Positive Definite Completion Problems For DAG Models

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Fields Institute: Workshop on Graphical Models

April 16, 2012
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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** $\mathcal{P}$: a subset of positions in an $n \times n$ matrix in which the entries are present.

- A (symmetric) **incomplete matrix** $\Upsilon$: the entries corresponding to the positions in $\mathcal{P}$ 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 $4 \times 4$ pattern:

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

- An incomplete matrix:

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

- A positive definite completion of $\Upsilon$

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

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

Theorem

Every incomplete matrix \( \Upsilon \) corresponding to a given pattern \( \mathcal{P} \) has a positive definite completion iff

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

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

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

\[
\Sigma^{-1}_{ij} = 0 \quad \forall \{i, j\} \in \mathcal{P}.
\]

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

- When \( G \) 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 \( \varphi \) can be explicitly computed [Dawid & Lauritzen (1993), Roverato (2000), Letac & Massam (2007)].
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).
- Flexible covariance estimation for decomposable graphs, Rajaratnam, Massam et al. (2008).
- Wishart distributions for decomposable covariance graph models, Khare & Rajaratnam (2011).
**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 $D$. 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 $G = (V, \mathcal{V})$
- An **(undirected) edge** in $\mathcal{V}$: denoted by an unordered pair $\{i, j\}$
- A **directed acyclic graph** $DAG$: denoted by $D = (V, \mathcal{E})$
- A **(directed) edge** in $\mathcal{E}$: denoted by a ordered pair $(i, j)$
  - $(i, j) \in \mathcal{E}$: denoted by $i \rightarrow j$, say $i$ a **parent** of $j$
- The set of parents of $j$: denoted by $\text{pa}(j) = \{i : i \rightarrow j\}$
- The **family** of $j$: denoted by $\text{fa}(j) = \text{pa}(j) \cup \{j\}$
- The **undirected version** of $D$: denoted by $D^u$
- An **immorality** in $D$: an induced subgraph of the form $i \rightarrow j \leftarrow k$
- The **moral graph** of $D$: denoted by $D^m$
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 $i \rightarrow j \implies i > j$

- For a parent ordered DAG $\mathcal{D}$, $i$ is a **predecessor** of $j$ if $i > j$ but $i \not\rightarrow j$ (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
Let $X = (X_1, \ldots, X_p)$ be a random vector in $\mathbb{R}^p$, with $p = |V|$.

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

  $$X_i \perp X_{\text{pr}(i) \setminus \text{pa}(i)}|X_{\text{pa}(i)} \quad \forall i \in V$$

- The **Gaussian DAG model** $\mathcal{N}(\mathcal{D})$ is the family of multivariate normal distributions $\mathcal{N}_p(\mu, \Sigma)$, $\mu \in \mathbb{R}^p$, $\Sigma > 0$ 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: $\mathcal{N}_p(\mu, \Sigma) \in \mathcal{N}(\mathcal{D})$ iff $\Sigma > 0$ and

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

- 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
  \[ X_1 \perp X_4|(X_2, X_3) \quad \text{and} \quad X_2 \perp X_3|(X_1, X_4) \]

- 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
  \[ X_1 \perp X_4|(X_2, X_3) \quad \text{and} \quad X_2 \perp X_3|X_4 \]
Preliminary notation

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

- A $\mathcal{D}$-incomplete matrix is a symmetric function
  
  $$\Gamma : \{i,j\} \mapsto \Gamma_{ij} \in \mathbb{R}, \text{ s.t. } \Gamma_{ij} = \Gamma_{ji} \quad \forall (i,j) \in \mathcal{E}.$$  

- $\Gamma$ is partially positive definite, denoted by $\Gamma >_{\mathcal{D}} 0$, if $\Gamma_C > 0$ for each clique $C$ of $\mathcal{D}^u$.

- The space of covariance and the inverse-covariance matrices over $\mathcal{D}$ are defined as

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

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

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

Let $L_D$ denote the linear space of all lower triangular matrices with unit diagonal entries such that

$$L \in L_D \implies L_{ij} = 0 \quad \forall (i, j) \notin E.$$ 

Then $\Omega \in P_D \iff \exists L \in L_D$ and a diagonal matrix $\Lambda$, with strictly positive diagonal entries s.t. in the modified Cholesky decomposition $\Omega = L\Lambda L'$, Wermuth (1980).

PD$_D$ $\subseteq$ PD$_D^m$, Wermuth (1980).

PD$_D$ = PD$_D^u \iff D$ is a perfect DAG.

Convention

Unless otherwise stated, hereafter $G = (V, \mathcal{V})$ denotes the undirected version of $D = (V, E)$. 
A formal definition of matrix completion

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

- We say that a $\mathcal{D}$-incomplete matrix $\Gamma$ can be completed in $\mathcal{M}$ if
  \[ \exists T \in \mathcal{M} \text{ s.t. } T_{ij} = \Gamma_{ij} \quad \forall (i,j) \in \mathcal{E} \]

- We refer to $T$ as a completion of $\Gamma$ in $\mathcal{M}$, or

- simply a completion of $\Gamma$, if $\mathcal{M}$ is the whole space $S_p(\mathbb{R})$. 
**Positive definite completion in \( \mathbb{P}_D \)**

- Let \( \mathcal{I}_D \) denote the set of \( \mathcal{D} \)-incomplete matrices.

**Proposition**

Let \( \Gamma \) be a \( \mathcal{D} \)-incomplete matrix in \( \mathcal{I}_D \). If \( \Gamma_{11} \neq 0 \), then

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

\[
\hat{\Gamma} = LL' \quad \text{is a completion of } \quad \Gamma
\]

- Part (b) The matrix \( \hat{\Gamma} \) is the unique positive definite completion of \( \Gamma \) in \( \mathbb{P}_D \) iff the diagonal entries of \( \Lambda \) are all strictly positive.
Sketch of the proof

1. Set $L_{ij} = 0$ for each $(i, j) \notin \mathcal{E}$.

2. Set $\Lambda_{11} = \Gamma_{11}$, $L_{i1} = \Lambda_{11}^{-1} \Gamma_{i1}$ for each $i \in \text{pa}(1)$ and set $j = 1$.

3. If $j < p$, then set $j = j + 1$ and proceed to step iv), otherwise $L$ and $\Lambda$ 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 $i \in \text{pa}(j)$ 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 $\Gamma$ exists that satisfies the condition in part (a). Consequently, $\Gamma$ cannot also be completed in $P_D$. 
Example

Let $\mathcal{D}$ and $\Gamma$ 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 $\Gamma$ we obtain

\[ \Lambda = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 0 & 0 \\
0 & 0 & 0 & -3 & 0 & 0 \\
0 & 0 & 0 & 0 & -2 & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}, \quad L = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 2 & 1 & 0 & 0 & 0 \\
-3 & 0 & -5 & 1 & 0 & 0 \\
0 & 5 & 0 & -1 & 1 & 0 \\
4 & -2 & 0 & 0 & 0 & 1
\end{pmatrix} \]
This yields the completed matrix $\widetilde{\Gamma}$ given as follows:

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

As the diagonal elements of $\Lambda$ are not strictly positive, $\Gamma$ cannot be completed in $P_D$. 
**Proposition**

Let $\Gamma$ be a partial positive definite matrix. The following completion process (of polynomial complexity) determines if a completion in $\text{PD}_D$ exists, and if so, it uniquely constructs the completed matrix $\Sigma$.

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

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

\[
\begin{array}{c}
\text{Layer: } j=4. \text{ In step (1)}
\end{array}
\]

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

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

Layer: \( j=3 \). In step (2) let \( j = 4 - 1 = 3 \). In step (3) either
\[
\Sigma_{fa(3)} = \begin{pmatrix} \Sigma_{33} & \Sigma_{34} \\ \Sigma_{43} & \Sigma_{44} \end{pmatrix} > 0,
\]
otherwise the completion in PD\(\mathcal{D}\) does not exist. Assuming the former, we proceed to step (5). Since \( pr(3) = \emptyset \), 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
\[
\Sigma_{fa(2)} = \begin{pmatrix} \Sigma_{22} & \Sigma_{24} \\ \Sigma_{42} & \Sigma_{44} \end{pmatrix} > 0.
\]
Assuming \( \Sigma_{fa(2)} > 0 \), then in step (5), as \( pr(2) = \{3\} \), we set \( \Sigma_{32} = \Sigma_{34} \Sigma_{44}^{-1} \Sigma_{42} \) and the layer down to \( j = 2 \) is thus completed.
Layer: \( j = 1 \). Process is returned to step (2) with \( j = 2 - 1 = 1 \). In step (3) we first check whether

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

Assuming \( \Sigma_{fa(1)} > 0 \), then in step (5), as \( pr(1) = \{4\} \) 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 \( \Sigma \) is the completion of \( \Gamma \) in \( PD_D \).
AN ALTERNATIVE PROCEDURE

- Step (1) We construct a finite sequence of DAGs, $D_0, \ldots, D_n$ such that $D_n$ at the end of this sequence is perfect. Let $\Gamma_n$ denote the incomplete matrix over $D_n$.
- Step (2) Set $D = D_n$ and $\Gamma = \Gamma_n$.
- Step (3) If $\Gamma > 0$, then proceed as follows.
  1. Set $\Sigma_{ij} = \Gamma_{ij}$ for each $\{i, j\} \in \mathcal{V}$,
  2. Set $\Sigma_{\text{pr}(j), j} = \Sigma_{\text{pr}(j), \text{pa}(j)} \Sigma_{\text{pa}(j), j}^{-1} \Sigma_{\text{pa}(j), j}$ and $\Sigma_{j, \text{pr}(j)} = \Sigma'_{\text{pr}(j), j}$ for each $j = p - 1, \ldots, 1$

Remark

- Let $D$ be a perfect DAG and $\Gamma \in I_D$

  $\Gamma$ can be competed in $\text{PD}_D \iff \Gamma \in Q_D \ (i.e., \ \Gamma >_D 0)$

- Thus the alternative procedure yields a completion iff $\Gamma_n >_D 0$. 
Example

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

- Starting from $\mathcal{D}_0 = \mathcal{D}$, the only immorality in this DAG is $5 \rightarrow 1 \leftarrow 2$. By adding the directed edge $5 \rightarrow 2$ we obtain $\mathcal{D}_1$.
- Next we obtain the perfect DAG $\mathcal{D}_2$ by adding the directed edge $5 \rightarrow 3$ corresponding to the immorality $5 \rightarrow 2 \leftarrow 3$ 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 \( D_2 \)

\[ \Gamma^{(2)} = \begin{pmatrix} \Gamma_{11} & \Gamma_{12} & * & * & \Gamma_{15} \\ \Gamma_{21} & \Gamma_{22} & \Gamma_{23} & * & \Gamma_{54} \Gamma_{44}^{-1} \Gamma_{43} \\ * & \Gamma_{32} & \Gamma_{33} & \Gamma_{34} & \Gamma_{53} \Gamma_{33}^{-1} \Gamma_{32} \\ * & * & \Gamma_{43} & \Gamma_{44} & \Gamma_{45} \\ \Gamma_{15} & \Gamma_{54} \Gamma_{44}^{-1} \Gamma_{43} & \Gamma_{53} \Gamma_{33}^{-1} \Gamma_{32} & \Gamma_{54} & \Gamma_{55} \end{pmatrix}. \]
Completable DAGs and generalization of Grone et al’s result

Theorem

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

Corollary

Suppose $\mathcal{G}$ is a decomposable graph. Then every partially positive definite matrix $\Gamma$ over $\mathcal{G}$ can be completed to a unique $\Sigma$ in 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 PD$_{\mathcal{D}}$ implies completion in PD$_{\mathcal{D}^u}$
Some insights

- Interesting contrast between completing a given partial positive definite matrix $\Gamma \in Q_D$ in $PD_G$ vs. completing it in $PD_D$.

- Grone et al. (1984) asserts that $\Gamma \in Q_G$ can be completed in $PD_G$ if any positive completion exists.

- A completion in $PD_D$ is therefore sufficient to guarantee a completion in $PD_G$.

- The other way around is unfortunately not true.

- In particular, $\Gamma$ may not be completed in $PD_D$ even when it can be completed in $PD_G$.

- This is because completion in $PD_D$ is more restrictive than completion in $PD_G$.

- We illustrate this distinction in the following example.
More formally, let $\Gamma$ be an incomplete matrix over $\mathcal{D}$ and let $\mathcal{G}$ be the undirected version of $\mathcal{D}$.

- If $\Gamma$ can be completed in $\text{PD}_G$, then can it be completed in $\text{PD}_D$ as well?

Consider the partial positive definite matrix $\Gamma$ 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 $\text{PD}_\mathcal{G}$.

- Completion of $\Gamma$ in $\text{PD}_\mathcal{D}$ 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, $\Gamma$ cannot be completed in $\text{PD}_\mathcal{D}$. 
Let $\Gamma$ be an incomplete matrix over $\mathcal{D}$ and let $\mathcal{G}$ be the undirected version of $\mathcal{D}$.

- If $\Gamma$ can be completed in $\text{PD}_G$, then can it be completed in $\text{PD}_D$ as well?

- The answer as we saw was negative.

- Then, can it at least be completed in $\text{PD}_{\mathcal{D}'}$ for a DAG version $\mathcal{D}'$ of $\mathcal{G}$?

The answer is still negative. We show this by constructing a counter example.
Consider the following partial matrix $\Gamma$ over the four cycle $C_4$.

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

- $\Gamma$ is a partial positive definite matrix over $C_4$ if $|a|, |b|, |c|, |d| < 1$.
- By Barrett et al. (1993), $\Gamma$ can be completed to a positive definite matrix $\Sigma$ 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)
We can show \( \Gamma \) can be completed in a DAG version above iff

\[
(1 - c^2)(1 - d^2) - (ab - cd)^2 > 0, \text{ or }
\]
\[
(1 - a^2)(1 - d^2) - (bc - ad)^2 > 0, \text{ or }
\]
\[
(1 - a^2)(1 - b^2) - (cd - ab)^2 > 0, \text{ or }
\]
\[
(1 - b^2)(1 - c^2) - (ad - bc)^2 > 0, \text{ or }
\]
\[
\min \left( (1 - b^2)(1 - c^2) - (bc)^2, (1 - a^2)(1 - d^2) - (ad)^2 \right) > 0, \text{ or }
\]
\[
\min \left( (1 - a^2)(1 - b^2) - (ab)^2, (1 - c^2)(1 - d^2) - (cd)^2 \right) > 0.
\]

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 $\Gamma$

**Definition**

Let $\mathcal{G} = (V, \mathcal{V})$ 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 $\Gamma$ be a $\mathcal{G}$-partial matrix. The zero-fill-in of $\Gamma$ in $\mathcal{G}$, denoted by $[\Gamma]^V$, is a $|V| \times |V|$ matrix $T$ s.t.

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

Let $\mathcal{D} = (V, \mathcal{E})$ be an arbitrary DAG. Let $\Sigma \in \text{PD}_\mathcal{D}$ 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. $\Sigma^{-1} = \left[ (\Sigma_{AUS})^{-1} \right]^V + \left[ (\Sigma_{BUS})^{-1} \right]^V - \left[ (\Sigma_S)^{-1} \right]^V$ and

2. $\det(\Sigma^{-1}) = \frac{\det(\Sigma_S)}{\det(\Sigma_{AUS}) \det(\Sigma_{BUS})}$.

Proof:

Since $\text{PD}_\mathcal{D} \subseteq \text{PD}_{\mathcal{D}^m}$ the proof directly follows from Lemma 5.5 in Lauritzen (1996).
Let $\Gamma$ be a partial positive definite matrix over $\mathcal{D}$ that can be completed to a positive definite matrix $\Sigma$ in $\text{PD}_\mathcal{D}$. Then

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

2. $\det(\Sigma^{-1}) = \frac{\prod_{i=1}^{p} \det(\Sigma_{pa(i)})}{\prod_{i=1}^{p} \det(\Sigma_{fa(i)})} = \prod_{i=1}^{p} \Sigma_{iil\mid \text{pa}(i)}^{-1}$. 
Example

Let $\mathcal{D}$ and $\Gamma$ 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 $\Gamma$, except for $\Sigma_{54}$ and $\Sigma_{42}$. 
Completing the computations we obtain

\[ \Sigma^{-1} = \left[ \begin{array}{ccc} 1 & \Sigma_{12} & \Sigma_{14} \\ \Sigma_{21} & 1 & 0 \\ \Sigma_{41} & 0 & 1 \end{array} \right]^{-1} + \left[ \begin{array}{ccc} 1 & \Sigma_{25} & 0 \\ \Sigma_{52} & 1 & 0 \\ \Sigma_{53} & 0 & 1 \end{array} \right]^{-1} \]

\[ = \frac{1}{1 - \Sigma_{12}^2 - \Sigma_{14}^2} \left[ \begin{array}{cccc} 1 & -\Sigma_{12} & 0 & -\Sigma_{14} \\ -\Sigma_{12} & 1 - \Sigma_{14}^2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\Sigma_{14} & 0 & 1 - \Sigma_{12}^2 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right] + \frac{1}{1 - \Sigma_{25}^2} \left[ \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]. \]

\[ + \frac{1}{1 - \Sigma_{34}^2 - \Sigma_{35}^2} \left[ \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\Sigma_{34} \\ 0 & 0 & -\Sigma_{34} & 1 - \Sigma_{35}^2 \end{array} \right] \]
Example continued

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

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

- 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 $\Sigma^{-1}$ 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 $\Sigma^{-1}$ has been evaluated without directly obtaining $\Sigma$, and then computing its inverse $\rightarrow$ fewer computations.
Thank You!