APPENDIX E

MULTIVARIATE GAUSSIAN INTEGRALS

Starting from the formula

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

it follows that

$$\int \ldots \int_{-\infty}^{\infty} dx_1 \ldots dx_n \exp \left\{ -\frac{1}{2} \sum_{i=1}^{n} a_i x_i^2 \right\} = \frac{(2\pi)^{n/2}}{\sqrt{a_1 a_2 \ldots a_n}} , \quad a_i > 0 . \quad (E-2)$$

Now carry out a real nonsingular linear transformation:

$$x_i = \sum_{j=1}^{n} B_{ij} q_j , \quad 1 \leq i \leq n , \quad (E-3)$$

where \( \det(B) \neq 0 \). Then, going into matrix notation,

$$\sum a_i x_i^2 = q^T B A B q = q^T M q \quad (E-4)$$

where

$$A_{ij} \equiv a_i \delta_{ij} \quad (E-5)$$

is a positive definite diagonal matrix. The volume element transforms according to the Jacobian rule

$$dx_1 \ldots dx_n = | \det(B) | dq_1 \ldots dq_n \quad (E-6)$$

and

$$\det(M) = \det(B^T A B) = | \det(B) |^2 \det(A) . \quad (E-7)$$

The matrix \( M \) is by definition real, symmetric, and positive definite; and by proper choice of \( A, B \) any such matrix may be generated in this way. The integral (E-2) may then be written as

$$\int \ldots \int \exp \left\{ -\frac{1}{2} q^T M q \right\} | \det(B) | dq_1 \ldots dq_n \quad (E-8)$$

and so the general multivariate Gaussian integral is

$$I = \int \ldots \int \exp\left[-\frac{1}{2} q^T M q\right] dq_1 \ldots dq_n = \frac{(2\pi)^{n/2}}{\sqrt{\det(M)}} . \quad (E-9)$$

**Partial Gaussian Integrals.** Suppose we don’t want to integrate over all the \( \{q_1 \ldots q_n\} \), but only the last \( r = n - m \) of them;

$$I_m = \int \ldots \int \exp\left[-\frac{1}{2} q^T M q\right] dq_{m+1} \ldots dq_n \quad (E-10)$$
to do this, break \( M \) down into submatrices

\[
M = \begin{pmatrix} U_0 & V \\ V^T & W_0 \end{pmatrix}
\]

and likewise separate the vector \( q \) in the same way:

\[
q = \begin{pmatrix} u \\ w \end{pmatrix}
\]

by writing \( \{ q_1 = u_1, \ldots, q_m = u_m \} \) and \( \{ q_{m+1} = w_1, \ldots, q_n = w_r \} \). Then

\[
Mq = \begin{pmatrix} U_0 & V \\ V^T & W_0 \end{pmatrix} \begin{pmatrix} u \\ w \end{pmatrix}
\]

and

\[
q^T Mq = u^T U_0 u + u^T V w + w^T V^T u + w^T W_0 w
\]

so that \( I_m \) becomes

\[
I_m = \exp \left( -\frac{1}{2} u^T U_0 u \right) \int \ldots \int \exp \left\{ -\frac{1}{2} \left[ w^T W_0 w + u^T V w + w^T V^T u \right] \right\} dw_1 \ldots dw_r
\]

To prepare to integrate out \( w \), first complete the square on \( w \) by writing the exponent as

\[
\left[ \begin{array}{c} w - \hat{w} \\ \hat{w} \end{array} \right] = (w - \hat{w})^T W_0 (w - \hat{w}) + C
\]

and equate terms in (E-14) and (E-16) to find \( \hat{w} \) and \( C \):

\[
w^T W_0 w + u^T V w + w^T V^T u = w^T W_0 w - \hat{w}^T W_0 w - \hat{w}^T W_0 \hat{w} + \hat{w}^T W_0 \hat{w} + C
\]

This requires (since it must be an identity in \( w \)):

\[
u^T V = -\hat{w}^T W_0
\]

\[
V^T u = -W_0 \hat{w}
\]

or,

\[
\hat{w}^T W_0 w + C = 0
\]

\[
\hat{w} = -W_0^{-1} V^T u
\]

\[
C = -(u^T V W_0^{-1}) W_0 (W_0^{-1} V^T u) = u^T V W_0^{-1} V^T u
\]

Then \( I_m \) becomes

\[
I_m = e^{-\frac{1}{2} (u^T U_0 u + C)} \int \ldots \int \exp \left\{ -\frac{1}{2} (w - \hat{w})^T W_0 (w - \hat{w}) \right\} dw_1 \ldots dw_r.
\]

But by (E-9) this integral is

\[
\frac{(2\pi)^{r/2}}{\sqrt{\det(W_0)}}
\]

and from (E-18)

\[
u^T U_0 u + C = u^T [U_0 - VW_0^{-1} V^T] u.
\]

The general partial Gaussian integral is therefore
\[ I_m = \int \cdots \int \exp\left[-\frac{1}{2} q^T M q\right] dq_{m+1} \cdots dq_n = \frac{(2\pi)^{m/2}}{\sqrt{\det(W_0)}} \exp \left\{ -\frac{1}{2} u^T U u \right\} \]  

(E-26)

where

\[ U \equiv U_0 - VW_0^{-1} V^T \]  

(E-27)

is a “renormalized” version of the first \((m \times m)\) block of the original matrix \(M\).

This result has a simple intuitive meaning in application to probability theory. The original \((n \times 1)\) vector \(q\) is composed of an \((m \times 1)\) vector \(u\) of “interesting” quantities that we wish to estimate, and an \((r \times 1)\) vector \(w\) of “uninteresting” quantities or “nuisance parameters” that we want to eliminate. Then \(U_0\) represents the inverse covariance matrix in the subspace of the interesting quantities, \(W_0\) is the corresponding matrix in the “uninteresting” subspace, and \(V\) represents an “interaction”, or correlation, between them.

It is clear from (E-27) that if \(V = 0\), then \(U = U_0\), and the pdf’s for \(u\) and \(w\) are independent. Our estimates of \(u\) are then the same whether or not we integrate \(w\) out of the problem. But if \(V \neq 0\), then the renormalized matrix \(U\) contains effects of the nuisance parameters. Two components, \(w_1\) and \(w_2\), that were uncorrelated in the original \(M^{-1}\) may become correlated in \(U^{-1}\) due to their common interactions (correlations) with the nuisance parameters \(w\).

**Inversion of a Block Form matrix.** The matrix \(U\) has another simple meaning, which we see when we try to invert the full matrix \(M\). Given an \((n \times n)\) matrix in block form

\[ M = \begin{pmatrix} U_0 & V \\ X & W_0 \end{pmatrix} \]  

(E-28)

where \(U_0\) is an \(m \times m\) submatrix, and \(W_0\) is \((r \times r)\) with \(m + r = n\), try to write \(M^{-1}\) in the same block form:

\[ M^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \]  

(E-29)

Writing out the equation \(MM^{-1} = 1\) in full, we have four relations of the form \(U_0 A + VC = 1, U_0 B + V D = 0\), etc. If \(U_0\) and \(W_0\) are nonsingular, there is a unique solution for \(A, B, C, D\) with the result

\[ M^{-1} = \begin{pmatrix} U_0^{-1} & -U_0^{-1} V W_0^{-1} \\ -W_0^{-1} X U_0^{-1} & W_0^{-1} \end{pmatrix} \]  

(E-30)

where

\[ U \equiv U_0 - VW_0^{-1} X \]  

(E-31)

\[ W \equiv W_0 - XU_0^{-1} V \]  

(E-32)

are “renormalized” forms of the diagonal blocks. Conversely, (E-30) can be verified by direct substitution into \(MM^{-1} = 1\) or \(M^{-1}M = 1\). If \(M\) is symmetric as it was above, then \(X = V^T\).

Another useful and nonobvious relation is found by integrating \(u\) out of (E-26). On the one hand we have from (E-9),

\[ \int \cdots \int \exp \left\{ -\frac{1}{2} u^T U u \right\} du_1 \cdots du_m = \frac{(2\pi)^{m/2}}{\sqrt{\det(U)}} \]  

(E-33)

but on the other hand, if we integrate \(\{u_1, \cdots, u_m\}\) out of (E-26), the final result must be the same as if we had integrated all the \(\{q_1, \cdots, q_n\}\) out of (E-9) directly; so (E-9), (E-26), (E-33) yield
\[ \det(M) = \det(U) \det(W_0) \quad (E-34) \]

Therefore we can eliminate \( W_0 \) and write the general partial Gaussian integral as

\[
\int \cdots \int \exp\left[-\frac{1}{2} q^T M q \right] dq_{m+1} \cdots dq_n = \left[ \frac{(2\pi)^{n/2}}{\det(M)} \right] \left[ \frac{\det(U)}{(2\pi)^{m/2}} \right] \exp \left\{ -\frac{1}{2} u^T U u \right\} \quad (E-35)
\]