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Graphical Gaussian Models**

by

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# Asymptotic Prior to Posterior Analysis for Graphical Gaussian Models

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**Abstract:** In this paper we derive the asymptotic posterior distribution, in a conjugate analysis, for the marginal and partial correlation coefficients in a graphical Gaussian model. An example of prior to posterior analysis is given and the problem of the specification of the hyper parameters discussed.

**Keywords:** Conditional Independence, Conjugate Prior, Correlation Coefficient, Graphical Model, Isserlis Matrix, Matrix Completion.

## 1. Introduction

Recent work established a class of statistical models, known as graphical models, that exploit the close relationship between conditional independence and separation in undirected graphs (see Lauritzen, 1996).

The conditional independence structure of a multivariate Normal distribution is dictated by the zero pattern of its concentration matrix  $\Sigma^{-1}$ . The use of the concentration matrix in the parametrisation of the normal distribution has many advantages. However non-zero elements of  $\Sigma^{-1}$  are difficult to interpret since they are unnormalised quantities. Consequently, when the interest is on the strength of the association structure, these parameters have to be transformed to obtain partial correlation coefficients.

In this paper we apply the results of Roverato and Whittaker (1996, 1997) to derive the asymptotic posterior distributions, in a Bayesian conjugate analysis, of the marginal and of the partial correlation coefficients. We give an example of prior to posterior analysis based on real data where we discuss the difficulties concerned with the specification of the hyper parameters.

The notation is given in Section 2. In Section 3 we present some basic theory relating to graphical Gaussian model and in Section 4 we describe the HIV data used in the application. In Section 5 we derive the required asymptotic distributions. Finally in Section 6 we carry out the application and discuss the problem of the specification of the hyper parameters.

## 2. Notation

Let  $V$  be a finite set with  $|V| = p$ , and let  $\Gamma$  be a  $p \times p$  symmetric in-

vertible matrix. The rows and columns of  $\Gamma$  are indexed by the elements of  $V$ , so that  $\Gamma$  itself is indexed by  $V \times V$ . When  $V = \{1, \dots, p\}$ ,  $\Gamma$  is indexed by row and column numbers.

The Isserlis matrix of  $\Gamma$ ,  $\text{Iss}(\Gamma)$ , (Isserlis, 1918; Roverato and Whittaker, 1997) is the symmetric matrix indexed by  $\mathcal{W} \times \mathcal{W}$  where  $\mathcal{W} = \{(i, j) : i, j \in V, i \leq j\}$ , with elements  $\{\text{Iss}(\Gamma)\}_{(i,j),(r,s)} = \gamma_{ir}\gamma_{js} + \gamma_{is}\gamma_{jr}$ .

The graph theory requisite for graphical models may be found in Lauritzen (1996). We use the convention that, for an arbitrary undirected graph  $G = (V, \mathcal{V})$  where  $V$  is the vertex set and  $\mathcal{V}$  is the set of edges, for all  $i \in V$  the pair  $(i, i)$  is included in  $\mathcal{V}$  and that if  $(i, j) \in \mathcal{V}$  then  $i \leq j$ . The set  $\mathcal{W}$  is therefore the edge set of the complete graph and we denote by  $\bar{\mathcal{V}} = \mathcal{W} \setminus \mathcal{V}$  the set of edges not in  $G$ .

*EXAMPLE 1* With  $V = \{1, 2, 3\}$  and graph  $G$   $\textcircled{1} \text{---} \textcircled{2} \text{---} \textcircled{3}$  the edge set is  $\mathcal{V} = \{(1, 1), (2, 2), (3, 3), (1, 2), (2, 3)\}$  while  $\bar{\mathcal{V}} = \{(1, 3)\}$ .  $\square$

For any undirected graph  $G = (V, \mathcal{V})$  the pair  $(\mathcal{V}, \bar{\mathcal{V}})$  is a partition of  $\mathcal{W}$ . To this correspond the submatrices  $\text{Iss}(\Gamma)_{\mathcal{V}\mathcal{V}}$ ,  $\text{Iss}(\Gamma)_{\mathcal{V}\bar{\mathcal{V}}}$  and  $\text{Iss}(\Gamma)_{\bar{\mathcal{V}}\bar{\mathcal{V}}}$  as well as the partial matrix  $\text{Iss}(\Gamma)_{\mathcal{V}\mathcal{V}|\bar{\mathcal{V}}} = \text{Iss}(\Gamma)_{\mathcal{V}\mathcal{V}} - \text{Iss}(\Gamma)_{\mathcal{V}\bar{\mathcal{V}}}[\text{Iss}(\Gamma)_{\bar{\mathcal{V}}\bar{\mathcal{V}}}]^{-1}\text{Iss}(\Gamma)_{\bar{\mathcal{V}}\mathcal{V}}$ .

For a set  $\mathcal{C} \subseteq \mathcal{W}$  we define the  $\mathcal{C}$ -incomplete matrix  $\Gamma^{\mathcal{C}}$  as the symmetrised matrix indexed by  $V \times V$  with elements  $\{\gamma_{ij}\}$  for all  $(i, j) \in \mathcal{C}$ , and with the remaining elements unspecified. In the Example 1 above the incomplete matrices corresponding to the sets  $\mathcal{V}$  and  $\bar{\mathcal{V}}$  are respectively

$$\Gamma^{\mathcal{V}} = \begin{pmatrix} \gamma_{11} & \gamma_{12} & * \\ \gamma_{21} & \gamma_{22} & \gamma_{23} \\ * & \gamma_{32} & \gamma_{33} \end{pmatrix} \quad \text{and} \quad \Gamma^{\bar{\mathcal{V}}} = \begin{pmatrix} * & * & \gamma_{13} \\ * & * & * \\ \gamma_{31} & * & * \end{pmatrix},$$

where asterisks denote unspecified elements. The matrix  $\Gamma^{-\mathcal{V}}$  is a shorthand for  $(\Gamma^{-1})^{\mathcal{V}}$ . If it is possible to fill an incomplete matrix  $\Gamma^{\mathcal{C}}$  to obtain a (full) positive definite matrix we say that  $\Gamma^{\mathcal{C}}$  admits a positive completion.

Let  $\Gamma^{\mathcal{V}}$  be a  $\mathcal{V}$ -incomplete matrix, with  $G = (V, \mathcal{V})$ , which admits a positive completion. We say that  $\Gamma_G$  is *the completion of  $\Gamma^{\mathcal{V}}$*  if it is the unique positive definite matrix such that

$$(\Gamma_G)^{\mathcal{V}} = \Gamma^{\mathcal{V}} \quad \text{and} \quad \{\Gamma_G^{-1}\}_{ij} = 0 \quad \text{for all } (i, j) \in \bar{\mathcal{V}}. \quad (1)$$

See Grone *et al.* (1984) for a proof of the existence and uniqueness of such matrix.

We denote by  $\text{diag}(\Gamma^{\mathcal{V}})_{\mathcal{V}\mathcal{V}}$  the matrix indexed by  $\mathcal{V} \times \mathcal{V}$  with the distinct specified elements of  $\Gamma^{\mathcal{V}}$  in the main diagonal and zero elsewhere.

For an undirected graph  $G = (V, \mathcal{V})$ , we denote by  $\mathcal{M}_*(G)$  the set of all  $\mathcal{V}$ -incomplete matrices and by  $\mathcal{M}_*^+(G)$  the set of all  $\mathcal{V}$ -incomplete matrices that admit positive completion. Furthermore we denote by  $\mathcal{M}_0(G)$  the set of all symmetric matrices indexed by  $V \times V$  with element  $(i, j)$  equal to zero

whenever  $(i, j) \in \bar{\mathcal{V}}$ . The intersection of  $\mathcal{M}_0(G)$  with the set of all positive definite matrices is denoted by  $\mathcal{M}_0^+(G)$ .

The trace of the product of two square matrices is  $\text{tr}(\Phi\Gamma) = \sum_{i=1}^p \sum_{j=1}^p \phi_{ij}\gamma_{ij}$ . If  $\Phi \in \mathcal{M}_0(G)$  only the specified elements of  $\Gamma^{\mathcal{V}}$  enter into this sum, and so we can write  $\text{tr}(\Phi\Gamma) = \text{tr}(\Phi\Gamma^{\mathcal{V}})$ .

### 3. Graphical Gaussian models

We consider graphical models for a random vector  $X_{\mathcal{V}}$  with distribution  $P_{\mathcal{V}}$  on an undirected graph  $G = (V, \mathcal{V})$ . We say that the distribution  $P_{\mathcal{V}}$  is Markov with respect to  $G$  if  $X_A$  is independent of  $X_B$  given  $X_S$ ,  $X_A \perp\!\!\!\perp X_B | X_S [P_{\mathcal{V}}]$ , whenever  $S$  separates  $A$  from  $B$  in  $G$ . (For the Gaussian case that interests us, the global, local and pairwise Markov properties are identical, see Lauritzen 1996.)

A graphical Gaussian model is defined as the intersection of the set of Markov distributions relative to  $G$  and the set of  $p$ -variate normal distributions with mean equal to zero and variance matrix  $\Sigma$ , which we assume positive definite. An off-diagonal element  $\sigma^{ij}$  of  $\Sigma^{-1}$  is zero if and only if  $X_i \perp\!\!\!\perp X_j | X_{V \setminus \{i, j\}} [P_{\mathcal{V}}]$ . Thus in graphical Gaussian models the pairwise conditional independence structure of  $X_{\mathcal{V}}$  is dictated by the zero structure of  $\Sigma^{-1}$  so that  $\Sigma = \Sigma_G$  is a  $G$ -completed matrix.

A natural measure of the interaction represented by the edge  $(i, j)$  of the graph is given by the partial correlation coefficient

$$\rho_{ij, \mathcal{V} \setminus \{i, j\}} = -\frac{\sigma^{ij}}{\sqrt{\sigma^{ii}\sigma^{jj}}} \quad (2)$$

which is zero if and only if  $(i, j) \notin \mathcal{V}$ .

The moment parameter of the distribution is  $\Sigma^{\mathcal{V}} \in \mathcal{M}_*^+(G)$  while the canonical parameter is  $\Sigma^{-1} \in \mathcal{M}_0^+(G)$ , the inverse of the completion of  $\Sigma^{\mathcal{V}}$ . The likelihood function of  $\Sigma^{-1}$  based on a random sample  $X^{(n)} = (X^1, \dots, X^n)$  from  $P_{\mathcal{V}}$  is

$$L(\Sigma^{-1}) \propto \exp \left\{ -\frac{n}{2} \text{tr}(\Sigma^{-1}S) + \frac{n}{2} \log |\Sigma^{-1}| \right\}, \quad (3)$$

where  $S$  is the sample variance matrix. In our notation, the maximum likelihood estimate  $\hat{\Sigma}^{-1}$  (Speed and Kiiveri, 1986) is the inverse of the completion of  $S^{\mathcal{V}}$ .

## 4. The HIV study

Table 1 presents some summary statistics for six variables measured in Genoa and Padua paediatric hospitals on 107 three month old babies. These data

Table 1: *Summary statistics for the HIV data: sample variances (main diagonal), correlations (lower triangle) and partial correlations (upper triangle).*

$X_1$	8.8374	0.479	-0.043	-0.033	0.356	-0.236
$X_2$	0.483	0.1919	0.068	-0.084	-0.224	-0.110
$X_3$	0.220	0.057	8924231.9	0.085	0.552	-0.330
$X_4$	-0.040	-0.133	0.149	20392.4	0.091	0.013
$X_5$	0.253	-0.124	0.523	0.179	1952795.2	0.384
$X_6$	-0.276	-0.314	-0.183	0.064	0.213	1.378
	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$

come from a larger Italian study (Boccuzzo, 1991) investigating early diagnosis of HIV infection in children from HIV positive mothers. The variables are related to various measures on blood and its components:  $X_1$  and  $X_2$  immunoglobulin G and A, respectively;  $X_4$  the platelet count;  $X_3, X_5$  lymphocyte B and T4, respectively; and  $X_6$  the T4/T8 lymphocyte ratio.

Discussion with the experts running the study suggests the presence of a strong association between variables  $X_1, X_2$  and between variables  $X_3, X_5, X_6$ ; together with an association structure of these variables compatible with the graph of Figure 1.

An essential quantity to be computed in a Bayesian analysis of the proposed graphical model is a posterior distribution for the relevant association coefficients which, in the Gaussian case, are the marginal and the partial correlations corresponding to the edges of the graph. In the next Section we consider an asymptotic approach to this problem.

## 5. Asymptotic distributions

Exact prior to posterior analysis for the correlation coefficients of an arbitrary graphical Gaussian model still poses difficulties concerned with the algebraic derivation of a tractable posterior distribution. In this Section we derive the asymptotic distributions for the marginal and the partial correlations in a conjugate analysis.

The conjugate prior density for  $\Sigma^{-1}$ , with respect to the product of Lebesgue measures on the diagonal and non-zero super-diagonal elements of  $\Sigma^{-1}$ , can be deduced from (3) (see Bernardo and Smith, 1994, p.269) and has form

$$\pi(\Sigma^{-1}|A^{\mathcal{V}}, h) \propto \exp\left\{-\frac{h}{2}\text{tr}(\Sigma^{-1}A^{\mathcal{V}}) + \frac{h}{2}\log|\Sigma^{-1}|\right\}, \quad (4)$$

for  $\Sigma^{-1} \in \mathcal{M}_0^+(G)$ . The hyper parameters are an incomplete matrix  $A^\nu \in \mathcal{M}_*^+(G)$  and a positive constant  $h$ . The posterior distribution has density function of the same form with hyper parameters  $T = (hA^\nu + nS^\nu)/(h+n)$  and  $m = h+n$ . By the similarity between (3) and (4) it can be shown that the posterior density has maximum at  $\Sigma^{-1} = T_G^{-1}$ , the inverse of the completion of  $T^\nu$ .

Let  $R^\nu$  be the incomplete matrix with main diagonal equal to that of  $\Sigma^\nu$  and with marginal correlations in the specified off-diagonal positions. Clearly  $R^\nu$  can be written as a (bijective) function of  $\Sigma^\nu$ ,  $R^\nu = g(\Sigma^\nu)$ , so that, by (2),  $P^\nu = -g(\Sigma^{-\nu})$  is the incomplete matrix with main diagonal equal to that of  $-\Sigma^{-\nu}$  and partial correlations in the specified off-diagonal positions. Roverato and Whittaker (1997) showed that the asymptotic posterior distributions for  $\Sigma^{-\nu}$  and  $\Sigma^\nu$  are

$$\Sigma^{-\nu} \stackrel{a}{\sim} N\left(T_G^{-\nu}, m^{-1} \text{Iss}(T_G^{-1})_{\nu\nu|\bar{\nu}}\right) \quad \text{and} \quad \Sigma^\nu \stackrel{a}{\sim} N\left(T^\nu, m^{-1} \text{Iss}(T_G)_{\nu\nu}\right) \quad (5)$$

respectively. The asymptotic posterior distribution of the transformed parameters can be obtained by applying standard delta-type methods (see Bernardo and Smith, 1994, p.295). The transformation  $g(\cdot)$  can be shown to have Jacobian

$$J(\Sigma^\nu)_{\nu\nu} = \frac{\partial g(\Sigma^\nu)}{\partial \Sigma^\nu} = \text{diag}(g(\Sigma^\nu))_{\nu\nu} H_{\nu\nu} \text{diag}(\Sigma^\nu)_{\nu\nu}^{-1} \quad (6)$$

where  $H_{\nu\nu}$  is the matrix indexed by  $\mathcal{V} \times \mathcal{V}$  with elements  $\{H_{\nu\nu}\}_{(i,j),(r,s)}$  equal to 1 if  $i=r$  and  $j=s$ , to  $-1/2$  if either  $i=r=s \neq j$  or  $j=r=s \neq i$  and 0 elsewhere. As usual, in taking the derivative in (6) the denominator is assumed to be a row vector, the numerator a column vector and the off diagonal elements are considered only once. Applying  $J(\cdot)$ , evaluated at the mode of the posterior density, to (5) we obtain

$$P^\nu \stackrel{a}{\sim} N\left(-g(T_G^{-\nu}), m^{-1} J(T_G^{-\nu})_{\nu\nu} \text{Iss}(T_G^{-1})_{\nu\nu|\bar{\nu}} J(T_G^{-\nu})'_{\nu\nu}\right) \quad (7)$$

and

$$R^\nu \stackrel{a}{\sim} N\left(g(T^\nu), m^{-1} J(T^\nu)_{\nu\nu} \text{Iss}(T_G)_{\nu\nu} J(T^\nu)'_{\nu\nu}\right) \quad (8)$$

which are the required asymptotic distributions.

## 7. Application

In this Section we carry out a prior to posterior analysis of the HIV data based on the results of Section 6.

A critical point in the conjugate Bayesian analysis of the graphical Gaussian model is the specification of the prior hyper parameters  $h$  and  $A^\nu$ . The

posterior distribution is very sensitive to different prior specifications. Furthermore note that the number of hyper parameters exceeds the number of parameters.

The positive constant  $h$  can be thought of as the number of imaginary data points establishing the prior belief, consequently in absence of genuine prior expert views it should be small.

The incomplete matrix  $A^\nu$  reflects the prior belief on the real value of  $\Sigma^\nu$ . Dealing with the saturated model,  $A^\nu = A$ , some authors (Chen, 1979; Dickey *et al.*, 1985) proposed to reduce the number of hyper parameters by constraining  $A$  to have lower dimension structure such as  $A = \Delta^{1/2}\Phi\Delta^{1/2}$ , where  $\Phi = (1 - \phi)I + 1_p 1_p'$  has intraclass correlation structure (with  $-1/(p-1) < \phi < 1$  so as to assure  $\Phi > 0$ ) and  $\Delta = \text{diag}(\delta_1, \dots, \delta_p)$ .

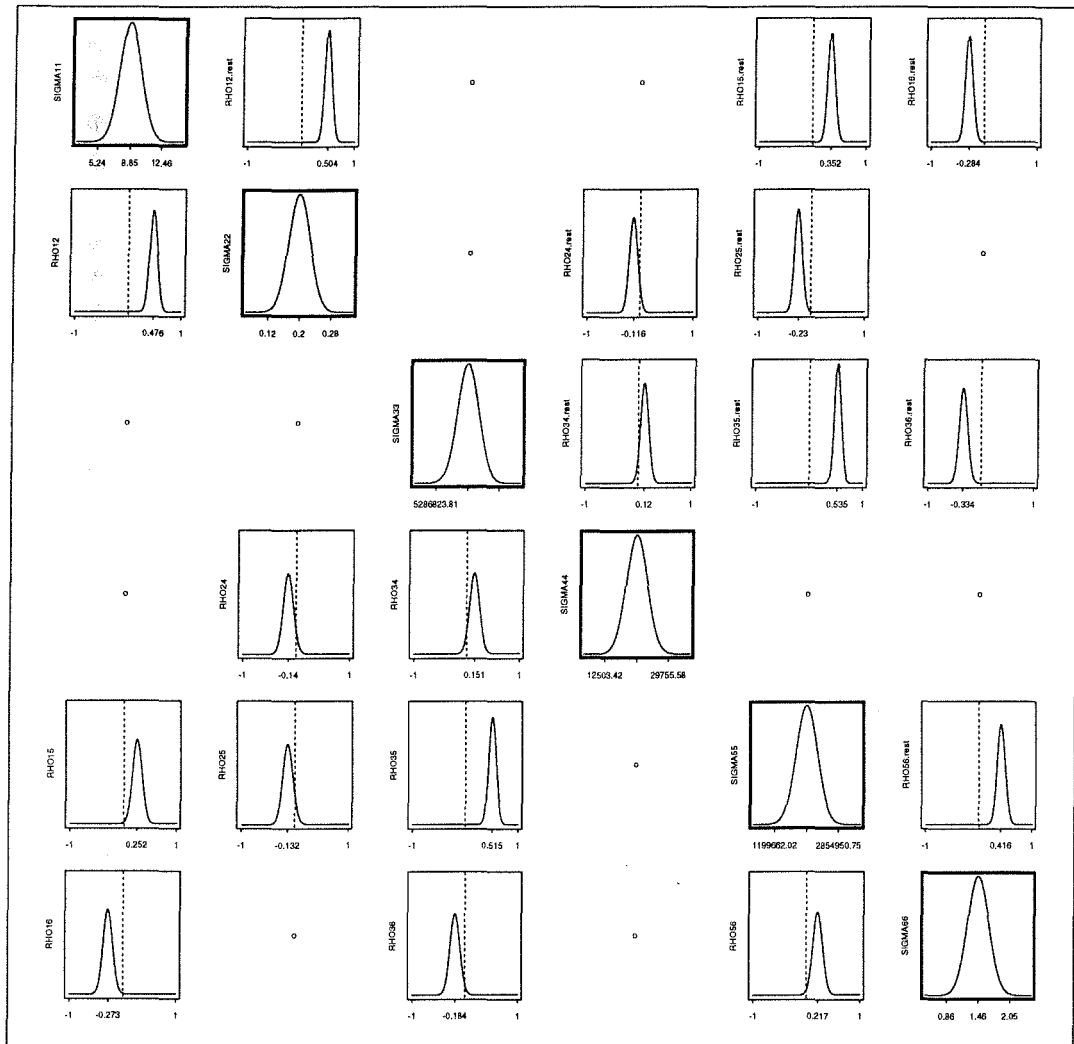
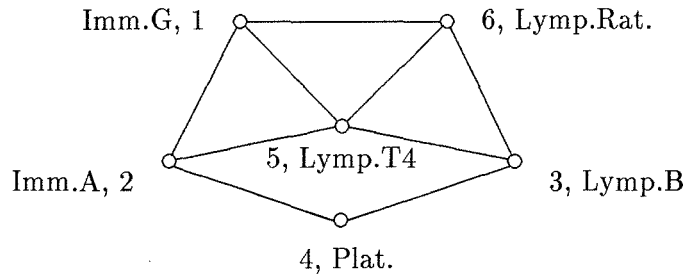
We remark that a similar choice of  $\Phi^\nu$  induces a systematic bias in the mean of the asymptotic posterior distributions here considered. To see this, consider two sample correlations  $r_{ij}$  and  $r_{ls}$  such that  $r_{ij} > 0$  and  $r_{ij} = -r_{ls}$ . In this case the evidence provided by the data is of equal strength in the associations relative to  $\rho_{ij}$  and  $\rho_{ls}$ . In such a situation it is desirable, when no otherwise specified in the prior, that this characteristic is maintained in the posterior distribution. However, it can be easily checked in  $g(T^\nu)$  that any choice of  $\phi > 0$  leads to a asymptotic posterior mean of  $\rho_{ls}$  closer to zero than that of  $\rho_{ij}$ . Furthermore a similar behaviour can be empirically observed in  $-g(T_G^{-\nu})$ . Therefore an intraclass correlation structure of  $\Phi^\nu$  implies an asymmetrical inference depending on the signs of the single correlation coefficients. Note that setting  $\phi$  to 0 would overtake this difficulty but at the price of a strong prior information of independence between all variables, which is seldom justified.

Our proposed solution to this problem is to set the specified  $(i, j)$ -element ( $i \neq j$ ) of  $\Phi^\nu$  to  $\phi \times \text{sign}(r_{ij})$ . Although this is not a pure Bayesian approach to the problem, it keeps the hyper parameter dimension low without introducing a systematic bias in the analysis. For the HIV data we set  $\phi = 0.3$  which assure  $\Phi^\nu$  to have positive completion. The hyper parameter  $h$  is set to 1 and  $\Delta = \text{diag}(10, 10^0, 10^7, 10^5, 10^7, 10)$ .

The resulting asymptotic marginal posterior densities are presented in Figure 1. The given marginal distributions are completely specified by their mean and variance values. Nevertheless the plot of the posterior densities in the  $[-1, 1]$  interval is useful since it allows an immediate visualisation of the densities behaviour around zero. For instance, it can be noted that all the correlations involving variable  $X_4$  (forth row and column in the picture) have high density values at zero. A more detailed analysis showed that all of the four corresponding 90% confidence intervals include zero, suggesting that the model may be overparametrised.



Figure 1: Independence graph of the hypothesised model for HIV diagnostic data and marginal asymptotic posterior densities for variances (main diagonal), partial correlations (upper triangle) and marginal correlations (lower triangle).



## 8. Conclusions

Graphical models are specified by set of pairwise conditional independencies and this leads to a parametrisation in terms of partial association coefficients. Nevertheless also the marginal independence pattern is of relevance in the comprehension of the problem under consideration. Figure 1, including both marginal and partial correlations, seems to be an effective device to summarise the data structure under a graphical Gaussian model.

The Splus functions relative to the work of this paper are available from the author.

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