Decomposable and Directed Graphical Gaussian Models

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The Wishart distribution is the sampling distribution of the matrix of sums of squares and products. More precisely:

A random $d \times d$ matrix W has a *d-dimensional Wishart distribution* with parameter Σ and n *degrees of freedom* if

$$W \overset{\mathcal{D}}{=} \sum_{i=1}^{n} X^{\nu}(X^{\nu})^{\top}$$

where $X^{\nu} \sim \mathcal{N}_d(0, \Sigma)$. We then write

$$W \sim \mathcal{W}_d(n, \Sigma).$$

The Wishart is the multivariate analogue to the χ^2:

$$\mathcal{W}_1(n, \sigma^2) = \sigma^2 \chi^2(n).$$

If $W \sim \mathcal{W}_d(n, \Sigma)$ its mean is $\mathbf{E}(W) = n\Sigma$.

If W_1 and W_2 are independent with $W_i \sim \mathcal{W}_d(n_i, \Sigma)$, then

$$W_1 + W_2 \sim \mathcal{W}_d(n_1 + n_2, \Sigma).$$

If A is an $r \times d$ matrix and $W \sim \mathcal{W}_d(n, \Sigma)$, then

$$AWA^\top \sim \mathcal{W}_r(n, A\Sigma A^\top).$$

For $r = 1$ we get that when $W \sim \mathcal{W}_d(n, \Sigma)$ and $\lambda \in R^d$,

$$\lambda^\top W \lambda \sim \sigma_\lambda^2 \chi^2(n),$$

where $\sigma_\lambda^2 = \lambda^\top \Sigma \lambda$.

If $W \sim \mathcal{W}_d(n, \Sigma)$, where Σ is regular, then *W is regular with probability one if and only if $n \geq d$*.

When $n \geq d$ the Wishart distribution has density

$$\begin{aligned} & f_d(w \mid n, \Sigma) \\ & \quad = \quad c(d,n)^{-1} (\det \Sigma)^{-n/2} (\det w)^{(n-d-1)/2} e^{-\operatorname{tr}(\Sigma^{-1} w)/2} \end{aligned}$$

for w positive definite, and 0 otherwise.

The *Wishart constant* $c(d, n)$ is

$$c(d,n) = 2^{nd/2} (2\pi)^{d(d-1)/4} \prod_{i=1}^{d} \Gamma\{(n+1-i)/2\}.$$

Consider $X = (X_v, v \in V) \sim \mathcal{N}_V(0, \Sigma)$ with Σ regular and $K = \Sigma^{-1}$.

The concentration matrix of the conditional distribution of (X_α, X_β) given $X_{V \setminus \{\alpha,\beta\}}$ is

$$K_{\{\alpha,\beta\}} = \begin{pmatrix} k_{\alpha\alpha} & k_{\alpha\beta} \\ k_{\beta\alpha} & k_{\beta\beta} \end{pmatrix}.$$

Hence

$$\alpha \perp\!\!\!\perp \beta \,|\, V \setminus \{\alpha, \beta\} \iff k_{\alpha\beta} = 0.$$

Thus *the dependence graph $\mathcal{G}(K)$ of a regular Gaussian distribution is given by*

$$\alpha \not\sim \beta \iff k_{\alpha\beta} = 0.$$

$\mathcal{S}(\mathcal{G})$ denotes the symmetric matrices A with $a_{\alpha\beta} = 0$ unless $\alpha \sim \beta$ and $\mathcal{S}^+(\mathcal{G})$ their positive definite elements.

A *Gaussian graphical model* for X specifies X as multivariate normal with $K \in \mathcal{S}^+(\mathcal{G})$ and otherwise unknown.

The likelihood function based on a sample of size n is

$$L(K) \propto (\det K)^{n/2} e^{-\operatorname{tr}(KW)/2},$$

where W is the Wishart matrix of sums of squares and products, $W \sim \mathcal{W}_{|V|}(n, \Sigma)$ with $\Sigma^{-1} = K \in \mathcal{S}^+(\mathcal{G})$.

Define the matrices $A^u, u \in V \cup E$ as those with elements

$$a^u_{ij} = \left\{ \begin{array}{ll} 1 & \text{if } u \in V \text{ and } i = j = u \\ 1 & \text{if } u \in E \text{ and } u = \{i,j\} \\ 0 & \quad\quad\text{otherwise.} \end{array} \right) .$$

Then, as $K \in \mathcal{S}(\mathcal{G})$,

$$K = \sum_{v \in V} k_v A^v + \sum_{e \in E} k_e A^e \tag{1}$$

and hence

$$\operatorname{tr}(KW) = \sum_{v \in V} k_v \operatorname{tr}(A^v W) + \sum_{e \in E} k_e \operatorname{tr}(A^e W)$$

Hence we can identify the family as a (regular and canonical) *exponential family with* $-\operatorname{tr}(A^u W)/2, u \in V \cup E$ *as canonical sufficient statistics.*

This yields the likelihood equations

$$\operatorname{tr}(A^u W) = n \operatorname{tr}(A^u \Sigma), \quad u \in V \cup E.$$

which can also be expressed as

$$n\hat{\sigma}_{vv} = w_{vv}, \quad n\hat{\sigma}_{\alpha\beta} = w_{\alpha\beta}, \quad v \in V, \{\alpha, \beta\} \in E.$$

or, equivalently

$$n\hat{\Sigma}_{cc} = w_{cc} \text{ for all cliques } c \in \mathcal{C}(\mathcal{G}),$$

We should remember the model restriction $\Sigma^{-1} \in \mathcal{S}^+(\mathcal{G})$.

For $K \in \mathcal{S}^+(\mathcal{G})$ and $c \in \mathcal{C}$, define the operation of 'adjusting the c-marginal' as follows. Let $a = V \setminus c$ and

$$T_c K = \begin{pmatrix} n(w_{cc})^{-1} + K_{ca}(K_{aa})^{-1}K_{ac} & K_{ca} \\ K_{ac} & K_{aa} \end{pmatrix}. \qquad (2)$$

The C-marginal covariance $\tilde{\Sigma}_{cc}$ corresponding to the adjusted concentration matrix becomes

$$\begin{aligned} \tilde{\Sigma}_{cc} &= \{(T_c K)^{-1}\}_{cc} \\ &= \left\{n(w_{cc})^{-1} + K_{ca}(K_{aa})^{-1}K_{ac} - K_{ca}(K_{aa})^{-1}K_{ac}\right\}^{-1} \\ &= w_{cc}/n, \end{aligned}$$

hence *$T_c K$ does indeed adjust the marginals*. From (2) it is seen that the pattern of zeros in K is preserved under the operation T_c, and it can also be seen to stay positive definite.

Next we choose any ordering $(c_1, \ldots, c_k)$ of the cliques in $\mathcal{G}$. Choose further $K_0 = I$ and define for $r = 0, 1, \ldots$

$$K_{r+1} = (T_{c_1} \cdots T_{c_k})K_r.$$

Then we have: *Consider a sample from a covariance selection model with graph $\mathcal{G}$. Then*

$$\hat{K} = \lim_{r \to \infty} K_r,$$

provided the maximum likelihood estimate $\hat{K}$ of K exists.

If the graph $\mathcal{G}$ is chordal, we say that the graphical model is *decomposable*.

In this case, *the IPS-algorithm converges in a finite number of steps*, as in the discrete case.

We also have the familiar *factorization of densities*

$$f(x \mid \Sigma) = \frac{\prod_{C \in \mathcal{C}} f(x_C \mid \Sigma_C)}{\prod_{S \in \mathcal{S}} f(x_S \mid \Sigma_S)^{\nu(S)}} \tag{3}$$

where $\nu(S)$ is the number of times S appear as intersection between neighbouring cliques of a junction tree for $\mathcal{C}$.

Relations for trace and determinant

Using the factorization (3) we can for example match the expressions for the trace and determinant of Σ

$$\operatorname{tr}(KW) = \sum_{C \in \mathcal{C}} \operatorname{tr}(K_C W_C) - \sum_{S \in \mathcal{S}} \nu(S) \operatorname{tr}(K_S W_S)$$

and further

$$\det \Sigma \quad = \quad \{\det(K)\}^{-1} = \frac{\prod_{C \in \mathcal{C}} \det\{\Sigma_C\}}{\prod_{S \in \mathcal{S}} \{\det(\Sigma_S)\}^{\nu(S)}}$$

These are some of many relations that can be derived using the decomposition property of chordal graphs.

The same factorization clearly holds for the maximum likelihood estimates:

$$f(x\,|\,\hat{\Sigma}) = \frac{\prod_{C\in\mathcal{C}} f(x_C\,|\,\hat{\Sigma}_C)}{\prod_{S\in\mathcal{S}} f(x_S\,|\,\hat{\Sigma}_S)^{\nu(S)}} \tag{4}$$

Moreover, it follows from the general likelihood equations that

$$\hat{\Sigma}_A = W_A/n \text{ whenever } A \text{ is complete.}$$

Exploiting this, we can obtain an explicit formula for the maximum likelihood estimate in the case of a chordal graph.

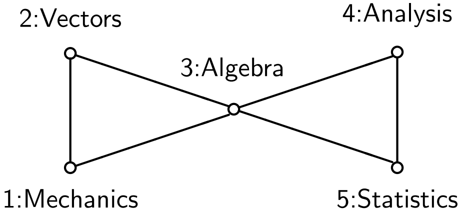
For a $|d| \times |e|$ matrix $A = \{a_{\gamma\mu}\}_{\gamma\in d,\mu\in e}$ we let $[A]^V$ denote the matrix obtained from A by filling up with zero entries to obtain full dimension $|V| \times |V|$, i.e.

$$\left([A]^V\right)_{\gamma\mu} = \begin{cases} a_{\gamma\mu} & \text{if } \gamma \in d, \mu \in e \\ 0 & \text{otherwise.} \end{cases}$$

The maximum likelihood estimates exists if and only if $n \geq C$ for all $C \in \mathcal{C}$. Then the following simple formula holds for the maximum likelihood estimate of K:

$$\hat{K} = n\left\{\sum_{C\in\mathcal{C}}\left[(w_C)^{-1}\right]^V - \sum_{S\in\mathcal{S}}\nu(S)\left[(w_S)^{-1}\right]^V\right\}.$$

Mathematics marks



This graph is chordal with cliques $\{1, 2, 3\}$, $\{3, 4, 5\}$ with separator $S = \{3\}$ having $\nu(\{3\}) = 1$.

Since one degree of freedom is lost by subtracting the average, we get in this example

$$\hat{K} = 87 \begin{pmatrix} w^{11}_{[123]} & w^{12}_{[123]} & w^{13}_{[123]} & 0 & 0 \\ w^{21}_{[123]} & w^{22}_{[123]} & w^{23}_{[123]} & 0 & 0 \\ w^{31}_{[123]} & w^{32}_{[123]} & w^{33}_{[123]} + w^{33}_{[345]} - 1/w_{33} & w^{34}_{[345]} & w^{35}_{[345]} \\ 0 & 0 & w^{43}_{[345]} & w^{44}_{[345]} & w^{45}_{[345]} \\ 0 & 0 & w^{53}_{[345]} & w^{54}_{[345]} & w^{55}_{[345]} \end{pmatrix}$$

where $w^{ij}_{[123]}$ is the ijth element of the inverse of

$$W_{[123]} = \begin{pmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{pmatrix}$$

and so on.

Consider a directed acyclic graph $\mathcal{D}$ and associate for every vertex a random variable X_v. Consider now the equation system

$$X_v \leftarrow \alpha_v^\top X_{\mathrm{pa}(v)} + \beta_v + U_v, v \in V \tag{5}$$

where $U_v, v \in V$ are independent random disturbances with $U_v \sim \mathcal{N}(0, \sigma_v^2)$.

Such an equation system is known as a *recursive structural equation system*.

Structural equation systems are used heavily in social sciences and in economics. The term *structural* refers to the fact that the equations are assumed to be *stable under intervention* so that fixing a value of x_v^* would change the system only by removing the line in the equation system (5) defining x_v^*.

A recursive structural equation system defines a multivariate Gaussian distribution which satisfies the directed Markov property of $\mathcal{D}$ since the joint density becomes

$$\begin{aligned} f(x \,|\, \alpha, \sigma) &= \prod_v (2\pi)^{-1/2} \sigma_v^{-1} e^{-\frac{(x_v - \alpha_v^\top x_{\mathrm{pa}(v)} - \beta_v)^2}{2\sigma_v^2}} \\ &= (2\pi)^{-|V|/2} \left(\prod_v \sigma_v^{-1} \right) \\ &\quad \times e^{-\sum_v \frac{(x_v - \alpha_v^\top x_{\mathrm{pa}(v)} - \beta_v)^2}{2\sigma_v^2}}, \end{aligned}$$

from which the joint concentration matrix K can easily be derived.

Consider the system

$$\begin{aligned} X_1 &\leftarrow U_1 \\ X_2 &\leftarrow U_2 \\ X_3 &\leftarrow \alpha_{31}X_1 + U_3 \\ X_4 &\leftarrow \alpha_{42}X_2 + \alpha_{43}X_3 + U_4. \end{aligned}$$

The quadratic expression in the exponent becomes

$$\frac{x_1^2}{\sigma_1^2} + \frac{x_2^2}{\sigma_2^2} + \frac{(x_3 - \alpha_{31}x_1)^2}{\sigma_3^2} + \frac{(x_4 - \alpha_{42}x_2 - \alpha_{43}x_3)^2}{\sigma_4^2}.$$

Expanding the squares and identifying terms yields the concentration matrix

$$\begin{pmatrix} \frac{1}{\sigma_1^2}+\frac{\alpha_{31}^2}{\sigma_3^2} & 0 & \frac{-\alpha_{31}}{\sigma_3^2} & 0 \\ 0 & \frac{1}{\sigma_2^2}+\frac{\alpha_{42}^2}{\sigma_4^2} & \frac{\alpha_{42}\alpha_{43}}{\sigma_4^2} & \frac{-\alpha_{42}}{\sigma_4^2} \\ \frac{-\alpha_{31}}{\sigma_3^2} & \frac{\alpha_{42}\alpha_{43}}{\sigma_4^2} & \frac{1}{\sigma_3^2}+\frac{\alpha_{43}^2}{\sigma_4^2} & \frac{-\alpha_{43}}{\sigma_4^2} \\ 0 & \frac{-\alpha_{42}}{\sigma_4^2} & \frac{-\alpha_{43}}{\sigma_4^2} & \frac{1}{\sigma_4^2} \end{pmatrix}.$$

The covariance matrix can in principle be found by inverting the above. However, it is easier to express X in terms of the Us as

$$\begin{aligned} X_1 &= U_1 \\ X_2 &= U_2 \\ X_3 &= \alpha_{31} U_1 + U_3 \\ X_4 &= \alpha_{43}\alpha_{31} U_1 + \alpha_{42} U_2 + \alpha_{43} U_3 + U_4 \end{aligned}$$

and then calculate the covariances directly to obtain

$$\begin{pmatrix} \sigma_1^2 & 0 & \alpha_{31}\sigma_1^2 & \alpha_{43}\alpha_{31}\sigma_1^2 \\ 0 & \sigma_2^2 & 0 & \alpha_{42}\sigma_2^2 \\ \alpha_{31}\sigma_1^2 & 0 & \sigma_3^2 + \alpha_{31}^2\sigma_1^2 & \alpha_{43}\alpha_{31}^2\sigma_1^2 + \alpha_{43}\sigma_3^2 \\ \alpha_{43}\alpha_{31}\sigma_1^2 & \alpha_{42}\sigma_2^2 & \alpha_{43}\alpha_{31}^2\sigma_1^2 + \alpha_{43}\sigma_3^2 & \omega_4^2 \end{pmatrix},$$

where

$$\omega_4^2 = \alpha_{43}^2\alpha_{31}^2\sigma_1^2 + \alpha_{42}^2\sigma_2^2 + \alpha_{43}^2\sigma_3^2 + \sigma_4^2.$$

Systems of structural equations of the type considered are called *recursive* in contrast to *feedback systems* of equations where directed cycles in the corresponding graph are allowed.

It is also customary to allow correlations between the disturbance terms. This leads to violation of the directed Markov property, so other types of graph and Markov properties must be considered to deal correctly with such models.

This type of model and analysis goes back to the geneticist Sewall Wright who coined the term *path analysis* to the calculus of effects based on this kind of models.
This is one of the early precursors for modern graphical modelling.

A directed graphical Gaussian model generated by a linear recursive structural equation system is equivalent to a corresponding undirected graphical model *if and only if $\mathcal{D}$ is perfect,* in which case its skeleton $\sigma(\mathcal{D})$ is chordal.

Still, even for non-perfect DAGs the MLE is easy to find for linear recursive structural equation systems:

For each v, linear regression of data $X_v^\nu, \nu = 1, \ldots N$ onto parents $X_{\mathrm{pa}(v)}$ is performed and corresponding regression coefficients $\hat{\alpha}_v$ and residual variance estimates $\hat{\sigma}_v^2$ are calculated in the usual way.