

CHAPTER 8

GENERATING MULTIVARIATE NORMALS

§1. The Joint Normal Density

The vector of random variables $\mathbf{Y} = (Y_1, \dots, Y_n)^T$ has a mean-zero n -dimensional multivariate normal distribution if, for some invertible linear transformation $\mathbf{A} = (a_{ij})_{n \times n}$, the vector of random variables $\mathbf{X} = (X_1, \dots, X_n)^T$ defined by $\mathbf{X} = \mathbf{A}^{-1}\mathbf{Y}$ are iid standard (mean 0, variance 1) normals. Then $\mathbf{Y} = \mathbf{A}\mathbf{X}$ and matrix multiplication yields

$$Y_i = \sum_{j=1}^n a_{ij} X_j, \quad 1 \leq i \leq n.$$

We are interested in calculating the joint probability density of \mathbf{Y} . We begin by calculating the joint density of \mathbf{X} . This is much easier as the X_i s are independent Normal $(0, 1)$ s. With $\mathbf{x} = (x_1, \dots, x_n)^T$ we have

$$\begin{aligned} f_{\mathbf{X}}(\mathbf{x}) &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-x_i^2/2} \\ &= \frac{1}{(2\pi)^{n/2}} \exp\left(-\sum_{i=1}^n x_i^2/2\right) = \frac{1}{(2\pi)^{n/2}} e^{-(\mathbf{x}^T \mathbf{x})/2}, \end{aligned} \quad (1)$$

where the matrix multiplication $\mathbf{x}^T \mathbf{x}$ gives the inner product (i.e., dot product) of \mathbf{x} with itself.

Now suppose $I \subset \mathbb{R}^n$ is a tiny n -dimensional cube and let $\mathbf{y} = (y_1, \dots, y_n)^T$ be a point in I . The joint density function $f_{\mathbf{Y}}(\cdot)$ is characterized by the property that

$$P[\mathbf{Y} \in I] \approx f_{\mathbf{Y}}(\mathbf{y}) \cdot \text{Vol}(I),$$

where $\text{Vol}(\cdot)$ denotes n -dimensional volume. Working on the left side of this and letting $\mathbf{x} = \mathbf{A}^{-1}\mathbf{y} \in \mathbf{A}^{-1}I$, we have

$$\begin{aligned} P[\mathbf{Y} \in I] &= P[\mathbf{A}\mathbf{X} \in I] = P[\mathbf{X} \in \mathbf{A}^{-1}I] \\ &\approx f_{\mathbf{X}}(\mathbf{x}) \cdot \text{Vol}(\mathbf{A}^{-1}I) \\ &= \frac{1}{(2\pi)^{n/2}} e^{-(\mathbf{x}^T \mathbf{x})/2} \cdot |\det \mathbf{A}^{-1}| \cdot \text{Vol}(I) \\ &= \frac{1}{(2\pi)^{n/2} |\det \mathbf{A}|} e^{-(\mathbf{x}^T \mathbf{x})/2} \cdot \text{Vol}(I). \end{aligned} \quad (2)$$

See Chapter 2 for a discussion of the determinant function and its relation to volume.

The next step is to restate this result in terms of the covariance matrix $\mathbf{V} = (v_{ij})$ for \mathbf{Y} , which is denoted by $\text{Cov}(\mathbf{Y})$ and defined by $v_{ij} = \text{Cov}(Y_i, Y_j)$. Then we have

$$\begin{aligned} \mathbf{V}_{ij} &= \text{Cov} \left(\sum_{s=1}^n a_{is} X_s, \sum_{t=1}^n a_{jt} X_t \right) \\ &= \sum_s \sum_t a_{is} a_{jt} \text{Cov}(X_s, X_t) \\ &= \sum_s a_{is} a_{js} = \sum_s a_{is} a_{sj}^T = (\mathbf{A}\mathbf{A}^T)_{ij}, \end{aligned}$$

where the third equality holds since $\text{Cov}(X_s, X_t) = 0$ if $t \neq s$ and 1 if $t = s$ — the inner summation (in t) has only one non-zero term. We therefore have $\text{Cov}(\mathbf{Y}) = \mathbf{V} = \mathbf{A}\mathbf{A}^T$. It follows then that

$$\mathbf{x}^T \mathbf{x} = (\mathbf{A}^{-1} \mathbf{y})^T \mathbf{A}^{-1} \mathbf{y} = \mathbf{y}^T [(\mathbf{A}^{-1})^T \mathbf{A}^{-1}] \mathbf{y} = \mathbf{y}^T \mathbf{V}^{-1} \mathbf{y},$$

where we have used that $(\mathbf{A}^{-1})^T \mathbf{A}^{-1} = (\mathbf{A}^T)^{-1} \mathbf{A}^{-1} = (\mathbf{A}\mathbf{A}^T)^{-1}$. Furthermore, since $\det \mathbf{A} = \det \mathbf{A}^T$ we have $\det \mathbf{V} = (\det \mathbf{A})^2$ and hence $|\det \mathbf{A}| = \sqrt{\det \mathbf{V}}$. Substituting this back into (2) gives

$$P[\mathbf{Y} \in I] \approx \frac{1}{(2\pi)^{n/2} \sqrt{\det \mathbf{V}}} e^{-(\mathbf{y}^T \mathbf{V}^{-1} \mathbf{y})/2} \cdot \text{Vol}(I),$$

and, therefore,

$$f_{\mathbf{Y}}(\mathbf{y}) = \frac{1}{(2\pi)^{n/2} \sqrt{\det \mathbf{V}}} e^{-(\mathbf{y}^T \mathbf{V}^{-1} \mathbf{y})/2}. \quad (3)$$

It is of significance that the distribution of \mathbf{Y} depends only on the correlation matrix \mathbf{V} , and not on the particular transformation \mathbf{A} . (See Exercises 2 and 3 below where it is shown that many different \mathbf{A} s produce the same \mathbf{V}). In particular this implies that, for joint normals \mathbf{Y} , if they are uncorrelated then they are independent. To see this, suppose that $\text{Cov}(Y_i, Y_j) = 0$ for $i \neq j$ and let $\text{Var } Y_i = \sigma_i^2$. Then \mathbf{V} is 0 off the diagonal and $V_{ii} = \sigma_i^2$. To simplify calculations, take each $\tilde{Y}_i = Y_i/\sigma_i$, which is a standard normal, and put $\tilde{\mathbf{Y}} = (\tilde{Y}_1, \dots, \tilde{Y}_n)^T$. Clearly the Y_i are independent if and only if the \tilde{Y}_i are independent and $\tilde{\mathbf{V}} = \text{Cov}(\tilde{\mathbf{Y}}) = \mathbf{I}$, the $n \times n$ identity matrix. But by (3)

$$f_{\tilde{\mathbf{Y}}}(\mathbf{y}) = \frac{1}{(2\pi)^{n/2}} e^{-(\mathbf{y}^T \mathbf{y})/2},$$

which factors into the marginals — just reverse the steps in (1).

Exercise 1. We saw above that if $\text{Cov}(\mathbf{X}) = \mathbf{I}$, then $\text{Cov}(\mathbf{AX}) = \mathbf{AA}^T$. Show that, more generally, $\text{Cov}(\mathbf{AX}) = \mathbf{ACov}(\mathbf{X})\mathbf{A}^T$.

Exercise 2. Suppose $\mathbf{X} = (X_1, X_2)^T$ are independent standard normals, $|\rho| < 1$, $\mathbf{A} = \begin{pmatrix} 1 & 0 \\ \rho & \pm\sqrt{1-\rho^2} \end{pmatrix}$, and $\mathbf{Y} = \mathbf{AX}$. Show that $\text{Cov}(\mathbf{Y}) = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$.

Exercise 3. With \mathbf{X} , ρ , and \mathbf{Y} as in Exercise 2, fix any a and b with $0 < a < 1$ and $a^2 + b^2 = 1$. Now put $c = a\rho \pm b\sqrt{1-\rho^2}$, $d = b\rho \mp a\sqrt{1-\rho^2}$, and $\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$. Show that $\text{Cov}(\mathbf{Y}) = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$.

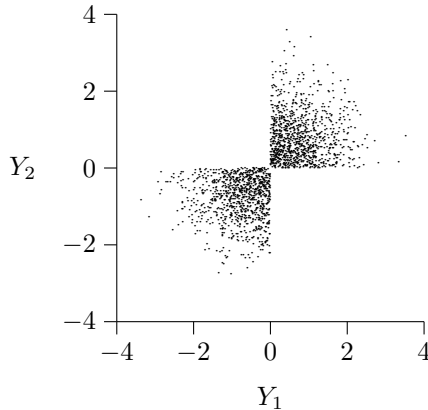
§2. Not all Pairs of Normals are Joint Normals

Consider the following construction. Let X_1 and X_2 be independent standard normals. Now put $Y_1 = X_1$ and let

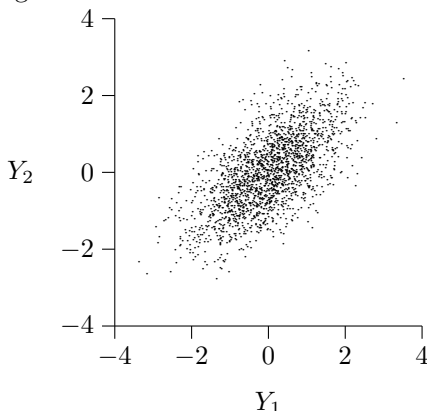
$$Y_2 = \begin{cases} |X_2| & \text{if } X_1 \geq 0 \\ -|X_2| & \text{if } X_1 < 0 \end{cases}$$

Observe that if Y_1 is positive so is Y_2 , and if Y_1 is negative so is Y_2 . Thus $f_{\mathbf{Y}}(\cdot)$ is positive only in the first and third quadrants. The scatter plot below (Figure 1) shows 2000 realizations of this construction. It turns out that Y_1 and Y_2 are both standard normals and their correlation is $2/\pi$. However, they are not *joint* normals, as can be seen by the fact that the density function for joint normals as given in (3) is positive *everywhere*.

Figure 1. Non-joint standard normals with $\rho = 2/\pi \approx 0.637$.



To construct *joint* normals with this correlation, we put $Y_1 = X_1$ and $Y_2 = (2/\pi)X_1 + \sqrt{1-(2/\pi)^2}X_2$ (the recipe given in Exercise 2). Figure 2 below shows a scatter plot corresponding to this construction.

Figure 2. Joint standard normals with $\rho = 2/\pi$.

Exercise 4. Show that the construction above for Figure 1 (the non-joint case) produces standard normals Y_1 and Y_2 with correlation $2/\pi$.

§3. Generating Dependent Joint Normals

If the pair of joint normals (X, Y) have mean 0 and variance 1 (they are standard normals), then their joint density function is specified by their correlation ρ , where $|\rho| < 1$:

$$f_\rho(x, y) = \frac{1}{2\pi\sqrt{1-\rho^2}} \exp \left[-\frac{x^2 - 2\rho xy + y^2}{2(1-\rho^2)} \right]. \quad (4)$$

To see this we note that their covariance matrix is $\mathbf{V} = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$, so

$$\det \mathbf{V} = 1 - \rho^2, \quad \mathbf{V}^{-1} = \frac{1}{1-\rho^2} \begin{pmatrix} 1 & -\rho \\ -\rho & 1 \end{pmatrix}, \text{ and}$$

$$\begin{pmatrix} x & y \end{pmatrix} \mathbf{V}^{-1} \begin{pmatrix} x \\ y \end{pmatrix} = (x^2 - 2\rho xy + y^2)/(1 - \rho^2);$$

refer back to equation (3). To better understand (4), complete the square in y :

$$x^2 - 2\rho xy + y^2 = (y - \rho x)^2 + x^2(1 - \rho^2).$$

Setting this into (4) yields, after a little algebra, that

$$f_\rho(x, y) = \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{x^2}{2} \right] \cdot \frac{1}{\sqrt{2\pi(1-\rho^2)}} \exp \left[-\frac{(y - \rho x)^2}{2(1-\rho^2)} \right]. \quad (5)$$

We recognize the first factor above as the density function of a standard normal. In fact, we have factored the joint distribution into the marginal distribution

of X evaluated at x times the conditional distribution of Y , given $X = x$, evaluated at y , that is, $f_X(x) \cdot f_{(Y|X=x)}(y)$. From this factorization, we see that, conditioned on $X = x$, $Y \sim \text{Normal}(\rho x, 1 - \rho^2)$. If we had completed the square for x instead of y , we would have found that Y is a standard normal and, conditioned on $Y = y$, $X \sim \text{Normal}(\rho y, 1 - \rho^2)$. This follows also from the symmetry of (4) in x and y .

We know how to generate two *independent* standard normals, X and Y . Suppose we put

$$Y_\rho = \rho X + \sqrt{1 - \rho^2} Y. \quad (6)$$

Since X and Y are independent with mean 0 and variance 1, $EY_\rho = \rho EX + \sqrt{1 - \rho^2} EY = 0$ and $\text{Var } Y_\rho = \rho^2 \text{Var } X + (1 - \rho^2) \text{Var } Y = 1$, both as desired. Furthermore, conditioned on $X = x$, we see that

$$\begin{aligned} Y_\rho &= \rho x + \sqrt{1 - \rho^2} Y \sim \rho x + \sqrt{1 - \rho^2} \text{Normal}(0, 1) \\ &\sim \text{Normal}(\rho x, 1 - \rho^2). \end{aligned}$$

Here we have used that the conditional distribution of Y does not depend on the particular realization of X since Y is independent of X . Since $X \sim \text{Normal}(0, 1)$ we see that the pair (X, Y_ρ) has the joint density function given in (5) (or (4)). Figure 3 below shows a scatter plot of 1000 realizations of the pair (X, Y_ρ) produced via (6) for various values of the correlation parameter ρ .

More Than Two Dependent Normals. In this section, we generalize this to more than two joint normals. Suppose we wish to generate n correlated normals $(Y_1, \dots, Y_n)^T$. Let $v_{ij} = \text{Cov}(Y_i, Y_j)$ denote the desired covariance between Y_i and Y_j , so $\mathbf{V} = (v_{ij})_{n \times n}$ is the desired correlation matrix corresponding to $(Y_1, \dots, Y_n)^T$. Not every square matrix may serve as a legitimate covariance matrix. Our first order of business is to characterize those that can:

Theorem 1. Let $\mathbf{V} = (v_{ij})$ be an $n \times n$ matrix. Then there are joint random variables $(Y_1, \dots, Y_n)^T$ whose covariance matrix is \mathbf{V} if and only if \mathbf{V} is symmetric and positive semi-definite.

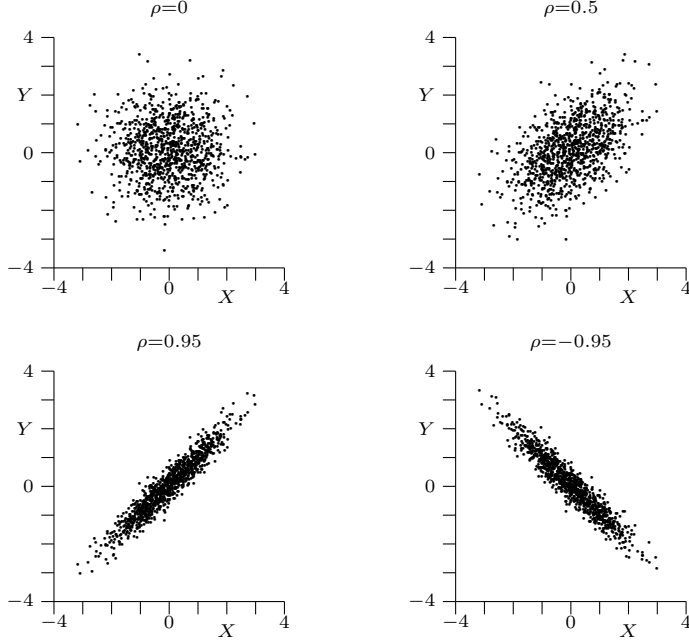
Proof. Suppose $(Y_1, \dots, Y_n)^T$ have covariance matrix \mathbf{V} , so $\text{Cov}(Y_i, Y_j) = v_{ij}$. Then \mathbf{V} is symmetric as $\text{Cov}(Y_i, Y_j) = \text{Cov}(Y_j, Y_i)$. Let $\mathbf{x} = (x_1, \dots, x_n)^T$ be any column vector and put $Z = x_1 Y_1 + \dots + x_n Y_n$. Then

$$\begin{aligned} 0 \leq \text{Var } Z &= \sum_{i=1}^n \sum_{j=1}^n \text{Cov}(x_i Y_i, x_j Y_j) \\ &= \sum_{i=1}^n \sum_{j=1}^n x_i x_j v_{ij} = \mathbf{x}^T \mathbf{V} \mathbf{x}. \end{aligned} \quad (7)$$

Hence \mathbf{V} is positive semi-definite. This proves the “only if” part.

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Figure 3. Scatter plots for joint standard normals with various correlations.



Now suppose \mathbf{V} is symmetric and positive semi-definite. Then \mathbf{V} factors as $\mathbf{V} = \mathbf{L}\mathbf{L}^T$, where $\mathbf{L} = (\ell_{ij})_{n \times n}$ is a lower triangular matrix with non-negative entries on the diagonal (each $\ell_{ii} \geq 0$). (See Chapter 4 for the Cholesky decomposition.) Now suppose $\mathbf{X} = (X_1, \dots, X_n)^T$ are independent standard normals and put

$$\begin{aligned}
 Y_1 &= \ell_{11}X_1 \\
 Y_2 &= \ell_{21}X_1 + \ell_{22}X_2 \\
 Y_3 &= \ell_{31}X_1 + \ell_{32}X_2 + \ell_{33}X_3 \\
 &\dots \\
 Y_n &= \ell_{n1}X_1 + \ell_{n2}X_2 + \ell_{n3}X_3 + \dots + \ell_{nn}X_n,
 \end{aligned} \tag{8}$$

so $\mathbf{Y} = \mathbf{L}\mathbf{X}$ where $\mathbf{Y} = (Y_1, \dots, Y_n)^T$. It follows immediately from §1 that $\text{Cov}(\mathbf{Y}) = \mathbf{L}\mathbf{L}^T = \mathbf{V}$. \square

Remark. If \mathbf{V} is only PSD, then at least one of the diagonal entries of \mathbf{L} is 0, hence $\det \mathbf{L} = \prod_{i=1}^n \ell_{ii} = 0$ and \mathbf{L} is not invertible. In this case \mathbf{Y} does not follow an n -dimensional joint normal distribution. See §4 for more on this.

We return to the problem of generating n normals $\mathbf{Y} = (Y_1, \dots, Y_n)^T$ with covariance matrix $\mathbf{V} = (v_{ij})_{n \times n}$. Assume that \mathbf{V} is PD — we'll handle the PSD case in the the next section. Presently we illustrate how to compute the ℓ_{ij} s

of (8) that yield the covariance matrix \mathbf{V} . We note that Theorem 1 guarantees their existence and, since \mathbf{V} is PD, we may take each $\ell_{ii} > 0$ (see Chapter 4).

First we illustrate with $n = 3$. Since we wish $\ell_{11}^2 = \text{Var}(Y_1) = v_{11}$, we take $\ell_{11} = \sqrt{v_{11}}$. Moving to Y_2 , we compute $\text{Cov}(Y_2, Y_1) = \ell_{11}\ell_{21}$. (We will repeatedly use the bi-linearity of covariance and the independence of the X_i s.) Since we seek $\text{Cov}(Y_2, Y_1) = v_{21}$, take $\ell_{21} = v_{21}/\ell_{11}$. Now $\text{Var}(Y_2) = \ell_{21}^2 + \ell_{22}^2$ and since we wish $\text{Var}(Y_2) = v_{22}$ we take $\ell_{22} = \sqrt{v_{22} - \ell_{21}^2}$. So far, in terms of the v_{ij} s, we have

$$\begin{aligned} Y_1 &= \sqrt{v_{11}}X_1 \\ Y_2 &= (v_{21}/\sqrt{v_{11}})X_1 + \sqrt{v_{22} - (v_{21}^2/v_{11})}X_2, \end{aligned}$$

which generalizes (6) where $v_{11} = v_{22} = 1$ and $v_{21} = \rho$. As for Y_3 , begin with $\text{Cov}(Y_3, Y_1) = \ell_{11}\ell_{31}$, which we wish to be v_{31} — so we take $\ell_{31} = v_{31}/\ell_{11}$. Moving across, $\text{Cov}(Y_3, Y_2) = \ell_{21}\ell_{31} + \ell_{22}\ell_{32}$, which we wish to be v_{32} . Now we've already computed ℓ_{21} , ℓ_{31} , and ℓ_{22} , so take $\ell_{32} = (v_{32} - \ell_{21}\ell_{31})/\ell_{22}$. Finally, since $\text{Var} Y_3 = \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2$ (which we wish to be v_{33}), take $\ell_{33} = \sqrt{v_{33} - (\ell_{31}^2 + \ell_{32}^2)}$. (Note that we've already computed ℓ_{31} and ℓ_{32}). This completes the exercise for $n = 3$.

This can be extended to arbitrary n as follows. Suppose we've computed the ℓ_{ij} s up to line $k - 1$. We show how to compute line k , i.e., how to compute the ℓ_{kj} for $1 \leq j \leq k$. Start with $\text{Cov}(Y_k, Y_1) = \ell_{11}\ell_{k1}$, which we wish to be v_{k1} . We take $\ell_{k1} = v_{k1}/\ell_{11}$. Now, working across row k , assume $\ell_{k1}, \ell_{k2}, \dots, \ell_{k,j-1}$ have been computed, where $j < k$. We may then compute ℓ_{kj} by solving

$$v_{kj} = \text{Cov}(Y_k, Y_j) = \ell_{j1}\ell_{k1} + \ell_{j2}\ell_{k2} + \dots + \ell_{j,j-1}\ell_{k,j-1} + \ell_{jj}\ell_{kj}. \quad (9)$$

The only ℓ_{**} that is unknown at this step is ℓ_{kj} and we may solve (9) for ℓ_{kj} because we know that $\ell_{jj} > 0$, as \mathbf{V} is PD. Finally, when $\ell_{k1}, \ell_{k2}, \dots, \ell_{k,k-1}$ have been computed, we may obtain ℓ_{kk} from

$$v_{kk} = \text{Var} Y_k = \ell_{k1}^2 + \ell_{k2}^2 + \dots + \ell_{k,k-1}^2 + \ell_{kk}^2,$$

yielding

$$\ell_{kk} = \sqrt{v_{kk} - (\ell_{k1}^2 + \ell_{k2}^2 + \dots + \ell_{k,k-1}^2)}. \quad (10)$$

A key point is that if the wished-for correlation matrix \mathbf{V} is PD, then the number under the radical in (10) will be strictly positive for each k . This is because Theorem 1 guarantees the existence of the requisite ℓ_{ij} s, and the computations of (9) and (10) are forced (there is no choice) line by line beginning with line 1 where we must have $\ell_{11} = \sqrt{v_{11}}$.

Remark. Actually, there appears to be a choice of *sign* to be made in (10). However Theorem 1 guarantees the existence of an $\mathbf{L} = (\ell_{ij})$ with strictly positive diagonal entries. To produce this \mathbf{L} , we *must* take the positive solution in (10).

Exercise 5. Suppose you wish to generate 5 standard normals Y_1, \dots, Y_5 so that $\text{Cov}(Y_i, Y_j) = 0.2$ if $i \neq j$ (of course $\text{Cov}(Y_i, Y_i) = 1$). Compute to five decimal places the ℓ_{ij} s that accomplish this. When applying (10), take the positive square root. Verify your computations by executing the program `CholeskyExample1.cpp`.

Exercise 6. Do the same thing, but this time take the *negative* square root when computing ℓ_{22} . What do you observe?

Exercise 7. Starting with six independent standard normals X_0, X_1, \dots, X_6 , there is an easier way to generate five Y s with the covariance matrix of Exercise 5. Can you find it? Hint: Display (6).

§4. When \mathbf{V} is Only PSD

With $\mathbf{V} = \mathbf{L}\mathbf{L}^T$, so $\det \mathbf{V} = (\det \mathbf{L})^2$, we have

$$\begin{aligned} \mathbf{V} \text{ is only PSD} &\iff \text{some } \ell_{ii} = 0 \\ &\iff \det \mathbf{L} = 0 \\ &\iff \det \mathbf{V} = 0 \\ &\iff \mathbf{V} \text{ is not invertible.} \end{aligned}$$

In this situation, for some non-zero vector $\mathbf{x} = (x_1, \dots, x_n)^T$ we have $\mathbf{x}^T \mathbf{V} \mathbf{x} = 0$ and the random variable $Z = x_1 Y_1 + \dots + x_n Y_n$ has $\text{Var } Z = 0$ (see (7)). It follows that $Z = c$ for some constant c . Since our random variables are mean zero, we have $c = 0$. Since \mathbf{x} is non-zero, at least one of the x_i s, say x_n , is not zero. This means that

$$Y_n = \left(\frac{-x_1}{x_n} \right) Y_1 + \dots + \left(\frac{-x_{n-1}}{x_n} \right) Y_{n-1}, \quad (11)$$

i.e., at least one of the Y_i s is a linear combination of the others.

Re-order the Y_i s, if necessary so that Y_1, \dots, Y_k are linearly independent (none are linear functions of the others) but each of Y_{k+1}, \dots, Y_n may be written as a linear function of Y_1, \dots, Y_k as in (11). Let $\tilde{\mathbf{V}}_{k \times k}$ denote the covariance matrix for $(Y_1, \dots, Y_k)^T$. Then $\tilde{\mathbf{V}}$ is PD and the random variables Y_{k+1}, \dots, Y_n can be expressed as linear functions of Y_1, \dots, Y_k .

Exercise 8. Analyze the case $\mathbf{V} = \begin{pmatrix} 1.0 & 1.4 & 0.2 \\ 1.4 & 5.8 & 2.2 \\ 0.2 & 2.2 & 1.0 \end{pmatrix}$ using (9) and (10).

Calculate to five decimal places. Verify your computations by executing the program `CholeskyExample2.cpp`. (Observe that \mathbf{V} is not of full rank, as $\text{row } 1 = \text{row } 2 - 2 \times \text{row } 3$.)

Accompanying Code

`CholeskyExample1.cpp` and `CholeskyExample2.cpp` illustrate Cholesky decomposition for the covariance matrices of Exercises 5 and 8, respectively. The matrix product \mathbf{LL}^T is computed to verify the decomposition.