Lecture 1: Intro/refresher in Matrix Algebra

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SISG - Mixed Model Course
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Matrix/ linear algebra

- Compact way for treating the algebra of systems of linear equations
- Most common statistical methods can be written in matrix form
  - $\mathbf{y} = \mathbf{X}\beta + \mathbf{e}$ is the general linear model
  - OLS solution: $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
  - $\mathbf{Y} = \mathbf{X}\beta + \mathbf{Z}\alpha + \mathbf{e}$ is the general mixed model

Topics

- Definitions, dimensionality, addition, subtraction
- Matrix multiplication
- Inverses, solving systems of equations
- Quadratic products and covariances
- The multivariate normal distribution
- Ordinary least squares
- Vector/matrix calculus (taking derivatives)

Matrices: An array of elements

Vectors: A matrix with either one row or one column. Usually written in bold lowercase, e.g. $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$

$$\mathbf{a} = \begin{pmatrix} 12 \\ 13 \\ 47 \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} 2 \\ 0 \\ 5 \\ 21 \end{pmatrix}$$

Column vector  Row vector

(3 x 1)  (1 x 4)

Dimensionality of a matrix: $r \times c$ (rows x columns)

think of Railroad Car
General Matrices

Usually written in bold uppercase, e.g. \( \mathbf{A}, \mathbf{C}, \mathbf{D} \)

\[
\mathbf{C} = \begin{pmatrix} 3 & 1 & 2 \\ 2 & 5 & 4 \\ 1 & 1 & 2 \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 0 & 1 \\ 3 & 4 \\ 2 & 9 \end{pmatrix}
\]

(3 x 3) \quad (3 x 2)

Square matrix

Dimensionality of a matrix: \( r \times c \) (rows x columns)

think of \textit{Railroad Car}

A matrix is defined by a list of its elements.

\( \mathbf{B} \) has \( ij \)-th element \( B_{ij} \)-- the element in row \( i \) and column \( j \)

Addition and Subtraction of Matrices

If two matrices have the same dimension (same number of rows and columns), then matrix addition and subtraction simply follows by adding (or subtracting) on an element by element basis

**Matrix addition:** \((\mathbf{A}+\mathbf{B})_{ij} = A_{ij} + B_{ij}\)

**Matrix subtraction:** \((\mathbf{A}-\mathbf{B})_{ij} = A_{ij} - B_{ij}\)

Examples:

\[
\mathbf{A} = \begin{pmatrix} 3 & 0 \\ 1 & 2 \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}
\]

\[
\mathbf{C} = \mathbf{A} + \mathbf{B} = \begin{pmatrix} 4 & 2 \\ 3 & 3 \end{pmatrix} \quad \text{and} \quad \mathbf{D} = \mathbf{A} - \mathbf{B} = \begin{pmatrix} 2 & -2 \\ -1 & 1 \end{pmatrix}
\]

Partitioned Matrices

It will often prove useful to divide (or partition) the elements of a matrix into a matrix whose elements are itself matrices.

\[
\mathbf{C} = \begin{pmatrix} 3 & 1 & 2 \\ 2 & 5 & 4 \\ 1 & 1 & 2 \end{pmatrix} = \begin{pmatrix} 3 & \cdots & 1 & 2 \\ \cdots & \cdots & \cdots & \cdots \\ 2 & \cdots & 5 & 4 \\ 1 & \cdots & 1 & 2 \end{pmatrix} = \begin{pmatrix} a & b \\ d & B \end{pmatrix}
\]

\[a = (3), \quad b = (1 \ 2), \quad d = \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \quad B = \begin{pmatrix} 5 & 4 \\ 1 & 2 \end{pmatrix}\]

One useful partition is to write the matrix as either a \textit{row vector of column vectors} or a \textit{column vector of row vectors}

\[
\mathbf{C} = \begin{pmatrix} 3 & 1 & 2 \\ 2 & 5 & 4 \\ 1 & 1 & 2 \end{pmatrix} = \begin{pmatrix} r_1 & r_2 & r_3 \end{pmatrix} \quad \text{A column vector whose elements are row vectors}
\]

\[
\begin{align*}
r_1 &= (3 \ 1 \ 2) \\
r_2 &= (2 \ 5 \ 4) \\
r_3 &= (1 \ 1 \ 2)
\end{align*}
\]

\[
\mathbf{C} = \begin{pmatrix} 3 & 1 & 2 \\ 2 & 5 & 4 \\ 1 & 1 & 2 \end{pmatrix} = \begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix} \quad \text{A row vector whose elements are column vectors}
\]

\[
\begin{align*}
c_1 &= \begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix}, \quad c_2 = \begin{pmatrix} 1 \\ 5 \\ 1 \end{pmatrix}, \quad c_3 = \begin{pmatrix} 2 \\ 4 \\ 2 \end{pmatrix}
\end{align*}
\]
Towards Matrix Multiplication: dot products

The dot (or inner) product of two vectors (both of length \( n \)) is defined as follows:

\[
\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^{n} a_i b_i
\]

Example:

\[
\mathbf{a} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad \text{and} \quad \mathbf{b} = (4 \ 5 \ 7 \ 9)
\]

\[
\mathbf{a} \cdot \mathbf{b} = 1 \times 4 + 2 \times 5 + 3 \times 7 + 4 \times 9 = 71
\]

Matrices are compact ways to write systems of equations

\[
5x_1 + 6x_2 + 4x_3 = 6 \\
7x_1 - 3x_2 + 5x_3 = -9 \\
-2x_1 - x_2 + 6x_3 = 12
\]

\[
\begin{pmatrix} 5 & 6 & 4 \\ 7 & -3 & 5 \\ -1 & -1 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ -9 \\ 12 \end{pmatrix}
\]

\[\mathbf{A} \mathbf{x} = \mathbf{c}, \quad \text{or} \quad \mathbf{x} = \mathbf{A}^{-1} \mathbf{c}\]

The least-squares solution for the linear model

\[
y = \mu + \beta_1 z_1 + \cdots + \beta_n z_n
\]

yields the following system of equations for the \( \beta_i \)

\[
\sigma(y, z_1) = \beta_1 \sigma(z_1, z_1) + \cdots + \beta_n \sigma(z_1, z_n)
\]

\[
\sigma(y, z_2) = \beta_1 \sigma(z_1, z_2) + \cdots + \beta_n \sigma(z_2, z_n)
\]

\[\vdots \]

\[
\sigma(y, z_n) = \beta_1 \sigma(z_1, z_n) + \cdots + \beta_n \sigma(z_n, z_n)
\]

This can be more compactly written in matrix form as

\[
\begin{pmatrix}
\sigma^2(z_1) & \sigma(z_1, z_2) & \cdots & \sigma(z_1, z_n) \\
\sigma(z_1, z_2) & \sigma^2(z_2) & \cdots & \sigma(z_2, z_n) \\
\vdots & \vdots & \ddots & \vdots \\
\sigma(z_1, z_n) & \sigma(z_2, z_n) & \cdots & \sigma^2(z_n)
\end{pmatrix}
\begin{pmatrix}
\beta_1 \\
\beta_2 \\
\vdots \\
\beta_n
\end{pmatrix}
= 
\begin{pmatrix}
\sigma(y, z_1) \\
\sigma(y, z_2) \\
\vdots \\
\sigma(y, z_n)
\end{pmatrix}
\]

\[\mathbf{X}^\top \mathbf{X} \quad \beta \quad \mathbf{X}^\top \mathbf{y}\]

or, \( \hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \)

Matrix Multiplication:

The order in which matrices are multiplied affects the matrix product, e.g. \( \mathbf{AB} \neq \mathbf{BA} \)

For the product of two matrices to exist, the matrices must conform. For \( \mathbf{AB} \), the number of columns of \( \mathbf{A} \) must equal the number of rows of \( \mathbf{B} \).

The matrix \( \mathbf{C} = \mathbf{AB} \) has the same number of rows as \( \mathbf{A} \) and the same number of columns as \( \mathbf{B} \).

\[
\mathbf{C}_{(r \times c)} = \mathbf{A}_{(r \times k)} \mathbf{B}_{(k \times c)}
\]

\( ij \)-th element of \( \mathbf{C} \) is given by

\[
C_{ij} = \sum_{l=1}^{k} A_{il} B_{lj}
\]

Elements in the \( j \)-th column of \( \mathbf{B} \)

Elements in the \( i \)-th row of \( \mathbf{A} \)
\[ C_{(rxc)} = A_{(rxk)} B_{(kxc)} \]

Outer indices given dimensions of resulting matrix, with \( r \) rows (A) and \( c \) columns (B)

Inner indices must match, columns of A = rows of B

Example: Is the product ABCD defined? If so, what is its dimensionality? Suppose

\[ A_{3x5} B_{5x9} C_{9x6} D_{6x23} \]

Yes, defined, as inner indices match. Result is a \( 3 \times 23 \) matrix (3 rows, 23 columns)

More formally, consider the product \( L = MN \)

Express the matrix \( M \) as a column vector of row vectors

\[ M = \begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ m_r \end{pmatrix} \text{ where } m_i = (M_{i1} M_{i2} \ldots M_{ic}) \]

Likewise express \( N \) as a row vector of column vectors

\[ N = (n_1 n_2 \ldots n_b) \text{ where } n_j = \begin{pmatrix} N_{1j} \\ N_{2j} \\ \vdots \\ N_{nj} \end{pmatrix} \]

The \( ij \)-th element of \( L \) is the inner product of \( M \)'s row \( i \) with \( N \)'s column \( j \)

\[ L = \begin{pmatrix} m_1 \cdot n_1 & m_1 \cdot n_2 & \ldots & m_1 \cdot n_b \\ m_2 \cdot n_1 & m_2 \cdot n_2 & \ldots & m_2 \cdot n_b \\ \vdots & \vdots & \ddots & \vdots \\ m_r \cdot n_1 & m_r \cdot n_2 & \ldots & m_r \cdot n_b \end{pmatrix} \]

Example

\[ AB = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} ae + bg & af + bh \\ ce + dg & cf + dh \end{pmatrix} \]

Likewise

\[ BA = \begin{pmatrix} ae + cf & eb + df \\ ga + ch & gd + dh \end{pmatrix} \]

ORDER of multiplication matters! Indeed, consider \( C_{3x5} D_{5x5} \) which gives a \( 3 \times 5 \) matrix, versus \( D_{5x5} C_{3x5} \), which is not defined

The Transpose of a Matrix

The transpose of a matrix exchanges the rows and columns, \( A^T_{ij} = A_{ji} \)

Useful identities

\[ (AB)^T = B^T A^T \]
\[ (ABC)^T = C^T B^T A^T \]

Inner product = \( a^T b = a \, (1 \times n) \, b \, (n \times 1) \)

Indices match, matrices conform

Dimension of resulting product is \( 1 \times 1 \) (i.e. a scalar)

\[ (a_1 \ldots a_n) \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = a^T b = \sum_{i=1}^{n} a_i b_i \]

Note that \( b^T a = (b^T a)^T = a^T b \)
Outer product = \( ab^T = a_{(n \times 1)} b_{(1 \times n)}^T \) 

Resulting product is an \( n \times n \) matrix

\[
\begin{pmatrix}
  a_1 \\
  a_2 \\
  \vdots \\
  a_n
\end{pmatrix}
\begin{pmatrix}
  b_1 & b_2 & \cdots & b_n
\end{pmatrix}
= 
\begin{pmatrix}
  a_1b_1 & a_1b_2 & \cdots & a_1b_n \\
  a_2b_1 & a_2b_2 & \cdots & a_2b_n \\
  \vdots & \vdots & \ddots & \vdots \\
  a_nb_1 & a_nb_2 & \cdots & a_nb_n
\end{pmatrix}
\]

### Solving equations

- **The identity matrix** \( I \)
  - Serves the same role as 1 in scalar algebra, e.g., \( a^*1=1^*a=a \), with \( AI=IA=A \)
- **The inverse matrix** \( A^{-1} \) (IF it exists)
  - Defined by \( A A^{-1} = I, \ A^{-1}A = I \)
  - Serves the same role as scalar division
    - To solve \( ax = c \), multiply both sides by \( (1/a) \) to give \( (1/a)ax = (1/a)c \) or \( (1/a)a^*x = 1^*x = x \),
    - Hence \( x = (1/a)c \)
    - To solve \( Ax = c \), \( A^{-1}Ax = A^{-1}c \)
    - Or \( A^{-1}Ax = Ix = x = A^{-1}c \)

### The Identity Matrix, \( I \)

The identity matrix serves the role of the number 1 in matrix multiplication: \( AI = A, \ IA = A \)

\( I \) is a square diagonal matrix, with all diagonal elements being one, all off-diagonal elements zero.

\[
I_{ij} = \begin{cases} 
1 & \text{for } i = j \\
0 & \text{otherwise}
\end{cases}
\]

\[
I_{3 \times 3} = \begin{pmatrix} 1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \end{pmatrix}
\]

### The Inverse Matrix, \( A^{-1} \)

For a square matrix \( A \), define is **Inverse** \( A^{-1} \), as the matrix satisfying

\[
A^{-1}A = AA^{-1} = I
\]

For \( A = \begin{pmatrix} a & b \\
                 c & d \end{pmatrix} \)

\[
A^{-1} = \frac{1}{ad-bc} \begin{pmatrix} d & -b \\
                                  -c & a \end{pmatrix}
\]

If this quantity (the **determinant**) is zero, the inverse does not exist.
If \( \det(A) \) is not zero, \( A^{-1} \) exists and \( A \) is said to be non-singular. If \( \det(A) = 0 \), \( A \) is singular, and no unique inverse exists (generalized inverses do)

Generalized inverses, and their uses in solving systems of equations, are discussed in Appendix 3 of Lynch & Walsh

\( A^+ \) is the typical notation to denote the \( G \)-inverse of a matrix

When a \( G \)-inverse is used, provided the system is consistent, then some of the variables have a family of solutions (e.g., \( x_1 = 2 \), but \( x_2 + x_3 = 6 \))

Example: solve the OLS for \( \beta \) in \( y = \alpha + \beta_1 z_1 + \beta_2 z_2 + e \)

\[
\beta = V^{-1} c \quad c = \begin{pmatrix} \sigma(y, z_1) \\ \sigma(y, z_2) \end{pmatrix} \quad V = \begin{pmatrix} \sigma^2(z_1) & \sigma(z_1, z_2) \\ \sigma(z_1, z_2) & \sigma^2(z_2) \end{pmatrix}
\]

It is more compact to use \( \sigma(z_1, z_2) = \rho_{12} \sigma(z_1) \sigma(z_2) \)

\[
V^{-1} = \frac{1}{\sigma^2(z_1) \sigma^2(z_2)(1 - \rho_{12}^2)} \begin{pmatrix} \sigma^2(z_2) & -\sigma(z_1, z_2) \\ -\sigma(z_1, z_2) & \sigma^2(z_1) \end{pmatrix}
\]

\[
\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = \frac{1}{\sigma^2(z_1) \sigma^2(z_2)(1 - \rho_{12}^2)} \begin{pmatrix} \sigma^2(z_2) & -\sigma(z_1, z_2) \\ -\sigma(z_1, z_2) & \sigma^2(z_1) \end{pmatrix} \begin{pmatrix} \sigma(y, z_1) \\ \sigma(y, z_2) \end{pmatrix}
\]

\[
\beta_1 = \frac{1}{1 - \rho_{12}^2} \left[ \frac{\sigma(y, z_1) \sigma(z_1) - \rho_{12} \sigma(y, z_2) \sigma(z_1)}{\sigma^2(z_1)} \right]
\]

\[
\beta_2 = \frac{1}{1 - \rho_{12}^2} \left[ \frac{\sigma(y, z_2) \sigma(z_2) - \rho_{12} \sigma(y, z_1) \sigma(z_2)}{\sigma^2(z_2)} \right]
\]

If \( \rho_{12} = 0 \), these reduce to the two univariate slopes,

\[
\beta_1 = \frac{\sigma(y, z_1)}{\sigma^2(z_1)} \quad \text{and} \quad \beta_2 = \frac{\sigma(y, z_2)}{\sigma^2(z_2)}
\]

Likewise, if \( \rho_{12} = 1 \), this reduces to a univariate regression,

Useful identities

\[
(A^T)^{-1} = (A^{-1})^T
\]

\[
(AB)^{-1} = B^{-1} A^{-1}
\]

For a diagonal matrix \( D \), then \( \text{Det} = |D| = \text{product of the diagonal elements} \)

Also, the determinant of any square matrix \( A \), \( \det(A) \), is simply the product of the eigenvalues \( \lambda \) of \( A \), which satisfy

\[
A e = \lambda e
\]

If \( A \) is \( n \times n \), solutions to \( \lambda \) are an \( n \)-degree polynomial.

If any of the roots to the equation are zero, \( A^{-1} \) is not defined. Further, some linear combination \( b \), we have \( Ab = 0 \). \( e \) is the eigenvector associated with \( \lambda_e \).
Variance-Covariance matrix

- A very important square matrix is the variance-covariance matrix $V$ associated with a vector $x$ of random variables.
- $V_{ij} = \text{Cov}(x_i, x_j)$, so that the $i$-th diagonal element of $V$ is the variance of $x_i$, and off-diagonal elements are covariances.
- $V$ is a symmetric, square matrix.

Quadratic and Bilinear Forms

**Quadratic product:** for $A_{n \times n}$ and $x_{n \times 1}$

$$x^T A x = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i x_j \quad \text{Scalar (1 \times 1)}$$

**Bilinear Form** (generalization of quadratic product)

for $A_{m \times n}$, $a_{n \times 1}$, $b_{m \times 1}$ their bilinear form is $b^T_{1 \times m} A_{m \times n} a_{n \times 1}$

$$b^T A a = \sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} b_i a_j$$

Note that $b^T A a = a^T A^T b$

Covariance Matrices for Transformed Variables

What is the variance of the linear combination, $c_1 X_1 + c_2 X_2 + \ldots + c_n X_n$? (note this is a scalar)

$$\sigma^2 (c^T x) = \sigma^2 \left( \sum_{i=1}^{n} c_i x_i \right) = \sigma \left( \sum_{i=1}^{n} c_i x_i \right) \left( \sum_{j=1}^{n} c_j x_j \right)$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \sigma(c_i x_i, c_j x_j) = \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \sigma(x_i, x_j)$$

$$= c^T V c$$

Likewise, the covariance between two linear combinations can be expressed as a bilinear form,

$$\sigma(a^T x, b^T x) = a^T V b$$
Example: Suppose the variances of $x_1$, $x_2$, and $x_3$ are 10, 20, and 30. $x_1$ and $x_2$ have a covariance of -5, $x_1$ and $x_3$ of 10, while $x_2$ and $x_3$ are uncorrelated.

What are the variances of the new variables $y_1 = x_1 - 2x_2 + 5x_3$ and $y_2 = 6x_2 - 4x_3$?

\[
V = \begin{pmatrix} 10 & -5 & 10 \\ -5 & 20 & 0 \\ 10 & 0 & 30 \end{pmatrix}, \quad c_1 = \begin{pmatrix} 1 \\ -2 \\ 5 \end{pmatrix}, \quad c_2 = \begin{pmatrix} 0 \\ 6 \\ -4 \end{pmatrix}
\]

\[
\text{Var}(y_1) = \text{Var}(c_1^T x) = c_1^T \text{Var}(x) c_1 = 960
\]

\[
\text{Var}(y_2) = \text{Var}(c_2^T x) = c_2^T \text{Var}(x) c_2 = 1200
\]

\[
\text{Cov}(y_1, y_2) = \text{Cov}(c_1^T x, c_2^T x) = c_1^T \text{Var}(x) c_2 = -910
\]

Now suppose we transform one vector of random variables into another vector of random variables.

Transform $x$ into

(i) $y_{k \times 1} = A_{k \times n} x_{n \times 1}$

(ii) $z_{m \times 1} = B_{m \times n} x_{n \times 1}$

The covariance between the elements of these two transformed vectors of the original is a $k \times m$ covariance matrix $= A V A^T$

For example, the covariance between $y_i$ and $y_j$ is given by the $ij$-th element of $A V A^T$

Likewise, the covariance between $y_i$ and $z_j$ is given by the $ij$-th element of $A V B^T$

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**Positive-definite matrix**

- A matrix $V$ is positive-definite if for all vectors $c$ contained at least one non-zero member, $c^T V c > 0$.
- A non-negative definite matrix satisfies $c^T V c \geq 0$.
- Any covariance-matrix is (at least) non-negative definite, as $\text{Var}(c^T x) = c^T V c > 0$.
- Any nonsingular covariance matrix is positive-definite
  - Nonsingular means $\det(V) > 0$
  - Equivalently, all eigenvalues of $V$ are positive, $\lambda_i > 0$.

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**The Multivariate Normal Distribution (MVN)**

Consider the pdf for $n$ independent normal random variables, the $i$th of which has mean $\mu_i$ and variance $\sigma^2_i$:

\[
p(x) = \prod_{i=1}^{n} (2\pi)^{-1/2} \sigma^{-1}_i \exp \left( -\frac{(x_i - \mu_i)^2}{2 \sigma_i^2} \right)
\]

\[
= (2\pi)^{-n/2} \left( \prod_{i=1}^{n} \sigma_i \right)^{-1} \exp \left( -\sum_{i=1}^{n} \frac{(x_i - \mu_i)^2}{2 \sigma_i^2} \right)
\]

This can be expressed more compactly in matrix form.
Define the **covariance matrix** $V$ for the vector $x$ of the $n$ normal random variable by

$$V = \begin{pmatrix}
s_1^2 & 0 & \cdots & 0 \\
0 & s_2^2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & \cdots & \cdots & s_n^2
\end{pmatrix}$$

$$|V| = \prod_{i=1}^{n} \sigma_i^2$$

Define the mean vector $\mu$ by

$$\mu = \begin{pmatrix}
\mu_1 \\
\mu_2 \\
\vdots \\
\mu_n
\end{pmatrix}$$

Hence in matrix form the MVN pdf becomes

$$p(x) = (2\pi)^{-n/2} |V|^{-1/2} \exp \left[ -\frac{1}{2} (x - \mu)^T V^{-1} (x - \mu) \right]$$

Notice this holds for any vector $\mu$ and symmetric **positive-definite** matrix $V$, as $|V| > 0$.

### The multivariate normal

- Just as a univariate normal is defined by its mean and spread, a multivariate normal is defined by its mean vector $\mu$ (also called the centroid) and variance-covariance matrix $V$.

Vector of means $\mu$ determines location

Spread (geometry) about $\mu$ determined by $V$

$\mu$

$\mu^*$

$x_1, x_2$ equal variances, positively correlated

$x_1, x_2$ equal variances, uncorrelated

**Eigenstructure** (the eigenvectors and their corresponding eigenvalues) determines the geometry of $V$.

Positive tilt = positive correlations

Negative tilt = negative correlation

No tilt = uncorrelated
Eigenstructure of $V$

The direction of the largest axis of variation is given by the unit-length vector $e_1$, the 1st eigenvector of $V$.

The next largest axis of orthogonal (at 90 degrees from) $e_1$, is given by $e_2$, the 2nd eigenvector.

Properties of the MVN - I

1) If $x$ is MVN, any subset of the variables in $x$ is also MVN.

2) If $x$ is MVN, any linear combination of the elements of $x$ is also MVN. If $x \sim \text{MVN}(\mu, V)$

\begin{align*}
\text{for } y &= x + a, \quad y \sim \text{MVN}_n(\mu + a, V) \\
\text{for } y &= a^T x = \sum_{k=1}^{n} a_k x_k, \quad y \sim N(a^T \mu, a^T V a) \\
\text{for } y &= Ax, \quad y \sim \text{MVN}_m(A \mu, A^T V A)
\end{align*}

Properties of the MVN - II

3) Conditional distributions are also MVN. Partition $x$ into two components, $x_1$ (m dimensional column vector) and $x_2$ (n-m dimensional column vector)

\[
x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad \text{and} \quad V = \begin{pmatrix} V_{x_1|x_2} & V_{x_1|x_2} \\ V_{x_1|x_2}^T & V_{x_2|x_2} \end{pmatrix}
\]

$x_1 | x_2$ is MVN with m-dimensional mean vector

\[
\mu_{x_1|x_2} = \mu_1 + V_{x_1|x_2} V_{x_2|x_2}^{-1} (x_2 - \mu_2)
\]

and m x m covariance matrix

\[
V_{x_1|x_2} = V_{x_1|x_1} - V_{x_1|x_2} V_{x_2|x_2}^{-1} V_{x_1|x_2}^T
\]

Properties of the MVN - III

4) If $x$ is MVN, the regression of any subset of $x$ on another subset is linear and homoscedastic

\[
x_1 = \mu_{x_1|x_2} + e = \mu_1 + V_{x_1|x_2} V_{x_2|x_2}^{-1} (x_2 - \mu_2) + e
\]

Where $e$ is MVN with mean vector 0 and variance-covariance matrix $V_{x_1|x_2}$.
The regression is linear because it is a linear function of $x_2$.

The regression is homoscedastic because the variance-covariance matrix for $e$ does not depend on the value of the $x$'s.

$$V_{X_1|X_2} = V_{X_1X_1} - V_{X_1X_2}V_{X_2X_2}^{-1}V_{X_1X_2}$$

All these matrices are constant, and hence the same for any value of $x$.

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**Example: Regression of Offspring value on Parental values**

Assume the vector of offspring value and the values of both its parents is MVN. Then from the correlations among (outbred) relatives,

$$
\begin{pmatrix}
  z_o \\
  z_s \\
  z_d 
\end{pmatrix} \sim \text{MVN}\left(\begin{pmatrix}
  \mu_o \\
  \mu_s \\
  \mu_d 
\end{pmatrix}, \begin{pmatrix}
  \sigma_z^2 & h^2/2 & h^2/2 \\
  h^2/2 & 1 & 0 \\
  h^2/2 & 0 & 1 
\end{pmatrix}\right)
$$

Let $x_1 = \begin{pmatrix} z_o \\ z_s \\ z_d \end{pmatrix}$, $x_2 = \begin{pmatrix} z_s \\ z_d \end{pmatrix}$.

$$V_{X_1X_1} = \sigma_z^2, \quad V_{X_1X_2} = \frac{h^2 \sigma_z^2}{2} \begin{pmatrix} 1 & 1 \end{pmatrix}, \quad V_{X_2X_2} = \sigma_z^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \mu_1 + V_{X_1X_2} V_{X_2X_2}^{-1} (x_2 - \mu_2) + e$$

---

**Regression of Offspring value on Parental values (cont.)**

$$= \mu_1 + V_{X_1X_2} V_{X_2X_2}^{-1} (x_2 - \mu_2) + e$$

$$V_{X_1X_1} = \sigma_z^2, \quad V_{X_1X_2} = \frac{h^2 \sigma_z^2}{2} \begin{pmatrix} 1 & 1 \end{pmatrix}, \quad V_{X_2X_2} = \sigma_z^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Hence,

$$z_o = \mu_o + \frac{h^2 \sigma_z^2}{2} (1 1) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} (z_s - \mu_s) + e$$

$$= \mu_o + \frac{h^2}{2} (z_s - \mu_s) + \frac{h^2}{2} (z_d - \mu_d) + e$$

Where $e$ is normal with mean zero and variance

$$V_{X_1X_2} = V_{X_1X_1} - V_{X_1X_2} V_{X_2X_2}^{-1} V_{X_1X_2}$$

$$\sigma_e^2 = \sigma_z^2 - \frac{h^2 \sigma_z^2}{2} (1 1) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \frac{h^2 \sigma_z^2}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \sigma_z^2 \left(1 - \frac{h^4}{2}\right)$$

Hence, the regression of offspring trait value given the trait values of its parents is

$$z_o = \mu_o + \frac{h^2}{2} (z_s - \mu_s) + \frac{h^2}{2} (z_d - \mu_d) + e$$

where the residual $e$ is normal with mean zero and

$$\text{Var}(e) = \sigma_e^2 (1-h^4)/2$$

Similar logic gives the regression of offspring breeding value on parental breeding value as

$$A_o = \mu_o + (A_s - \mu_s)/2 + (A_d - \mu_d)/2 + e$$

$$= A_s/2 + A_d/2 + e$$

where the residual $e$ is normal with mean zero and

$$\text{Var}(e) = \sigma_A^2/2$$
Ordinary least squares

For the general linear model

\[ y = X\beta + e \]

The predicted values given \( \beta \) and the resulting residuals are given by

\[ \hat{y} = X\beta, \quad e = y - X\beta \]

Ordinary least squares (OLS) finds the value \( \beta \) that minimizes the sum of squared residuals

\[ \sum c_i^2 - e^T e \]

or

\[ (y - X\beta)^T (y - X\beta) \]

The solution is given by setting the derivative of this function with respect to \( \beta \) equal to zero and solving.

Hence, we need to discuss vector/matrix derivatives

\[ \nabla_x [a^T x] = \nabla_x [x^T a] = a \]

\[ \nabla_x [Ax] = A^T \]

Turning to quadratic forms, if \( A \) is symmetric, then

\[ \nabla_x [x^T Ax] = 2 \cdot Ax \]

\[ \nabla_x [(x - a)^T A(x - a)] = 2 \cdot A(x - A) \]

\[ \nabla_x [(a - x)^T A(a - x)] = -2 \cdot A(a - x) \]

Taking \( A = I \),

\[ \nabla_x [x^T x] - \nabla_x [x^T I x] = 2 \cdot I x - 2 \cdot x \]

Some common derivatives

\[ \sum_{i=1}^{n} c_i^2 = c^T e = (y - X\beta)^T (y - X\beta) \]

\[ = y^T y - \beta^T X^T y - y^T X\beta + \beta^T X^T X\beta \]

\[ = y^T y - 2\beta^T X^T y + \beta^T X^T X\beta \]

where the last step follows since the matrix product \( \beta^T X^T y \) yields a scalar and hence it equals its transpose,

\[ \beta^T X^T y = (\beta^T X^T y)^T = y^T X\beta \]

To find the vector \( \beta \) that minimizes \( e^T e \), taking the derivative with respect to \( \beta \) and using Equations 45.1a through e gives

\[ \frac{\partial e^T e}{\partial \beta} = -2X^T y + 2X^T X\beta \]

Setting this equal to zero gives \( X^T \beta = X^T y \) giving

\[ \beta = (X^T X)^{-1} X^T y \]
Simple matrix commands in R

- R is case-sensitive!
- t(A) = transpose of A
- A %*% B = matrix product AB
- %*% command = matrix multiplication
- `solve(A)` = compute inverse of A
- x <- = assigns the variable `x` what is to the right of the arrow
  - e.g., `x <- 3.15`

Example: Solve the equation
\[
\begin{pmatrix}
  5 & 6 & 4 \\
  7 & -3 & 5 \\
 -1 & -1 & 6
\end{pmatrix}
\begin{pmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{pmatrix}
= \begin{pmatrix}
  -6 \\
  -9 \\
  12
\end{pmatrix}
\]

\[\mathbf{Ax} = \mathbf{c}, \quad \text{or} \quad \mathbf{A}^{-1}\mathbf{c}\]

First, input the matrix A. In R, `c` denotes a list, and we built the matrix by columns,

\[
\begin{pmatrix}
  5 & 6 & 4 \\
  7 & -3 & 5 \\
 -1 & -1 & 6
\end{pmatrix}
\]

Next, input the vector `c`.

\[
\begin{pmatrix}
  5 \\
  6 \\
  4
\end{pmatrix}
\]

Finally, compute \(\mathbf{A}^{-1}\mathbf{c}\).

\[
\begin{pmatrix}
  \text{det}(A) \quad \text{returns the determinant of } A \\
  \text{eigen}(A) \quad \text{returns the eigenvalues and vectors of } A
\end{pmatrix}
\]

Example 2: Compute \(\text{Var}(y_1), \text{Var}(y_2), \text{and} \text{Cov}(y_1, y_2)\), where \(y_i = \mathbf{c}_i^T \mathbf{x}\).

\[
\begin{pmatrix}
  \mathbf{c}_1^T \mathbf{V} \mathbf{c}_1 \\
  \mathbf{c}_2^T \mathbf{V} \mathbf{c}_2 \\
  \mathbf{c}_1^T \mathbf{V} \mathbf{c}_2
\end{pmatrix}
\]

For example, second eigenvalue is \(\lambda_2 = 21.11734\), second eigenvector

\[
\mathbf{e}_2 = \begin{pmatrix}
  0.2111734 \\
 -0.9477830 \\
 -0.2381340
\end{pmatrix}
\]
Additional references

- Lynch & Walsh Chapter 8 (intro to matrices)
- In notes package:
  - Appendix 4 (Matrix geometry)
  - Appendix 5 (Matrix derivatives)
  - Matrix Calculations in R