APPENDIX E

MULTIVARIATE GAUSSIAN INTEGRALS

Starting from the formula

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} \tag{E–1}$$

it follows that

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

Now carry out a real nonsingular linear transformation:

$$x_i = \sum_{j=1}^{n} B_{ij}\, q_j , \qquad 1 \le i \le n , \tag{E–3}$$

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

$$\sum a_i\, x_i^2 = q^T B^T A B q = q^T M q \tag{E–4}$$

where

$$A_{ij} \equiv a_i\, \delta_{ij} \tag{E–5}$$

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

$$dx_1 \ldots dx_n = |\det(B)|\, dq_1 \ldots dq_n \tag{E–6}$$

and

$$\det(M) = \det(B^T A B) = [\det(B)]^2 \det(A). \tag{E–7}$$

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

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

and so the general multivariate Gaussian integral is

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

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;

$$I_m \equiv \int \ldots \int \exp\left\{-\frac{1}{2}\, q^T M q\right\} dq_{m+1} \ldots dq_n \tag{E–10}$$

to do this, break M down into submatrices

$$M = \begin{pmatrix} U_0 & V \\ V^T & W_0 \end{pmatrix} \tag{E–11}$$

and likewise separate the vector q in the same way:

$$q = \begin{pmatrix} u \\ w \end{pmatrix} . \tag{E–12}$$

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

$$Mq = \begin{pmatrix} U_0 & V \\ V^T & W_0 \end{pmatrix} \begin{pmatrix} u \\ w \end{pmatrix} \tag{E–13}$$

and

$$q^T M q = u^T U_0 u + u^T V w + w^T V^T u + w^T W_0 w \tag{E–14}$$

so that I_m becomes

$$I_m = \exp\left(-\frac{1}{2}\, u^T U_0 u\right) \int \ldots \int \exp\left\{-\frac{1}{2}\,[w^T W_0 w + u^T V w + w^T V^T u]\right\} dw_1 \ldots dw_r \tag{E–15}$$

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

$$[\quad] = (w - \hat{w})^T W_0 (w - \hat{w}) + C \tag{E–16}$$

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

$$w^T W w + u^T V w + w^T V^T u = w^T W_0 w - \hat{w}^T W_0 w - w^T W_0 \hat{w} + \hat{w}^T W_0 \hat{w} + C \tag{E–17}$$

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

$$u^T V = -\hat{w}^T W_0 \tag{E–18}$$

$$V^T u = -W_0 \hat{w} \tag{E–19}$$

$$\hat{w}^T W_0 w + C = 0 \tag{E–20}$$

or,

$$\hat{w} = -W_0^{-1} V^T u \tag{E–21}$$

$$C = -(u^T V W_0^{-1})\, W_0\, (W_0^{-1} V^T u) = u^T V\, W_0^{-1}\, V^T u \tag{E–22}$$

Then I_m becomes

$$I_m = e^{-\frac{1}{2}(u^T U_0 u + C)} \int \ldots \int \exp\left\{-\frac{1}{2}\,(w - \hat{w})^T W_0 (w - \hat{w})\right\} dw_1 \ldots dw_r\,. \tag{E–23}$$

But by (E–9) this integral is

$$\frac{(2\pi)^{r/2}}{\sqrt{\det(W_0)}} \tag{E–24}$$

and from (E–18)

$$u^T U_0 u + C = u^T [U_0 - V W_0^{-1} V^T] u\,. \tag{E–25}$$

The general partial Gaussian integral is therefore

$$I_m = \int \dots \int \exp[-\frac{1}{2}\, q^T M q]\, dq_{m+1} \dots dq_n = \frac{(2\pi)^{\frac{n-m}{2}}}{\sqrt{\det(W_0)}} \exp\left\{-\frac{1}{2}\, u^T U u\right\} \tag{E–26}$$

where

$$U \equiv U_0 - V W_0^{-1} V^T \tag{E–27}$$

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, u_1 and u_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

$$M = \begin{pmatrix} U_0 & V \\ X & W_0 \end{pmatrix} \tag{E–28}$$

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:

$$M^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{E–29}$$

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

$$M^{-1} = \begin{pmatrix} U^{-1} & -U_0^{-1} V W^{-1} \\ -W_0^{-1} X U^{-1} & W^{-1} \end{pmatrix} \tag{E–30}$$

where

$$U \equiv U_0 - V W_0^{-1} X \tag{E–31}$$

$$W \equiv W_0 - X U_0^{-1} V \tag{E–32}$$

are "renormalized" forms of the diagonal blocks. Conversely, (E–30) can be verified by direct substitution into $M M^{-1} = 1$ 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),

$$\int \cdots \int \exp\left\{-\frac{1}{2}\, u^T\, U\, u\right\} du_1 \cdots du_m = \frac{(2\pi)^{m/2}}{\sqrt{\det(U)}} \tag{(E–33)}$$

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

$$\det(M) = \det(U)\,\det(W_0) \tag{E–34}$$

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

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