

# Lecture 1: Intro/refresher in Matrix Algebra

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SISG -Mixed Model Course  
version 28 June 2012

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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
  - $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$  is the general linear model
    - OLS solution:  $\boldsymbol{\beta} = (\mathbf{X}^T\mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$
  - $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{a} + \mathbf{e}$  is the general mixed model

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## 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)

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## Matrices: An array of elements

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

Usually written in bold lowercase, e.g.  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$

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

Column vector

(3 x 1)

Row vector

(1 x 4)

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

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## 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) (3 x 2)

Square matrix

Dimensionality of a matrix:  $r \times c$  (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  $j$

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## Partitioned Matrices

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

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

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

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

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## 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:  $(\mathbf{A}+\mathbf{B})_{ij} = \mathbf{A}_{ij} + \mathbf{B}_{ij}$

Matrix subtraction:  $(\mathbf{A}-\mathbf{B})_{ij} = \mathbf{A}_{ij} - \mathbf{B}_{ij}$

Examples:

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

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

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$$\mathbf{C} = \begin{pmatrix} 3 & 1 & 2 \\ 2 & 5 & 4 \\ 1 & 1 & 2 \end{pmatrix} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \mathbf{r}_3 \end{pmatrix} \quad \text{A column vector whose elements are row vectors}$$

$$\mathbf{r}_1 = (3 \ 1 \ 2)$$

$$\mathbf{r}_2 = (2 \ 5 \ 4)$$

$$\mathbf{r}_3 = (1 \ 1 \ 2)$$

$$\mathbf{C} = \begin{pmatrix} 3 & 1 & 2 \\ 2 & 5 & 4 \\ 1 & 1 & 2 \end{pmatrix} = (\mathbf{c}_1 \ \mathbf{c}_2 \ \mathbf{c}_3) \quad \text{A row vector whose elements are column vectors}$$

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

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## 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:

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

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

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Matrices are compact ways to write systems of equations

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

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

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

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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  $\beta_i$

$$\sigma(y, z_1) = \beta_1 \sigma^2(z_1) + \beta_2 \sigma(z_1, z_2) + \cdots + \beta_n \sigma(z_1, z_n)$$

$$\sigma(y, z_2) = \beta_1 \sigma(z_1, z_2) + \beta_2 \sigma^2(z_2) + \cdots + \beta_n \sigma(z_2, z_n)$$

$$\vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \ddots \quad \quad \quad \vdots$$

$$\sigma(y, z_n) = \beta_1 \sigma(z_1, z_n) + \beta_2 \sigma(z_2, z_n) + \cdots + \beta_n \sigma^2(z_n)$$

This can be more compactly written in matrix form as

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

$\mathbf{X}^T \mathbf{X}$

$\boldsymbol{\beta}$

$\mathbf{X}^T \mathbf{y}$

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

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## 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  $\mathbf{B}$ .

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

$i$ -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 matrix  $\mathbf{A}$

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

$$C_{(rxc)} = A_{(rxk)} B_{(kxc)}$$

Inner indices must match  
columns of A = rows of B

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

$$A_{3 \times 5} B_{5 \times 9} C_{9 \times 6} D_{6 \times 23}$$

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

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## 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  $C_{3 \times 5} D_{5 \times 5}$  which gives a 3 x 5 matrix, versus  $D_{5 \times 5} C_{3 \times 5}$ , which is not defined

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More formally, consider the product  $L = MN$

Express the matrix M as a column vector of row vectors

$$M = \begin{pmatrix} \mathbf{m}_1 \\ \mathbf{m}_2 \\ \vdots \\ \mathbf{m}_r \end{pmatrix} \quad \text{where} \quad \mathbf{m}_i = (M_{i1} \quad M_{i2} \quad \dots \quad M_{ic})$$

Likewise express N as a row vector of column vectors

$$N = (\mathbf{n}_1 \quad \mathbf{n}_2 \quad \dots \quad \mathbf{n}_b) \quad \text{where} \quad \mathbf{n}_j = \begin{pmatrix} N_{1j} \\ N_{2j} \\ \vdots \\ N_{cj} \end{pmatrix}$$

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

$$L = \begin{pmatrix} \mathbf{m}_1 \cdot \mathbf{n}_1 & \mathbf{m}_1 \cdot \mathbf{n}_2 & \dots & \mathbf{m}_1 \cdot \mathbf{n}_b \\ \mathbf{m}_2 \cdot \mathbf{n}_1 & \mathbf{m}_2 \cdot \mathbf{n}_2 & \dots & \mathbf{m}_2 \cdot \mathbf{n}_b \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{m}_r \cdot \mathbf{n}_1 & \mathbf{m}_r \cdot \mathbf{n}_2 & \dots & \mathbf{m}_r \cdot \mathbf{n}_b \end{pmatrix}$$

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## The Transpose of a Matrix

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

Useful identities

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

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

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

$$\text{Inner product} = \mathbf{a}^T \mathbf{b} = \mathbf{a}_{(1 \times n)}^T \mathbf{b}_{(n \times 1)}$$

**Indices match, matrices conform**

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

$$(a_1 \quad \dots \quad a_n) \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} = \mathbf{a}^T \mathbf{b} = \sum_{i=1}^n a_i b_i \quad \text{Note that } \mathbf{b}^T \mathbf{a} = (\mathbf{b}^T \mathbf{a})^T = \mathbf{a}^T \mathbf{b}$$

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

Resulting product is an  $n \times n$  matrix

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

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## Solving equations

- The identity matrix **I**
  - Serves the same role as 1 in scalar algebra, e.g.,  $a \cdot 1 = 1 \cdot a = a$ , 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  $(1/a) \cdot ax = (1/a)c$  or  $(1/a) \cdot a \cdot x = 1 \cdot x = x$ ,
    - Hence  $x = (1/a)c$
    - To solve  $\mathbf{Ax} = \mathbf{c}$ ,  $\mathbf{A}^{-1} \mathbf{Ax} = \mathbf{A}^{-1} \mathbf{c}$
    - Or  $\mathbf{A}^{-1} \mathbf{Ax} = \mathbf{Ix} = \mathbf{x} = \mathbf{A}^{-1} \mathbf{c}$

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## The Identity Matrix, **I**

The identity matrix serves the role of the number 1 in matrix multiplication:  $\mathbf{AI} = \mathbf{A}$ ,  $\mathbf{IA} = \mathbf{A}$

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

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

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

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## The Inverse Matrix, $\mathbf{A}^{-1}$

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

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

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.

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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  $x_2 + x_3 = 6$ )

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

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

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,

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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  $\sigma(z_1, z_2) = \rho_{12} \sigma(z_1)\sigma(z_2)$

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

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

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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

$$Ae = \lambda e$$

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 some linear combination  $b$ , we have  $Ab = 0$ .  $e$  is the **eigenvector** associated with  $\lambda^2$

## Variance-Covariance matrix

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

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## The trace

The **trace**,  $\text{tr}(\mathbf{A})$  or **trace**( $\mathbf{A}$ ), of a square matrix  $\mathbf{A}$  is simply the sum of its diagonal elements

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

For a covariance matrix  $\mathbf{V}$ ,  $\text{tr}(\mathbf{V})$  measures the total amount of variation in the variables

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

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## Quadratic and Bilinear Forms

**Quadratic product**: for  $\mathbf{A}_{n \times n}$  and  $\mathbf{x}_{n \times 1}$

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

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

for  $\mathbf{A}_{m \times n}$ ,  $\mathbf{a}_{n \times 1}$ ,  $\mathbf{b}_{m \times 1}$  their bilinear form is  $\mathbf{b}^T \mathbf{A} \mathbf{a}$

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

Note that  $\mathbf{b}^T \mathbf{A} \mathbf{a} = \mathbf{a}^T \mathbf{A}^T \mathbf{b}$

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## Covariance Matrices for Transformed Variables

What is the variance of the linear combination,  $c_1 x_1 + c_2 x_2 + \dots + c_n x_n$ ? (note this is a scalar)

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

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

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

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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

$$y_1 = x_1 - 2x_2 + 5x_3 \text{ and } y_2 = 6x_2 - 4x_3?$$

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

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

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

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

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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 =  $AVB^T$

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

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

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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  $\text{Var}(c^T x) = c^T V c \geq 0$ .
- 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  $\sigma_i^2$

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

This can be expressed more compactly in matrix form

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Define the **covariance matrix**  $V$  for the vector  $x$  of the  $n$  normal random variable by

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

Define the mean vector  $\mu$  by

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{pmatrix} \quad \sum_{i=1}^n \frac{(x_i - \mu_i)^2}{\sigma_i^2} = (x - \mu)^T V^{-1} (x - \mu)$$

Hence in matrix form from 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  $|V| > 0$ .

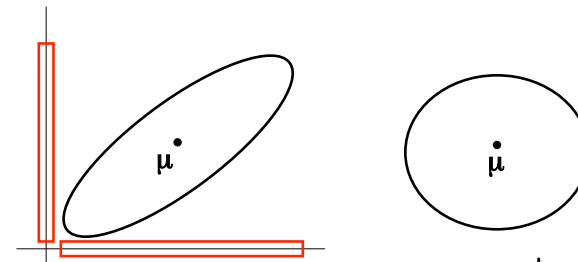
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## The multivariate normal

- 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  $V$

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Vector of means  $\mu$  determines location  
Spread (geometry) about  $\mu$  determined by  $V$



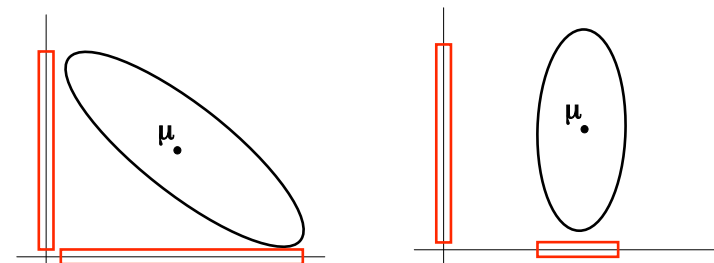
$x_1, x_2$  equal variances,  
positively correlated

$x_1, x_2$  equal variances,  
uncorrelated

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

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Vector of means  $\mu$  determines location  
Spread (geometry) about  $\mu$  determined by  $V$



$x_1, x_2$  equal variances,  
negatively correlated

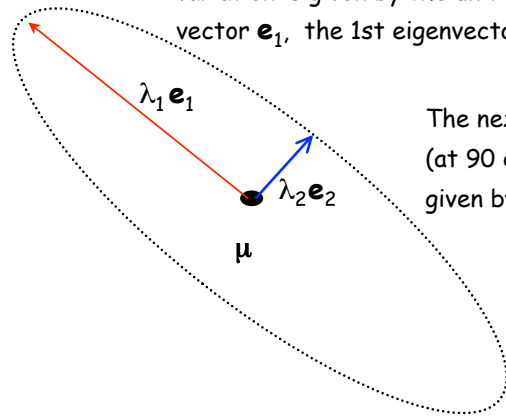
$\text{Var}(x_1) < \text{Var}(x_2)$ ,  
uncorrelated

Positive tilt = positive correlations  
Negative tilt = negative correlation  
No tilt = uncorrelated

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## 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

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## Properties of the MVN - I

1) If  $\mathbf{x}$  is MVN, any subset of the variables in  $\mathbf{x}$  is also MVN

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

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

for  $y = \mathbf{a}^T \mathbf{x} = \sum_{k=1}^n a_k x_k$ ,  $y$  is  $N(\mathbf{a}^T \boldsymbol{\mu}, \mathbf{a}^T \mathbf{V} \mathbf{a})$

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

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## Properties of the MVN - II

3) Conditional distributions are also MVN. Partition  $\mathbf{x}$  into two components,  $\mathbf{x}_1$  (m dimensional column vector) and  $\mathbf{x}_2$  (n-m dimensional column vector)

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} \quad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix} \quad \text{and} \quad \mathbf{V} = \begin{pmatrix} \mathbf{V}_{\mathbf{x}_1 \mathbf{x}_1} & \mathbf{V}_{\mathbf{x}_1 \mathbf{x}_2} \\ \mathbf{V}_{\mathbf{x}_1 \mathbf{x}_2}^T & \mathbf{V}_{\mathbf{x}_2 \mathbf{x}_2} \end{pmatrix}$$

$\mathbf{x}_1 | \mathbf{x}_2$  is MVN with m-dimensional mean vector

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

and m x m covariance matrix

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

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## Properties of the MVN - III

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

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

Where  $\mathbf{e}$  is MVN with mean vector  $\mathbf{0}$  and variance-covariance matrix  $\mathbf{V}_{\mathbf{x}_1 | \mathbf{x}_2}$

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$$\mu_1 + \mathbf{V}_{\mathbf{X}_1\mathbf{X}_2} \mathbf{V}_{\mathbf{X}_2\mathbf{X}_2}^{-1} (\mathbf{x}_2 - \mu_2) + e$$

The regression is **linear** because it is a linear function of  $\mathbf{x}_2$

The regression is **homoscedastic** because the variance-covariance matrix for  $e$  does not depend on the value of the  $\mathbf{x}$ 's

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

All these matrices are constant, and hence the same for any value of  $\mathbf{x}$

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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,

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

Let  $\mathbf{x}_1 = (z_o)$ ,  $\mathbf{x}_2 = \begin{pmatrix} z_s \\ z_d \end{pmatrix}$

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

$$= \mu_1 + \mathbf{V}_{\mathbf{X}_1\mathbf{X}_2} \mathbf{V}_{\mathbf{X}_2\mathbf{X}_2}^{-1} (\mathbf{x}_2 - \mu_2) + e$$

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Regression of Offspring value on Parental values (cont.)

$$= \mu_1 + \mathbf{V}_{\mathbf{X}_1\mathbf{X}_2} \mathbf{V}_{\mathbf{X}_2\mathbf{X}_2}^{-1} (\mathbf{x}_2 - \mu_2) + e$$

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

Hence,

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

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

Where  $e$  is normal with mean zero and variance

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

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

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

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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

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

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

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

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# Ordinary least squares

For the general linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$$

The predicted values given  $\boldsymbol{\beta}$  and the resulting residuals are given by

$$\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\beta}, \quad \mathbf{e} = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}$$

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

$$\sum e_i^2 = \mathbf{e}^T \mathbf{e}$$

or

$$(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

The solution is given by setting the derivative of this function with respect to  $\boldsymbol{\beta}$  equal to zero and solving.

Hence, we need to discuss vector/matrix derivatives

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## The gradient, the derivative of a vector-valued function

$$\nabla_{\mathbf{x}}[f] = \frac{\partial f}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

Compute the gradient for

$$f(\mathbf{x}) = \sum_{i=1}^n x_i^2 = \mathbf{x}^T \mathbf{x}$$

Since  $\partial f / \partial x_i = 2x_i$ , the gradient vector is just  $\nabla_{\mathbf{x}}[f(\mathbf{x})] = 2\mathbf{x}$ .

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## Some common derivatives

$$\begin{aligned} \nabla_{\mathbf{x}}[\mathbf{a}^T \mathbf{x}] &= \nabla_{\mathbf{x}}[\mathbf{x}^T \mathbf{a}] = \mathbf{a} \\ \nabla_{\mathbf{x}}[\mathbf{A}\mathbf{x}] &= \mathbf{A}^T \end{aligned}$$

Turning to quadratic forms, if  $\mathbf{A}$  is symmetric, then

$$\begin{aligned} \nabla_{\mathbf{x}}[\mathbf{x}^T \mathbf{A}\mathbf{x}] &= 2 \cdot \mathbf{A}\mathbf{x} \\ \nabla_{\mathbf{x}}[(\mathbf{x} - \mathbf{a})^T \mathbf{A}(\mathbf{x} - \mathbf{a})] &= 2 \cdot \mathbf{A}(\mathbf{x} - \mathbf{a}) \\ \nabla_{\mathbf{x}}[(\mathbf{a} - \mathbf{x})^T \mathbf{A}(\mathbf{a} - \mathbf{x})] &= -2 \cdot \mathbf{A}(\mathbf{a} - \mathbf{x}) \end{aligned}$$

Taking  $\mathbf{A} = \mathbf{I}$ ,

$$\nabla_{\mathbf{x}}[\mathbf{x}^T \mathbf{x}] = \nabla_{\mathbf{x}}[\mathbf{x}^T \mathbf{I}\mathbf{x}] = 2 \cdot \mathbf{I}\mathbf{x} = 2 \cdot \mathbf{x}$$

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$$\begin{aligned} \sum_{i=1}^n e_i^2 &= \mathbf{e}^T \mathbf{e} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \\ &= \mathbf{y}^T \mathbf{y} - \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\beta} \\ &= \mathbf{y}^T \mathbf{y} - 2\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\beta} \end{aligned}$$

where the last step follows since the matrix product  $\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y}$  yields a scalar, and hence it equals its transpose,

$$\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} = (\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y})^T = \mathbf{y}^T \mathbf{X}\boldsymbol{\beta}$$

To find the vector  $\boldsymbol{\beta}$  that minimizes  $\mathbf{e}^T \mathbf{e}$ , taking the derivative with respect to  $\boldsymbol{\beta}$  and using Equations A5.1a/c gives

$$\frac{\partial \mathbf{e}^T \mathbf{e}}{\partial \boldsymbol{\beta}} = -2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X}\boldsymbol{\beta}$$

Setting this equal to zero gives  $\mathbf{X}^T \mathbf{X}\boldsymbol{\beta} = \mathbf{X}^T \mathbf{y}$  giving

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

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# 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.,  $x <- 3.15$

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

Example 2: Compute  $Var(y_1)$ ,  $Var(y_2)$ , and  $Cov(y_1, y_2)$ , where  $y_i = c_i^T x$ .

```
> 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
> c1<-matrix(c(1,-2,5),nrow=3)
> c2<-matrix(c(0,6,-4),nrow=3)
> c1
     [,1]
[1,]   1
[2,]  -2
[3,]   5
> c2
     [,1]
[1,]   0
[2,]   6
[3,]  -4
> t(c1)%*%V*c1      c1^T V c1
     [,1]
[1,]  960
> t(c2)%*%V*c2      c2^T V c2
     [,1]
[1,] 1200
> t(c1)%*%V*c2      c1^T V c2
     [,1]
[1,] -910
```

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

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

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

```
> A <- matrix(c(5,7,-1,6,-3,-1,4,5,6),nrow=3)
> A
     [,1] [,2] [,3]
[1,]   5   6   4
[2,]   7  -3   5
[3,]  -1  -1   6
>
> c<-matrix(c(6,-9,12),nrow=3)
> c
     [,1]
[1,]   6
[2,]  -9
[3,]  12
```

Next, input the vector  $c$

```
> solve(A)%*%c
     [,1]
[1,] -2.031008
[2,]  1.426357
[3,]  1.899225
```

Finally, compute  $A^{-1}c$ .

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$\det(A)$  returns the determinant of A

```
> det(V)
[1] 3250
```

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

```
> 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
```

For example, second eigenvalue is  $\lambda_2 = 21.117310$ , second eigenvector

$$e_2 = \begin{pmatrix} 0.2117936 \\ -0.9477830 \\ -0.2384340 \end{pmatrix}$$

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## Additional references

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

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

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

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