Gaussian Graphical Models

Steffen Lauritzen
University of Oxford

CIMPA Summerschool, Hammamet 2011, Tunisia

September 8, 2011

A d-dimensional random vector $X = (X_1, \ldots, X_d)$ has a *multivariate Gaussian distribution* or *normal* distribution on $\mathcal{R}^d$ if there is a vector $\xi \in \mathcal{R}^d$ and a $d \times d$ matrix Σ such that

$$\lambda^\top X \sim \mathcal{N}(\lambda^\top \xi, \lambda^\top \Sigma \lambda) \quad \text{for all } \lambda \in R^d. \tag{1}$$

We then write $X \sim \mathcal{N}_d(\xi, \Sigma)$.

Taking $\lambda = e_i$ or $\lambda = e_i + e_j$ where e_i is the unit vector with i-th coordinate 1 and the remaining equal to zero yields:

$$X_i \sim \mathcal{N}(\xi_i, \sigma_{ii}), \quad \mathrm{Cov}(X_i, X_j) = \sigma_{ij}.$$

Hence ξ is the *mean vector* and Σ the *covariance matrix* of the distribution.

The definition (1) makes sense if and only if $\lambda^\top \Sigma \lambda \geq 0$, i.e. if Σ is *positive semidefinite*. Note that we have allowed distributions with variance zero.

The multivariate moment generating function of X can be calculated using the relation (1) as

$$m_d(\lambda) = E\{e^{\lambda^\top X}\} = e^{\lambda^\top \xi + \lambda^\top \Sigma \lambda / 2}$$

where we have used that the univariate moment generating function for $\mathcal{N}(\mu, \sigma^2)$ is

$$m_1(t) = e^{t\mu + \sigma^2 t^2 / 2}$$

and let $t = 1$, $\mu = \lambda^\top \xi$, and $\sigma^2 = \lambda^\top \Sigma \lambda$.

In particular this means that *a multivariate Gaussian distribution is determined by its mean vector and covariance matrix.*

Assume $X^\top = (X_1, X_2, X_3)$ with X_i independent and $X_i \sim \mathcal{N}(\xi_i, \sigma_i^2)$. Then

$$\lambda^\top X = \lambda_1 X_1 + \lambda_2 X_2 + \lambda_3 X_3 \sim \mathcal{N}(\mu, \tau^2)$$

with

$$\mu = \lambda^\top \xi = \lambda_1 \xi_1 + \lambda_2 \xi_2 + \lambda_3 \xi_3, \quad \tau^2 = \lambda_1^2 \sigma_1^2 + \lambda_2^2 \sigma_2^2 + \lambda_3^2 \sigma_3^2.$$

Hence $X \sim \mathcal{N}_3(\xi, \Sigma)$ with $\xi^\top = (\xi_1, \xi_2, \xi_3)$ and

$$\Sigma = \begin{pmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{pmatrix}.$$

If Σ is *positive definite*, i.e. if $\lambda^\top \Sigma \lambda > 0$ for $\lambda \neq 0$, the distribution has density on $\mathcal{R}^d$

$$f(x \mid \xi, \Sigma) = (2\pi)^{-d/2} (\det K)^{1/2} e^{-(x-\xi)^\top K (x-\xi)/2}, \qquad (2)$$

where $K = \Sigma^{-1}$ is the *concentration matrix* of the distribution. Since a positive semidefinite matrix is positive definite if and only if it is invertible, we then also say that Σ is *regular*.

If $X_1, \ldots, X_d$ are independent and $X_i \sim \mathcal{N}(\xi_i, \sigma_i^2)$ their joint density has the form (2) with $\Sigma = \mathrm{diag}(\sigma_i^2)$ and $K = \Sigma^{-1} = \mathrm{diag}(1/\sigma_i^2)$.

Hence *vectors of independent Gaussians are multivariate Gaussian.*

In the bivariate case it is traditional to write

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho \\ \sigma_1\sigma_2\rho & \sigma_2^2 \end{pmatrix},$$

with ρ being the *correlation* between X_1 and X_2. Then

$$\det(\Sigma) = \sigma_1^2\sigma_2^2(1-\rho^2) = \det(K)^{-1}$$

and

$$K = \frac{1}{\sigma_1^2\sigma_2^2(1-\rho^2)} \begin{pmatrix} \sigma_2^2 & -\sigma_1\sigma_2\rho \\ -\sigma_1\sigma_2\rho & \sigma_1^2 \end{pmatrix}.$$

Thus the density becomes

$$f(x \mid \xi, \Sigma) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{(1-\rho^2)}}$$
$$\times e^{-\frac{1}{2(1-\rho^2)}\left\{\frac{(x_1-\xi_1)^2}{\sigma_1^2} - 2\rho\frac{(x_1-\xi_1)(x_2-\xi_2)}{\sigma_1\sigma_2} + \frac{(x_2-\xi_2)^2}{\sigma_2^2}\right\}}.$$

The contours of this density are ellipses and the corresponding density is bell-shaped with maximum in (ξ_1, ξ_2).

The marginal distributions of a vector X can all be Gaussian without the joint being multivariate Gaussian:

For example, let $X_1 \sim \mathcal{N}(0, 1)$, and define X_2 as

$$X_2 = \begin{cases} X_1 & \text{if } |X_1| > c \\ -X_1 & \text{otherwise.} \end{cases}$$

Then, using the symmetry of the univariate Gausssian distribution, X_2 is also distributed as $\mathcal{N}(0, 1)$.

However, the joint distribution is not Gaussian unless $c = 0$ since, for example, $Y = X_1 + X_2$ satisfies

$$P(Y = 0) = P(X_2 = -X_1) = P(|X_1| \leq c) = \Phi(c) - \Phi(-c).$$

Note that for $c = 0$, the correlation ρ between X_1 and X_2 is 1 whereas for $c = \infty$, $\rho = -1$.

It follows that *there is a value of c so that X_1 and X_2 are uncorrelated,* and still not jointly Gaussian.

Adding two independent Gaussians yields a Gaussian:

If $X \sim \mathcal{N}_d(\xi_1, \Sigma_1)$ and $X_2 \sim \mathcal{N}_d(\xi_2, \Sigma_2)$ and $X_1 \perp\!\!\!\perp X_2$

$$X_1 + X_2 \sim \mathcal{N}_d(\xi_1 + \xi_2, \Sigma_1 + \Sigma_2).$$

To see this, just note that

$$\lambda^\top (X_1 + X_2) = \lambda^\top X_1 + \lambda^\top X_2$$

and use the univariate addition property.

Linear transformations preserve multivariate normality:

If A is an $r \times d$ matrix, $b \in \mathcal{R}^r$ and $X \sim \mathcal{N}_d(\xi, \Sigma)$, then

$$Y = AX + b \sim \mathcal{N}_r(A\xi + b, A\Sigma A^\top).$$

Again, just write

$$\gamma^\top Y = \gamma^\top (AX + b) = (A^\top \gamma)^\top X + \gamma^\top b$$

and use the corresponding univariate result.

Partition X into into X_1 and X_2, where $X_1 \in \mathcal{R}^r$ and $X_2 \in \mathcal{R}^s$ with $r + s = d$.

Partition mean vector, concentration and covariance matrix accordingly as

$$\xi = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}, \quad K = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

so that Σ_{11} is $r \times r$ and so on. *Then, if* $X \sim \mathcal{N}_d(\xi, \Sigma)$

$$X_2 \sim \mathcal{N}_s(\xi_2, \Sigma_{22}).$$

This follows simply from the previous fact using the matrix

$$A = \left(0_{sr} \; I_s\right).$$

where 0_{sr} is an $s \times r$ matrix of zeros and I_s is the $s \times s$ identity matrix.

If Σ_{22} is regular, it further holds that

$$X_1 \mid X_2 = x_2 \sim \mathcal{N}_r(\xi_{1|2}, \Sigma_{1|2}),$$

where

$$\xi_{1|2} = \xi_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \xi_2) \quad \text{and} \quad \Sigma_{1|2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}.$$

In particular, $\Sigma_{12} = 0$ *if and only if X_1 and X_2 are independent.*

To see this, we simply calculate the conditional density.

$$f(x_1 \mid x_2) \propto f_{\xi,\Sigma}(x_1, x_2)$$
$$\propto \exp\left\{-(x_1 - \xi_1)^\top K_{11}(x_1 - \xi_1)/2 - (x_1 - \xi_1)^\top K_{12}(x_2 - \xi_2)\right\}.$$

The linear term involving x_1 has coefficient equal to

$$K_{11}\xi_1 - K_{12}(x_2 - \xi_2) = K_{11}\left\{\xi_1 - K_{11}^{-1}K_{12}(x_2 - \xi_2)\right\}.$$

Using the matrix identities

$$K_{11}^{-1} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} \tag{3}$$

and

$$K_{11}^{-1}K_{12} = -\Sigma_{12}\Sigma_{22}^{-1}, \tag{4}$$

we find

$$f(x_1 \mid x_2) \propto \exp\left\{-(x_1 - \xi_{1|2})^\top K_{11}(x_1 - \xi_{1|2})/2\right\}$$

and the result follows.

From the identities (3) and (4) it follows in particular that then the conditional expectation and concentrations also can be calculated as

$$\xi_{1|2} = \xi_1 - K_{11}^{-1} K_{12}(x_2 - \xi_2) \quad \text{and} \quad K_{1|2} = K_{11}.$$

Note that the *marginal covariance is simply expressed in terms of* Σ whereas the *conditional concentration is simply expressed in terms of* K. Further, X_1 *and* X_2 *are independent if and only if* $K_{12} = 0$, giving $K_{12} = 0$ *if and only if* $\Sigma_{12} = 0$.

Consider $\mathcal{N}_3(0, \Sigma)$ with covariance matrix

$$\Sigma = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}.$$

The concentration matrix is

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

The marginal distribution of (X_2, X_3) has covariance and concentration matrix

$$\Sigma_{23} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}, \quad (\Sigma_{23})^{-1} = \frac{1}{3}\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}.$$

The conditional distribution of (X_1, X_2) given X_3 has concentration and covariance matrix

$$K_{12} = \begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix}, \quad \Sigma_{12|3} = (K_{12})^{-1} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 3 \end{pmatrix}.$$

Similarly, $\mathbf{V}(X_1 \mid X_2, X_3) = 1/k_{11} = 1/3$, etc.

A square matrix A has *trace*

$$\operatorname{tr}(A) = \sum_i a_{ii}.$$

The trace has a number of properties:

1. $\operatorname{tr}(\gamma A + \mu B) = \gamma \operatorname{tr}(A) + \mu \operatorname{tr}(B)$ for γ, μ being scalars;
2. $\operatorname{tr}(A) = \operatorname{tr}(A^\top)$;
3. $\operatorname{tr}(AB) = \operatorname{tr}(BA)$
4. $\operatorname{tr}(A) = \sum_i \lambda_i$ where λ_i are the *eigenvalues* of A.

For symmetric matrices the last statement follows from taking an orthogonal matrix O so that $OAO^\top = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$ and using

$$\mathrm{tr}(OAO^\top) = \mathrm{tr}(AO^\top O) = \mathrm{tr}(A).$$

The trace is thus *orthogonally invariant*, as is the determinant:

$$\det(OAO^\top) = \det(O)\det(A)\det(O^\top) = 1\det(A)1 = \det(A).$$

There is an important trick that we shall use again and again: For $\lambda \in \mathcal{R}^d$

$$\lambda^\top A\lambda = \mathrm{tr}(\lambda^\top A\lambda) = \mathrm{tr}(A\lambda\lambda^\top)$$

since $\lambda^\top A\lambda$ is a scalar.

Consider the case where $\xi = 0$ and a sample $X^1 = x^1, \ldots, X^n = x^n$ from a multivariate Gaussian distribution $\mathcal{N}_d(0, \Sigma)$ with Σ regular. Using (2), we get the likelihood function

$$\begin{aligned} L(K) &= (2\pi)^{-nd/2} (\det K)^{n/2} e^{-\sum_{\nu=1}^n (x^\nu)^\top K x^\nu /2} \\ &\propto (\det K)^{n/2} e^{-\sum_{\nu=1}^n \operatorname{tr}\{K x^\nu (x^\nu)^\top\}/2} \\ &= (\det K)^{n/2} e^{-\operatorname{tr}\{K \sum_{\nu=1}^n x^\nu (x^\nu)^\top\}/2} \\ &= (\det K)^{n/2} e^{-\operatorname{tr}(Kw)/2}. \end{aligned} \tag{5}$$

where

$$W = \sum_{\nu=1}^n X^\nu (X^\nu)^\top$$

is the matrix of *sums of squares and products*.

Writing the trace out

$$\operatorname{tr}(KW) = \sum_i \sum_j k_{ij} W_{ji}$$

emphasizes that it is linear in both K and W and we can recognize this as a linear and canonical exponential family with K as the canonical parameter and $-W/2$ as the canonical sufficient statistic. Thus, the likelihood equation becomes

$$\mathbf{E}(-W/2) = -n\Sigma/2 = -w/2$$

since $\mathbf{E}(W) = n\Sigma$. Solving, we get

$$\hat{K}^{-1} = \hat{\Sigma} = w/n$$

in analogy with the univariate case.

Rewriting the likelihood function as

$$\log L(K) = \frac{n}{2} \log(\det K) - \operatorname{tr}(Kw)/2$$

we can of course also differentiate to find the maximum, leading to

$$\frac{\partial}{\partial k_{ij}} \log(\det K) = w_{ij}/n,$$

which in combination with the previous result yields

$$\frac{\partial}{\partial K} \log(\det K) = K^{-1}.$$

The latter can also be derived directly by writing out the determinant, and it holds for any non-singular square matrix, i.e. one which is not necessarily positive definite.

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

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

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.

Note that the density then factorizes as

$$\log f(x) = \text{constant} - \frac{1}{2}\sum_{\alpha\in V} k_{\alpha\alpha}x_\alpha^2 - \sum_{\{\alpha,\beta\}\in E} k_{\alpha\beta}x_\alpha x_\beta,$$

hence *no interaction terms involve more than pairs.*.

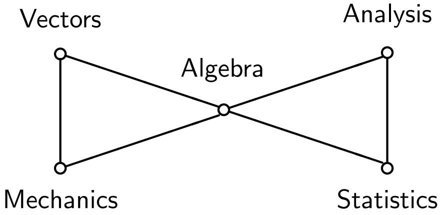
This is different from the discrete case and generally makes things easier.

Mathematics marks

Examination marks of 88 students in 5 different mathematical subjects. The empirical concentrations (on or above diagonal) and partial correlations (below diagonal) are

	Mechanics	Vectors	Algebra	Analysis	Statistics
Mechanics	5.24	−2.44	−2.74	0.01	−0.14
Vectors	0.33	10.43	−4.71	−0.79	−0.17
Algebra	0.23	0.28	26.95	−7.05	−4.70
Analysis	−0.00	0.08	0.43	9.88	−2.02
Statistics	0.02	0.02	0.36	0.25	6.45

Graphical model for mathmarks



This analysis is from Whittaker (1990).

We have An, Stats $\perp\!\!\!\perp$ Mech,Vec | Alg.

Frets' heads

This example is concerned with a study of heredity of head dimensions (Frets 1921). Lengths L_i and breadths B_i of the heads of 25 pairs of first and second sons are measured. Previous analyses by Whittaker (1990) support the graphical model: