Positive Definite Completion Problems For DAG Models

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MATRIX COMPLETION PROBLEMS

- A **matrix completion problem**: asks whether for a given pattern the unspecified entries of each incomplete matrix can be chosen in such a way that the resulting conventional matrix is of a desired type.

- An $n \times n$ **pattern** $\mathscr{P}$: a subset of positions in an $n \times n$ matrix in which the entries are present.

- A (symmetric) **incomplete matrix** Υ: the entries corresponding to the positions in $\mathscr{P}$ specified, the rest unspecified (free to be chosen).

- **Positive definite completion problem**: asks which incomplete matrices have positive definite completions, with or without additional features.

Example

- A 4×4 pattern:

$$\mathscr{P} = \{\{1,1\},\{2,2\},\{4,4\},\{1,4\},\{2,3\}\}$$

- An incomplete matrix:

$$\Upsilon = \begin{pmatrix} 3.0 & ? & ? & 2.00 \\ ? & 6.25 & 4.00 & ? \\ ? & 4.00 & ? & ? \\ 2.0 & ? & ? & 2.25 \end{pmatrix}$$

- A positive definite completion of Υ

$$\begin{pmatrix} 3.0 & 1.50 & 3.50 & 2.00 \\ 1.5 & 6.25 & 4.00 & 3.00 \\ 3.5 & 4.00 & 6.25 & 3.00 \\ 2.0 & 3.00 & 3.00 & 2.25 \end{pmatrix}$$

The Grone et al's Theorem (1984)

- Υ is a partial positive definite matrix if $\Upsilon_C > 0$ for each clique C of $\mathcal{G}$.
- A chordal (decomposable) graph is an undirected graph $\mathcal{G}$ that has no induced cycle of length greater than or equal to 4.

Theorem

Every incomplete matrix Υ corresponding to a given pattern $\mathscr{P}$ has a positive definite completion iff

1. *Υ is a partial positive definite matrix.*
2. *The pattern $\mathscr{P}$ considered as a set of edges, forms a chordal (or equivalently decomposable) graph $\mathcal{G}$.*

Grone et al.'s theorem (1984) has had a significant impact in graphical models research.

Remarks

- Υ has a unique positive definite completion $\Sigma = \Sigma(\Upsilon)$ if we require

$$\Sigma^{-1}_{ij} = 0 \qquad \forall \{i, j\} \in \mathscr{P}.$$

- Equivalently, positive definite completion in the space of covariance matrices corresponding to a concentration graph model is unique.

- When $\mathcal{G}$ is decomposable
  - $\Sigma(\Upsilon)$ can be completed via a polynomial time process.
  - There exists an explicit one-to-one mapping $\varphi : \Upsilon \mapsto \Sigma(\Upsilon)^{-1}$.
  - The Jacobian of the mapping φ can be explicitly computed [Dawid & Lauritzen (1993), Roverato (2000), Letac & Massam (2007)].

Applications in Graphical Models

Positive definite completion problems frequently arise (explicitly or implicitly) in the study of Graphical Models. For example:

- Maximum likelihood estimation for Gaussian graphical models, Dempster (1972).
- Hyper-Markov laws for decomposable graphs, Dawid & Lauritzen (1993).
- Wishart distributions for decomposable graphs, Letac & Massam (2007).
- Flexible covariance estimation for decomposable graphs, Rajaratnam, Massam et al. (2008).
- Wishart distributions for decomposable covariance graph models, Khare & Rajaratnam (2011).
- Generalized hyper Markov laws for directed acyclic graphs, Ben-David & Rajaratnam (2012).

Motivation for current work

- **DAG models** (or Bayesian networks): one of the widely used classes of graphical models.

Completion problems for DAGs

In the DAG setting, we consider positive definite completions of incomplete matrices specified by a directed acyclic graph $\mathcal{D}$. Here the incomplete matrices are desired to be completed in

- the space of covariance, or
- the space of inverse covariance / concentration matrices

corresponding to the DAG model.

- The need for studying this new class of problems naturally arises when studying spaces of covariance & concentration matrices corresponding to DAG models, Ben-David & Rajaratnam (2011).

Graph theoretic notation

- An **undirected graph** UG: denoted by $\mathcal{G} = (V, \mathscr{V})$
- An **(undirected) edge** in $\mathscr{V}$: denoted by an unordered pair $\{i, j\}$
- A **directed acyclic graph** DAG: denoted by $\mathcal{D} = (V, \mathscr{E})$
- A **(directed) edge** in $\mathscr{E}$: denoted by a ordered pair (i, j)
- $(i, j) \in \mathscr{E}$: denoted by $i \to j$, say i a **parent** of j
- The set of parents of j: denoted by $\mathrm{pa}(j) = \{i : \; i \to j\}$
- The **family** of j: denoted by $\mathrm{fa}(j) = \mathrm{pa}(j) \cup \{j\}$
- The **undirected version** of $\mathcal{D}$: denoted by $\mathcal{D}^u$
- An **immorality** in $\mathcal{D}$: an induced subgraph of the form $i \to j \leftarrow k$
- The **moral graph** of $\mathcal{D}$: denoted by $\mathcal{D}^m$

Basic definitions

- A perfect DAG is a DAG $\mathcal{D}$ that has no **immoralities**, i.e., $\mathcal{D}^u = \mathcal{D}^m$
- A DAG is **parent ordered** if $i \to j \implies i > j$
- For a parent ordered DAG $\mathcal{D}$, i is a **predecessor** of j if

$$i > j \quad \text{but} \quad i \nrightarrow j \quad \text{(notational convenience)}$$

- The set of predecessors of j is denoted by $\text{pr}(j)$

Remarks

- If $\mathcal{D}$ is perfect then $\mathcal{D}^u$ is decomposable
- If $\mathcal{G}$ is decomposable, then it has a perfect DAG version $\mathcal{D}$
- We can assume w.l.o.g. that each DAG $\mathcal{D}$ is parent ordered

Gaussian DAG models

Let $\mathbf{X} = (X_1, \dots, X_p)$ be a random vector in $\mathbb{R}^p$, with $p = |V|$.

- $\mathbf{X}$ obeys the **ordered Markov property** w.r.t. $\mathcal{D}$ if

$$X_i \perp\!\!\!\perp \mathbf{X}_{\mathrm{pr}(i)\setminus\mathrm{pa}(i)} | \mathbf{X}_{\mathrm{pa}(i)} \qquad \forall i \in V$$

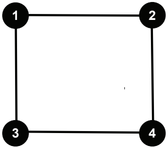
- The **Gaussian DAG model** $\mathcal{N}(\mathcal{D})$ is the family of multivariate normal distributions $\mathrm{N}_p(\mu, \Sigma)$, $\mu \in \mathbb{R}^p$, $\Sigma \succ 0$ that obey the ordered Markov property w.r.t. $\mathcal{D}$.
- For an undirected graph $\mathcal{G}$, the **Gaussian UG model** $\mathcal{N}(\mathcal{G})$ is the family of Gaussian Markov random fields over $\mathcal{G}$.

Remark

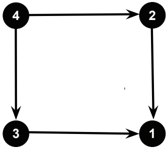
- A key observation: $\mathrm{N}_p(\mu, \Sigma) \in \mathcal{N}(\mathcal{D})$ iff $\Sigma \succ 0$ and

$$\Sigma_{\mathrm{pr}(j),j} = \Sigma_{\mathrm{pr}(j),\mathrm{pa}(j)}(\Sigma_{\mathrm{pa}(j)})^{-1}\Sigma_{\mathrm{pa}(j),j} \quad \forall j \in V, \quad \text{(Andersson (1998))}$$

Examples



(a)



(b)

- Let $\mathcal{G}$ be given by Figure (a). If $(X_1, \ldots, X_4) \in \mathbb{R}^4$ obeys the local Markov property w.r.t. $\mathcal{G}$, then

$$X_1 \perp\!\!\!\perp X_4 | (X_2, X_3) \quad \text{and} \quad X_2 \perp\!\!\!\perp X_3 | (X_1, X_4)$$

- Let $\mathcal{D}$ be given by Figure (b). If $(X_1, \ldots, X_4)$ obeys the ordered Markov property w.r.t. $\mathcal{D}$, then

$$X_1 \perp\!\!\!\perp X_4 | (X_2, X_3) \quad \text{and} \quad X_2 \perp\!\!\!\perp X_3 | X_4$$

Preliminary notation

Let $\mathcal{D} = (V, \mathscr{E})$ be a DAG.

- A $\mathcal{D}$**-incomplete matrix** is a symmetric function

$$\Gamma : \{i, j\} \mapsto \Gamma_{ij} \in \mathbb{R}, \text{ s.t. } \Gamma_{ij} = \Gamma_{ji} \quad \forall (i, j) \in \mathscr{E}.$$

- Γ is **partially positive definite**, denoted by $\Gamma \succ_{\mathcal{D}} 0$, if $\Gamma_C \succ 0$ for each clique C of $\mathcal{D}^u$.
- The space of covariance and the inverse-covariance matrices over $\mathcal{D}$ are defined as

$$\mathrm{PD}_{\mathcal{D}} = \left\{\Sigma : \mathrm{N}_p(0, \Sigma) \in \mathscr{N}(\mathcal{D})\right\} \quad \text{and} \quad \mathrm{P}_{\mathcal{D}} = \left\{\Omega : \Omega^{-1} \in \mathrm{PD}_{\mathcal{D}}\right\}.$$

- Similar spaces for an undirected graph $\mathcal{G}$ are

$$\mathrm{PD}_{\mathcal{G}} = \left\{\Sigma : \mathrm{N}_p(0, \Sigma) \in \mathscr{N}(\mathcal{G})\right\} \quad \text{and} \quad \mathrm{P}_{\mathcal{G}} = \left\{\Omega : \Omega^{-1} \in \mathrm{PD}_{\mathcal{G}}\right\}.$$

A FEW OBSERVATIONS

- Let $\mathcal{L}_{\mathcal{D}}$ denote the linear space of all lower triangular matrices with unit diagonal entries such that

$$L \in \mathcal{L}_{\mathcal{D}} \Longrightarrow L_{ij} = 0 \quad \forall (i,j) \notin \mathscr{E}.$$

  Then $\Omega \in \mathrm{P}_{\mathcal{D}} \Longleftrightarrow \exists L \in \mathcal{L}_{\mathcal{D}}$ and a diagonal matrix Λ, with strictly positive diagonal entries s.t. in the modified Cholesky decomposition $\Omega = L\Lambda L'$, Wermuth (1980).

- $\mathrm{PD}_{\mathcal{D}} \subseteq \mathrm{PD}_{\mathcal{D}^m}$, Wermuth (1980).
- $\mathrm{PD}_{\mathcal{D}} = \mathrm{PD}_{\mathcal{D}^u} \Longleftrightarrow \mathcal{D}$ is a perfect DAG.

Convention

Unless otherwise stated, hereafter $\mathcal{G} = (V, \mathscr{V})$ denotes the undirected version of $\mathcal{D} = (V, \mathscr{E})$.

A FORMAL DEFINITION OF MATRIX COMPLETION

Let $\mathcal{M} \subseteq \mathrm{S}_p(\mathbb{R})$, the space of $p \times p$ symmetric matrices.

- We say that a $\mathcal{D}$-incomplete matrix Γ can be completed in $\mathcal{M}$ if

$$\exists T \in \mathcal{M} \quad \text{s.t.} \quad T_{ij} = \Gamma_{ij} \quad \forall (i,j) \in \mathcal{E}$$

- We refer to T as a **completion** of Γ in $\mathcal{M}$, or
- simply a completion of Γ, if $\mathcal{M}$ is the whole space $\mathrm{S}_p(\mathbb{R})$.

Positive definite completion in $\mathrm{P}_{\mathcal{D}}$

- Let $\mathrm{I}_{\mathcal{D}}$ denote the set of $\mathcal{D}$-incomplete matrices.

Proposition

Let Γ be a $\mathcal{D}$-incomplete matrix in $\mathrm{I}_{\mathcal{D}}$. If $\Gamma_{11} \neq 0$, then

- Part (a) Almost everywhere (w.r.t. Lebesgue measure on $\mathrm{I}_{\mathcal{D}}$), there exist a unique lower triangular matrix $L \in \mathcal{L}_{\mathcal{D}}$ and a unique diagonal matrix $\Lambda \in \mathbb{R}^{p \times p}$ s.t.

$$\widehat{\Gamma} = L \Lambda L' \quad \text{is a completion of} \quad \Gamma$$

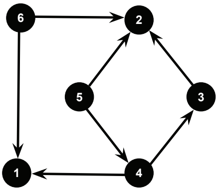
- Part (b) The matrix $\widehat{\Gamma}$ is the unique positive definite completion of Γ in $\mathrm{P}_{\mathcal{D}}$ iff the diagonal entries of Λ are all strictly positive.

Sketch of the proof

1. Set $L_{ij} = 0$ for each $(i,j) \notin \mathscr{E}$.
2. Set $\Lambda_{11} = \Gamma_{11},\ L_{i1} = \Lambda_{11}^{-1}\Gamma_{i1}$ for each $i \in \mathrm{pa}(1)$ and set $j = 1$.
3. If $j < p$, then set $j = j + 1$ and proceed to step *iv*), otherwise L and Λ are constructed such that they satisfy the condition in part (a).
4. Set $\Lambda_{jj} = \Gamma_{jj} - \sum_{k=1}^{j-1} \Lambda_{kk} L_{jk}^2$ and proceed to the next step.
5. For each $i \in \mathrm{pa}(j)$ if $\Lambda_{jj} \neq 0$, then set $L_{ij} = \Lambda_{jj}^{-1}(\Gamma_{ij} - \sum_{k=1}^{j-1} \Lambda_{kk} L_{ik} L_{jk})$, and return to step *iii*). If $\Lambda_{jj} = 0$, then no completion of Γ exists that satisfies the condition in part (a). Consequently, Γ cannot also be completed in $\mathrm{P}_{\mathcal{D}}$.

Example

Let $\mathcal{D}$ and Γ be given as follows:



$$\Gamma = \begin{pmatrix} 1 & * & * & -3 & * & 4 \\ * & -1 & -2 & * & -5 & 2 \\ * & -2 & -2 & -10 & * & * \\ -3 & * & -10 & 56 & 3 & * \\ * & -5 & * & 3 & -30 & * \\ 4 & 2 & * & * & * & 13 \end{pmatrix}$$

Now by applying the completion process to Γ we obtain

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -3 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \qquad L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 & 0 & 0 \\ -3 & 0 & -5 & 1 & 0 & 0 \\ 0 & 5 & 0 & -1 & 1 & 0 \\ 4 & -2 & 0 & 0 & 0 & 1 \end{pmatrix},$$

Example continued

This yields the completed matrix $\widehat{\Gamma}$ given as follows:

$$\widehat{\Gamma} = \begin{pmatrix} 1 & 0 & 0 & -3 & 0 & 4 \\ 0 & -1 & -2 & 0 & -5 & 2 \\ 0 & -2 & -2 & -10 & -10 & 4 \\ -3 & 0 & -10 & 56 & 3 & -12 \\ 0 & -5 & -10 & 3 & -30 & 10 \\ 4 & 2 & 4 & -12 & 10 & 13 \end{pmatrix}.$$

As the diagonal elements of Λ are not strictly positive, Γ cannot be completed in $P_{\mathcal{D}}$.

Positive definite completion in $\mathrm{PD}_{\mathcal{D}}$

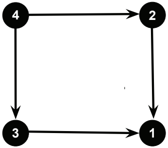
Proposition

Let Γ be a partial positive definite matrix. The following completion process (of polynomial complexity) determines if a completion in $\mathrm{PD}_{\mathcal{D}}$ exists, and if so, it uniquely constructs the completed matrix Σ.

1. Set $\Sigma_{ij} = \Gamma_{ij}$ for each $\{i, j\} \in \mathscr{V}$ and set $j = p$.
2. If $j > 1$, then set $j = j - 1$ and proceed to the next step, otherwise Σ is successfully completed.
3. If $\Sigma_{\mathrm{fa}(j)} \succ 0$, then proceed to the next step, otherwise the completion in $\mathrm{PD}_{\mathcal{D}}$ does not exist.
4. If $\mathrm{pr}(j)$ is empty, then return to step (2), otherwise proceed to the next step.
5. If $\mathrm{pa}(j)$ is non-empty, then set $\Sigma_{\mathrm{pr}(j),j} = \Sigma_{\mathrm{pr}(j),\mathrm{pa}(j)}(\Sigma_{\mathrm{pa}(j)})^{-1}\Sigma_{\mathrm{pa}(j),j}$, $\Sigma_{j,\mathrm{pr}(j)} = \Sigma'_{\mathrm{pr}(j),j}$ and return to step (2). If $\mathrm{pa}(j)$ is empty, then set $\Sigma_{\mathrm{pr}(j),j} = 0$ and return to step (2).

Example

Let $\mathcal{D}$ and Γ be given as follows.



$$\Gamma = \begin{pmatrix} \Gamma_{11} & \Gamma_{12} & \Gamma_{13} & * \\ \Gamma_{21} & \Gamma_{22} & * & \Gamma_{24} \\ \Gamma_{31} & * & \Gamma_{33} & \Gamma_{34} \\ * & \Gamma_{42} & \Gamma_{43} & \Gamma_{44} \end{pmatrix}$$

- Layer: j=4. In step (1)

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \Sigma_{13} & ? \\ \Sigma_{21} & \Sigma_{22} & ? & \Sigma_{24} \\ \Sigma_{31} & ? & \Sigma_{33} & \Sigma_{34} \\ ? & \Sigma_{42} & \Sigma_{43} & \Sigma_{44} \end{pmatrix}$$

Example continued

- Layer: j=3. In step (2) let $j = 4 - 1 = 3$. In step (3) either $\Sigma_{\mathrm{fa}(3)} = \begin{pmatrix} \Sigma_{33} & \Sigma_{34} \\ \Sigma_{43} & \Sigma_{44} \end{pmatrix} \succ 0$, otherwise the completion in $\mathrm{PD}_{\mathcal{D}}$ does not exist. Assuming the former, we proceed to step (5). Since $\mathrm{pr}(3) = \emptyset$, the layer down to $j = 3$ is thus completed.

- Layer: j=2. Return to step (2) with $j = 3 - 1 = 2$. In step (3) we check whether $\Sigma_{\mathrm{fa}(2)} = \begin{pmatrix} \Sigma_{22} & \Sigma_{24} \\ \Sigma_{42} & \Sigma_{44} \end{pmatrix} \succ 0$. Assuming $\Sigma_{\mathrm{fa}(2)} \succ 0$, then in step (5), as $\mathrm{pr}(2) = \{3\}$, we set $\Sigma_{32} = \Sigma_{34}\Sigma_{44}^{-1}\Sigma_{42}$ and the layer down to $j = 2$ is thus completed.

Example continued

- Layer: j=1. Process is returned to step (2) with $j = 2 - 1 = 1$. In step (3) we first check whether

$$\Sigma_{\mathrm{fa}(1)} = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \Sigma_{13} \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{34}\Sigma_{44}^{-1}\Sigma_{42} \\ \Sigma_{31} & \Sigma_{34}\Sigma_{44}^{-1}\Sigma_{42} & \Sigma_{33} \end{pmatrix} \succ 0.$$

- Assuming $\Sigma_{\mathrm{fa}(1)} \succ 0$, then in step (5), as $\mathrm{pr}(1) = \{4\}$ we set

$$\Sigma_{41} = (\Sigma_{42}, \Sigma_{43}) \begin{pmatrix} \Sigma_{22} & \Sigma_{34}\Sigma_{44}^{-1}\Sigma_{42} \\ \Sigma_{34}\Sigma_{44}^{-1}\Sigma_{42} & \Sigma_{33} \end{pmatrix}^{-1} \begin{pmatrix} \Sigma_{21} \\ \Sigma_{31} \end{pmatrix}.$$

- The processed yields a completion. The matrix Σ is the completion of Γ in $\mathrm{PD}_{\mathcal{D}}$.

An alternative procedure

- Step (1) We construct a finite sequence of DAGs, $\mathcal{D}_0, \ldots, \mathcal{D}_n$ such that $\mathcal{D}_n$ at the end of this sequence is perfect. Let Γ_n denote the incomplete matrix over $\mathcal{D}_n$.
- Step (2) Set $\mathcal{D} = \mathcal{D}_n$ and $\Gamma = \Gamma_n$.
- Step (3) If $\Gamma \succ 0$, then proceed as follows.
  1. Set $\Sigma_{ij} = \Gamma_{ij}$ for each $\{i, j\} \in \mathscr{V}$,
  2. Set $\Sigma_{\mathrm{pr}(j),j} = \Sigma_{\mathrm{pr}(j),\mathrm{pa}(j)}\Sigma^{-1}_{\mathrm{pa}(j)}\Sigma_{\mathrm{pa}(j),j}$ and $\Sigma_{j,\mathrm{pr}(j)} = \Sigma'_{\mathrm{pr}(j),j}$ for each $j = p - 1, \ldots, 1$

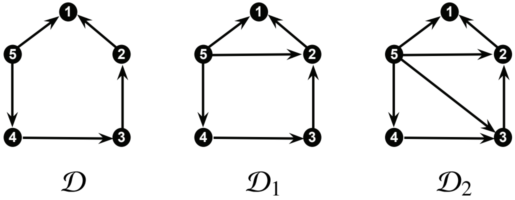
Remark

- Let $\mathcal{D}$ be a perfect DAG and $\Gamma \in \mathrm{I}_{\mathcal{D}}$

$$\Gamma \text{ can be competed in } \mathrm{PD}_{\mathcal{D}} \Longleftrightarrow \Gamma \in Q_{\mathcal{D}} \quad (i.e., \quad \Gamma \succ_{\mathcal{D}} 0)$$

- Thus the alternative procedure yields a completion iff $\Gamma_n \succ_{\mathcal{D}_n} 0$.

Example



Let $\mathcal{D}$ be as above.

- Starting from $\mathcal{D}_0 = \mathcal{D}$, the only immorality in this DAG is $5 \to 1 \leftarrow 2$. By adding the directed edge $5 \to 2$ we obtain $\mathcal{D}_1$.
- Next we obtain the perfect DAG $\mathcal{D}_2$ by adding the directed edge $5 \to 3$ corresponding to the immorality $5 \to 2 \leftarrow 3$ in $\mathcal{D}_1$.
- Now consider the completion of the following $\mathcal{D}$-incomplete matrix.

Example continued

$$\Gamma = \begin{pmatrix} \Gamma_{11} & \Gamma_{12} & * & * & \Gamma_{15} \\ \Gamma_{21} & \Gamma_{22} & \Gamma_{23} & * & * \\ * & \Gamma_{32} & \Gamma_{33} & \Gamma_{34} & * \\ * & * & \Gamma_{43} & \Gamma_{44} & \Gamma_{45} \\ \Gamma_{15} & * & * & \Gamma_{54} & \Gamma_{55} \end{pmatrix}.$$

- $\Gamma_{53} = \Gamma_{54}\Gamma_{44}^{-1}\Gamma_{43}$, and $\Gamma_{52} = \Gamma_{53}\Gamma_{33}^{-1}\Gamma_{32} = \Gamma_{54}\Gamma_{44}^{-1}\Gamma_{43}\Gamma_{33}^{-1}\Gamma_{32}$
- Thus we obtain the following incomplete matrix over the perfect DAG $\mathcal{D}_2$

$$\Gamma^{(2)} = \begin{pmatrix} \Gamma_{11} & \Gamma_{12} & * & * & \Gamma_{15} \\ \Gamma_{21} & \Gamma_{22} & \Gamma_{23} & * & \Gamma_{54}\Gamma_{44}^{-1}\Gamma_{43} \\ * & \Gamma_{32} & \Gamma_{33} & \Gamma_{34} & \Gamma_{53}\Gamma_{33}^{-1}\Gamma_{32} \\ * & * & \Gamma_{43} & \Gamma_{44} & \Gamma_{45} \\ \Gamma_{15} & \Gamma_{54}\Gamma_{44}^{-1}\Gamma_{43} & \Gamma_{53}\Gamma_{33}^{-1}\Gamma_{32} & \Gamma_{54} & \Gamma_{55} \end{pmatrix}.$$

Completable DAGs and generalization of Grone et al's result

Theorem

Every partial positive definite matrix over $\mathcal{D}$ can be completed in $\mathrm{PD}_{\mathcal{D}}$ iff $\mathcal{D}$ is a perfect DAG.

Corollary

Suppose $\mathcal{G}$ is a decomposable graph. Then every partially positive definite matrix Γ over $\mathcal{G}$ can be completed to a unique Σ in $\mathrm{PD}_{\mathcal{G}}$. Consequently, every partial positive definite matrix over a decomposable graph has a positive definite completion.

- The proof the theorem is based on an inductive argument assuming the statement of the theorem is true for any DAG s.t. $|V| < p$.
- For ANY DAG $\mathcal{D}$, completion in $\mathrm{PD}_{\mathcal{D}}$ implies completion in $\mathrm{PD}_{\mathcal{D}^u}$

Some insights

- Interesting contrast between completing a given partial positive definite matrix $\Gamma \in Q_{\mathcal{D}}$ in $PD_{\mathcal{G}}$ vs. completing it in $PD_{\mathcal{D}}$.
- Grone et al. (1984) asserts that $\Gamma \in Q_{\mathcal{G}}$ can be completed in $PD_{\mathcal{G}}$ if *any* positive completion exists.
- A completion in $PD_{\mathcal{D}}$ is therefore sufficient to guarantee a completion in $PD_{\mathcal{G}}$.
- The other way around is unfortunately not true.
- In particular, Γ may not be completed in $PD_{\mathcal{D}}$ even when it can be completed in $PD_{\mathcal{G}}$.
- This is because completion in $PD_{\mathcal{D}}$ is more restrictive than completion in $PD_{\mathcal{G}}$.
- We illustrate this distinction in the following example.

Few Questions

More formally, let Γ be an incomplete matrix over $\mathcal{D}$ and let $\mathcal{G}$ be the undirected version of $\mathcal{D}$.

- If Γ can be completed in $PD_{\mathcal{G}}$, then can it be completed in $PD_{\mathcal{D}}$ as well?

Consider the partial positive definite matrix Γ over the DAG $\mathcal{D}$.

$$\Gamma = \begin{pmatrix} 7 & 12 & 12 & 16 \\ 12 & 30 & 28 & * \\ 12 & 28 & 37 & 32 \\ 16 & * & 32 & 38 \end{pmatrix}$$

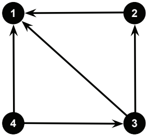


Figure: A non-perfect DAG $\mathcal{D}$

Few Questions

- Although $\mathcal{D}$ is not a perfect DAG we have that $\mathcal{G}$, the undirected version of $\mathcal{D}$, is decomposable.
- By Corollary above it can be completed to a positive definite matrix in $\mathrm{PD}_{\mathcal{G}}$.
- Completion of Γ in $\mathrm{PD}_{\mathcal{D}}$ requires $\Sigma_{42} = \Gamma_{43}\Gamma_{33}^{-1}\Gamma_{32} = 24.2162$
- The completed matrix (below) however is not positive definite.

$$\begin{pmatrix} 7 & 12 & 12 & 16 \\ 12 & 30 & 28 & 24.2162 \\ 12 & 28 & 37 & 32 \\ 16 & 24.2162 & 32 & 38 \end{pmatrix}$$

- Consequently, Γ cannot be completed in $\mathrm{PD}_{\mathcal{D}}$.

Few Questions

Let Γ be an incomplete matrix over $\mathcal{D}$ and let $\mathcal{G}$ be the undirected version of $\mathcal{D}$.

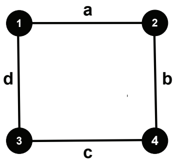
- If Γ can be completed in $\mathrm{PD}_{\mathcal{G}}$, then can it be completed in $\mathrm{PD}_{\mathcal{D}}$ as well?
- The answer as we saw was negative.
- Then, can it at least be completed in $\mathrm{PD}_{\mathcal{D}'}$ for a DAG version $\mathcal{D}'$ of $\mathcal{G}$?

The answer is still negative. We show this by constructing a counter example.

Counterexample

Consider the following partial matrix Γ over the four cycle C_4.

$$\Gamma = \begin{pmatrix} 1 & a & d & * \\ a & 1 & * & b \\ d & * & 1 & c \\ * & b & c & 1 \end{pmatrix}$$

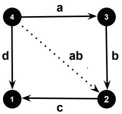


- Γ is a partial positive definite matrix over C_4 if $|a|, |b|, |c|, |d| < 1$.
- By Barrett et al. (1993), Γ can be completed to a positive definite matrix Σ iff

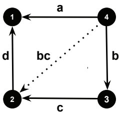
$$f(a, b, c, d) = \sqrt{(1 - a^2)(1 - b^2)} + \sqrt{(1 - c^2)(1 - d^2)} - |ab - cd| > 0$$

- An enumeration of the DAG versions of C_4 are given as follows.

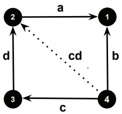
COUNTEREXAMPLE CONTINUED



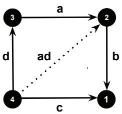
(1)



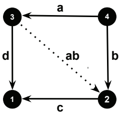
(2)



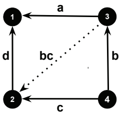
(3)



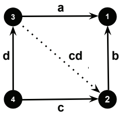
(4)



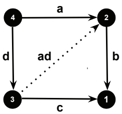
(5)



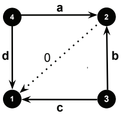
(6)



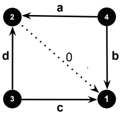
(7)



(8)



(9)



(10)

COUNTEREXAMPLE CONTINUED

- We can show Γ can be completed in a DAG version above iff

$$
\begin{aligned}
&(1-c^2)(1-d^2)-(ab-cd)^2 > 0, \text{ or}\\
&(1-a^2)(1-d^2)-(bc-ad)^2 > 0, \text{ or}\\
&(1-a^2)(1-b^2)-(cd-ab)^2 > 0, \text{ or}\\
&(1-b^2)(1-c^2)-(ad-bc)^2 > 0, \text{ or}\\
&\min\left((1-b^2)(1-c^2)-(bc)^2, (1-a^2)(1-d^2)-(ad)^2\right) > 0, \text{ or}\\
&\min\left((1-a^2)(1-b^2)-(ab)^2, (1-c^2)(1-d^2)-(cd)^2\right) > 0.
\end{aligned}
$$

- If $a = 0.6$, $b = 0.9$, $c = 0.1$, and $d = 0.9$, then we have $f(0.6, 0.9, 0.1, 0.9) = 0.3324 > 0$, but none of the inequalities above is satisfied.

Computing $\Sigma(\Gamma)^{-1}$ and $\det \Sigma(\Gamma)$ without completing Γ

Definition

Let $\mathcal{G} = (V, \mathscr{V})$ be an arbitrary undirected graph.

- For three disjoint subsets A, B and S of V we say that S separates A from B in $\mathcal{G}$ if every path from a vertex in A to a vertex in B intersects a vertex in S.
- Let Γ be a $\mathcal{G}$-partial matrix. The zero-fill-in of Γ in $\mathcal{G}$, denoted by $[\Gamma]^V$, is a $|V| \times |V|$ matrix T s.t.

$$T_{ij} = \begin{cases} \Gamma_{ij} & \text{if } \{i,j\} \in \mathscr{V}, \\ 0 & \text{otherwise.} \end{cases}$$

A KEY LEMMA

Lemma

Let $\mathcal{D} = (V, \mathscr{E})$ be an arbitrary DAG. Let $\Sigma \in \mathrm{PD}_{\mathcal{D}}$ and let (A, B, S) be a partition of V s.t. S separates A from B in $\mathcal{D}^m$. Then we have

1. $\Sigma^{-1} = \left[(\Sigma_{A\cup S})^{-1}\right]^V + \left[(\Sigma_{B\cup S})^{-1}\right]^V - \left[(\Sigma_S)^{-1}\right]^V$ and
2. $\det(\Sigma^{-1}) = \dfrac{\det(\Sigma_S)}{\det(\Sigma_{A\cup S})\det(\Sigma_{B\cup S})}$.

Proof:

Since $\mathrm{PD}_{\mathcal{D}} \subseteq \mathrm{PD}_{\mathcal{D}^m}$ the proof directly follows from Lemma 5.5 in Lauritzen (1996).

Formulae

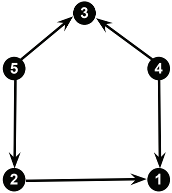
- Let Γ be a partial positive definite matrix over $\mathcal{D}$ that can be completed to a positive definite matrix Σ in $PD_{\mathcal{D}}$. Then

1. $\Sigma^{-1} = \sum_{i=1}^{p} \left(\left[(\Sigma_{\mathrm{fa}(i)})^{-1} \right]^{V} - \left[(\Sigma_{\mathrm{pa}(i)})^{-1} \right]^{V} \right)$

2. $\det(\Sigma^{-1}) = \dfrac{\prod_{i=1}^{p} \det(\Sigma_{\mathrm{pa}(i)})}{\prod_{i=1}^{p} \det(\Sigma_{\mathrm{fa}(i)})} = \prod_{i=1}^{p} \Sigma_{ii|\mathrm{pa}(i)}^{-1}.$

Example

Let $\mathcal{D}$ and Γ be given as follows.



$$\Gamma = \begin{pmatrix} 1 & \Sigma_{12} & * & \Sigma_{14} & * \\ \Sigma_{21} & 1 & * & * & \Sigma_{25} \\ * & * & 1 & \Sigma_{34} & \Sigma_{35} \\ \Sigma_{41} & * & \Sigma_{43} & 1 & * \\ * & \Sigma_{52} & \Sigma_{53} & * & 1 \end{pmatrix}$$

- By applying the first formula we obtain

$$\Sigma^{-1} = \left[(\Sigma_{\{1,2,4\}})^{-1}\right]^V + \left[(\Sigma_{\{2,5\}})^{-1}\right]^V + \left[(\Sigma_{\{3,4,5\}})^{-1}\right]^V + \left[\Sigma_{44}^{-1}\right]^V$$
$$+ \left[\Sigma_{55}^{-1}\right]^V - \left[(\Sigma_{\{2,4\}})^{-1}\right]^V - \left[\Sigma_{55}^{-1}\right]^V - \left[(\Sigma_{\{4,5\}})^{-1}\right]^V .$$

- Note that all the involved entries are given by Γ, except for Σ_{54} and Σ_{42}.

Example continued

Completing the computations we obtain

$$\Sigma^{-1} = \left[\begin{pmatrix} 1 & \Sigma_{12} & \Sigma_{14} \\ \Sigma_{21} & 1 & 0 \\ \Sigma_{41} & 0 & 1 \end{pmatrix}^{-1}\right]^V + \left[\begin{pmatrix} 1 & \Sigma_{25} \\ \Sigma_{52} & 1 \end{pmatrix}^{-1}\right]^V + \left[\begin{pmatrix} 1 & \Sigma_{34} & \Sigma_{35} \\ \Sigma_{43} & 1 & 0 \\ \Sigma_{53} & 0 & 1 \end{pmatrix}^{-1}\right]^V$$

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

$$= \frac{1}{1 - \Sigma_{12}^2 - \Sigma_{14}^2} \begin{pmatrix} 1 & -\Sigma_{12} & 0 & -\Sigma_{14} & 0 \\ -\Sigma_{12} & 1 - \Sigma_{14}^2 & 0 & \Sigma_{12}\Sigma_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\Sigma_{14} & \Sigma_{12}\Sigma_{14} & 0 & 1 - \Sigma_{12}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} + \frac{1}{1 - \Sigma_{25}^2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -\Sigma_{25} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -\Sigma_{25} & 0 & 0 & 1 \end{pmatrix}$$

$$+ \frac{1}{1 - \Sigma_{34}^2 - \Sigma_{35}^2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\Sigma_{34} & -\Sigma_{35} \\ 0 & 0 & -\Sigma_{34} & 1 - \Sigma_{35}^2 & \Sigma_{34}\Sigma_{35} \\ 0 & 0 & -\Sigma_{35} & \Sigma_{34}\Sigma_{35} & 1 - \Sigma_{34}^2 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

Example continued

By combining these terms into one matrix we have Σ^{-1} is equal to

$$\begin{pmatrix}
\frac{1}{1-\Sigma_{12}^2-\Sigma_{14}^2} & \frac{-\Sigma_{12}}{1-\Sigma_{12}^2-\Sigma_{14}^2} & 0 & \frac{-\Sigma_{14}}{1-\Sigma_{12}^2-\Sigma_{14}^2} & 0 \\
\frac{-\Sigma_{12}}{1-\Sigma_{12}^2-\Sigma_{14}^2} & \frac{1-\Sigma_{14}^2}{1-\Sigma_{12}^2-\Sigma_{14}^2} + \frac{1}{1-\Sigma_{25}^2} - 1 & 0 & \frac{\Sigma_{12}\Sigma_{14}}{1-\Sigma_{12}^2-\Sigma_{14}^2} & \frac{-\Sigma_{25}}{1-\Sigma_{25}^2} \\
0 & 0 & \frac{1}{1-\Sigma_{34}^2-\Sigma_{35}^2} & \frac{-\Sigma_{34}}{1-\Sigma_{34}^2-\Sigma_{35}^2} & \frac{-\Sigma_{35}}{1-\Sigma_{34}^2-\Sigma_{35}^2} \\
\frac{-\Sigma_{14}}{1\Sigma_{12}^2-\Sigma_{14}^2} & \frac{\Sigma_{12}\Sigma_{14}}{1-\Sigma_{12}^2-\Sigma_{14}^2} & \frac{-\Sigma_{34}}{1-\Sigma_{34}^2-\Sigma_{35}^2} & \frac{1-\Sigma_{12}^2}{1-\Sigma_{12}^2-\Sigma_{14}^2} + \frac{1-\Sigma_{35}^2}{1-\Sigma_{34}^2-\Sigma_{35}^2} - 1 & \frac{\Sigma_{34}\Sigma_{35}}{1-\Sigma_{34}^2-\Sigma_{35}^2} \\
0 & \frac{-\Sigma_{25}}{1-\Sigma_{25}^2} & \frac{-\Sigma_{35}}{1-\Sigma_{34}^2-\Sigma_{35}^2} & \frac{\Sigma_{34}\Sigma_{35}}{1-\Sigma_{34}^2-\Sigma_{35}^2} & \frac{1-\Sigma_{34}^2}{1-\Sigma_{34}^2-\Sigma_{35}^2} + \frac{1}{1-\Sigma_{25}^2} - 1
\end{pmatrix}$$

- Using the second formula we obtain

$$\det(\Sigma^{-1}) = \left[(1-\Sigma_{12}^2-\Sigma_{14}^2)(1-\Sigma_{25}^2)(1-\Sigma_{34}^2-\Sigma_{35}^2)\right]^{-1}.$$

A NUMERICAL EXAMPLE

- We apply the result for commuting the Σ^{-1} to the the following specific $\mathcal{D}$-partial matrix

$$\Gamma = \begin{pmatrix} 4 & -2 & * & 1 & * \\ -2 & 2 & * & * & -1 \\ * & * & 3 & 1 & -1 \\ 1 & * & 1 & 1 & * \\ * & -1 & -1 & * & 1 \end{pmatrix}.$$

- We obtain

$$\Sigma^{-1} = \begin{pmatrix} 1 & 1 & 0 & -1 & 0 \\ 1 & 2 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 & 1 \\ -1 & -1 & -1 & 3 & -1 \\ 0 & 1 & 1 & -1 & 3 \end{pmatrix}$$

- Note that Σ^{-1} has been evaluated without directly obtaining Σ, and then computing its inverse $\longrightarrow$ fewer computations.

Thank You!