = \{1,4,5\}$

$\mathcal{K} \vee_{\mathcal{S}} \mathcal{L}$:

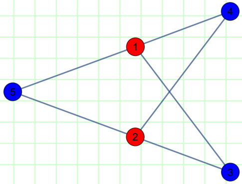


Set-Joins: Familiar Examples

- Stars: $\{v\} \vee \mathcal{K}$



- Complete bipartite graphs: $\mathcal{L} \vee \mathcal{K}$, $\mathcal{L} \cap \mathcal{K} = \emptyset$.



Set-join cover

G a simple graph with loops, $\mathcal{K}_i, \mathcal{L}_i \subseteq V(G)$.

$$\mathscr{C} = \{\mathcal{K}_i \vee_{V(G)} \mathcal{L}_i, i \in [t]\}$$

is a set-join cover of G if $E(G) = \bigcup_{i=1}^{t} E(\mathcal{K}_i \vee_{V(G)} \mathcal{L}_i)$.

The graph $G(\mathscr{C})$:

- the component set: $V(\mathscr{C}) = \{\mathcal{K}_i; i \in [t]\} \cup \{\mathcal{L}_i; i \in [t]\}$
- the order: $|V(\mathscr{C})|$
- $G(\mathscr{C})$ is the graph with
  - $V(G(\mathscr{C})) = V(\mathscr{C})$
  - $\{\mathcal{K}_i, \mathcal{K}_j\} \in E(G(\mathscr{C}))$ if and only if $\mathcal{K}_i \vee_{V(G)} \mathcal{K}_j \in \mathscr{C}$.

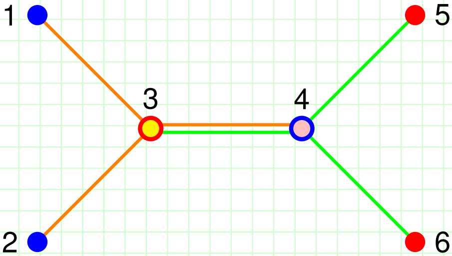
Optimal set-join cover

$$\mathrm{st}_+(G) = \min\{|V(\mathscr{C})|;\ \mathscr{C} \text{ a set-join cover of } G\}.$$

An optimal set-join (OSJ) cover for G is a set-join cover $\mathscr{C}$ of G with $|V(\mathscr{C})| = \mathrm{st}_+(G)$.

We are optimising $|V(\mathscr{C})|$ not $|\mathscr{C}|$.

Example: Set-join cover



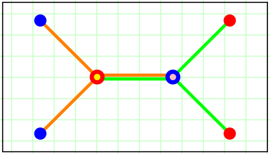
$$B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}, C = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, A = BCB^T = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\mathcal{K}_1 = \{1, 2, 4\}, \mathcal{K}_2 = \{3\}, \mathcal{K}_3 = \{4\}, \mathcal{K}_4 = \{3, 5, 6\}$$

$$\mathscr{C} = \{\mathcal{K}_1 \vee_{[6]} \mathcal{K}_2, \mathcal{K}_3 \vee_{[6]} \mathcal{K}_4\},\ G(\mathscr{C}) = 2K_2,\ |V(\mathscr{C})| = 4$$

$$\mathscr{C}_1 = \{\mathcal{K}_1 \vee_{[6]} \mathcal{K}_2, \mathcal{K}_2 \vee_{[6]} \mathcal{K}_3, \mathcal{K}_3 \vee_{[6]} \mathcal{K}_4\},\ G(\mathscr{C}_1) = P_4,\ |V(\mathscr{C}_1)| = 4$$

Interpretation



$$\mathcal{K}_1 = \{1, 2, 4\}, \mathcal{K}_2 = \{3\}, \mathcal{K}_3 = \{4\}, \mathcal{K}_4 = \{3, 5, 6\}$$

$$\mathscr{C} = \{\mathcal{K}_1 \vee_{[6]} \mathcal{K}_2, \mathcal{K}_3 \vee_{[6]} \mathcal{K}_4\},\ G(\mathscr{C}) = 2K_2$$

- $u, v \in V$ are either required or forbidden to interact: restrictions are recorded in G.
- The interactions are organised by meetings of certain subgroups of V: $\mathcal{K}, \mathcal{L} \subseteq V$ meet $\Rightarrow$ all the items from $\mathcal{K}$ interact with all the items from $\mathcal{L}$.
- What is the minimal number of subgroups that need to be formed, to be able to organise all the desired interactions in such a way that no forbidden interactions occur?

Unique optimal set-join cover

Unique OSJ cover: there is a unique OSJ cover of G of order $\mathrm{st}_{+}(G)$.

Essentially unique OSJ cover: $\mathscr{C}$ and $\mathscr{C}'$ OSJ covers of $G \Rightarrow$ there exists an automorphism $\sigma : V(G) \to V(G)$ of G so that $\sigma(\mathscr{C}) = \mathscr{C}'$.

Unique OSJ cover graph: all OSJ covers $\mathscr{C}$ of G have the same $G(\mathscr{C})$ up to isomorphism of graphs.

Twins

- $v, w \in V(G)$ are called twins if they have the same neighbourhoods.
- A graph G is twin-free, if no pair of vertices in $V(G)$ are twins.
- $F_{tw}(G)$ denotes the biggest twin free sub-graph of G.

$$\mathrm{st}_+(G) = \mathrm{st}_+(F_{tw}(G))$$

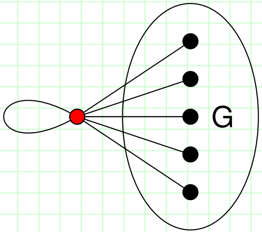
G has unique OSJ cover if and only if $F_{tw}(G)$ has.

Twins can appear in the same components of the cover.

Joins

$\widehat{G} = G \vee K_1^{\ell}$. Then:

$$\mathrm{st}_+(\widehat{G}) = \begin{cases} \mathrm{st}_+(G); & \text{if G has no isolated vertices,} \\ \mathrm{st}_+(H) + 2; & \text{if } G = H \cup tK_1. \end{cases}$$



If G has no isolated vertices, then $\hat{G}$ has unique OSJ cover graph if and only if G has.

The new vertex can be added to all components.

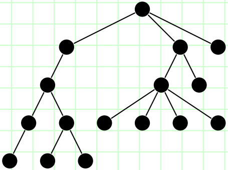
Graphs of OSJ covers

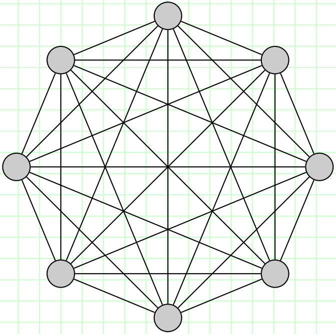
Let $\mathscr{C}$ be an OSJ cover of G. Then:

- $|V(\mathscr{C})| = \mathrm{st}_+(G) = \mathrm{st}_+(G(\mathscr{C}))$.
- $G(\mathscr{C})$ is twin-free.
- G contains a subgraph that is isomorphic to $G(\mathscr{C})$.
- G has a monotone property $P \Rightarrow G(\mathscr{C})$ has a monotone property P.

P: acyclic, triangle free, bipartite, etc.

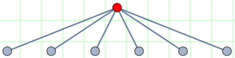
Finding optimal covers





Star Covers

Star: $S = \{v\} \vee \mathcal{K}$



Let G be a simple graph without loops.

- An edge star cover of G is a family of simple stars $\{S_1, S_2, \ldots, S_k\}$ satisfying $E(G) = \cup_{i=1}^{k} E(S_i)$.
- The edge star cover number $\mathrm{star}(G)$ of G is the minimal number of stars in any edge star cover of G.

$$\mathrm{st}_+(G) \leq 2\,\mathrm{star}(G)$$

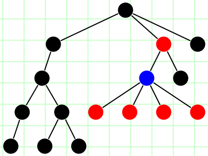
Trees

Let T be a tree (without loops) with $|V(T)| \geq 3$. Then

- $\mathrm{st}_+(T) = 2\,\mathsf{star}(T)$
- T has unique OSJ cover if and only if the distance between any two leaves in T is even.

For $A \in \mathcal{S}^+(T)$:

$$\mathsf{rk}(A) = \mathrm{st}_+(A) = \mathrm{st}_+(T) = 2\,\mathsf{star}(T).$$



Separating Cover

$\mathcal{T}$ - a collection of k subsets of $[n] := \{1, 2, \ldots, n\}$.

$\mathcal{T}$ is called a separating cover of $[n]$ if for any pair $i, j \in [n]$, $i \neq j$, there exists $\mathcal{A}, \mathcal{B} \in \mathcal{T}$ so that $i \in \mathcal{A}$, $j \in \mathcal{B}$ and $\mathcal{A} \cap \mathcal{B} = \emptyset$.

$$n = 9: \quad \mathcal{K}_1 = \{1, 2, 3\}, \qquad \mathcal{L}_1 = \{1, 4, 7\}$$
$$\mathcal{K}_2 = \{4, 5, 6\}, \qquad \mathcal{L}_2 = \{2, 5, 8\}$$
$$\mathcal{K}_3 = \{7, 8, 9\}, \qquad \mathcal{L}_3 = \{3, 6, 9\}$$

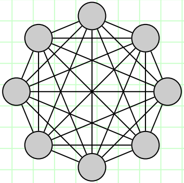
OSJ Cover of Complete Graphs

If $\mathscr{C}$ is a set-join cover of K_n, then $V(\mathscr{C})$ is a separating cover of n elements with $|V(\mathscr{C})|$ sets.

The minimal number of sets in a separating cover of n elements is equal to $\mathrm{st}_+(K_n)$.

$$n = 9: \ \mathcal{K}_1 = \{1, 2, 3\}, \qquad \mathcal{L}_1 = \{1, 4, 7\}$$
$$\mathcal{K}_2 = \{4, 5, 6\}, \qquad \mathcal{L}_2 = \{2, 5, 8\}$$
$$\mathcal{K}_3 = \{7, 8, 9\}, \qquad \mathcal{L}_3 = \{3, 6, 9\}$$

$$\mathscr{C} = \{\mathcal{K}_i \vee \mathcal{K}_j, \mathcal{L}_i \vee \mathcal{L}_j, i \neq j\}$$



Katona's Problem

G.O.H. Katona, 1973: What is the minimal number of sets in a separating cover of n elements? Determine $\mathrm{st}_+(K_n)$.

A. C. C. Yao, 1976 and M. C. Cai, 1984

$$\mathrm{st}_+(K_n) = \begin{cases} 3i & \text{for } 2 \cdot 3^{i-1} < n \leq 3^i, \\ 3i+1 & \text{for } 3^i < n \leq 4 \cdot 3^{i-1}, \\ 3i+2 & \text{for } 4 \cdot 3^{i-1} < n \leq 2 \cdot 3^i. \end{cases}$$

$6 < n \leq 9$	$\mathrm{st}_+(K_n) = 6$
$9 < n \leq 12$	$\mathrm{st}_+(K_n) = 7$
$12 < n \leq 18$	$\mathrm{st}_+(K_n) = 8$
$18 < n \leq 27$	$\mathrm{st}_+(K_n) = 9$

Asymptotically: $\mathrm{st}_+(K_n) \sim \frac{3}{\log 3} \log n$, ($\mathrm{rk}_{0,1}(K_n) \sim \frac{1}{\log 2} \log n$).

$\mathrm{st}_+(K_n)$

$$\mathrm{st}_+(K_n) = \begin{cases} 3i & \text{if } 2 \cdot 3^{i-1} < n \leq 3^i \\ 3i+1 & \text{if } 3^i < n \leq 4 \cdot 3^{i-1} \\ 3i+2 & \text{if } 4 \cdot 3^{i-1} < n \leq 2 \cdot 3^i \end{cases}$$

$$= \min \left\{ \sum_{i=1}^{t} q_i ; n \leq \prod_{i=1}^{t} q_i,\ q_i \in \mathbb{N} \right\}$$

$$= \min \left\{ k + \mathrm{st}_+ \left(K_{\lceil \frac{n}{k} \rceil} \right) ; k = 2, 3, 4, 5 \right\}.$$

Constructing separating covers of $\{1, 2, \dots, n\}$

$n = p \cdot q$ with $p, q \geq 2$

- $\mathcal{K}_i = \{(i-1)p + s; s = 1, \dots, p\}$ for $i \in \{1, 2, \dots, q\}$
- $\mathcal{L}_j = \{j + tp; t = 0, \dots, q-1\}$ for $j \in \{1, 2, \dots, p\}$

$\mathcal{K}_1 = \{1, 2, \dots, p\}$

$\mathcal{K}_2 = \{p+1, \dots, 2p\}$

$\vdots$

$\mathcal{K}_q = \{(q-1)p + 1, \dots, q \cdot p\}$

$\mathcal{L}_1 = \{1, 1+p, 1+2p, \dots, 1+(q-1)p\}$

$\mathcal{L}_2 = \{2, 2+p, \dots, 2+(q-1)p\}$

$\vdots$

$\mathcal{L}_p = \{p, 2p, \dots, q \cdot p\}$

$$\mathscr{C} = \{\mathcal{K}_i \vee_{[n]} \mathcal{K}_j, i, j \in [q], i \neq j\} \cup \{\mathcal{L}_i \vee_{[n]} \mathcal{L}_j, i, j \in [p], i \neq j\}$$

$\mathscr{C}$ is a set-join of K_n with $G(\mathscr{C}) = K_p \cup K_q \Rightarrow \mathrm{st}_+(K_n) \leq p + q$.

Co-normal products of graphs

Co-normal product of $G * H$:

- $V(G * H) = V(G) \times V(H)$
- $E(G * H) = \{\{(g,h),(g',h')\}; \{g,g'\} \in E(G) \text{ or } \{h,h'\} \in E(H)\}$.

$$\mathrm{st}_+(G * H) \leq \mathrm{st}_+(G) + \mathrm{st}_+(H)$$

Complete graphs - uniquness

$\mathrm{st}_+(K_6) = 5$, K_6 has essentially unique OSJ cover.

$\mathrm{st}_+(K_4) = 4$, K_4 has two essentially different OSJ covers:

- a cover where all the components are singletons
- $\mathcal{C} = \{\{1,2\} \vee_{[4]} \{3,4\}, \{1,3\} \vee_{[4]} \{2,4\}\}$

The graph K_n has essentially unique OSJ cover if and only if

- $n = 3^i$ for some $i \geq 1$,
- $n = 2 \cdot 3^i$ for some $i \geq 1$,
- $n = 3^i - 1$ for some $i \geq 3$, or
- $n = 2 \cdot 3^i - 1$ for some $i \geq 2$.

Thank you!

- *Symmetric nonnegative matrix trifactorization*, *Linear Algebra Appl.*, 2023. (10.1016/j.laa.2023.01.027)
- *Symmetric Nonnegative Trifactorization of Pattern Matrices* (https://arxiv.org/abs/2308.12399)

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