Lecture 1: Intro/refresher in Matrix Algebra

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Introduction to Mixed Models

SISG (Module 12), Seattle

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Topics

- Definitions, dimensionality, addition, subtraction
- Matrix multiplication
- Inverses, solving systems of equations
- Quadratic products and covariances
- The multivariate normal distribution
- Eigenstructure
- Basic matrix calculations in R
- The Singular Value Decomposition (SVD)
  - First PAUSE slide 16

Matrices: An array of elements

Vectors: A matrix with either one row or one column.

Usually written in bold lowercase, e.g. **a, b, 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 x c (rows x columns)
think of Railroad Car

General Matrices

Usually written in bold uppercase, e.g. **A, C, 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)

Square matrix

(3 x 2)

Dimensionality of a matrix: r x c (rows x columns)
think of Railroad Car

A matrix is defined by a list of its elements.
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 (both are r x c), then matrix addition and subtraction simply follows by adding (or subtracting) on an element by element basis

Matrix addition: $(A+B)_{ij} = A_{ij} + B_{ij}$

Matrix subtraction: $(A-B)_{ij} = A_{ij} - B_{ij}$

Examples:

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

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

Partitioned Matrices

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

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

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

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

$$\mathbf{C} = \begin{pmatrix} 3 & 1 & 2 \\ 2 & 5 & 4 \\ 1 & 1 & 2 \end{pmatrix} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \mathbf{r}_3 \end{pmatrix}$$

A column vector whose elements are row vectors

$$\mathbf{r}_1 = \begin{pmatrix} 3 & 1 & 2 \end{pmatrix}$$
$$\mathbf{r}_2 = \begin{pmatrix} 2 & 5 & 4 \end{pmatrix}$$
$$\mathbf{r}_3 = \begin{pmatrix} 1 & 1 & 2 \end{pmatrix}$$

$$\mathbf{C} = \begin{pmatrix} 3 & 1 & 2 \\ 2 & 5 & 4 \\ 1 & 1 & 2 \end{pmatrix} = \begin{pmatrix} \mathbf{c}_1 & \mathbf{c}_2 & \mathbf{c}_3 \end{pmatrix}$$

A row vector whose elements are column vectors

$$\mathbf{c}_1 = \begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix}, \quad \mathbf{c}_2 = \begin{pmatrix} 1 \\ 5 \\ 1 \end{pmatrix}, \quad \mathbf{c}_3 = \begin{pmatrix} 2 \\ 4 \\ 2 \end{pmatrix}$$

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:

$$\mathbf{a} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \quad \text{and} \quad \mathbf{b} = \begin{pmatrix} 4 & 5 & 7 & 9 \end{pmatrix}$$

a ˙b = 1*4 + 2*5 + 3*7 + 4*9 = 71

Matrices are compact ways to write systems of equations

$$
\begin{aligned}
5x_1 + 6x_2 + 4x_3 &= 6 \\
7x_1 - 3x_2 + 5x_3 &= -9 \\
-x_1 - x_2 + 6x_3 &= 12
\end{aligned}
$$

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

$$
\mathbf{A}\mathbf{x} = \mathbf{c}, \qquad \text{or} \quad \mathbf{x} = \mathbf{A}^{-1}\mathbf{c}
$$

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 β_i

$$\begin{aligned}
\sigma(y, z_1) &= \beta_1 \sigma^2(z_1) + \beta_2 \sigma(z_1, z_2) + \cdots + \beta_n \sigma(z_1, z_n) \\
\sigma(y, z_2) &= \beta_1 \sigma(z_1, z_2) + \beta_2 \sigma^2(z_2) + \cdots + \beta_n \sigma(z_2, z_n) \\
\vdots \quad & \qquad \vdots \qquad\qquad\qquad \vdots \qquad\qquad \ddots \qquad \vdots \\
\sigma(y, z_n) &= \beta_1 \sigma(z_1, z_n) + \beta_2 \sigma(z_2, z_n) + \cdots + \beta_n \sigma^2(z_n)
\end{aligned}$$

This can be more compactly written in matrix form as

$$\underbrace{\begin{pmatrix} \sigma^2(z_1) & \sigma(z_1, z_2) & \ldots & \sigma(z_1, z_n) \\ \sigma(z_1, z_2) & \sigma^2(z_2) & \ldots & \sigma(z_2, z_n) \\ \vdots & \vdots & \ddots & \vdots \\ \sigma(z_1, z_n) & \sigma(z_2, z_n) & \ldots & \sigma^2(z_n) \end{pmatrix}}_{X^T X} \underbrace{\begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{pmatrix}}_{\boldsymbol{\beta}} = \underbrace{\begin{pmatrix} \sigma(y, z_1) \\ \sigma(y, z_2) \\ \vdots \\ \sigma(y, z_n) \end{pmatrix}}_{X^T y}$$

or, $\boldsymbol{\beta} = (X^T X)^{-1} X^T y$

Matrix Multiplication:

The order in which matrices are multiplied affects the matrix product, e.g. $AB \neq BA$

For the product of two matrices to exist, the matrices must conform. For AB, the number of columns of A must equal the number of rows of B.

The matrix C = AB has the same number of rows as A and the same number of columns as B.

$$C_{(r\times c)} = A_{(r\times k)}\ B_{(k\times c)}$$

ij-th element of C is given by

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

Elements in the jth column of B

Elements in the ith row of matrix A

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

$$C_{(r x c)} = A_{(r x k)} \quad B_{(k x c)}$$

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 x 23 matrix (3 rows, 23 columns)

More formally, consider the product L = MN

Express the matrix M as a column vector of row vectors

$$\mathbf{M} = \begin{pmatrix} \mathbf{m_1} \\ \mathbf{m_2} \\ \vdots \\ \mathbf{m_r} \end{pmatrix} \qquad \text{where} \qquad \mathbf{m_i} = \begin{pmatrix} M_{i1} & M_{i2} & \cdots & M_{ic} \end{pmatrix}$$

Likewise express N as a row vector of column vectors

$$\mathbf{N} = \begin{pmatrix} \mathbf{n_1} & \mathbf{n_2} & \cdots & \mathbf{n_b} \end{pmatrix} \qquad \text{where} \qquad \mathbf{n_j} = \begin{pmatrix} N_{1j} \\ N_{2j} \\ \vdots \\ N_{cj} \end{pmatrix}$$

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

$$\mathbf{L} = \begin{pmatrix} \mathbf{m_1} \cdot \mathbf{n_1} & \mathbf{m_1} \cdot \mathbf{n_2} & \cdots & \mathbf{m_1} \cdot \mathbf{n_b} \\ \mathbf{m_2} \cdot \mathbf{n_1} & \mathbf{m_2} \cdot \mathbf{n_2} & \cdots & \mathbf{m_2} \cdot \mathbf{n_b} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{m_r} \cdot \mathbf{n_1} & \mathbf{m_r} \cdot \mathbf{n_2} & \cdots & \mathbf{m_r} \cdot \mathbf{n_b} \end{pmatrix}$$

Example

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

Likewise

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

ORDER of multiplication matters! Indeed, consider C_{3x5} D_{5x5} which gives a 3 x 5 matrix, versus D_{5x5} C_{3x5} , which is not defined.

Matrix multiplication in R

```
> A<-matrix(c(1,2,3,4),nrow=2)
> B<-matrix(c(4,5,6,7),nrow=2)
> A
     [,1] [,2]
[1,]    1    3
[2,]    2    4
> B
     [,1] [,2]
[1,]    4    6
[2,]    5    7
> A %*% B
     [,1] [,2]
[1,]   19   27
[2,]   28   40
```

R fills in the matrix from the list c by filling in as columns, here with 2 rows (nrow=2)

Entering A or B displays what was entered (always a good thing to check)

The command %*% is the R code for the multiplication of two matrices

On your own: What is the matrix resulting from BA?
What is A if nrow=1 or nrow=4 is used?

PAUSE

- Matrix multiplication arises as a way to compactly write systems of equations
- Indeed, much of linear algebra has deep roots in systems of equations, as we will now explore.
- Next pause at slide 27

The Transpose of a Matrix

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

Useful identities

$(AB)^T = B^T A^T$

$(ABC)^T = C^T B^T A^T$

$$\mathbf{a} = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}$$

Inner product = $a^T b = a^T_{(1 \times n)} b_{(n \times 1)}$

Indices match, matrices conform

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

$$\begin{pmatrix} a_1 & \cdots & a_n \end{pmatrix} \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} = \mathbf{a}^T \mathbf{b} = \sum_{i=1}^{n} a_i b_i$$

Note that $b^T a = (b^T a)^T = a^T b$

Outer product = ab^T = a $_{(n \times 1)}$ b^T $_{(1 \times n)}$

Resulting product is an n x n matrix

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \begin{pmatrix} b_1 & b_2 & \cdots & b_n \end{pmatrix}$$

$$= \begin{pmatrix} a_1 b_1 & a_1 b_2 & \dots & a_1 b_n \\ a_2 b_1 & a_2 b_2 & \dots & a_2 b_n \\ \vdots & \vdots & \ddots & \vdots \\ a_n b_1 & a_n b_2 & \dots & a_n b_{bn} \end{pmatrix}$$

R code for transposition

```
> t(A)
     [,1] [,2]
[1,]    1    2
[2,]    3    4
>
```

t(A) = transpose of A

```
> a<-matrix(c(1,2,3),nrow=3)
> a
     [,1]
[1,]    1
[2,]    2
[3,]    3
> t(a) %*% a
     [,1]
[1,]   14
> a %*% t(a)
     [,1] [,2] [,3]
[1,]    1    2    3
[2,]    2    4    6
[3,]    3    6    9
```

Enter the column vector a

Compute inner product $\mathbf{a}^T\mathbf{a}$

Compute outer product $\mathbf{a}\mathbf{a}^T$

Solving equations

- The identity matrix **I**
  - Serves the same role as 1 in scalar algebra, e.g., $a*1=1*a=a$, with $\mathbf{AI}=\mathbf{IA}=\mathbf{A}$
- The inverse matrix $\mathbf{A}^{-1}$ (IF it exists)
  - Defined by $\mathbf{A}\,\mathbf{A}^{-1} = \mathbf{I}$, $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$
  - 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 $\mathbf{Ax} = \mathbf{c}$, $A^{-1}\mathbf{Ax} = A^{-1}\,\mathbf{c}$
    - Or $\mathbf{A}^{-1}\mathbf{Ax} = \mathbf{Ix} = \mathbf{x} = A^{-1}\,\mathbf{c}$

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.

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

$$\mathbf{I}_{3x3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The Identity Matrix in R

diag(k), where k is an integer, return the k x k I matrix

```
> I<-diag(4)
> I
     [,1] [,2] [,3] [,4]
[1,]    1    0    0    0
[2,]    0    1    0    0
[3,]    0    0    1    0
[4,]    0    0    0    1
> I2 <-diag(2)
> I2
     [,1] [,2]
[1,]    1    0
[2,]    0    1
```

The Inverse Matrix, A^{-1}

For a square matrix A, define its Inverse A^{-1}, as the matrix satisfying

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$$

For $\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ $\mathbf{A}^{-1} = \frac{1}{ad - bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

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 $x_2 + x_3 = 6$)

Inversion in R

solve(A) computes A^{-1}

det(A) computes determinant of **A**

Using **A** entered earlier

```
> A
     [,1] [,2]
[1,]    1    3
[2,]    2    4
> solve(A)
     [,1] [,2]
[1,]   -2  1.5
[2,]    1 -0.5
> solve(A) %*% A
     [,1]          [,2]
[1,]    1 -8.881784e-16
[2,]    0  1.000000e+00
> det(A)
[1] -2
```

Compute A^{-1}

Showing that $A^{-1} A = I$

Computing determinant of A

Homework

Put the following system of equations in matrix form, and solve using R

$$
\begin{aligned}
3x_1 + 4x_2 + 4\,x_3 + 6x_4 &= -10 \\
9x_1 + 2x_2 - x_3 - 6x_4 &= 20 \\
x_1 + x_2 + x_3 - 10x_4 &= 2 \\
2x_1 + 9x_2 + 2x_3 - x_4 &= -10
\end{aligned}
$$

PAUSE

- One can think of the inverse of a square matrix **A** as the unique solution to its corresponding set of equations.
- The determinant of **A** informs us as to whether such a unique solution exists
- As we will now see, the eigenstructure (geometry) of **A** provides a deeper understanding of nature of solutions, especially when det(**A**)= 0.
- Next pause at slide 35

Useful identities

$$(\mathbf{A}^T)^{-1} = (\mathbf{A}^{-1})^T$$

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\,\mathbf{A}^{-1}$$

For a diagonal matrix **D**, then det (**D**), which is also denoted by |**D**|, = product of the diagonal elements

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

$$\mathbf{Ae} = \lambda\mathbf{e}$$

If A is n x n, solutions to λ are an n-degree polynomial. **e** is the eigenvector associated with λ. If any of the roots to the equation are zero, A^{-1} is not defined. In this case, for some linear combination **b**, we have **Ab** = 0.

Variance-Covariance matrix

- A very important square matrix is the variance-covariance matrix **V** associated with a vector **x** of random variables.
- $V_{ij} = Cov(x_i, x_j)$, 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

The trace

The trace, tr(**A**) or trace(**A**), of a square matrix A is simply the sum of its diagonal elements

The importance of the trace is that it equals the sum of the eigenvalues of **A**, tr(**A**) = $\sum \lambda_i$

For a covariance matrix **V**, tr(V) measures the total amount of variation in the variables

λ_i / tr(**V**) is the fraction of the total variation in x contained in the linear combination $\mathbf{e}_i^T\mathbf{x}$, where $\mathbf{e}_i$, the i-th principal component of **V** is also the i-th eigenvector of **V** ($\mathbf{V}\mathbf{e}_i = \lambda_i\, \mathbf{e}_i$)

Eigenstructure in R

`eigen(A)` returns the eigenvalues and vectors of A

```
> V<-matrix(c(10,-5,10,-5,20,0,10,0,30),nrow=3)
> V
     [,1] [,2] [,3]
[1,]   10   -5   10
[2,]   -5   20    0
[3,]   10    0   30
> eigen(V)
$values
[1] 34.410103 21.117310  4.472587

$vectors
           [,1]       [,2]       [,3]
[1,]  0.3996151  0.2117936  0.8918807
[2,] -0.1386580 -0.9477830  0.2871955
[3,]  0.9061356 -0.2384340 -0.3493816
```

PC 1   PC 2

Trace = 60

PC 1 accounts for 34.4/60 = 57% of all the variation

$0.400^* x_1 - 0.139^* x_2 + 0.906^* x_3$

$0.212^* x_1 - 0.948^* x_2 - 0.238^* x_3$

Quadratic and Bilinear Forms

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

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i x_j$$

Scalar (1 x 1)

Bilinear Form (generalization of quadratic product)
for $A_{m \times n}$, $a_{n \times 1}$, $b_{m \times 1}$ their bilinear form is $b^T_{1 \times m} A_{m \times n} a_{n \times 1}$

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

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

Covariance Matrices for Transformed Variables

What is the variance of the linear combination, $c_1x_1 + c_2x_2 + \ldots + c_nx_n$? (note this is a scalar)

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

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

$$= \mathbf{c}^T\mathbf{V}\,\mathbf{c}$$

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

$$\sigma(\mathbf{a}^T\mathbf{x}, \mathbf{b}^T\mathbf{x}) = \mathbf{a}^T\mathbf{V}\,\mathbf{b}$$

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 indices
$y_1 = x_1 - 2x_2 + 5x_3$ and $y_2 = 6x_2 - 4x_3$?

$$\mathbf{V} = \begin{pmatrix} 10 & -5 & 10 \\ -5 & 20 & 0 \\ 10 & 0 & 30 \end{pmatrix}, \quad \mathbf{c}_1 = \begin{pmatrix} 1 \\ -2 \\ 5 \end{pmatrix}, \quad \mathbf{c}_2 = \begin{pmatrix} 0 \\ 6 \\ -4 \end{pmatrix}$$

$\mathrm{Var}(y_1) = \mathrm{Var}(c_1^T x) = c_1^T \mathrm{Var}(x)\, c_1 = 960$

$\mathrm{Var}(y_2) = \mathrm{Var}(c_2^T x) = c_2^T \mathrm{Var}(x)\, c_2 = 1200$

$\mathrm{Cov}(y_1, y_2) = \mathrm{Cov}(c_1^T x, c_2^T x) = c_1^T \mathrm{Var}(x)\, c_2 = -910$

Homework: use R to compute the above values

PAUSE

The concepts of inverses, quadratic products, eigenstructure, and covariance matrices form the foundation to explore the multivariate normal (MVN) distribution

- This distribution underpins much of linear and mixed models theory and we will extensively use it properties
  - PCs
  - Regressions and conditional expectations
- Next pause at slide 53

The Multivariate Normal Distribution (MVN)

Consider the pdf for n independent normal random variables, the ith of which has mean μ_i and variance σ^2_i

$$p(\mathbf{x}) = \prod_{i=1}^{n} (2\pi)^{-1/2} \sigma_i^{-1} \exp\left(- \frac{(x_i - \mu_i)^2}{2\,\sigma_i^2} \right)$$

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

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

$$\mathbf{V} = \begin{pmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \cdots & \sigma_n^2 \end{pmatrix} \qquad |\mathbf{V}| = \prod_{i=1}^{n} \sigma_i^2$$

Define the mean vector μ by gives

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

$$\sum_{i=1}^{n} \frac{(x_i - \mu_i)^2}{\sigma_i^2} = (\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

Hence in matrix from the MVN pdf becomes

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

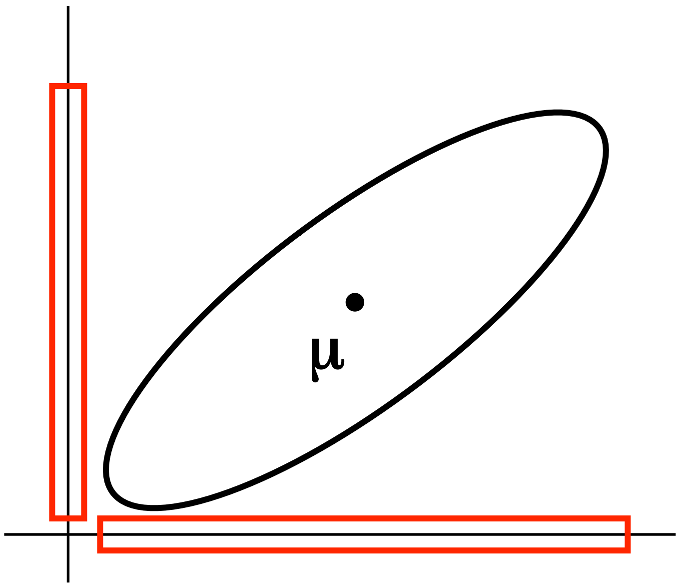
Notice this holds for any vector μ and symmetric positive -definite matrix V, as | V | > 0.

The multivariate normal

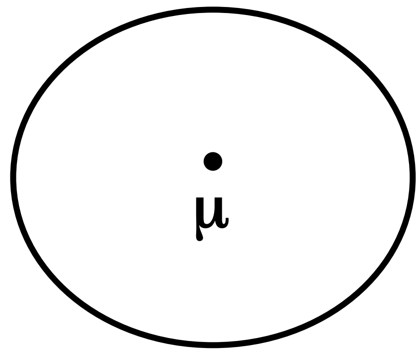
- Just as a univariate normal is defined by its mean and spread, a multivariate normal is defined by its mean vector $\boldsymbol{\mu}$ (also called the centroid) and variance -covariance matrix **V**

Vector of means $\boldsymbol{\mu}$ determines location

Spread (geometry) about $\boldsymbol{\mu}$ determined by **V**



x_1, x_2 equal variances, positively correlated

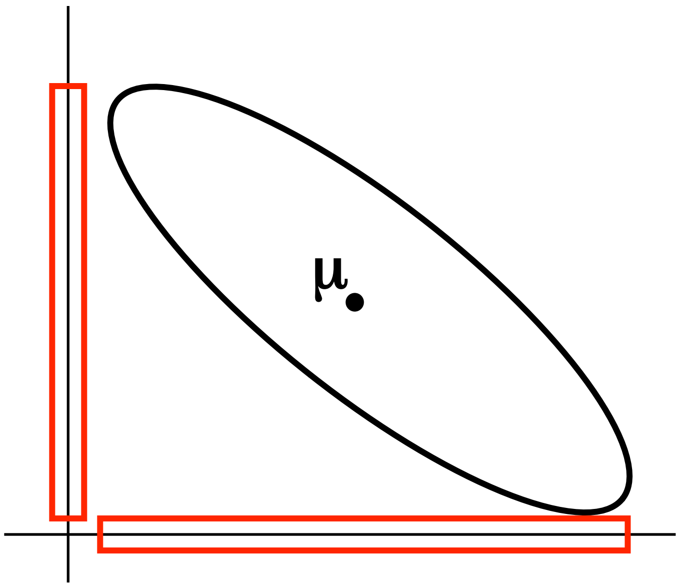


x_1, x_2 equal variances, uncorrelated

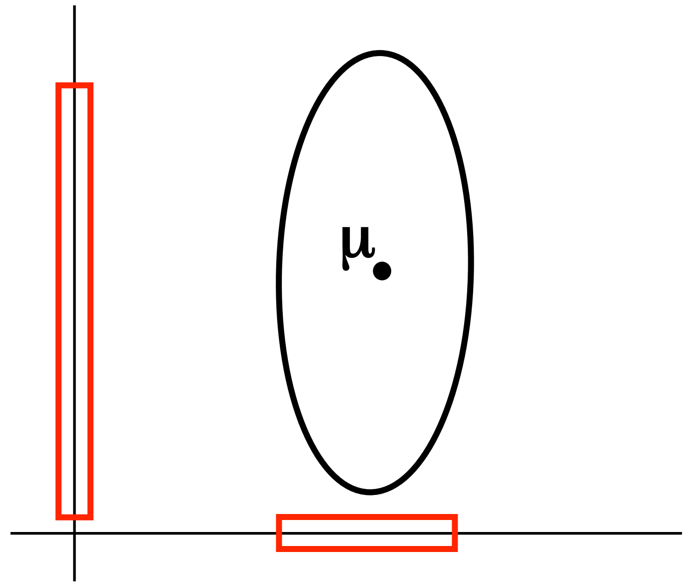
Eigenstructure (the eigenvectors and their corresponding eigenvalues) determines the geometry of **V**.

Vector of means $\boldsymbol{\mu}$ determines location

Spread (geometry) about $\boldsymbol{\mu}$ determined by **V**



x_1, x_2 equal variances, negatively correlated

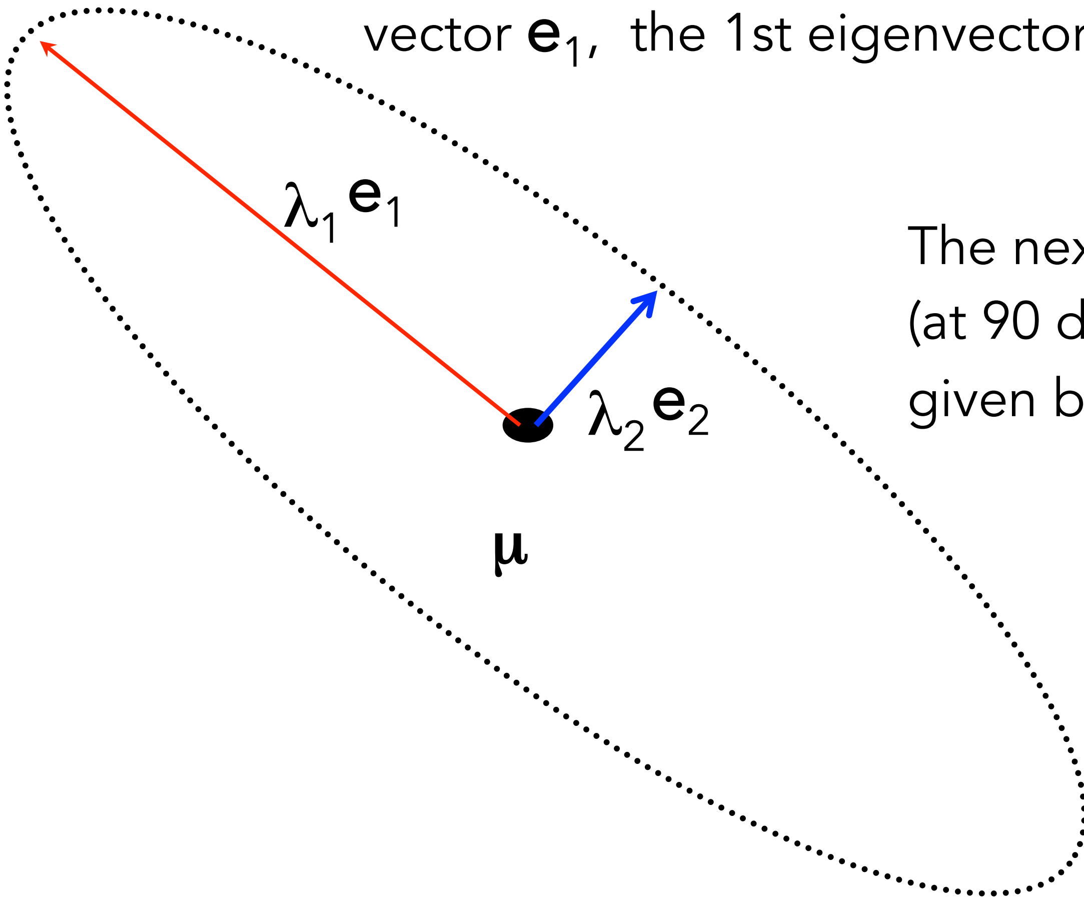


$\mathrm{Var}(x_1) < \mathrm{Var}(x_2)$, uncorrelated

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 $\mathbf{e}_1$, the 1st eigenvector of V.



The next largest axis of orthogonal (at 90 degrees from) $\mathbf{e}_1$, is given by $\mathbf{e}_2$, the 2nd eigenvector

Principal components

- The principal components (or PCs) of a covariance matrix define the axes of variation.
  - PC1 is the direction (linear combination $\mathbf{c}^T\mathbf{x}$) that explains the most variation.
  - PC2 is the next largest direction (at 90 degree from PC1), and so on
- PC_i = ith eigenvector of V
- Fraction of variation accounted for by PCi = λ_i / trace(V)
- If V has a few large eigenvalues, most of the variation is distributed along a few linear combinations (axis of variation)
- The singular value decomposition is the generalization of this idea to nonsquare matrices

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** ~ MVN(μ,V)

$$\text{for} \quad \mathbf{y} = \mathbf{x} + \mathbf{a}, \qquad \mathbf{y} \text{ is } \mathrm{MVN}_n(\boldsymbol{\mu} + \mathbf{a}, \mathbf{V})$$

$$\text{for} \quad y = \mathbf{a}^T\mathbf{x} = \sum_{k=1}^{n} a_i x_i, \qquad y \text{ is } \mathrm{N}(\mathbf{a}^T\boldsymbol{\mu}, \mathbf{a}^T\mathbf{V}\,\mathbf{a})$$

$$\text{for} \quad \mathbf{y} = \mathbf{A}\mathbf{x}, \qquad \mathbf{y} \text{ is } \mathrm{MVN}_m\left(\mathbf{A}\boldsymbol{\mu}, \mathbf{A}^T\mathbf{V}\mathbf{A}\right)$$

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)

$$\mathbf{x} = \begin{pmatrix} \mathbf{x_1} \\ \mathbf{x_2} \end{pmatrix} \quad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu_1} \\ \boldsymbol{\mu_2} \end{pmatrix} \quad \text{and} \quad \mathbf{V} = \begin{pmatrix} \mathbf{V_{x_1x_1}} & \mathbf{V_{x_1x_2}} \\ \mathbf{V^T_{x_1x_2}} & \mathbf{V_{x_2x_2}} \end{pmatrix}$$

$x_1 \mid x_2$ is MVN with m-dimensional mean vector

$$\boldsymbol{\mu}_{\mathbf{x_1|x_2}} = \boldsymbol{\mu_1} + \mathbf{V_{x_1x_2}} \mathbf{V^{-1}_{x_2x_2}} (\mathbf{x_2} - \boldsymbol{\mu_2})$$

and m x m covariance matrix

$$\mathbf{V_{x_1|x_2}} = \mathbf{V_{x_1x_1}} - \mathbf{V_{x_1x_2}} \mathbf{V^{-1}_{x_2x_2}} \mathbf{V^T_{x_1x_2}}$$

Properties of the MVN - III

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

$$\mathbf{x_1} = \boldsymbol{\mu}_{\mathbf{x_1}|\mathbf{x_2}} + \mathbf{e}$$
$$= \boldsymbol{\mu}_\mathbf{1} + \mathbf{V}_{\mathbf{x_1 x_2}} \mathbf{V}^{-1}_{\mathbf{x_2 x_2}} (\mathbf{x_2} - \boldsymbol{\mu}_\mathbf{2}) + \mathbf{e}$$

Where e is MVN with mean vector **0** and variance-covariance matrix $\mathbf{V}_{\mathbf{x_1}|\mathbf{x_2}}$

$$\boldsymbol{\mu_1} + \mathbf{V_{x_1x_2}} \mathbf{V^{-1}_{x_2x_2}} (\mathbf{x_2} - \boldsymbol{\mu_2}) + \mathbf{e}$$

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

$$\mathbf{V_{x_1|x_2}} = \mathbf{V_{x_1x_1}} - \mathbf{V_{x_1x_2}} \mathbf{V^{-1}_{x_2x_2}} \mathbf{V^{T}_{x_1x_2}}$$

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

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,

$$\begin{pmatrix} z_o \\ z_s \\ z_d \end{pmatrix} \sim \mathrm{MVN}\left[\begin{pmatrix} \mu_0 \\ \mu_s \\ \mu_d \end{pmatrix}, \sigma_z^2 \begin{pmatrix} 1 & h^2/2 & h^2/2 \\ h^2/2 & 1 & 0 \\ h^2/2 & 0 & 1 \end{pmatrix} \right]$$

Let $\mathbf{x_1} = (\, z_o \,), \quad \mathbf{x_2} = \begin{pmatrix} z_s \\ z_d \end{pmatrix}$

$$\mathbf{V}_{\mathbf{x}_1,\mathbf{x}_1} = \sigma_z^2, \quad \mathbf{V}_{\mathbf{x}_1,\mathbf{x}_2} = \frac{h^2\sigma_z^2}{2}(\,1 \quad 1\,), \quad \mathbf{V}_{\mathbf{x}_2,\mathbf{x}_2} = \sigma_z^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \boldsymbol{\mu}_1 + \mathbf{V}_{\mathbf{x}_1\mathbf{x}_2}\mathbf{V}_{\mathbf{x}_2\mathbf{x}_2}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2) + \mathbf{e}$$

Regression of Offspring value on Parental values (cont.)

$$= \boldsymbol{\mu}_1 + \mathbf{V}_{\mathbf{x}_1\mathbf{x}_2}\mathbf{V}^{-1}_{\mathbf{x}_2\mathbf{x}_2}(\mathbf{x}_2 - \boldsymbol{\mu}_2) + \mathbf{e}$$

$$\mathbf{V}_{\mathbf{x}_1,\mathbf{x}_1} = \sigma_z^2, \quad \mathbf{V}_{\mathbf{x}_1,\mathbf{x}_2} = \frac{h^2\sigma_z^2}{2}\begin{pmatrix} 1 & 1 \end{pmatrix}, \quad \mathbf{V}_{\mathbf{x}_2,\mathbf{x}_2} = \sigma_z^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Hence,

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

Where e is normal with mean zero and variance

$$\mathbf{V}_{\mathbf{x}_1|\mathbf{x}_2} = \mathbf{V}_{\mathbf{x}_1\mathbf{x}_1} - \mathbf{V}_{\mathbf{x}_1\mathbf{x}_2}\mathbf{V}^{-1}_{\mathbf{x}_2\mathbf{x}_2}\mathbf{V}^{T}_{\mathbf{x}_1\mathbf{x}_2}$$

$$\begin{aligned} \sigma_e^2 &= \sigma_z^2 - \frac{h^2\sigma_z^2}{2}\begin{pmatrix} 1 & 1 \end{pmatrix}\sigma_z^{-2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\frac{h^2\sigma_z^2}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ &= \sigma_z^2\left(1 - \frac{h^4}{2}\right) \end{aligned}$$

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

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

where the residual e is normal with mean zero and $\text{Var}(e) = \sigma_z^2(1-h^4/2)$

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

$$\begin{aligned} A_o &= \mu_o + (A_s - \mu_s)/2 + (A_d - \mu_d)/2 + e \\ &= A_s/2 + A_d/2 + e \end{aligned}$$

where the residual e is normal with mean zero and $\text{Var}(e) = \sigma_A^2/2$

Additional R matrix commands

Operator or Function	Description
A * B	Element-wise multiplication
A %*% B	Matrix multiplication
A %o% B	Outer product. **AB'**
crossprod(A,B) **crossprod(A)**	**A'B** and **A'A** respectively.
t(A)	Transpose
diag(x)	Creates diagonal matrix with elements of **x** in the principal diagonal
diag(A)	Returns a vector containing the elements of the principal diagonal
diag(k)	If k is a scalar, this creates a k x k identity matrix. Go figure.
solve(A, b)	Returns vector **x** in the equation **b** = **Ax** (i.e., **A**$^{-1}$**b**)
solve(A)	Inverse of **A** where A is a square matrix.
ginv(A)	Moore-Penrose Generalized Inverse of **A**. ginv(A) requires loading the **MASS** package.
y<-eigen(A)	**y$val** are the eigenvalues of **A** **y$vec** are the eigenvectors of **A**
y<-svd(A)	Single value decomposition of **A**. **y$d** = vector containing the singular values of **A** **y$u** = matrix with columns contain the left singular vectors of **A** **y$v** = matrix with columns contain the right singular vectors of **A**

Additional R matrix commands (cont)

R <- chol(A)	Choleski factorization of **A**. Returns the upper triangular factor, such that **R'R** = **A**.
y <- qr(A)	QR decomposition of **A**. **y$qr** has an upper triangle that contains the decomposition and a lower triangle that contains information on the Q decomposition. **y$rank** is the rank of A. **y$qraux** a vector which contains additional information on Q. **y$pivot** contains information on the pivoting strategy used.
cbind(A,B,...)	Combine matrices(vectors) horizontally. Returns a matrix.
rbind(A,B,...)	Combine matrices(vectors) vertically. Returns a matrix.
rowMeans(A)	Returns vector of row means.
rowSums(A)	Returns vector of row sums.
colMeans(A)	Returns vector of column means.
colSums(A)	Returns vector of coumn means.

Additional references

- Lynch & Walsh Chapter 8 (intro to matrices)
- Walsh and Lynch,
  - Appendix 5 (Matrix geometry)
  - Appendix 6 (Matrix derivatives)

PAUSE

- Many of the key results in linear and mixed models arise by considering the regression of one subset of a vector of random variable on another (slides 44-46)
- We conclude with a few optional slides on the singular value decomposition, the generalization of eigenstructure to any matrix (such as nonsquare matrices).
- The SVD arises when consider certain G x E problems.

The Singular-Value Decomposition (SVD)

An $n \times p$ matrix $\mathbf{A}$ can always be decomposed as the product of three matrices: an $n \times p$ diagonal matrix $\boldsymbol{\Lambda}$ and two unitary matrices, $\mathbf{U}$ which is $n \times n$ and $\mathbf{V}$ which is $p \times p$. The resulting **singular value decomposition** (SVD) of $\mathbf{A}$ is given by

$$\mathbf{A}_{n\times p} = \mathbf{U}_{n\times n}\boldsymbol{\Lambda}_{n\times p}\mathbf{V}^T_{p\times p} \tag{39.16a}$$

We have indicated the dimensionality of each matrix to allow the reader to verify that each matrix multiplication conforms. The diagonal elements $\lambda_1, \cdots, \lambda_s$ of $\boldsymbol{\Lambda}$ correspond to the **singular values** of $\mathbf{A}$ and are ordered by decreasing magnitude. Returning to the unitary matrices $\mathbf{U}$ and $\mathbf{V}$, we can write each as a row vector of column vectors,

$$\mathbf{U} = (\mathbf{u}_1, \cdots, \mathbf{u}_i, \cdots \mathbf{u}_n), \qquad \mathbf{V} = (\mathbf{v}_1, \cdots, \mathbf{v}_i, \cdots \mathbf{v}_p) \tag{39.16b}$$

where $\mathbf{u}_i$ and $\mathbf{v}_i$ are n and p-dimensional column vectors (often called the **left** and **right singular vectors**, respectively). Since both $\mathbf{U}$ and $\mathbf{V}$ are unitary, by definition (Appendix 4) each column vector has length one and are mutually orthogonal (i.e., if $i \neq j$, $\mathbf{u}_i\mathbf{u}_j^T = \mathbf{v}_i\mathbf{v}_j^T = 0$). Since $\boldsymbol{\Lambda}$ is diagonal, it immediately follows from matrix multiplication that we can write any element in $\mathbf{A}$ as

$$A_{ij} = \sum_{k=1}^{s} \lambda_k \, u_{ik} \, v_{kj} \tag{39.16c}$$

where λ_k is the kth singular value and $s \leq \min(p, n)$ is the number of non-zero singular values.

The importance of the singular value decomposition in the analysis of G×E arises from the **Eckart-Young theorem** (1938), which relates the best approximation of a matrix by some lower-rank (say k) matrix with the SVD. Define as our measure of goodness of fit between a matrix $\mathbf{A}$ and a lower rank approximation $\widehat{\mathbf{A}}$ as the sum of squared differences over all elements,

$$\sum_{ij} (A_{ij} - \hat{A}_{ij})^2$$

Eckart and Young show that the best fitting approximation $\widehat{\mathbf{A}}$ of rank $m < s$ is given from the first m terms of the singular value decomposition (the **rank-m SVD**),

$$\hat{A}_{ij} = \sum_{k=1}^{m} \lambda_k \, u_{ik} \, v_{kj} \tag{39.17a}$$

For example, the best rank-2 approximation for the G×E interaction is given by

$$GE_{ij} \simeq \lambda_1 \, u_{i1} \, v_{j1} + \lambda_2 \, u_{i2} \, v_{j2} \tag{39.17b}$$

where λ_i is the ith singular value of the $\mathbf{GE}$ matrix, $\mathbf{u}$ and $\mathbf{v}$ are the associated singular vectors (see Example 39.3). The fraction of total variation of a matrix accounted for by taking the first m terms in its SVD is

$$\sum_{k=1}^{m} \lambda_k^2 \Big/ \sum_{ij} A_{ij}^2 = \frac{\lambda_1^2 + \cdots + \lambda_m^2}{\lambda_1^2 + \cdots + \lambda_s^2}$$

A data set for soybeans grown in New York (Gauch 1992) gives the GE matrix as

$$\mathbf{GE} = \begin{pmatrix} 57 & 176 & -233 \\ -36 & -196 & 233 \\ -45 & -324 & 369 \\ -66 & 178 & -112 \\ 89 & 165 & -254 \end{pmatrix}$$

Where GE_{ij} = value for Genotype i in envir. j

In **R**, the compact SVD (Equation 39.16d) of a matrix X is given by **svd(X)**, returning the SVD of $\mathbf{GE}$ as

$$\begin{pmatrix} 0.40 & 0.21 & 0.18 \\ -0.41 & 0.00 & 0.91 \\ -0.66 & 0.12 & -0.30 \\ 0.26 & -0.83 & 0.11 \\ 0.41 & 0.50 & 0.19 \end{pmatrix} \begin{pmatrix} 746.10 & 0 & 0 \\ 0 & 131.36 & 0 \\ 0 & 0 & 0.53 \end{pmatrix} \begin{pmatrix} 0.12 & 0.64 & -0.76 \\ 0.81 & -0.51 & -0.30 \\ 0.58 & 0.58 & 0.58 \end{pmatrix}$$

The first singular value accounts for $746.10^2/(743.26^2 + 131.36^2 + 0.53^2) = 97.0\%$ of the total variation of $\mathbf{GE}$, while the second singular value accounts for 3.0%, so that together they account for essentially all of the total variation. The rank-1 SVD approximation of $\mathbf{GE}$ is given by setting all of the diagonal elements of $\boldsymbol{\Lambda}$ except the first entry to zero,

$$\mathbf{GE}_1 = \begin{pmatrix} 0.40 & 0.21 & 0.18 \\ -0.41 & 0.00 & 0.91 \\ -0.66 & 0.12 & -0.30 \\ 0.26 & -0.83 & 0.11 \\ 0.41 & 0.50 & 0.19 \end{pmatrix} \begin{pmatrix} 746.10 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0.12 & 0.64 & -0.76 \\ 0.81 & -0.51 & -0.30 \\ 0.58 & 0.58 & 0.58 \end{pmatrix}$$

Similarly, the rank-2 SVD is given by setting all but the first two singular values to zero,

$$\mathbf{GE}_2 = \begin{pmatrix} 0.40 & 0.21 & 0.18 \\ -0.41 & 0.00 & 0.91 \\ -0.66 & 0.12 & -0.30 \\ 0.26 & -0.83 & 0.11 \\ 0.41 & 0.50 & 0.19 \end{pmatrix} \begin{pmatrix} 746.10 & 0 & 0 \\ 0 & 131.36 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0.12 & 0.64 & -0.76 \\ 0.81 & -0.51 & -0.30 \\ 0.58 & 0.58 & 0.58 \end{pmatrix}$$

For example, the rank-1 SVD approximation for GE_{32} is $g_{31}\lambda_1 e_{12}$ = 746.10*(-0.66)*0.64 = -315

While the rank-2 SVD approximation is $g_{31}\lambda_2 e_{12} + g_{32}\lambda_2 e_{22}$ = 746.10*(-0.66)*0.64 + 131.36* 0.12*(-0.51) = -323

Actual value is -324

Generally, the rank-2 SVD approximation for GE_{ij} is $g_{i1}\lambda_1 e_{1j} + g_{i2}\lambda_2 e_{2j}$