Algebraic Sparse Factor Analysis

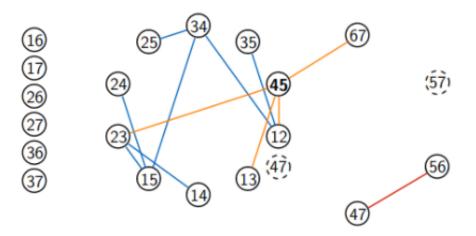
International Congress on Mathematical Software 2024

Classical Algebraic Geometry and Modern Computer Algebra: Innovative Software Design and its Applications

İrem Portakal (🌖

Max Planck Institute for Mathematics in the Sciences Leipzig

(joint work with Mathias Drton, Alexandros Grosdos and Nils Sturma)



Factor Analysis Models

Graph $G = (V \cup \mathcal{H}, E)$, only edges from latent to observed variables. Usually, V = [p]. The factor analysis model postulates that the observed variables are linear functions of the factors and noise, i.e., $X_V = \Lambda X_H + \varepsilon$.



• Covariance matrix:

$$\mathsf{Cov}\left[\begin{pmatrix} X_V \\ X_{\mathcal{H}} \end{pmatrix}\right] = (I - \Lambda)^{-1} \Omega (I - \Lambda)^{-\top} = \begin{pmatrix} \Omega_{VV} + \Lambda_{V\mathcal{H}} \Omega_{\mathcal{H}\mathcal{H}} \Lambda_{V\mathcal{H}}^\top & \Lambda_{V\mathcal{H}} \Omega_{\mathcal{H}\mathcal{H}} \\ \Omega_{\mathcal{H}\mathcal{H}} \Lambda_{V\mathcal{H}}^\top & \Omega_{\mathcal{H}\mathcal{H}} \end{pmatrix}$$

• Observed covariance matrix (projection):

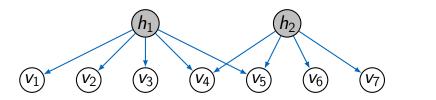
$$Cov[X_V] = \Omega_{VV} + \Lambda_{VH}\Omega_{HH}\Lambda_{VH}^{\top}$$

Observed covariance model:

$$F_G = \{ \Sigma := \widetilde{\Omega} + \widetilde{\Lambda} \widetilde{\Lambda}^\top \in \mathbb{R}^{|V| \times |V|} : \widetilde{\Omega} > 0 \text{ diagonal, } \widetilde{\Lambda} \in \mathbb{R}^{E_{VH}} \}$$

Factor Analysis Models

Graph $G = (V \cup \mathcal{H}, E)$, only edges from latent to observed variables. Usually, V = [p]. The factor analysis model postulates that the observed variables are linear functions of the factors and noise, i.e., $X_V = \Lambda X_H + \varepsilon$.



$$\Lambda = \begin{pmatrix} 0 & \Lambda_{\mathcal{VH}} \\ 0 & 0 \end{pmatrix} \qquad \qquad \Omega = \begin{pmatrix} \Omega_{\mathcal{VV}} & 0 \\ 0 & \Omega_{\mathcal{HH}} \end{pmatrix}$$

• Covariance matrix:

$$\mathsf{Cov}\left[\begin{pmatrix} X_V \\ X_{\mathcal{H}} \end{pmatrix}\right] = (I - \Lambda)^{-1} \Omega (I - \Lambda)^{-\top} = \begin{pmatrix} \Omega_{VV} + \Lambda_{V\mathcal{H}} \Omega_{\mathcal{H}\mathcal{H}} \Lambda_{V\mathcal{H}}^\top & \Lambda_{V\mathcal{H}} \Omega_{\mathcal{H}\mathcal{H}} \\ \Omega_{\mathcal{H}\mathcal{H}} \Lambda_{V\mathcal{H}}^\top & \Omega_{\mathcal{H}\mathcal{H}} \end{pmatrix}$$

• Observed covariance matrix (projection):

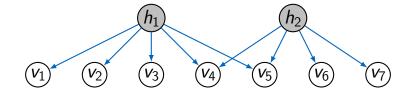
$$Cov[X_V] = \Omega_{VV} + \Lambda_{VH}\Omega_{HH}\Lambda_{VH}^{\top}$$

Observed covariance model:

$$F_{\mathcal{G}} = \{ \Sigma := \widetilde{\Omega} + \widetilde{\Lambda} \widetilde{\Lambda}^{\top} \in \mathbb{R}^{|V| \times |V|} : \widetilde{\Omega} > 0 \text{ diagonal, } \widetilde{\Lambda} \in \mathbb{R}^{E_{VH}} \}$$

Goals: $\dim(F_G)$? $I(F_G) \subseteq \mathbb{R}[\sigma_{ij}, i < j]$?

Example: Factor Analysis Models



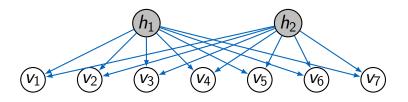
Parameter matrix:

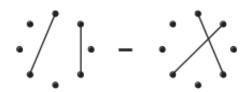
$$\widetilde{\Lambda} = egin{pmatrix} \lambda_{11} & \lambda_{21} & \lambda_{31} & \lambda_{41} & \lambda_{51} & 0 & 0 \ 0 & 0 & \lambda_{42} & \lambda_{52} & \lambda_{62} & \lambda_{72} \end{pmatrix}^{ op}, \qquad \widetilde{\Omega} = \mathsf{diag}(\omega_{11}, \omega_{22}, \omega_{33}, \omega_{44}, \omega_{55}, \omega_{66}, \omega_{77}).$$

Observed covariance matrix:

$$\Sigma = \begin{pmatrix} \omega_{11} + \lambda_{11}^2 & \lambda_{11}\lambda_{21} & \lambda_{11}\lambda_{31} & \lambda_{11}\lambda_{41} & \lambda_{11}\lambda_{51} & 0 & 0 \\ \lambda_{11}\lambda_{21} & \omega_{22} + \lambda_{21}^2 & \lambda_{21}\lambda_{31} & \lambda_{21}\lambda_{41} & \lambda_{21}\lambda_{51} & 0 & 0 \\ \lambda_{11}\lambda_{31} & \lambda_{21}\lambda_{31} & \omega_{33} + \lambda_{31}^2 & \lambda_{31}\lambda_{41} & \lambda_{31}\lambda_{51} & 0 & 0 \\ \lambda_{11}\lambda_{41} & \lambda_{21}\lambda_{41} & \lambda_{31}\lambda_{41} & \omega_{44} + \lambda_{41}^2 + \lambda_{42}^2 & \lambda_{41}\lambda_{51} + \lambda_{42}\lambda_{52} & \lambda_{42}\lambda_{62} & \lambda_{42}\lambda_{72} \\ \lambda_{11}\lambda_{51} & \lambda_{21}\lambda_{51} & \lambda_{31}\lambda_{51} & \lambda_{41}\lambda_{51} + \lambda_{42}\lambda_{52} & \omega_{55} + \lambda_{51}^2 + \lambda_{52}^2 & \lambda_{52}\lambda_{62} & \lambda_{52}\lambda_{72} \\ 0 & 0 & 0 & \lambda_{42}\lambda_{62} & \lambda_{52}\lambda_{62} & \omega_{66} + \lambda_{62}^2 & \lambda_{62}\lambda_{72} \\ 0 & 0 & 0 & \lambda_{42}\lambda_{72} & \lambda_{52}\lambda_{72} & \lambda_{62}\lambda_{72} & \omega_{77} + \lambda_{72}^2 \end{pmatrix}.$$

Previous work: Full Factor Analysis Models





Dimension: [Drton, Sullivant, Sturmfels, 2007]

$$\dim(F_G) = \min\{p(|\mathcal{H}|+1) - {|\mathcal{H}| \choose 2}, {p+1 \choose 2}\},$$

where |V| = p.

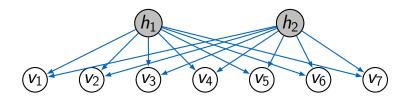
deal: [Drton, Sullivant, Sturmfels, 2007]

$$I(F_G) = M_{p,|\mathcal{H}|} \cap \mathbb{R}[\sigma_{ij}, i < j],$$

where $M_{p,|\mathcal{H}|} \subseteq \mathbb{R}[\sigma_{ij}, i \leq j]$ is the ideal generated by all $(|\mathcal{H}|+1) \times (|\mathcal{H}|+1)$ minors of a symmetric $p \times p$ matrix.

İrem Portakal | Algebraic Sparse Factor Analysis (arXiv: 2312.14762)

Previous work: Full Factor Analysis Models





Dimension: [Drton, Sullivant, Sturmfels, 2007]

$$\dim(F_G) = \min\{p(|\mathcal{H}|+1) - {|\mathcal{H}| \choose 2}, {p+1 \choose 2}\},$$

where |V| = p.

Ideal: [Drton, Sullivant, Sturmfels, 2007]

$$I(F_G) = M_{p,|\mathcal{H}|} \cap \mathbb{R}[\sigma_{ij}, i < j],$$

where $M_{p,|\mathcal{H}|} \subseteq \mathbb{R}[\sigma_{ij}, i \leq j]$ is the ideal generated by all $(|\mathcal{H}|+1) \times (|\mathcal{H}|+1)$ minors of a symmetric $p \times p$ matrix. Irem Portakal | Algebraic Sparse Factor Analysis (arXiv: 2312.14762)

Gröbner basis:

$$|\mathcal{H}| = 1$$
:

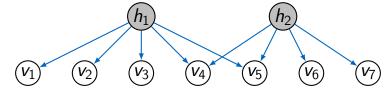
$$G_{p,1} = \{ \sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl}, \sigma_{il}\sigma_{jk} - \sigma_{ik}\sigma_{jl} \}$$

$$1 \le i < j < k < l \le p \}.$$

$$|\mathcal{H}|=2$$
:

- $\overline{F_G}$ secant variety of the 1-factor model.
- Delightful strategy. [Sullivant, 2009]

At least one edge is missing and under Zero Upper Triangular Assumption (ZUTA): ZUTA ensures that the rows and columns of the factor loading matrix Λ can be permuted such that the upper triangle of the matrix is zero. Generalizes k-pure children assumption.



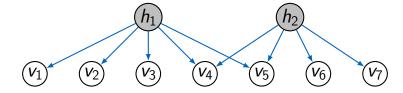
- $C(V, 2) := \{ \{v, w\} : v, w \in V, v \neq w \}.$
- $jpa(\{u,v\}) = \{h \in \mathcal{H} : h \in pa(u) \cap pa(v)\}$: set of *joint parents* of a pair $\{u,v\} \in C(V,2)$.
- For any latent node $h \in \mathcal{H}$, $C(V, 2)_h = \{ \{v, w\} \in C(V, 2) : h \in jpa(\{v, w\}) \}$.

Dimension:

Theorem[DG \bullet S]: Let $G = (V \cup \mathcal{H}, D)$ be a factor analysis graph such that ZUTA is satisfied. If there is a ZUTA-conform pairwise disjoint collection of subsets $\mathcal{A} = (A_h)_{h \in \mathcal{H}}$ of $C(V, 2)_h$ where $|A_h| \leq |\operatorname{ch}(h)|$ such that the sum of cardinalities $\sum_{h \in \mathcal{H}} |A_h|$ is maximal, then

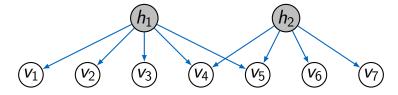
$$\dim(F(G)) = |V| + \sum_{h \in \mathcal{H}} |A_h|.$$

Example:



```
A_{h_1} = \{\{v_1, v_2\}, \{v_1, v_3\}, \{v_2, v_3\}, \{v_1, v_4\}, \{v_2, v_4\}\}\}
A_{h_2} = \{\{v_4, v_5\}, \{v_5, v_6\}, \{v_5, v_7\}, \{v_6, v_7\}\}\}
\dim(F(G)) = |V| + \sum_{h \in \mathcal{H}} |A_h| = 7 + 5 + 4 = 16.
```

Example:



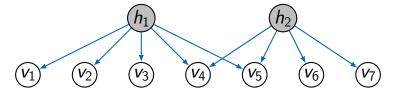
$$A_{h_1} = \{\{v_1, v_2\}, \{v_1, v_3\}, \{v_2, v_3\}, \{v_1, v_4\}, \{v_2, v_4\}\}\}$$

$$A_{h_2} = \{\{v_4, v_5\}, \{v_5, v_6\}, \{v_5, v_7\}, \{v_6, v_7\}\}\}$$

$$\dim(F(G)) = |V| + \sum_{h \in \mathcal{H}} |A_h| = 7 + 5 + 4 = 16.$$

Corollary [DG \bullet S]: If $p \ge 5$ and $|\mathcal{H}| = 2$ where any latent node has at least 3 children, then $\dim(F_G) = p + |E|$.

Example:



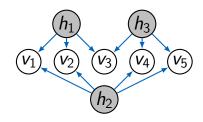
$$A_{h_1} = \{\{v_1, v_2\}, \{v_1, v_3\}, \{v_2, v_3\}, \{v_1, v_4\}, \{v_2, v_4\}\}\}$$

$$A_{h_2} = \{\{v_4, v_5\}, \{v_5, v_6\}, \{v_5, v_7\}, \{v_6, v_7\}\}\}$$

$$\dim(F(G)) = |V| + \sum_{h \in \mathcal{H}} |A_h| = 7 + 5 + 4 = 16.$$

Corollary[DG \bullet S]: If $p \ge 5$ and $|\mathcal{H}| = 2$ where any latent node has at least 3 children, then $\dim(F_G) = p + |E|$.

No ZUTA but MathRepo: $dim(F_G) = 14$.





Joins

What about $I(F_G)$?

- If $pa(u) \cap pa(v) = \emptyset$, then $\sigma_{uv} = 0$ (degree one monomials).
- Let U, $W \subseteq V$ be disjoint sets s.t. |U| = |W| = 2. $|pa(U) \cap pa(W)| \le 1$, then $det(\Sigma_{U,W}) = 0$ (tetrads).

Theorem[DG \bullet S]: Let| \mathcal{H} | = 2.

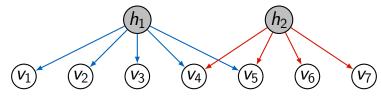
$$\mathbb{V}(I(F_G)) = \mathbb{V}(\{M_{p,2} + M_{\leq 1}(G)\} \cap \mathbb{R}[\sigma_{ij}, i < j]),$$

where $M_{\leq 1}(G)$ is the ideal generated by all degree one monomials and tetrads corresponding to G.

Join of Varieties:

$$W_1*W_2=\overline{\{\lambda w_1+(1-\lambda)w_2:w_1\in W_1,w_2\in W_2,\lambda\in\mathbb{R}\}}$$

(Sparse) Factor Models = Joins of (Sparse) One-Factor Models: For two ideals I_1 , I_2 , one defines the join ideal $I_1 * I_2$ such that $I_1 * I_2 = I(\mathbb{V}(I_1) * \mathbb{V}(I_2))$. $I(F_G) = I_1 * I_2$.



Delightful Strategy for Gröbner Basis

Observation:

 $\operatorname{in}_{\prec}(I_1*I_2)\subseteq\operatorname{in}_{\prec}(I_1)*\operatorname{in}_{\prec}(I_2)$ for any term order \prec . If equality holds, then \prec is *delightful* for I_1,I_2 .

"Delightful" strategy: [Sturmfels, Sullivant, 2006]

Find $G \subseteq I_1 * I_2$ such that $\langle \operatorname{in}_{\prec}(g) | g \in G \rangle = \operatorname{in}_{\prec}(I_1) * \operatorname{in}_{\prec}(I_2)$. Then G is a Gröbner basis.

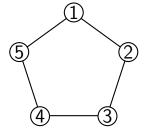
- 1. Find delightful term order \prec .
- 2. Understand $\operatorname{in}_{\prec}(I_1) * \operatorname{in}_{\prec}(I_2)$.
- 3. Define polynomials $g \in G$ with correct initial terms.

Circular Term Order

Circular order:

Any block-term order \prec such that $\sigma_{uv} \succ \sigma_{wz}$ whenever the circular distance between u and v is smaller than the circular distance of w and z.

Example:



- $\sigma_{15} \succ \sigma_{24}$,
- $\sigma_{34} \succ \sigma_{25}$.

- $\sigma_{15}\sigma_{24} \sigma_{25}\sigma_{14}$, $\sigma_{45}\sigma_{12} \sigma_{25}\sigma_{14}$
- $\sigma_{34}\sigma_{25} \sigma_{35}\sigma_{24}$, $\sigma_{45}\sigma_{23} \sigma_{35}\sigma_{24}$.

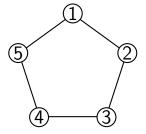
The ideal of the one-factor analysis model is the toric edge ideal of the complete graph on $A \subseteq [p]$ vertices with $B := [p] \setminus A$ isolated vertices. Its initial ideal is a monomial edge ideal.

Circular Term Order

Circular order:

Any block-term order \prec such that $\sigma_{uv} \succ \sigma_{wz}$ whenever the circular distance between u and v is smaller than the circular distance of w and z.

Example:



- $\sigma_{15} \succ \sigma_{24}$,
- $\sigma_{34} \succ \sigma_{25}$.

- $\sigma_{15}\sigma_{24} \sigma_{25}\sigma_{14}$, $\sigma_{45}\sigma_{12} \sigma_{25}\sigma_{14}$
- $\sigma_{34}\sigma_{25} \sigma_{35}\sigma_{24}$, $\sigma_{45}\sigma_{23} \sigma_{35}\sigma_{24}$.

The ideal of the one-factor analysis model is the toric edge ideal of the complete graph on $A \subseteq [p]$ vertices with $B := [p] \setminus A$ isolated vertices. Its initial ideal is a monomial edge ideal.

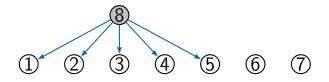
Gröbner basis: Let $B \subset [p]$ be the set of isolated vertices of the one-factor analysis graph and $A \sqcup B = V$.

The set of degree-one monomials and tetrads

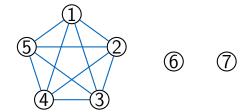
$$\{\sigma_{ij} \mid i \in B \text{ or } j \in B\} \cup \{\sigma_{ij}\sigma_{kl} - \sigma_{ik}\sigma_{jl}, \sigma_{il}\sigma_{jk} - \sigma_{ik}\sigma_{jl} \mid 1 \leq i < j < k < l \leq |A|\}.$$

is a reduced Gröbner basis for the sparse one-factor analysis model with respect to any circular term order.

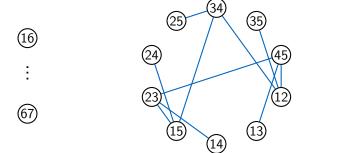
Non-Crossing Edge Graphs



Complete graph on $v \in V$ s.t. $pa(v) \neq \emptyset$:

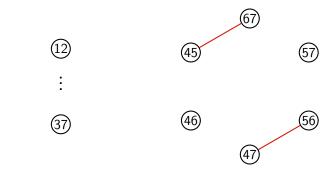


Non-crossing edge graph:





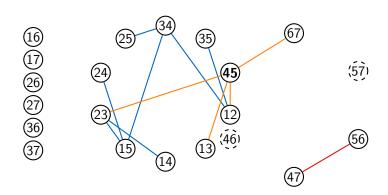




Gröbner Basis for "Overlap = 2"

 $in_{\prec}(I_1) * in_{\prec}(I_2)$ is given by the edge ideal of the hypergraph obtained by gluing the non-crossing edge graphs.

Glued Hypergraph



Gröbner basis of $I_1 * I_2 = I(F_G)$

- σ_{16} , σ_{17} , σ_{26} , σ_{27} , σ_{36} , σ_{37} .
- $\sigma_{47}\sigma_{56} \sigma_{57}\sigma_{46}$, $\sigma_{12}\sigma_{34} - \sigma_{13}\sigma_{24}$, $\sigma_{14}\sigma_{23} - \sigma_{13}\sigma_{24}$, $\sigma_{12}\sigma_{35} - \sigma_{13}\sigma_{25}$, $\sigma_{15}\sigma_{23} - \sigma_{13}\sigma_{25}$, $\sigma_{15}\sigma_{24} - \sigma_{14}\sigma_{25}$, $\sigma_{15}\sigma_{34} - \sigma_{14}\sigma_{35}$, $\sigma_{25}\sigma_{34} - \sigma_{24}\sigma_{35}$.
- $\sigma_{67}\sigma_{12}\sigma_{45} \sigma_{67}\sigma_{24}\sigma_{15} \sigma_{12}\sigma_{47}\sigma_{56}$, $\sigma_{67}\sigma_{13}\sigma_{45} - \sigma_{67}\sigma_{34}\sigma_{15} - \sigma_{13}\sigma_{47}\sigma_{56}$, $\sigma_{67}\sigma_{23}\sigma_{45} - \sigma_{67}\sigma_{34}\sigma_{25} - \sigma_{23}\sigma_{47}\sigma_{56}$.

Conclusion

Theorem [DG \bigcirc S]: The generators of a Gröbner basis for $I_{A_1,B_1,1}*I_{A_2,B_2,1}$ with respect to any circular term order for sparse two-factor analysis models where $A_1 \cap A_2 = \{j_1, j_2\}$ comes in three types:

- 1. Degree-one monomial: σ_{ik} is a generator, where $pa(i) \cap pa(j) = \emptyset$.
- 2. Tetrads: The binomial generators of the Gröbner basis of $I_{A_1,B_1,1}$ and $I_{A_2,B_2,1}$ with respect to any circular order that do not contain σ_{h_2} .
- 3. Hexads: Consider $i_1, i_2 \in A_1 \setminus \{j_1, j_2\}$ and $k_1, k_2 \in A_2 \setminus \{j_1, j_2\}$. Then

$$\underline{\sigma_{k_1k_2}\sigma_{i_1i_2}\sigma_{j_1j_2}}-\sigma_{k_1k_2}\sigma_{j_1i_2}\sigma_{j_2i_1}-\sigma_{i_1i_2}\sigma_{j_1k_2}\sigma_{j_2k_1},$$

is a degree three generator, where $\{i_1, i_2\}$, $\{j_1, j_2\}$ and $\{j_1, j_2\}$, $\{k_1, k_2\}$ are non-crossing edges of the complete graphs on the vertices $A_1 \setminus \{j_1, j_2\}$ and $A_2 \setminus \{j_1, j_2\}$ respectively.

Question: Is there a 2-delightful term order for sparse two-factor analysis models?

Conjecture: The ideal of the sparse two-factor analysis model corresponding to graph G is generated by off-diagonal 3×3 -minors, pentads, and the polynomials in $M_{<1}(G)$.