Multivariate Biostatistics
Biostat 251

Prereq: Satisfactory performance in 250a 250b

Initial topics

1. Course Info
2. Background Review
   - Matrix Algebra
   - Differentiation
   - Integration
   - Inference
     - ML
     - Bayes
3. Repeated Measures intro
   - Pictures
4. What is Multivariate Data?

~~Reading: Chapters 1–4 in Rencher~~

5. Multivariate Normal
6. Distributions

7. Repeated Measures

Review

Matrix Algebra

Let A be a matrix that is $p \times p$, symmetric, with elements a_{ij} $i=1 \ldots p$ $j=1 \ldots p$. We write

$$A = (a_{ij})$$

Let λ_i $i=1 \ldots p$ be the eigenvalues of A, that is, for some p-vector t_i we have

$$A t_i = \lambda_i t_i \, .$$

Then t_i is an eigenvector of A. Define the trace of A

$$tr(A) = \sum_{i=1}^{p} a_{ii}$$

and we have

$$tr(A) = \sum \lambda_i \, .$$

Also

$$tr(AB) = tr(BA)$$

assuming the multiplications AB and BA make sense.
The determinant of A is written

$$\det A = |A| = \prod_{i=1}^{p} \lambda_i$$

Matrix Decompositions

For a general matrix $X_{n\times p}$ the SVD, Singular Value Decomposition is

$$\underset{n\times p}{X} = LDU$$

where $L_{n\times n}$ $D_{n\times p}$ $U_{p\times p}$ and U is orthogonal, that is,

$$L'L = LL' = I = I_n,$$

the identity matrix of order n. The matrix U is also orthogonal. The matrix $D = (d_{ij})$ is all 0 (zero) except for elements d_{ii}, where

$$d_{11} \geq d_{22} \geq \cdots \geq d_{pp} \geq 0$$

The d_{ii} are called the singular values. The columns of U are eigenvectors of $X^T X$ and the rows of L are eigenvectors of XX^T.

If X is symmetric, call it $A_{p\times p}$ we have the spectral decomposition

$$A = T \Lambda T',$$

$$\Lambda = \mathrm{diag}(\lambda_i) \quad \lambda_1 \geq \lambda_2 \cdots \geq \lambda_p$$

and

$$TT' = T'T = I_p$$

Alternatively

$$A = \sum_{i=1}^{p} \lambda_i t_i t_i'$$

where t_i is the i^{th} column of T.

The <u>Cholesky</u> decomposition is

$$A = U'U$$

where U is an unique upper triangular matrix.

The <u>QR</u> <u>decomposition</u> ~~of~~ a matrix $X_{n \times p}$ is

$$X = QR$$

where $Q_{n \times p}$ and $R_{p \times p}$ satisfy

$$Q'Q = I_p, \quad QQ' \text{ is a projection}$$
$$R \text{ is upper triangular.}$$

The process of producing the Q matrix is often referred to as the Gram-Schmidt process.

The <u>rank</u> of a matrix $X_{n \times p}$ is the number of non-zero singular values. For A <u>symmetric</u> ($a_{ij} = a_{ji}$) it is also the number of non-zero eigenvalues.

We will rarely deal with matrices with negative eigenvalues.

A matrix P is a <u>projection</u> matrix if it is symmetric and idempotent

$$P = P^T$$
$$P^2 = P.$$

Inverse of Partitioned Matrix

The inverse of the matrix

$$\begin{pmatrix} A & B \\ B' & D \end{pmatrix}^{-1} = \begin{pmatrix} A^{-1}+A^{-1}BE^{-1}B'A^{-1} & -A^{-1}BE^{-1} \\ -E^{-1}B'A^{-1} & (D-B'A^{-1}B)^{-1} \end{pmatrix},$$

where $E = D - B'A^{-1}B$.

Also

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = |D|\,|A-BD^{-1}C| \quad \text{if } D^{-1} \text{ exists}$$

$$= |A|\,|D-CA^{-1}B| \quad \text{if } A^{-1} \text{ exists}$$

The updating formula for the inverse of a matrix is

$$(A+UBV)^{-1} = A^{-1} - A^{-1}UB(B+BVA^{-1}UB)^{-1}BUA^{-1}.$$

An important special case is for $X^TX = \sum_{i=1}^{n} x_i x_i^T$ where $U = V' = x_i$, $B = -1$

$$(X^TX - x_i x_i^T)^{-1} = (X^TX)^{-1} + \frac{(X^TX)^{-1}x_i x_i^T (X^TX)^{-1}}{1-h_i}$$

where x_i^T is the i^{th} row of X and $h_i = x_i^T(X^TX)^{-1}x_i$, assuming the inverse exists.

On inverses

Inverse of Compound Symmetric Matrix

$$A = \begin{pmatrix} a & b & \cdots & b \\ b & a & \ddots & \vdots \\ \vdots & \ddots & a & b \\ b & \cdots & b & a \end{pmatrix}_{K\times K} \qquad A^{-1} = \frac{1}{a-b}\left(I - \frac{b}{a+(k-1)b} J\right)$$

k is dimension

is Compound Symmetric. See Seber Appendix A3 part 5 for result.

Inverse of $^{J\times J}$ AR-1 matrix

$$A = \begin{pmatrix} 1 & \rho & \rho^2 & \cdots & \rho^{J-1} \\ & 1 & \ddots & & \rho^2 \\ & & 1 & \ddots & \rho \\ & & & \ddots & \\ & & & & 1 \end{pmatrix}$$

$$A_{jk} = \rho^{|j-k|} \qquad A^{-1} = \begin{pmatrix} 1 & -\rho & 0 & \cdots & 0 \\ -\rho & (1+\rho^2) & -\rho & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & (1+\rho^2) & -\rho \\ 0 & \cdots & 0 & -\rho & 1 \end{pmatrix}$$

A^{-1} is tridiagonal. $(A^{-1})_{jk} = 1, 0, -\rho$ or $(1+\rho^2)$.

General rule: patterned covariance matrices have patterned inverses,

Graybill Chapter 8.3 is helpful (Matrices with applications in statistics) (1983) Th^m 8.3.4 & Ex 8.3.8

Some Vector & Matrix Differentiation

Let a, β be $p \times 1$ vectors. Then

(1) $$\frac{d}{d\beta} = \left[\frac{\partial}{\partial \beta_i} \right]_{p \times 1}$$

(2) $$\frac{d}{d\beta} (\beta' a) = a$$

(3) $$\frac{d}{d\beta} (\beta' A \beta) = 2 A \beta \qquad (A \text{ symmetric})$$

Some Definitions

The Kronecker or direct product of A and B is

$$A \otimes B = \begin{pmatrix} a_{11} B & a_{12} B & \cdots & a_{1m} B \\ \vdots & a_{22} B & \cdots & \vdots \\ & & \ddots & \vdots \\ a_{m1} B & & & a_{mm} B \end{pmatrix}.$$

The most common use of this is when $Y = (Y_1^t, Y_2^t, \ldots Y_n^t)^t$ where $Y_i \mid \mu, \Sigma \sim N(\mu, \Sigma)$, then

$$Var(Y) = I_n \otimes \Sigma = \begin{pmatrix} \Sigma & 0 & \cdots & 0 \\ 0 & \Sigma & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \Sigma \end{pmatrix}.$$

The <u>Mahalanobis</u> <u>Distance</u>. Suppose $z_{p\times 1}$ has mean

$$E[z] = \mu$$

and variance

$$Var[z] = V[z] = \mathcal{D}(z) = \Sigma.$$

The Mahalanobis distance from z to μ is

$$D = (z-\mu)^t \Sigma^{-1} (z-\mu).$$

The matrix Σ^{-1} is the inner product. Often almost any quadratic form $(x-y)^T A^{-1} (x-y)$ are called Mahalanobis Distance.