

APPENDIX E

MULTIVARIATE GAUSSIAN INTEGRALS

Starting from the formula

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} \quad (\text{E-1})$$

it follows that

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

Now carry out a real nonsingular linear transformation:

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

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

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

where

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

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

$$dx_1 \dots dx_n = |\det(B)| dq_1 \dots dq_n \quad (\text{E-6})$$

and

$$\det(M) = \det(B^T A B) = [\det(B)]^2 \det(A). \quad (\text{E-7})$$

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

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

and so the general multivariate Gaussian integral is

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

Partial Gaussian Integrals. Suppose we don't want to integrate over all the $\{q_1 \dots q_n\}$, but only the last $r = n - m$ of them;

$$I_m \equiv \int \dots \int \exp \left\{ -\frac{1}{2} q^T M q \right\} dq_{m+1} \dots dq_n \quad (\text{E-10})$$

to do this, break M down into submatrices

$$M = \begin{pmatrix} U_0 & V \\ V^T & W_0 \end{pmatrix} \quad (\text{E-11})$$

and likewise separate the vector q in the same way:

$$q = \begin{pmatrix} u \\ w \end{pmatrix}. \quad (\text{E-12})$$

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

$$Mq = \begin{pmatrix} U_0 & V \\ V^T & W_0 \end{pmatrix} \begin{pmatrix} u \\ w \end{pmatrix} \quad (\text{E-13})$$

and

$$q^T M q = u^T U_0 u + u^T V w + w^T V^T u + w^T W_0 w \quad (\text{E-14})$$

so that I_m becomes

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

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

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

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

$$w^T W_0 w + u^T V w + w^T V^T u = w^T W_0 w - \hat{w}^T W_0 w - w^T W_0 \hat{w} + \hat{w}^T W_0 \hat{w} + C \quad (\text{E-17})$$

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

$$u^T V = -\hat{w}^T W_0 \quad (\text{E-18})$$

$$V^T u = -W_0 \hat{w} \quad (\text{E-19})$$

$$\hat{w}^T W_0 w + C = 0 \quad (\text{E-20})$$

or,

$$\hat{w} = -W_0^{-1} V^T u \quad (\text{E-21})$$

$$C = -(u^T V W_0^{-1}) W_0 (W_0^{-1} V^T u) = u^T V W_0^{-1} V^T u \quad (\text{E-22})$$

Then I_m becomes

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

But by (E-9) this integral is

$$\frac{(2\pi)^{r/2}}{\sqrt{\det(W_0)}} \quad (\text{E-24})$$

and from (E-18)

$$u^T U_0 u + C = u^T [U_0 - V W_0^{-1} V^T] u. \quad (\text{E-25})$$

The general partial Gaussian integral is therefore

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

where

$$U \equiv U_0 - V W_0^{-1} V^T \quad (\text{E-27})$$

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

$$M = \begin{pmatrix} U_0 & V \\ X & W_0 \end{pmatrix} \quad (\text{E-28})$$

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:

$$M^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad (\text{E-29})$$

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

$$M^{-1} = \begin{pmatrix} U^{-1} & -U_0^{-1} V W^{-1} \\ -W_0^{-1} X U^{-1} & W^{-1} \end{pmatrix} \quad (\text{E-30})$$

where

$$U \equiv U_0 - V W_0^{-1} X \quad (\text{E-31})$$

$$W \equiv W_0 - X U_0^{-1} V \quad (\text{E-32})$$

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),

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

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

$$\det(M) = \det(U) \det(W_0) \quad (\text{E-34})$$

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

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