Estimation of a Covariance Matrix with Zeros

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Abstract

We consider estimation of the covariance matrix of a multivariate random vector under the constraint that certain covariances are zero. We first present an algorithm, which we call Iterative Conditional Fitting, for computing the maximum likelihood estimator of the constrained covariance matrix, under the assumption of multivariate normality. In contrast to previous approaches, this algorithm has guaranteed convergence properties. Dropping the assumption of multivariate normality, we show how to estimate the covariance matrix in an empirical likelihood approach. These approaches are then compared via simulation and on an example of gene expression.

Some key words: Covariance graphs; Empirical likelihood; Graphical models; Marginal independence; Maximum likelihood estimation; Multivariate normal distribution

1 Introduction

In this paper we consider estimation of the covariance matrix of a random vector, subject to certain entries being set to zero. Such restrictions appear, for example, in recent work by Grzebyk et al. (2004) and Mao et al. (2004). Suppose we have a random vector

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Figure 1: The covariance graph for the matrix in (1.1).

\[ X = (X_1, X_2, X_3, X_4)' \in \mathbb{R}^4 \]

whose covariance matrix \( \Sigma \) exhibits the zero pattern

\[
\Sigma = \begin{pmatrix}
\sigma_{11} & 0 & \sigma_{13} & 0 \\
0 & \sigma_{22} & 0 & \sigma_{24} \\
\sigma_{13} & 0 & \sigma_{33} & \sigma_{34} \\
0 & \sigma_{24} & \sigma_{34} & \sigma_{44}
\end{pmatrix} \in \mathbb{R}^{4 \times 4}.
\] (1.1)

It is often helpful to visualize the pattern of zeros by a so-called covariance graph, especially for larger covariance matrices (Cox and Wermuth, 1993, 1996). A covariance graph has one vertex for each one of the random variables in the random vector. In the above example, the vertex set is \( V = \{1, 2, 3, 4\} \), where the random variable \( X_i \) is identified with its index \( i \). Next, each pair of vertices \( (i, j) \in V \times V, i \neq j \), is connected by an edge unless \( \sigma_{ij} = 0 \). Assuming that the covariance matrix in (1.1) has no zeros other than those indicated explicitly, its covariance graph is given in Figure 1. Here we use bi-directed edges in keeping with the path diagram notation used by Wright (1921); other authors have used dashed edges; see Cox and Wermuth (1993, 1996).

We define a covariance graph model as the set of joint distributions in which the associated zero restrictions hold in the covariance matrix. In the absence of an assumption of normality, the model does not have a Markov interpretation.

The Gaussian covariance graph model is the family of all multivariate normal distributions \( \mathcal{N}(\mu, \Sigma) \) such that \( \sigma_{ij} = 0 \) whenever \( i \neq j \) and \( i \neq j \). Clearly, \( \sigma_{ij} = 0 \) if and only if \( X_i \) and \( X_j \) are marginally independent; in symbols \( X_i \perp \perp X_j \). Hence a Gaussian covariance graph model is a graphical model based on marginal independence in contrast with graphical models based on undirected graphs (Markov random fields), directed acyclic graphs (DAGs, Bayesian networks), or chain graphs, where the absence of an edge between two vertices generally indicates some conditional independence between the associated variables (Edwards, 2000; Lauritzen, 1996; Whittaker, 1990).

Maximum likelihood (ML) estimation in Gaussian covariance graph models is not well developed: the conceptual simplicity of these models belies the fact that, in contrast to undirected graph models, they form curved exponential families. For instance, the graphical modelling software MIM (Edwards, 2000, §7.4) permits fitting of such models only by a heuristic “dual likelihood” method due to Kauermann (1996). There is, however, an algorithm due to Anderson (1969, 1970, 1973) that can be used to compute the ML estimate in models defined by linear hypotheses on covariance matrices, hence also...
in covariance graph models. However, it is unclear when this algorithm converges and when its limit points are positive semi-definite matrices. Such issues become more pressing when mis-specified models are fitted, as will be the case in a specification search. In this paper, we introduce a new algorithm for ML estimation in covariance graph models, called Iterative Conditional Fitting (ICF), which does not suffer from the same problems as Anderson’s algorithm.

For situations in which multivariate normality does not hold, estimates may still be obtained via procedures based on normality such as ICF and dual estimation but the behaviour of these methods is then unclear. As an alternative, we present an approach, based on empirical likelihood (Owen, 2001), which provides consistent estimates even without normality. We compare the different estimation methods on real and simulated data.

2 Covariance graph models

2.1 Non-parametric model

Suppose that we observe a random vector \( Y = (Y_i \mid i \in V)' \in \mathbb{R}^V \), indexed by \( V \), and with joint distribution \( P \). Let \( \Sigma(P) = (\sigma_{ij}) \in \mathbb{R}^{V \times V} \) be the unknown covariance matrix. Let \( G = (V, E) \) be a graph with the variable set \( V \) as vertex set and the edge set \( E \subseteq V \times V \setminus \{(i, i) \mid i \in V\} \) consisting exclusively of bi-directed edges \((i, j), (j, i) \in E\), denoted by \( i \leftrightarrow j \). Let \( P(V) \) be the cone of positive definite \( V \times V \) matrices and let \( P(G) \) be the cone of all matrices \( \Sigma \in P(V) \) which fulfill the linear restrictions

\[
i \not\leftrightarrow j \implies \sigma_{ij} = 0.
\]  

(2.1)

The covariance graph model \( M(G) \) associated with the bi-directed graph \( G \) is simply the family of joint distributions

\[
M(G) = \{P_V \mid \Sigma(P_V) \in P(G)\}. 
\]  

(2.2)

We consider estimation of the unknown parameter \( \Sigma = \Sigma(P_V) \) based on a sample of observations \( Y_V^{(k)} \in \mathbb{R}^V \), \( k \in N = \{1, \ldots, n\} \), that are i.i.d. according to \( P_V \in M(G) \). The set \( N \) can be interpreted as indexing the subjects on which we observe the variables in \( V \). We group the vectors in the sample as columns in the \( V \times N \) random matrix \( Y \) so that

\[
\text{Var}(Y) = \Sigma \otimes I_N.
\]  

(2.3)

Here, \( I_N \) is the \( N \times N \) identity matrix and \( \otimes \) is the Kronecker product. Thus the \( i \)-th row \( Y_i \in \mathbb{R}^N \) of the matrix \( Y \) contains the i.i.d. observations for variable \( i \in V \) on all the subjects in \( N \) and the \( k \)-th column \( Y_V^{(k)} \) holds all the observations made on subject \( k \in N \). Finally, the sample size is \( n = |N| \) and the number of variables is \( p = |V| \).
2.2 Gaussian model

We define a Gaussian covariance graph model as the multivariate normal submodel

$$N(G) = (N_V(\mu, \Sigma) \mid \Sigma \in \mathcal{P}(G)) \subset M(G).$$

(2.4)

The log-likelihood function $\ell$ of the covariance graph model $N(G)$ is a function from $\mathbb{R}^V \times \mathcal{P}(G)$ to $\mathbb{R}$ and can be expressed as

$$\ell(\mu, \Sigma) = -\frac{np}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{n}{2} \text{tr}(\Sigma^{-1} \tilde{S}),$$

(2.5)

see e.g. Edwards (2000, §3.1). Here $\tilde{S}$ is

$$\tilde{S} = \frac{1}{n} (Y - \mu \otimes 1_N)(Y - \mu \otimes 1_N)' \in \mathbb{R}^{V \times V},$$

(2.6)

where $1_N = (1, \ldots, 1)' \in \mathbb{R}^N$. For any given value of $\Sigma$, $\ell(\mu, \Sigma)$ is maximized by setting $\mu = \bar{Y} \in \mathbb{R}^V$, i.e., the vector of the row means of $Y$. Hence, the profile log-likelihood for $\Sigma$, $\ell(\Sigma)$ is obtained by replacing $\tilde{S}$ with

$$S = \frac{1}{n} (Y - \bar{Y} \otimes 1_N)(Y - \bar{Y} \otimes 1_N)' \in \mathbb{R}^{V \times V},$$

(2.7)

in (2.5). Working with the profile likelihood corresponds to fitting the submodel of $N(G)$ in which $\mu = 0$ and adjusting the sample size to $n - 1$.

If $S$ is positive definite, which will occur with probability 1 if $n \geq p+1$ (Eaton and Perlman, 1973), then the global maximum of $\ell(\Sigma)$ over $\mathcal{P}(G)$, i.e., the ML estimator of $\Sigma$, exists. In general, the condition $n \geq p+1$ is not necessary for almost sure existence of the ML estimator but we are not aware of any results in the literature which provide a necessary and sufficient condition (compare Buhl, 1993). In the sequel we will assume $S$ to be positive definite. Note that since the model $N(G)$ is a curved, but not necessarily regular, exponential family, the likelihood function may, and in fact can, have multiple local maxima (Drton, 2005; Drton and Richardson, 2004).

Let

$$F = \{(i, i) \mid i \in V\} \cup \{(i, j) \in V^2 \mid i < j \land i \leftrightarrow j\}$$

(2.8)

be the pairs of vertices indexing unrestricted elements in the matrix $\Sigma \in \mathcal{P}(G)$. The cardinality of $F$ is equal to the number of vertices plus the number of edges in the graph $G$. The unrestricted elements of $\Sigma$ form the vector

$$\sigma = (\sigma_{ij} \mid (i, j) \in F) \in \mathbb{R}^F.$$  

(2.9)

In order to write derivatives of the log-likelihood function in compact form we introduce the matrix $Q$ with entries in $\{0, 1\}$ that satisfies $\text{vec}(\Sigma) = Q\sigma$, where $\text{vec}$ is the operator of
column-wise matrix vectorization. The columns of $Q$ that are associated with a variance $\sigma_{ii}$ contain exactly one entry equal to one, whereas a column of $Q$ that is associated with a covariance $\sigma_{ij}$, $i \neq j$, $i \leftrightarrow j$, contains exactly two entries equal to one. If the graph $G$ is complete, i.e., all possible edges are present in $G$, then $Q$ is the duplication matrix described in Harville (1997, p.352).

The first derivative of the log-likelihood function, that is, the score function can then be written as

$$\frac{\partial \ell(\Sigma)}{\partial \sigma} = \frac{n}{2} Q' \left[ \text{vec}(\Sigma^{-1} S \Sigma^{-1}) - \text{vec}(\Sigma^{-1}) \right],$$

(2.10)

see Harville (1997, §15) for details on the necessary matrix differential calculus. It follows that the likelihood equations $\frac{\partial \ell(\Sigma)}{\partial \sigma} = 0$ are

$$(\Sigma^{-1})_{ij} = (\Sigma^{-1} S \Sigma^{-1})_{ij}, \quad (i, j) \in F;$$

(2.11)

compare also Anderson and Olkin (1985, §2.1.1). The full matrix $\Sigma$ is determined by $\sigma_{ij} = 0$ for $(i, j) \notin F$, that is for $i \neq j$ and $i \not\leftrightarrow j$.

The second derivative of $\ell(\Sigma)$ can be computed using results from Harville (1997, §15.9), and we find that the Hessian matrix equals

$$\frac{\partial^2 \ell(\Sigma)}{\partial \sigma^2} = \frac{n}{2} Q' \left\{ \left[ (\Sigma^{-1} \otimes \Sigma^{-1}) - \left[ (\Sigma^{-1} S \Sigma^{-1}) \otimes \Sigma^{-1} \right] - \left[ \Sigma^{-1} \otimes (\Sigma^{-1} S \Sigma^{-1}) \right] \right\} Q. $$

(2.12)

Its negated expectation under $\mathcal{N}_v(0, \Sigma)$, the Fisher-information, equals

$$-E \left[ \frac{\partial^2 \ell(\Sigma)}{\partial \sigma^2} \right] = \frac{n}{2} Q' (\Sigma^{-1} \otimes \Sigma^{-1}) Q$$

(2.13)

and can be used for normal approximation to the distribution of roots of the likelihood equations. Sections §§3-5 focus on the computations of such roots.

### 3 Existing estimation methods for Gaussian covariance graphs

We are aware of only one specialized algorithm for ML estimation applicable to covariance graph models. This algorithm is due to Anderson (1973) and will fit any Gaussian model obtained from a linear hypothesis on the covariance matrix (Anderson, 1969, 1970). In this section, we describe the incarnation of Anderson’s algorithm that fits covariance graph models. We also review a dual estimation method due to Kauermann (1996), which produces estimates that are unique and asymptotically efficient though, in general, not solutions to the likelihood equations. Note that Cox et al. (2004) have recently proposed moment based estimators in the special case where the graph is a chain, or equivalently, the covariance matrix is tri-diagonal under a suitable ordering.
3.1 Anderson’s algorithm for ML estimation

Each iteration of Anderson’s algorithm solves a system of linear equations built from the current estimate of $\Sigma$. In the case of covariance graphs, the linear equations are solved for the vector $\sigma$ of unrestricted elements in $\Sigma$, compare (2.11), and can be specified as follows. Let $\sigma^{ij} = (\Sigma^{-1})_{ij}$ and $A = A_\Sigma$ be the $F \times F$ matrix with entries

$$A_{(ij, k\ell)} = \begin{cases} \sigma^{ik}\sigma^{jk} & \text{if } k = \ell, \\ \sigma^{ik}\sigma^{j\ell} + \sigma^{j\ell}\sigma^{i\ell} & \text{if } k \neq \ell. \end{cases} \quad (3.1)$$

Here $(i, j)$ and $(k, \ell)$ are elements of $F$. Furthermore, let \( b = b_\Sigma \) be the $F \times 1$ vector with components

$$b_{ij} = (\Sigma^{-1}S\Sigma^{-1})_{ij}, \quad (i, j) \in F. \quad (3.2)$$

From Anderson (1973), it follows that $\Sigma \in P(G)$ solves $A_\Sigma \sigma = b_\Sigma$ if and only if $\Sigma$ solves the likelihood equations (2.11).

This motivates the following iterative scheme. Start with some $\Sigma^{(0)} \in P(G)$. Iteratively update the current estimate $\Sigma^{(r)}$ to $\Sigma^{(r+1)}$ determined by the linear equations

$$A_{\Sigma^{(r)}} \sigma^{(r+1)} = b_{\Sigma^{(r)}}. \quad (3.3)$$

A fixed point of this algorithm solves the likelihood equations (2.11). As starting value, Anderson suggests the identity matrix, i.e., $\Sigma^{(0)} = I_V$. In the first step, his algorithm constructs the empirical estimate $\Sigma^{(1)}$ with $\sigma^{(1)}_{ij} = S_{ij}, (i, j) \in F$. However, neither $\Sigma^{(1)}$ nor any subsequent estimate of $\Sigma$ has to be positive (semi-) definite and thus may not be a valid covariance matrix. Moreover, at any given stage, the likelihood function may decrease, and convergence of Anderson’s algorithm cannot be guaranteed.

3.2 Kauermann’s dual estimation

Dual estimation is based on the maximization of a dual likelihood function, which is motivated by interchanging the role of the parameter matrix $\Sigma$ and the empirical covariance matrix $S$ in (2.5) (Kauermann, 1996, §4). Procedurally, dual estimation, also called minimizing the discriminant information, amounts to finding the matrix $\hat{\Sigma}_{\text{dual}} \in P(G)$ that solves the equations

$$(\hat{\Sigma}_{\text{dual}}^{-1})_{ij} = (S^{-1})_{ij}, \quad \forall (i, j) \in F, \quad (3.4)$$

while satisfying that $(\hat{\Sigma}_{\text{dual}})_{ij} = 0$ for all $(i, j) \notin F$. Contrary to (2.11), the equation system (3.4) always has a unique solution that can be found by the iterative proportional fitting algorithm; see also Edwards (2001, §7.4). In particular, if the covariance graph is decomposable, then iterative proportional fitting will terminate in finitely many steps, and the dual estimator $\hat{\Sigma}_{\text{dual}}$ is available in closed form.
4 Iterative conditional fitting for Gaussian covariance graphs

In this section, we present the new Iterative Conditional Fitting (ICF) algorithm for ML estimation, which is guaranteed to produce positive definite roots of the likelihood equations of covariance graph models. We begin by explaining the idea of iteratively fitting conditional distributions that stands behind ICF, and then show how the algorithm can be implemented using simple least squares computations.

4.1 The idea of iterative conditional fitting

Starting with some initial estimate of the joint distribution, the idea of ICF is to repeatedly iterate through all vertices \( i \in V \), and

(i) Fix the marginal distribution for the variables different from \( i \), i.e., the variables \(-i = V \setminus \{i\}\);

(ii) Estimate, by maximum likelihood, the conditional distribution of variable \( i \) given the variables \(-i\) under the constraints implied by the covariance graph model \( \mathcal{N}(G) \);

(iii) Find a new estimate of the joint distribution by multiplying together the fixed marginal and the estimated conditional distribution.

Since we fix the marginal distribution of variables \(-i\) in the update for variable \( i \), all marginal independences amongst the variables \(-i\) still hold true after the update. Therefore, only the marginal independences involving variable \( i \) lead to constraints for the estimation in step (ii).

In order to make the idea more precise, let \( \Sigma_{A,B} \) denote the \( A \times B \) submatrix of \( \Sigma \) and \( Y_A \) denote the \( A \times N \) submatrix of \( Y \), where \( A, B \subseteq V \). Clearly,

\[ Y_{-i} \sim \mathcal{N}_{-i \times N}(0, \Sigma_{-i,-i} \otimes I_N). \]

Hence, step (i) simply fixes the value of \( \Sigma_{-i,-i} \), i.e., everything but the \( i \)-th row and column of \( \Sigma \). As \( \Sigma_{-i,-i} \) remains unchanged in the \( i \)-th update many of the zero constraints imposed on the covariance matrix trivially hold true also after the update.

The conditional distribution of \( Y_i \) given \( Y_{-i} \) is the normal distribution

\[ (Y_i \mid Y_{-i}) \sim \mathcal{N}_{\{i\} \times N}(B_iY_{-i}, \lambda_i I_N), \]

where

\[ B_i = \Sigma_{i,-i}(\Sigma_{-i,-i})^{-1} \in \mathbb{R}^{|i| \times -i} \]

is the \( \{i\} \times -i \) matrix of regression coefficients, and

\[ \lambda_i = \sigma_{ii} - \Sigma_{i,-i}(\Sigma_{-i,-i})^{-1}\Sigma_{-i,i} \in (0, \infty) \]
is the conditional variance. If the graph \( G \) was the complete graph \( \bar{G} \) in which an edge joins any pair of vertices then the mapping

\[
P(\bar{G}) = P(V) \to (0, \infty) \times \mathbb{R}^{(i) \times -i} \times P_{-i}(\bar{G}),
\]

\[
\Sigma \mapsto (\lambda_i, B_i, \Sigma_{-i,-i})
\]

(4.4)

would be bijective and the regression in (4.1) a standard least squares regression. Here, \( P_A(G) \) is the set of all \( A \times A \) submatrices of matrices in \( P(G) \), \( A \subseteq V \). For a general graph \( G \), (4.4) is no longer bijective and (4.1) is not a standard regression because we need to respect the restriction \( \Sigma \in P(G) \), i.e., the restrictions \( \sigma_{ij} = 0 \) if \( j \in -i \), \( j \not\leftrightarrow i \).

However, this can be circumvented using synthetic \textit{pseudo-variables} that are computed from the data \( Y_{-i} \) and the fixed matrix \( \Sigma_{-i,-i} \).

### 4.2 Pseudo-variable regressions

Instead of working with the regression coefficients \( B_i \), we exploit the fact that \( B_i \) equals \( \Sigma_{i,-i} \) multiplied by the inverse of the fixed submatrix \( \Sigma_{-i,-i} \). Let \( \text{sp}(i) = \{ j \mid i \leftrightarrow j \} \) be the set of \textit{spouses} of \( i \in V \) and let \( \text{nsp}(i) = V \setminus (\text{sp}(i) \cup \{ i \}) \) be the set of \textit{non-spouses}, yielding the partition \( V = \{ i \} \cup \text{sp}(i) \cup \text{nsp}(i) \). Then the conditional expectation of \( (Y_i \mid Y_{-i}) \) can be written as

\[
E[Y_i \mid Y_{-i}] = \Sigma_{i,-i}[(\Sigma_{-i,-i})^{-1} Y_{-i}] = \Sigma_{i,\text{sp}(i)} Z_{\text{sp}(i)}^{(i)} = \sum_{j \in \text{sp}(i)} \sigma_{ij} Z_j^{(i)},
\]

(4.5)

where the \textit{pseudo-variable} \( Z_j^{(i)} \) is equal to the \( j \)-th row in

\[
Z_{\text{sp}(i)}^{(i)} = [(\Sigma_{-i,-i})^{-1}]_{\text{sp}(i),-i} Y_{-i} \in \mathbb{R}^{\text{sp}(i) \times N}.
\]

(4.6)

In (4.6), we exploit that \( \sigma_{ij} = 0 \) if \( j \in \text{nsp}(i) \). From (4.5), we obtain

\[
(Y_i \mid Y_{-i}) \sim \mathcal{N}(\{ i \} \times N \left( \sum_{j \in \text{sp}(i)} \sigma_{ij} Z_j^{(i)}, \lambda_i I_N \right).
\]

(4.7)

Let \( P_{-i}(G) \) be the set of \(-i \times -i\) submatrices of the matrices in \( P(G) \). Then the mapping

\[
P(G) \to (0, \infty) \times \mathbb{R}^{(i) \times \text{sp}(i)} \times P_{-i}(G)
\]

\[
\Sigma \mapsto (\lambda_i, \Sigma_{i,\text{sp}(i)}, \Sigma_{-i,-i})
\]

(4.8)

is a bijection, which implies that the parameters \( \sigma_{ij}, j \in \text{sp}(i) \), and \( \lambda_i \) are variation independent in (4.7). Therefore, if \( \Sigma_{-i,-i} \) is fixed to equal some given matrix in \( P_{-i}(G) \),
then \((4.7)\) constitutes a standard normal regression model whose parameters \(\sigma_{ij}, j \in \text{sp}(i)\), and \(\lambda_i\) can be estimated by the usual least squares formula. The estimate of \(\lambda_i\) yields an estimate of \(\sigma_{ii}\) by solving \((4.3)\) for \(\sigma_{ii}\). Thus, we obtain the ML estimator of the \(i\)-th row and column of \(\Sigma\) when \(\Sigma_{-i,-i}\) is fixed. In particular, after updating the \(i\)-th row and column we are still left with a matrix \(\Sigma \in P(G)\).

### 4.3 The iterative conditional fitting algorithm

Let \(\hat{\Sigma}^{(r)}\) be the estimate of \(\Sigma\) after the \(r\)-th iteration and \(\hat{\Sigma}^{(r,i)}\) the estimate of \(\Sigma\) after the \(i\)-th update step of the \(r\)-th iteration in ICF, i.e., after estimating \((Y_i \mid Y_{-i})\).

**Algorithm 1.** The ICF algorithm can be implemented as:

1. (Initialization) Set the iteration counter \(r = 0\), and choose a starting value \(\hat{\Sigma}^{(0)} \in P(G)\), e.g. the identity matrix \(\hat{\Sigma}^{(0)} = I_V\).

2. (Updates) Order the variables as \(V = \{1, \ldots, p\}\), set \(\hat{\Sigma}^{(r,0)} = \hat{\Sigma}^{(r)}\), and repeat the following steps for all \(i = 1, \ldots, p\):
   
   (i) Let \(\hat{\Sigma}^{(r,i)}_{-i,-i} = \hat{\Sigma}^{(r,i-1)}_{-i,-i}\) and calculate from this submatrix the pseudo-variables \(Z^{(i)}_{\text{sp}(i)}\) according to \((4.6)\).

   (ii) Compute the ML estimators
   
   \[
   \hat{\Sigma}^{(r,i)}_{i,\text{sp}(i)} = Y_i (Z^{(i)}_{\text{sp}(i)})' [Z^{(i)}_{\text{sp}(i)} (Z^{(i)}_{\text{sp}(i)})']^{-1} ;
   \hat{\lambda}_i = \frac{1}{n} (Y_i - \hat{\Sigma}^{(r,i)}_{i,\text{sp}(i)} Z^{(i)}_{\text{sp}(i)}) (Y_i - \hat{\Sigma}^{(r,i)}_{i,\text{sp}(i)} Z^{(i)}_{\text{sp}(i)})' .
   \]

   for the linear regression \((4.7)\). The existence of the matrix inverse follows from the assumed non-singularity of the sample covariance matrix \(S\).

   (iii) Complete \(\hat{\Sigma}^{(r,i)}\) by setting
   
   \[
   \hat{\sigma}^{(r,i)}_{ii} = \hat{\lambda}_i + \hat{\Sigma}^{(r,i)}_{i,\text{sp}(i)} [\hat{\Sigma}^{(r,i)}_{-i,-i}]^{-1} \hat{\Sigma}^{(r,i)}_{\text{sp}(i),i} ;
   \]

   compare \((4.9)\).

3. (Repeat) Set \(\hat{\Sigma}^{(r+1)} = \hat{\Sigma}^{(r,p)}\). Increment the counter \(r\) to \(r + 1\). Go to 2.

The iterations can be stopped according to a criterion such as “the estimate of \(\Sigma\) is not changed” (in some pre-determined accuracy).
Example 2. Figure 2 illustrates ICF for the model $N(G)$ based on the graph $G$ shown in Figure 1. The algorithm cycles in arbitrary order through the four regressions $(Y_i \mid Y_{-i})$, $i = 1, 2, 3, 4$. In Figure 2 a filled circle represents variables in the conditioning set $-i$, and an unfilled circle stands for the variable $i$ forming the response variable in the considered regression. The directed edges coincide with bi-directed edges in the original graph in Figure 1 and indicate the pseudo-variable regressions to be carried out. The vertices that are joined to vertex $i$ by a directed edges are labelled with the pseudo-variables that act as covariates. The directed edges are labelled with the covariances that are estimated.

Remark 3 (Complexity). The algorithm can be restated only in terms of the empirical covariance matrix $S$ defined in (2.7). For example in (4.9),

$$Y_i(Z_{sp(i)}^{(i)})' = S_{i,-i}[(\Sigma_{-i,-i})^{-1}]_{-i,sp(i)},$$

$$Z_{sp(i)}^{(i)}(Z_{sp(i)}^{(i)})' = [(\Sigma_{-i,-i})^{-1}]_{sp(i),-i}S_{-i,-i}[(\Sigma_{-i,-i})^{-1}]_{-i,sp(i)}.$$

Other products between data matrices appearing in the sequel can be similarly expressed in terms of the empirical covariance matrix $S$. Thus, the sample size does not affect the complexity of the algorithm. The complexity of one of the algorithm’s pseudo-variable regression steps is dominated by the computation of the inverse of $\Sigma_{-i,-i}$ in (4.6), and the inversion of a matrix of size $sp(i) \times sp(i)$ (4.9). Note that $\Sigma_{-i,-i}$ may be sparse and special methods for inversion of sparse matrices might be useful. In particular, if the induced subgraph $G_{-i}$ has disconnected components then only the submatrices of $\Sigma$ over connected components containing spouses of $i$ have to be inverted.

4.4 Convergence

The key to prove convergence of ICF is to recognize that the algorithm consists of iterated partial maximizations over sections of the parameter space $P(G)$. In ICF we
repeatedly maximize the likelihood function of the covariance graph model partially by allowing only the entries in the $i$-th row and column of $\Sigma$ to vary. The remaining entries are fixed. A bit more formally, we consider the parameter space

$$\Theta = \{ \Sigma \in \mathcal{P}(G) \mid \ell(\Sigma) \geq \ell(\hat{\Sigma}^{(0)}) \}, \quad (4.12)$$

which is compact, though not necessarily connected, and contains the global maximizer of $\ell(\Sigma)$. Recall that we assume the empirical covariance matrix $S$ to be positive definite. Defining the section $\Theta_i(\bar{\Sigma}) \subseteq \Theta$ as

$$\Theta_i(\bar{\Sigma}) = \{ \Sigma \in \Theta \mid \Sigma_{-i,-i} = \bar{\Sigma}_{-i,-i} \}, \quad (4.13)$$

it becomes clear that the algorithm steps 2(i)-2(iii) maximize the log-likelihood function partially over the section $\Theta_i((\hat{\Sigma})^{(r,i-1)})$, i.e.

$$\hat{\Sigma}^{(r,i)} = \arg \max \{ \ell(\Sigma) \mid \Sigma \in \Theta_i((\hat{\Sigma})^{(r,i-1)}) \}. \quad (4.14)$$

This local and global maximizer over the section is unique. If a matrix $\Sigma \in \mathcal{P}(G)$ maximizes the log-likelihood function over all sections $\Theta_i(\Sigma)$, $i \in V$, simultaneously, then it solves the likelihood equations. Hence, the following theorem follows from results in Drton and Eichler (2005, Appendix).

**Theorem 4.** Suppose the sequence $(\hat{\Sigma}^{(r)})$ is constructed by the ICF algorithm. Then all accumulation points of $(\hat{\Sigma}^{(r)})$ are saddle points or local maxima of the log-likelihood function. Moreover, all accumulation points have the same likelihood value. In particular, if the likelihood equations have only finitely many solutions, then $(\hat{\Sigma}^{(r)})$ converges.

### 5 Iterative conditional fitting with multivariate updates

The algorithm presented in §4 is based on updating one row and column of an estimate of the covariance matrix $\Sigma \in \mathcal{P}(G)$ by carrying out a univariate regression. A natural modification of this approach is to update several rows and columns of the estimate $\Sigma \in \mathcal{P}(G)$ simultaneously using multivariate regression.

#### 5.1 Seemingly unrelated pseudo-variable regressions

Let $C \subseteq V$ be a subset of the vertices. In order to estimate all rows and columns of $\Sigma$ that are indexed by the vertices in $C$ in the ICF algorithm presented in §4 we have to carry out several univariate pseudo-variable regressions for $(Y_i \mid Y_{-i}), \ i \in C$. Instead, we would like to consider only one multivariate regression of the form $(Y_C \mid Y_{-C})$, where $-C = V \setminus C$. The conditional distribution

$$
(Y_C \mid Y_{-C}) \sim \mathcal{N}_{C \times N}(B_C Y_{-C}, \Lambda_C \otimes I_N)
$$

(5.1)
is specified by the matrix of regression coefficients
\[ B_C = \Sigma_{C,-C}(\Sigma_{-C,-C})^{-1} \in \mathbb{R}^{C \times -C}, \] (5.2)

and the conditional covariance matrix
\[ \Lambda_C = \Sigma_{C,C} - \Sigma_{C,-C}(\Sigma_{-C,-C})^{-1}\Sigma_{-C,C} \in P(C). \] (5.3)

In order for the conditional distribution (5.1) to be of a simple structure, there should be no constraints on the \( \Lambda_C \), in which case \( P(C) = P_G \). This holds if there are no constraints on the submatrix \( \Sigma_{C,C} \), which in turn holds if the set \( C \) is complete, i.e., if \( i \leftrightarrow j \) whenever \( i, j \in C \) and \( i \neq j \). Then the only constraints on the conditional distribution (5.1) are on the matrix of regression coefficients \( B_C \) and stem from restrictions that \( \sigma_{ij} = 0 \), if \( i \in C \), \( j \notin C \) and \( j \not\leftrightarrow i \).

Let \( \text{sp} \left( \mathcal{C} \right) = \left[ \bigcup \text{sp} \left( \mathcal{C} \right) \mid i \in \mathcal{C} \right] \setminus \mathcal{C} \) (5.4) be the spouses of \( \mathcal{C} \), that is the vertices that are not in \( \mathcal{C} \) but adjacent to some vertex in \( \mathcal{C} \), and let \( \text{nsp} \left( \mathcal{C} \right) = V \setminus \left( \text{sp} \left( \mathcal{C} \right) \cup \mathcal{C} \right) \) be the non-spouses of \( \mathcal{C} \), yielding the partition \( V = \mathcal{C} \cup \text{sp} \left( \mathcal{C} \right) \cup \text{nsp} \left( \mathcal{C} \right) \).

Then we can rewrite (5.1) as
\[ (Y_C \mid Y_{-C}) \sim \mathcal{N}_{C \times N}(\Sigma_{C,\text{sp}(C)} Z_{\text{sp}(C)}^{(C)} \Lambda_C \otimes I_N), \] (5.6)

because \( \Sigma_{C,\text{nsp}(C)} = 0 \). As \( \Sigma \) ranges through \( P(G) \), the submatrix \( \Sigma_{C,\text{sp}(C)} \) playing the role of regression coefficients in (5.6) ranges through the linear space
\[ P_{\text{C,sp}(C)}(G) = \{ A \in \mathbb{R}^{C \times \text{sp}(C)} \mid A_{ij} = 0 \text{ if } i \not\leftrightarrow j \}. \] (5.7)

Hence, (5.6) constitutes seemingly unrelated regressions (Zellner, 1962).

5.2 The iterative conditional fitting algorithm with multivariate updates
ML estimation in seemingly unrelated regressions itself generally requires iterative algorithms, such as iterating the two-step estimator of Zellner (1962). In the case of (5.6), the two-step estimator consists of first estimating \( \Sigma_{C,\text{sp}(C)} \) for some fixed \( \Lambda_C \) by generalized least squares, and then estimating \( \Lambda_C \) as the empirical covariance matrix of the residuals \( Y_i - \Sigma_{C,\text{sp}(C)} Z_{\text{sp}(C)}^{(C)} \) computed with the estimate of \( \Sigma_{C,\text{sp}(C)} \) obtained in the first
step. However, if the current estimate of $\Sigma$ is used to obtain starting values $\Sigma_{C,\text{sp}(C)}$ and $\Lambda_{C}$, then the two-step method does not have to be iterated in order to obtain estimates for the seemingly unrelated pseudo-regressions (5.6) that yield a convergent ICF algorithm with multivariate updates. For specification of the estimator of $\Sigma_{C,\text{sp}(C)}$ we need to introduce the matrix $P_{C}$ of the linear map that sends the vector of unrestricted elements in $\Sigma_{C,\text{sp}(C)}$ to the matrix $\Sigma_{C,\text{sp}(C)} \in \mathbf{P}_{C,\text{sp}(C)}(G)$. The vector of unrestricted elements of $\Sigma_{C,\text{sp}(C)}$ is the vector $\sigma_{C} = (\sigma_{ij} \mid i \in C, j \in \text{sp}(C), i \leftrightarrow j)$. The matrix $P_{C}$ has exactly one entry equal to one in each column, the other entries are zero, and it satisfies $\text{vec}(\Sigma_{C,\text{sp}(C)}) = P_{C}\sigma_{C}$ for $\Sigma \in \mathbf{P}(G)$; compare the definition of the matrix $Q$ in §2.

In order to run ICF with multivariate updates, we have to choose a family of complete sets $(C \mid C \in \mathcal{C})$ such that

$$\bigcup (C \mid C \in \mathcal{C}) = V,$$

(5.8)

where the sets $C$ do not have to be disjoint. For example the sets $C$ could be chosen as edges, but the largest possible choice for the sets $C$ would be the cliques, i.e., the maximal complete sets, in $G$.

**Algorithm 5.** For a given choice of $\mathcal{C}$, the ICF algorithm with multivariate updates can be implemented as:

1. (Initialization) Set the iteration counter $r = 0$, and choose a starting value $\hat{\Sigma}^{(0)} \in \mathbf{P}(G)$, e.g. the identity matrix $\hat{\Sigma}^{(0)} = I_{V}$. 

2. (Updates) Order the sets in the family $\mathcal{C}$ as $\mathcal{C} = \{C_{1}, \ldots, C_{q}\}$, set $\hat{\Sigma}^{(r,0)} = \hat{\Sigma}^{(r)}$, and repeat the following steps for all $C_{k} \in \mathcal{C}$:

   (i) Let $\hat{\Sigma}^{(r,k)}_{-C_{k},-C_{k}} = \hat{\Sigma}^{(r,k-1)}_{-C_{k},-C_{k}}$. From this submatrix, compute the conditional covariance matrix $\hat{\Lambda}_{C_{k}}$ according to (5.7) and the pseudo-variables $Z^{(k)}_{\text{sp}(C_{k})}$ according to (5.5). Calculate $\hat{\Omega}_{C_{k}} = (\hat{\Lambda}_{C_{k}})^{-1}$.

   (ii) Compute the (generalized least squares) matrix that satisfies $\text{vec}(\hat{\Sigma}^{(r,k)}_{C_{k},\text{sp}(C_{k})}) = P_{C_{k}}\hat{\sigma}_{C_{k}}$, where

   $$\hat{\sigma}_{C_{k}} = \left\{ P_{C_{k}}' \left\{ [Z^{(k)}_{\text{sp}(C_{k})}]ZY_{C_{k}} \right\} \odot \hat{\Omega}_{C_{k}} \right\}^{-1} \times \left\{ P_{C_{k}}' \text{vec}[\hat{\Omega}_{C_{k}} Y_{C} (Z^{(k)}_{\text{sp}(C_{k})})'] \right\}.$$  

   (5.9)

   (iii) Compute the empirical covariance matrix of residuals

   $$\hat{\Lambda}_{C_{k}} = \frac{1}{n}(Y_{C_{k}} - \hat{\Sigma}^{(r,k)}_{C_{k},\text{sp}(C_{k})}Z^{(k)}_{\text{sp}(C_{k})})(Y_{C_{k}} - \hat{\Sigma}^{(r,k)}_{C_{k},\text{sp}(C_{k})}Z^{(k)}_{\text{sp}(C_{k})})'.$$  

(5.10)
(iii) Complete $\hat{\Sigma}^{(r,k)}$ by setting

$$\hat{\Sigma}_{C_k,C_k}^{(r,k)} = \hat{\Lambda}_{C_k} + \hat{\Sigma}_{C_k,sp(C_k)}^{(r,k)} \left[ (\hat{\Sigma}_{C_k,C_k}^{(r,k)})^{-1} \right]_{sp(C_k),sp(C_k)} \hat{\Sigma}_{sp(C_k),C_k}^{(r,k)};$$

compare (5.3).

3. (Repeat) Set $\hat{\Sigma}^{(r+1)} = \hat{\Sigma}^{(r,q)}$. Increment the counter $r$ to $r+1$. Go to 2.

Note that if the family $\mathcal{C}$ consists of only singletons then Algorithm 5 reduces to Algorithm 1.

**Example 6.** We take up the covariance graph shown in Figure 1. For the family $\mathcal{C}$ of complete vertex sets, several choices are possible. If the cliques $\mathcal{C} = \{13, 34, 24\}$ are chosen, then all conditional distributions considered in ICF are bivariate, whereas for $\mathcal{C} = \{1, 2, 34\}$ two univariate distributions are estimated in conjunction with a bivariate distribution. For the clique choice $\mathcal{C} = \{13, 34, 24\}$, we illustrate the seemingly unrelated pseudo-variable regressions to be estimated in Figure 3, which is to be interpreted similarly as Figure 2. An additional feature are the bi-directed edges that connect the vertices in the sets $C \in \mathcal{C}$; see [Richardson and Spirtes 2002] for a formal definition of these graphs.

![Figure 3](image-url)

Figure 3: Illustration of the seemingly unrelated pseudo-variable regressions in ICF with multivariate updates, and $\mathcal{C} = \{13, 34, 24\}$.

### 5.3 Convergence

The ICF algorithm with multivariate updates is still an iterative partial maximization algorithm. However, the sections in the parameter space over which maximizations are performed are not quite as simple as the sections described in §4.4. Steps 2(ii) and 2(iii) of Algorithm 5 do not jointly maximize the log-likelihood function $\ell$ over sections of the form

$$\Theta_C(\Sigma) = \{\Sigma \in \Theta \mid \Sigma_{-C,-C} = \Sigma_{-C,-C}\}.$$  

(5.12)
Instead step 2(ii) maximizes $\ell$ over sections of the form

$$\Theta_{1,C}(\bar{\Sigma}) = \{ \Sigma \in \Theta \mid \Sigma_{-C,-C} = \bar{\Sigma}_{-C,-C}, \Lambda_C = \bar{\Lambda}_C \},$$

where $\Lambda_C$ is again the conditional covariance matrix from (5.3). The subsequent step 2(iii) maximizes $\ell$ over sections of the form

$$\Theta_{2,C}(\bar{\Sigma}) = \{ \Sigma \in \Theta \mid \Sigma_{-C,-C} = \bar{\Sigma}_{-C,-C}, \Sigma_{C,-C} = \bar{\Sigma}_{C,-C} \}.$$  

Nevertheless it holds under condition (5.8) that if $\Sigma$ maximizes the log-likelihood function $\ell$ over both section $\Theta_{1,C}(\bar{\Sigma})$ and $\Theta_{2,C}(\bar{\Sigma})$ simultaneously for all $C \in \mathcal{C}$, then $\Sigma$ is a solution to the likelihood equations. Thus, Theorem 4 holds also for ICF with multivariate updates as stated in Algorithm 5.

### 6 Empirical likelihood estimation

In contexts where it is not appropriate to assume multivariate normality, we may still wish to estimate a covariance matrix subject to various zero restrictions. Here we present an approach based on empirical likelihood (Owen, 2001). In the resulting method an estimate of the underlying distribution is obtained by maximizing a non-parametric likelihood under constraints that include the desired zero covariance restrictions; see Chaudhuri, Handcock, and Rendall (2005) and Hellerstein and Imbens (1999) for similar applications of empirical likelihood.

We associate a weight $w_k$ with the $k$-th sample observation $Y^{(k)}_k$, $k \in N$. Estimating the mean vector and covariance matrix simultaneously, we solve the nested constrained maximization problem

$$\max_{\mu} \left\{ \max_{w=(w_1, \ldots, w_n)} \prod_{k \in N} nw_k \right\}$$

subject to

$$w_k \geq 0, \quad k \in N,$$

$$\sum_{k \in N} w_k = 1,$$

$$\sum_{k \in N} w_k (Y^{(k)}_i - \mu_i) = 0, \quad \forall \ i \in V,$$

$$\sum_{k \in N} w_k (Y^{(k)}_i - \mu_i)(Y^{(k)}_j - \mu_j) = 0, \quad \forall \ i, j \in V \text{ s.t. } i \not\leftrightarrow j.$$  

Without the additional constraints (6.4) and (6.5), the empirical likelihood ratio $\prod_{k \in N} nw_k$ is maximized for $w_k = 1/n$, $k \in N$. The additional constraint (6.4) enforces that the
mean of the reweighted rows of $Y$ is equal to $\mu$. Constraint (6.5) ensures that the estimated weights $\hat{w}_k$ are such that the empirical covariance matrix of the reweighted sample satisfies the zero constraints specified by the graph $G$.

In order to avoid obvious problems with feasibility of the optimization problem, we assume that the sample size, i.e., the number of weights, is strictly larger than the number of constraints in (6.3) and (6.5). Note that the number of constraints (6.5) may grow quadratically as the number of variables increases. The nesting of the maximization steps in (6.1) is done to avoid cubic constraints in $w$, which would have resulted had we

$$
\mu_i = \sum_{k \in N} w_k Y_i^{(k)}, \quad \forall i \in V
$$

(6.6)

in (6.5) and made the constraints in (6.3) redundant. The constrained maximization problem can be solved through its dual problem, in which the number of unknowns is equal to the number of constraints of the original problem; see Owen (2001) and Chaudhuri et al. (2005) for details.

If $\hat{\mu}$ and $\hat{w}$ are, respectively, the vectors of mean and weights maximizing (6.1) under the constraints (6.2)-(6.5), then the estimated covariance matrix is given by

$$
\hat{\Sigma}_E = (Y - \hat{\mu} \otimes 1_N) \cdot \text{diag}(\hat{w}) \cdot (Y - \hat{\mu} \otimes 1_N)',
$$

(6.7)

where $\text{diag}(\hat{w})$ is an $n \times n$ diagonal matrix with $\hat{w}$ along its diagonal. Following Owen (2001) and Qin and Lawless (1994) one can show that asymptotically $\hat{\mu}$ and $\hat{\Sigma}_E$ are consistent.

7 Data and simulations

We now compare the three approaches to estimation of a covariance matrix with zeros in a data example and in simulations: (i) ML estimation relying on ICF, (ii) dual likelihood estimation as described in §3.2, and (iii) empirical likelihood estimation.

7.1 Gene expression in yeast

Gasch et al. (2000) present gene expression data from microarray experiments with yeast strands. We focus on $p = 8$ genes related to galactose utilization. The gene $GAL11$ is responsible for transcription. The genes $GAL4$ and $GAL80$ are involved in galactose regulation. Gene $GAL2$ is related to transport and the remaining four genes, $GAL1$, $GAL3$, $GAL7$, and $GAL10$, are involved in galactose metabolism. There are $n = 134$ experiments with gene expression measurements for all eight genes. The observed marginal correlations and standard deviations are shown in Table I where we denote the variables
Table 1: Observed marginal correlations and standard deviations.

|        | $X_{11}$ | $X_4$ | $X_{80}$ | $X_2$ | $X_1$ | $X_3$ | $X_7$ | $X_{10}$ |
|--------|----------|-------|----------|-------|-------|-------|-------|----------|
| $X_{11}$ |          |       |          |       |       |       |       |          |
| $X_4$   | 0.24     |       |          |       |       |       |       |          |
| $X_{80}$| 0.08     | 0.23  |          |       |       |       |       |          |
| $X_2$   | -0.18    | -0.03 | 0.26     |       |       |       |       |          |
| $X_1$   | -0.10    | -0.10 | 0.28     | 0.87  |       |       |       |          |
| $X_3$   | -0.18    | 0.12  | 0.20     | 0.44  | 0.39  |       |       |          |
| $X_7$   | -0.07    | -0.08 | 0.21     | 0.81  | 0.88  | 0.50  |       |          |
| $X_{10}$| -0.08    | -0.07 | 0.26     | 0.87  | 0.92  | 0.46  | 0.91  |          |
| SD     | 0.39     | 0.36  | 0.47     | 1.70  | 1.70  | 0.78  | 1.85  | 1.54     |

for the gene expression measurements by $X_i$, $i = 1, 2, 3, 4, 7, 10, 11, 80$, using the obvious correspondence.

By multiple testing of correlations as described in Drton and Perlman (2004, 2005) and implemented in the R package ‘SIN’, we selected the two covariance graphs $G_s \subset G_d$ that are illustrated in Figure 4. The larger graph $G_d$ contains all edges shown, i.e., both the solid and the dashed edges, whereas the sub-graph $G_s$ includes only the solid edges. In $G_s$ the vertices 1, 2, 3, 7, and 10 form a clique and in $G_d$ the clique is enlarged to include vertex 80. With the R package ‘ggm’ and additional code, we computed the ML, the dual, and the empirical likelihood estimates of the covariance matrix under the zero constraints specified in the graphs. The results for both $G_s$ and $G_d$ are shown in Table 2. We remark that we started ICF from the identity matrix and that Anderson’s algorithm gave the same results as ICF. However, although we refer to “ML estimates”, ICF is only guaranteed to find a stationary point which may not be the global maximizer of the likelihood.

Upon inspection of Table 2 we find that the three estimates are in better agreement for the graph $G_d$. This graph yields the better fitting covariance graph model. The deviance of the model $N(G_d)$ under comparison to the model based on the complete graph equals 9.98 over 9 degrees of freedom, whereas the deviance of the model $N(G_s)$ equals 33.07 over 13 degrees of freedom. This indicates a good fit of $N(G_d)$ and a poor fit of the more restrictive model $N(G_s)$. The difference in log-likelihood between ML and dual estimates equals 4.29 in $N(G_s)$ and reduces to 0.51 in $N(G_d)$. In contrast the difference in log-likelihood between ML and empirical likelihood estimates equals 20.54 in $N(G_s)$ and 5.67 in $N(G_d)$.
Table 2: Marginal correlations and standard deviations from ML (M), dual (D), and empirical likelihood (E) estimates for graph $G_s$ (lower half) and graph $G_d$ (upper italicized half).

|         | $X_{11}$ | $X_4$ | $X_{80}$ | $X_2$ | $X_1$ | $X_3$ | $X_7$ | $X_{10}$ | SD |
|---------|---------|-------|---------|-------|-------|-------|-------|---------|-----|
| $X_{11}$ | 0.28    | 0     | −0.12   | 0     | −0.21 | 0     | 0     | 0       | 0.40 M |
|         | 0.26    | 0     | −0.11   | 0     | −0.20 | 0     | 0     | 0       | 0.39 D |
|         | 0.25    | 0     | −0.11   | 0     | −0.20 | 0     | 0     | 0       | 0.39 E |
| $X_4$   | 0.22    | 0.20  | 0       | 0     | 0     | 0     | 0     | 0       | 0.36 M |
|         | 0.27    | 0.21  | 0       | 0     | 0     | 0     | 0     | 0       | 0.35 D |
|         | 0.28    | 0.27  | 0       | 0     | 0     | 0     | 0     | 0       | 0.36 E |
| $X_{80}$| 0       | 0.22  | 0.27    | 0.29  | 0.19  | 0.22  | 0.27  | 0.47    | M   |
|         | 0       | 0.20  | 0.28    | 0.31  | 0.19  | 0.23  | 0.28  | 0.47    | D   |
|         | 0       | 0.18  | 0.26    | 0.31  | 0.16  | 0.21  | 0.27  | 0.48    | E   |
| $X_2$   | 0       | 0     | 0.08    | 0.86  | 0.43  | 0.81  | 0.87  | 1.69    | M   |
|         | 0       | 0     | 0.09    | 0.86  | 0.43  | 0.81  | 0.87  | 1.68    | D   |
|         | 0       | 0     | 0.17    | 0.83  | 0.43  | 0.79  | 0.85  | 1.48    | E   |
| $X_1$   | 0       | 0     | 0.11    | 0.86  | 0.38  | 0.88  | 0.92  | 1.70    | M   |
|         | 0       | 0     | 0.12    | 0.86  | 0.39  | 0.88  | 0.91  | 1.69    | D   |
|         | 0       | 0     | 0.10    | 0.83  | 0.34  | 0.85  | 0.88  | 1.48    | E   |
| $X_3$   | 0       | 0     | 0       | 0.43  | 0.38  | 0.49  | 0.44  | 0.78    | M   |
|         | 0       | 0     | 0       | 0.39  | 0.37  | 0.51  | 0.46  | 0.78    | D   |
|         | 0       | 0     | 0       | 0.39  | 0.31  | 0.49  | 0.46  | 0.78    | E   |
| $X_7$   | 0       | 0     | 0       | 0.81  | 0.88  | 0.50  | 0.91  | 1.85    | M   |
|         | 0       | 0     | 0       | 0.80  | 0.87  | 0.50  | 0.91  | 1.84    | D   |
|         | 0       | 0     | 0       | 0.77  | 0.83  | 0.38  | 0.90  | 1.68    | E   |
| $X_{10}$| 0       | 0     | 0.08    | 0.87  | 0.91  | 0.45  | 0.91  | 1.54    | M   |
|         | 0       | 0     | 0.08    | 0.86  | 0.91  | 0.44  | 0.90  | 1.53    | D   |
|         | 0       | 0     | 0.13    | 0.86  | 0.87  | 0.36  | 0.88  | 1.36    | E   |

SD     | 0.39    | 0.36  | 0.47    | 1.70  | 1.70  | 0.78  | 1.85  | 1.54    | M   |
|        | 0.37    | 0.35  | 0.45    | 1.61  | 1.61  | 0.75  | 1.79  | 1.47    | D   |
|        | 0.38    | 0.33  | 0.47    | 1.41  | 1.37  | 0.74  | 1.57  | 1.22    | E   |
7.2 Simulations

Since the ML estimator $\hat{\Sigma}_M$ and Kauermann’s dual estimator $\hat{\Sigma}_D$ are based on a normality assumption, but the empirical likelihood based estimator $\hat{\Sigma}_E$ is not, it is of interest to compare their performance, both when the underlying distribution is, and is not, Gaussian. We simulated 1000 data sets for sample sizes $n = 10, 20, 25, 30, 50, 100$ from a multivariate normal distribution, and a multivariate $t$ distribution with 5 degrees of freedom ($t_5$). The mean vector was zero and the covariance matrix for the multivariate normal distribution was

$$\Sigma = \begin{pmatrix}
1 & 0 & \frac{1}{2} & 0 \\
0 & 1 & 0 & \frac{1}{2} \\
\frac{1}{2} & 0 & 1 & \frac{3}{4} \\
0 & \frac{1}{2} & \frac{3}{4} & 1
\end{pmatrix},$$

(7.1)

corresponding to the graph shown in Figure 4. For the $t_5$ distribution, we used $\Sigma$ as dispersion matrix, which results in the covariance matrix $\frac{5}{3}\Sigma$. In Figure 5 and 6 we present the bias and root-mean-squared error (RMSE) respectively for the three estimators (off-diagonal entries are considered once). For the heavier-tailed multivariate $t_5$ distribution, moments up to fourth order exist \cite{Kotz and Nadarajah 2004}, thus it makes sense to consider RMSE of the estimated variances and covariances. For sample size 10 we experienced problems with the empirical likelihood procedure, resulting from an inability to find feasible starting values. Consequently we do not present results for
Figure 5: Comparing the bias of the ML, DL and the EL estimator for various sample sizes. ML (---M---), DL (---D---) and EL (···E···).

\( \hat{\Sigma}_E \) when \( n = 10 \).

From Figures 5(a) and (b) it is evident that the biases of \( \hat{\Sigma}_E \) and \( \hat{\Sigma}_D \) are larger than the bias of \( \hat{\Sigma}_M \) for all values of \( n \). Whereas in the Gaussian case, \( \hat{\Sigma}_E \) behaves better in terms of bias than \( \hat{\Sigma}_D \) for \( n > 20 \), the opposite happens under the \( t_5 \) distribution. As would be expected the RMSE of \( \hat{\Sigma}_M \) is slightly lower than that of \( \hat{\Sigma}_D \) and \( \hat{\Sigma}_E \) under Gaussianity; cf. Figure 6(a). On the other hand \( \hat{\Sigma}_E \) performs better in terms of RMSE than \( \hat{\Sigma}_M \) for all sample sizes when the underlying distribution is \( t_5 \); see Figure 6(b). The RMSE of \( \hat{\Sigma}_E \) is also smaller than that of \( \hat{\Sigma}_D \) under \( t_5 \), for moderately large sample sizes (\( n > 20 \)).

8 Discussion

We have considered three methods for estimating a covariance matrix with pre-specified zeros. In a Gaussian covariance graph model both ML estimation and the dual likelihood method of Kauermann [1996] provide efficient estimates of the covariance matrix. If the assumption of multivariate normality is not reasonable, then non-parametric estimates can be obtained in an empirical likelihood approach.

For the problem of maximizing the likelihood function of a Gaussian covariance graph model we have introduced the new Iterative Conditional Fitting (ICF) algorithm, which
can be implemented in both a univariate as well as a multivariate version. The advantage of multivariate ICF is the maximization of the likelihood function over larger sections of the parameter space; the disadvantage is the overhead in carrying out generalized least squares computations as opposed to the standard least squares computations of univariate ICF. Future practical experience will show whether general recommendations in this trade off can be given, but the structure of the particular covariance graph considered will certainly be important.

Besides its clear convergence properties, strengths of ICF include the fact that the covariance matrix estimates are positive definite at any stage of the algorithm and that only tools from least squares regression are required for implementation. In addition, it is very appealing that ICF extends the duality between covariance graph and undirected (concentration) graph models (cf. Kauermann, 1996) to the level of fitting algorithms. The commonly used method for fitting undirected graph models, the iterative proportional fitting (IPF) algorithm (Whittaker, 1990, pp.182–185), fits marginal distributions while fixing conditionals. ICF does exactly the converse. The abstract idea behind ICF can be expressed in terms of marginal and conditional distributions which suggests that it is not limited in any way to Gaussian covariance graph models. In fact, work by the authors on applying ICF in binary graphical models for marginal independence appears promising.

Figure 6: Comparing the root mean squared errors of the ML, DL and the EL estimator for various sample sizes. ML (---M---) DL (--D--) and EL(· · ·E· · ·).
The ICF algorithm resembles the Iterative Conditional Modes (ICM) algorithm of Besag (1986). However, ICM obtains maximum a posteriori estimates in a Bayesian framework, whereas our ICF maximizes a likelihood function, which constitutes a very differently structured problem. Another related algorithm is the Conditional Iterative Proportional Fitting (CIPF) algorithm of Cramer (1998, 2000). CIPF can be used to maximize the likelihood function of a model that comprises joint distributions with prescribed conditional distributions. However, CIPF differs from ICF because the update steps of ICF do not simply equate a conditional distribution with a prescribed conditional, but rather maximize a conditional likelihood function that will generally not be the same in two different iterations of ICF.

It is obviously a most attractive feature of the empirical likelihood procedure that it does not require multivariate normality. Algorithmically, empirical likelihood estimation is more involved than maximum likelihood and dual estimation. In particular, we had difficulties obtaining empirical likelihood estimates for smaller sample sizes, which is related to a fundamental difference between empirical likelihood estimation and the other two methods based on multivariate normality. Both ML and dual estimation are possible whenever the sample covariance matrix is positive definite, which occurs with probability one if the sample size is larger than the number of variables, and may occur for smaller sample sizes if the covariance graph is disconnected. In contrast, the optimization problem to be solved for empirical likelihood estimation may become infeasible if the sample size is small compared to the number of constraints imposed. The number of constraints depends on the covariance graph, and seemingly simpler sparser structures impose more constraints and render the empirical likelihood approach more sample size-demanding.

Not surprisingly, our simulations show that the ML estimates computed with ICF are preferable if the underlying distribution is indeed multivariate normal. When simulating from a multivariate $t$ distribution instead non-parametric estimation via empirical likelihood gave the best results in terms of mean squared error.

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