
Linear Algebra

Edps/Soc 584 and Psych 594

Applied Multivariate Statistics

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I L L I N O I S

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Outline

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Motivation

Vectors

Matrices

Random Vectors and Matrices

Useful Matrix Formulas

Matrix Software

- Motivation
- Vectors
- Matrices
- Random Vectors & Matrices
- Useful Matrix Formulas
- Matrix Software (SAS/IML, MATLAB, & R)

Reading & Resources:

- Johnson & Wichern, Chapter 1, Chapter 2, supplement
- Chapter by Larry Hubert linked to course web-site
- Matrix reference manual at <http://www.ee.ic.ac.uk/hp/staff/dmb/matrix/intro.html>
- Matrix cookbook at <http://matrixcookbook.com>



Motivation

Data Array:

$n \times p$ matrix X (cases \times variables)

“size” of matrix X

Why learn about linear algebra (& geometry)?

- Provides a useful mathematical form.
- Simplifies: shorthand with which extensive material can be condenses into a compact form.
- Perform matrix operations in multivariate analysis.
- Needed for more advanced statistics and multivariate methods

So we need to study matrices & operations and properties of solutions.

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Vectors

Vectors: An array x of n real numbers is called a vector & written as

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \quad \text{or} \quad \mathbf{x}' = (x_1, x_2, \dots, x_n)$$

- Vectors are denoted by lower case bold letters (i.e., when hand written, put a \sim underneath the letter).
- Typically, vectors are columns
- **Transpose** of a (column) vector is x' is a row vector.
- A vector consists of n **scalars** (numbers).
- A vector is a matrix with one column, $(n \times 1)$.

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- Projection of a Vector
- Projection of a Vector



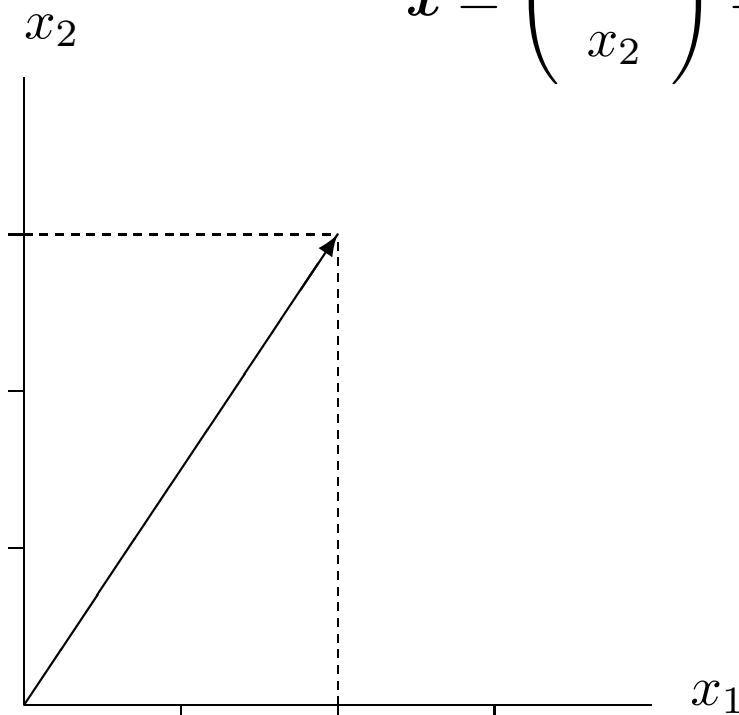
Vector as a Point

A Vector is a point in n -dimensional space represented by an arrow originating at zero.

All vectors have a Length and a Direction.

e.g.,

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$



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Definition of Equal Vectors

Two vectors (matrices) are equal if they have the same number of rows, the same number of columns, and the corresponding entries in each are equal

$$a = b \quad \text{means} \quad a_{ij} = b_{ij} \quad \text{for all } i \text{ \& } j$$

OR

Two vectors are equal (identical) if they both have the same length and direction.

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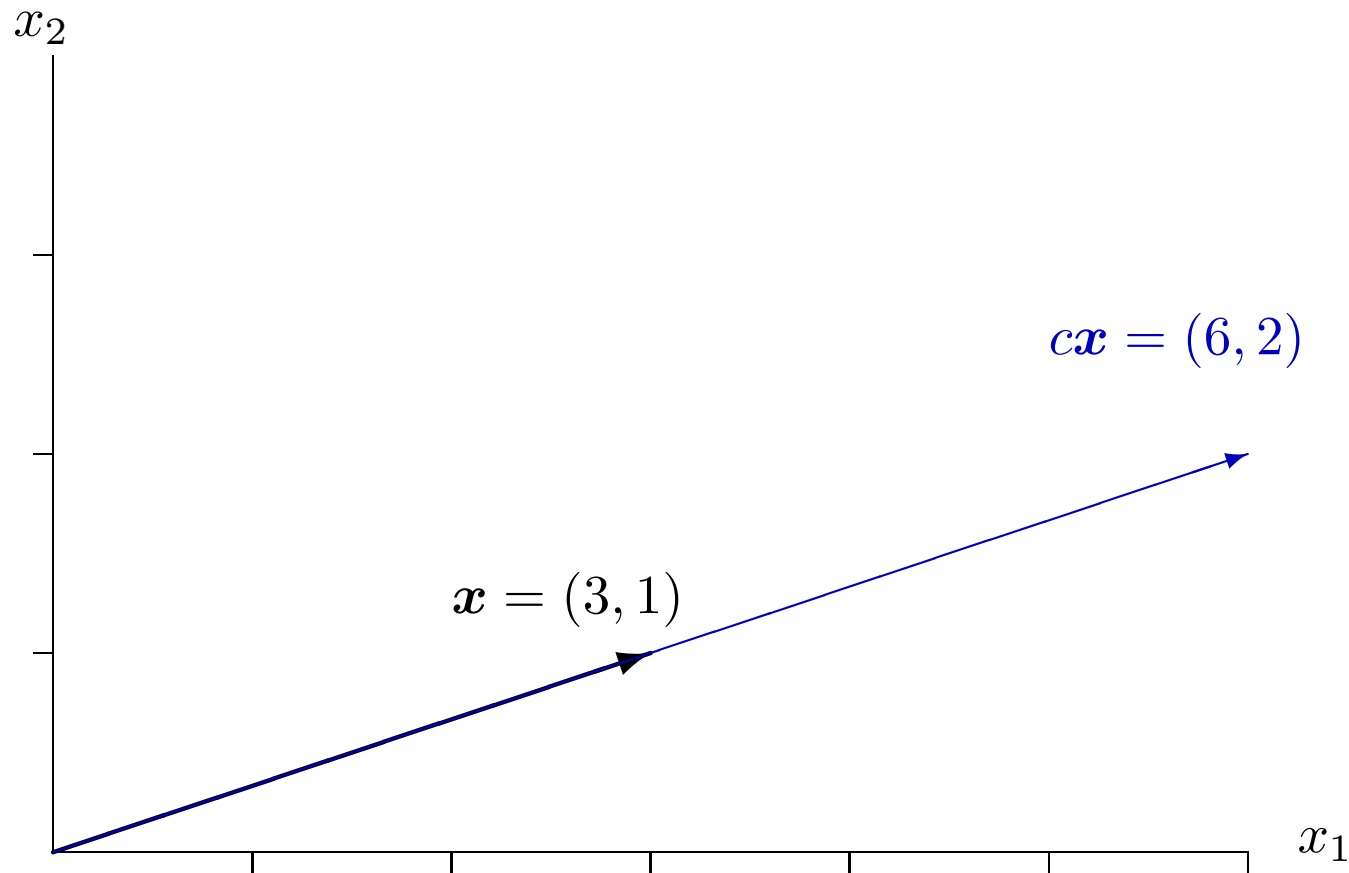


Multiplication of Vector by a Scalar

Suppose that c is some number (a scalar). For scalar multiplication, multiply each entry of x by c :

$$cx' = (cx_1, cx_2, \dots, cx_n)$$

Example: Let $x' = (3, 1)$ and $c = 2$



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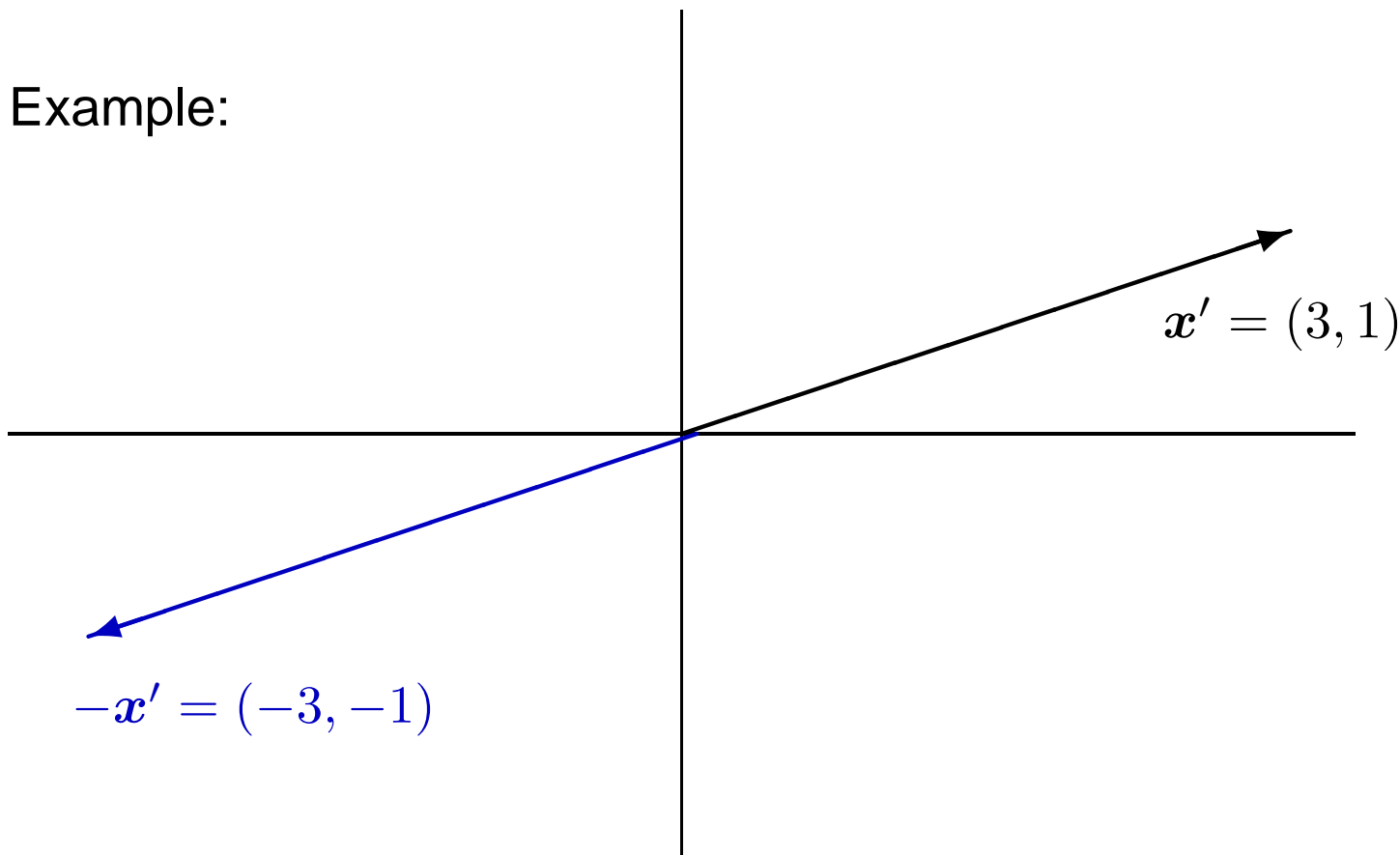


Reflection

Multiplication of a vector by $c = -1$

$$-\mathbf{x}' = (-x_1, -x_2, \dots, -x_n)$$

Example:



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Vector Addition

The sum of two vectors, each with the same number of elements (i.e., same size), element by element:

$$\mathbf{z} = \mathbf{x} + \mathbf{y} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{pmatrix}$$

e.g., $\mathbf{x}' = (3, 1)$ and $\mathbf{y}' = (2, 3)$

$$\mathbf{x} + \mathbf{y} = \begin{pmatrix} 3 \\ 1 \end{pmatrix} + \begin{pmatrix} 2 \\ 3 \end{pmatrix} =$$

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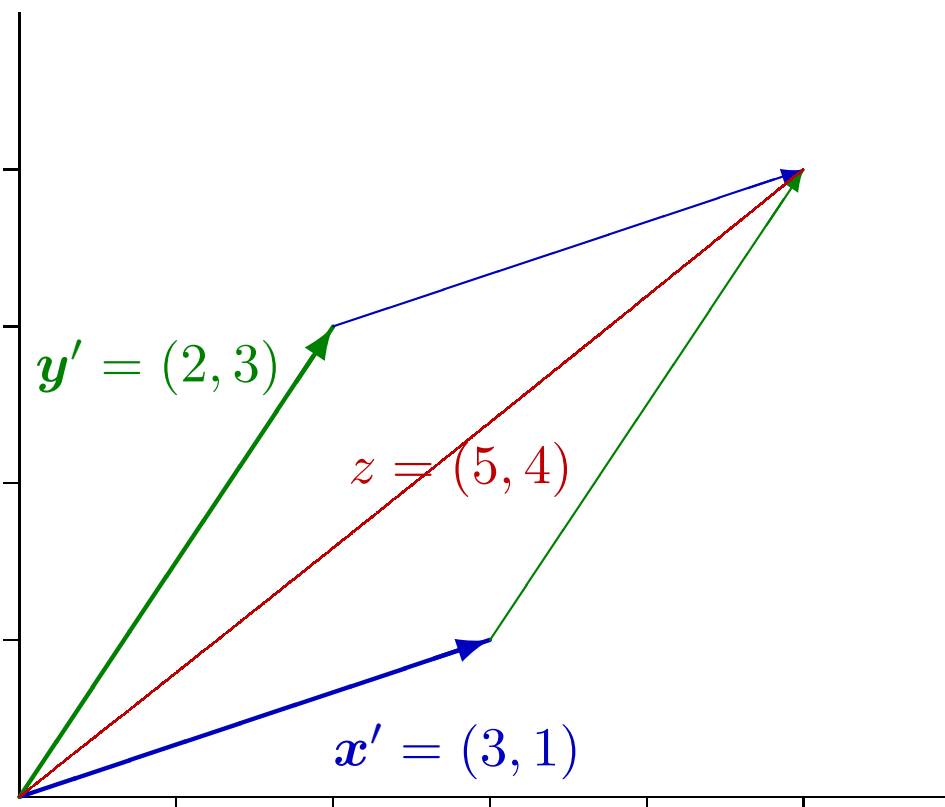
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Geometry of Vector Addition

Form a parallelogram by sliding the origin of one vector to the end of the other.

The sum is the diagonal of the parallelogram. e.g.,



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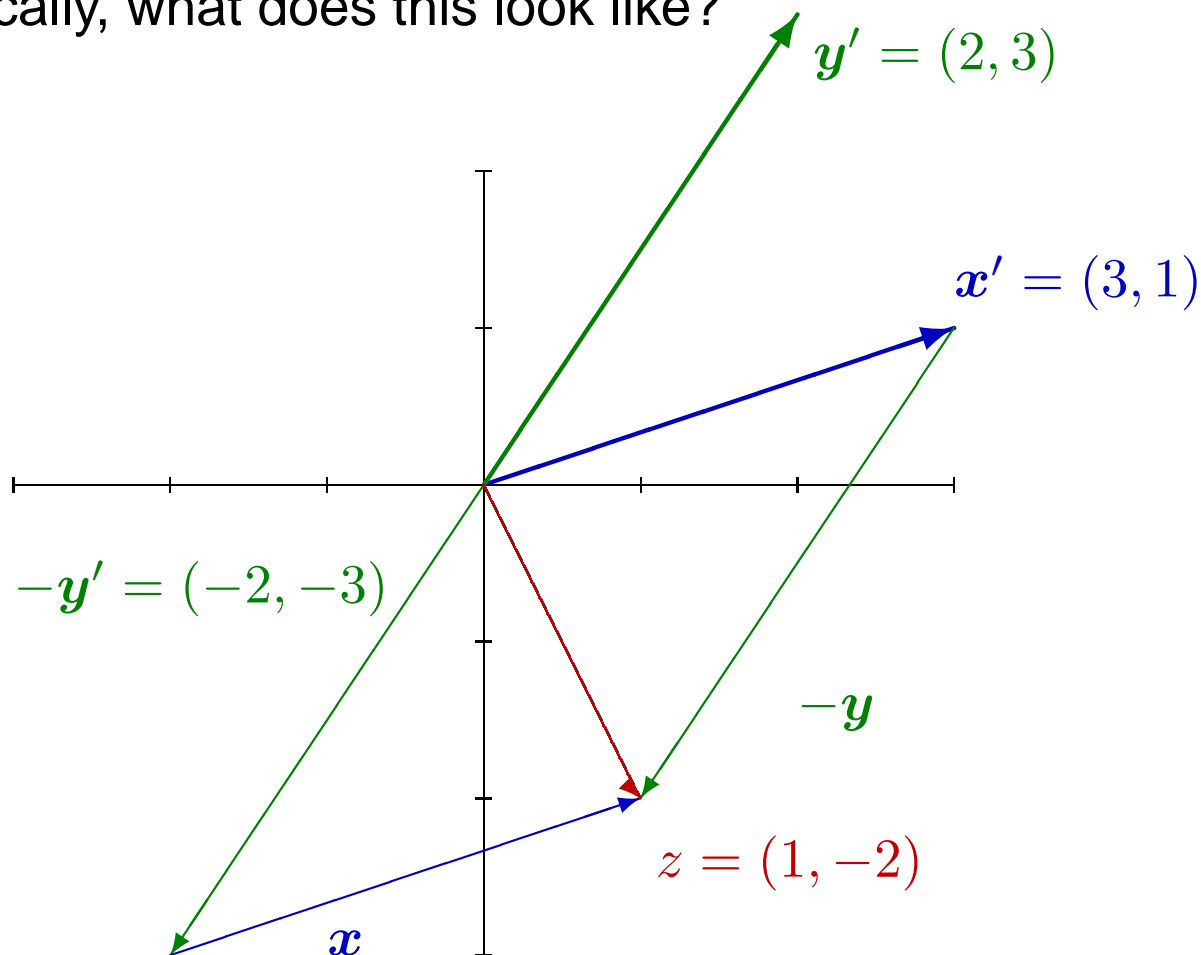


Vector Subtraction

Element by element addition

$$\mathbf{x}' - \mathbf{y}' = (x_1 - y_1, x_2 - y_2, \dots, x_I - y_I)$$

Geometrically, what does this look like?



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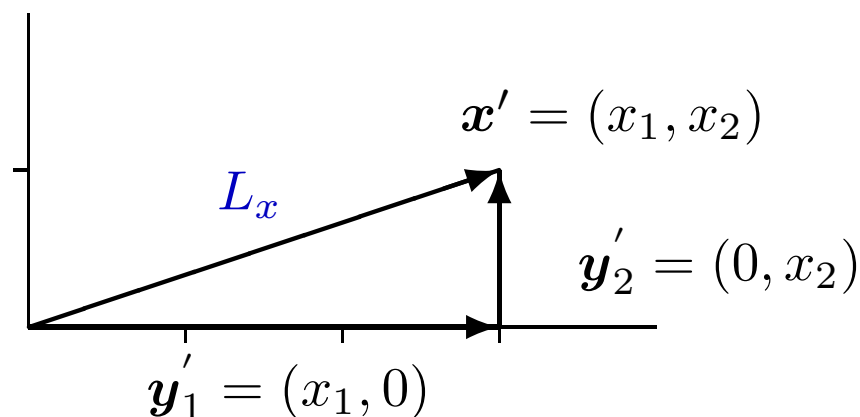


Length of Vector

Remember the Pythagorean Theorem?

Let

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ x_2 \end{pmatrix} = \mathbf{y}_1 + \mathbf{y}_2$$



$$L\mathbf{x} = \sqrt{x_1^2 + x_2^2}$$

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Generalization to n -Dimensional Space

Let

$$\mathbf{x}' = (x_1, x_2, \dots, x_n)$$

And the length of \mathbf{x} is

$$L_x = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2} = \sqrt{\sum_{j=1}^n x_j^2}$$

Implications for scalar multiplication:

$$\begin{aligned} c\mathbf{x} \longrightarrow L_{c\mathbf{x}} &= \sqrt{c^2 x_1^2 + c^2 x_2^2 + \dots + c^2 x_n^2} \\ &= |c| \sqrt{x_1^2 + x_2^2 + \dots + x_n^2} \\ &= |c| L_x \end{aligned}$$

■ If $c < 0$, then change direction.

■ If $c = -1$, then change direction but not length.

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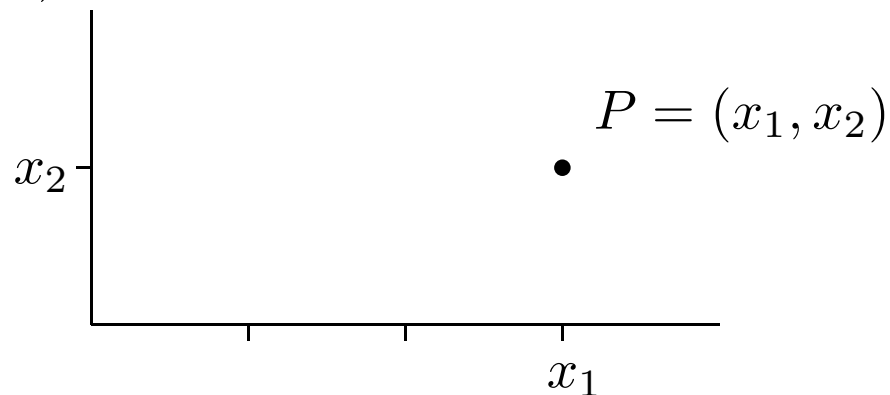
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Length \longrightarrow Distance

Distance between points.

Suppose we have a 2-dimensional space and a point $P = (x_1, x_2)$



Distance from the origin $0 = (0, 0)$ to point P is

$$d(0, P) = \sqrt{x_1^2 + x_2^2} = L_x$$

If point P has n coordinates, $P = (x_1, x_2, \dots, x_n)$ then the “straight-line” distance from the origin, $0 = (0, 0, \dots, 0)$ to P is

$$d(0, P) = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$$

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Distance between Two Arbitrary Points

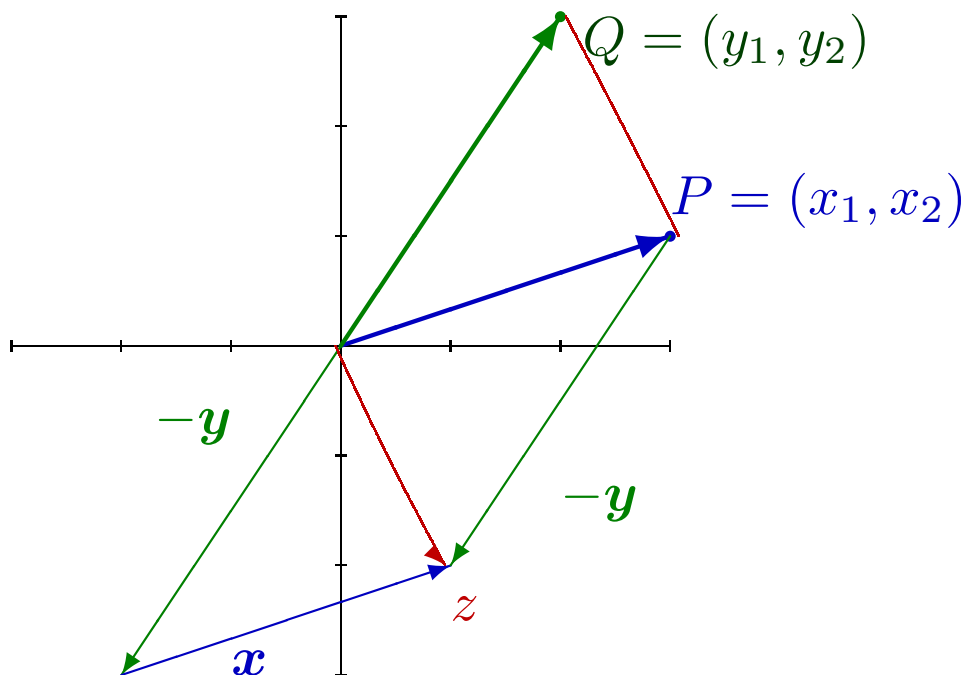
The “straight-line” distance between two arbitrary points

$P = (x_1, x_2, \dots, x_n)$ and $Q = (y_1, y_2, \dots, y_n)$ is

$$d(P, Q) = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \dots + (x_n - y_n)^2}$$

Why?

Show this for 2-Dimensional case:



The length of $x - y$ is the distance between $P - Q$.

e.g., $x = (3, 1)$, $y = (2, 3)$, and z

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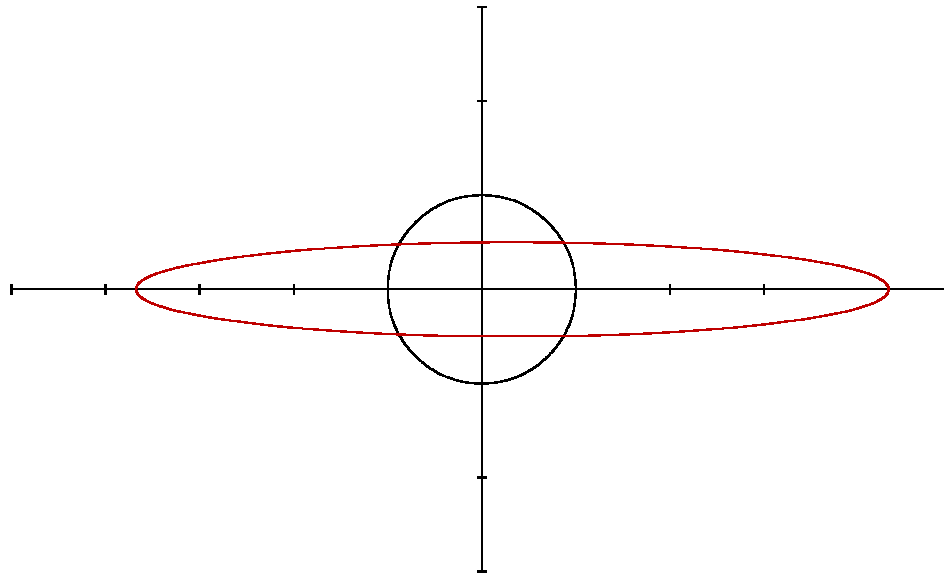


Squared Distances

All points that are a constant (squared) distance, say c^2 from the origin $\mathbf{0}$ satisfy the equation

$$d^2(\mathbf{0}, P) = x_1^2 + x_2^2 + \dots + x_n^2 = c^2$$

This is the equation for a sphere in n -dimensional space in (un-weighted) Euclidean space.



Statistical Distance: Weight scores by a variable's standard deviation (more about these later). This yields an ellipsoid, which has important statistical connections.

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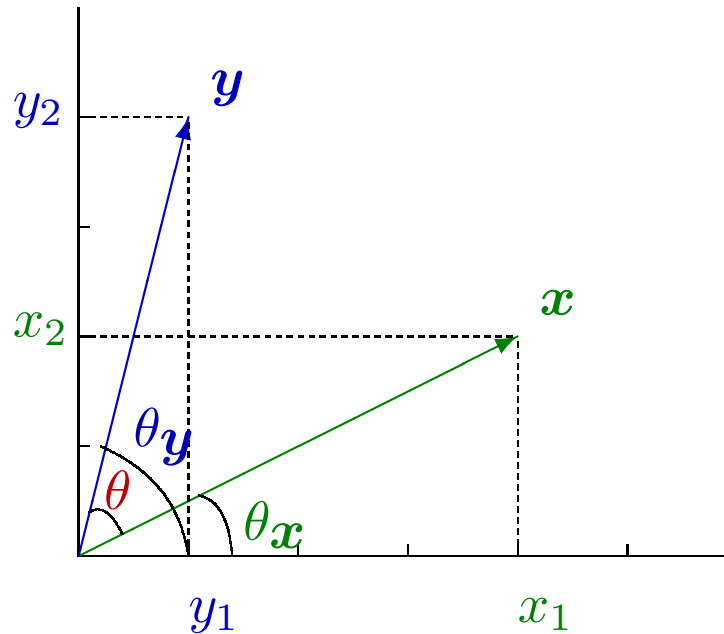
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Direction: Angles between two vectors

θ = the angle between x and y



What do we know or can compute?

- $x_1, x_2, y_1,$ and y_2
- Lx and Ly
- θ_y and θ_x .
- And $\theta = \theta_y - \theta_x$.

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Trigonometry Review

Remember this?

$$\cos(\theta_x) = \frac{x_1}{L_x}$$

$$\cos(\theta_y) = \frac{y_1}{L_y}$$

and

$$\sin(\theta_x) = \frac{x_2}{L_x}$$

$$\sin(\theta_y) = \frac{y_2}{L_y}$$

And

$$\begin{aligned} \cos(\theta) &= \cos(\theta_y - \theta_x) \\ &= \cos(\theta_y) \cos(\theta_x) + \sin(\theta_y) \sin(\theta_x) \end{aligned}$$

So

$$\begin{aligned} \cos(\theta) &= \left(\frac{y_1}{L_y} \right) \left(\frac{x_1}{L_x} \right) + \left(\frac{y_2}{L_y} \right) \left(\frac{x_2}{L_y} \right) \\ &= \frac{x_1 y_1 + x_2 y_2}{L_x L_y} \end{aligned}$$

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Example: Computing angle between vectors

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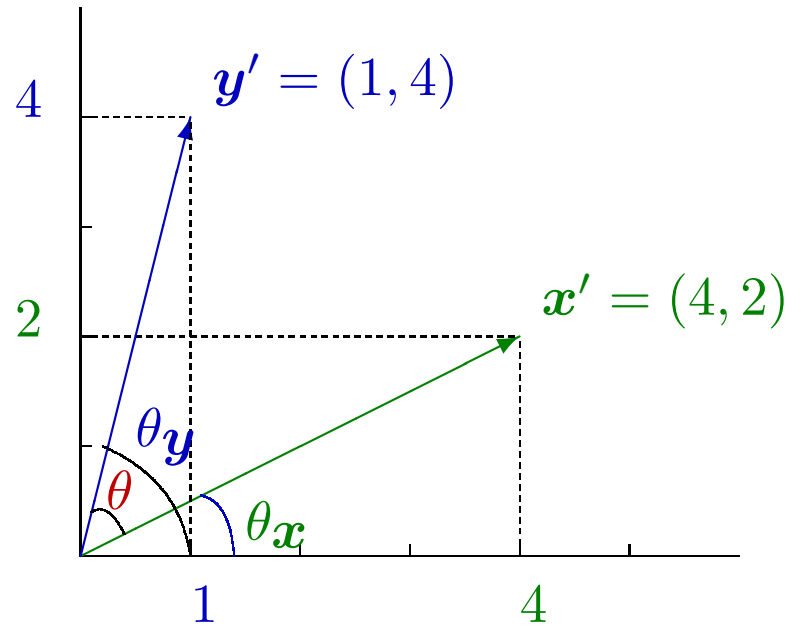
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$$L_x = \sqrt{4^2 + 2^2} = \sqrt{20} = 4.472136 \quad L_y = \sqrt{1^2 + 4^2} = \sqrt{17} = 4.12311$$

$$\cos(\theta) = \left(\frac{y_1}{L_y} \right) \left(\frac{x_1}{L_x} \right) + \left(\frac{y_2}{L_y} \right) \left(\frac{x_2}{L_x} \right)$$

=

Answer: $\cos^{-1}(.65079) = 49.40^\circ$



Inner Product of Two Vectors

Note:

$$\cos(\theta) = \frac{(x_1y_1 + x_2y_2)}{\sqrt{x_1^2 + x_2^2}\sqrt{y_1^2 + y_2^2}}$$

The “inner product” of vectors x and y equals $(x_1y_1 + x_2y_2)$.

- Also called the “dot product”.
- Denoted by $x'y$ or $y'x$ (order doesn't matter).
- $x'y = x_1y_1 + x_2y_2$
- $x'x = x_1^2 + x_2^2 = L_x^2$
- $y'y = y_1^2 + y_2^2 = L_y^2$
- $\cos(\theta) = 0$ when $\theta = 90^\circ \iff$
 x and y are perpendicular when $x'y = 0$.

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Generalization to n dimensions

If x and y are $(n \times 1)$ vectors , i.e.,

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \quad \text{and} \quad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

Then the inner product between x and y is

$$x'y = y'x = (x_1y_1 + x_2y_2 + \dots + x_ny_n) = \text{a scalar}$$

$$\text{Length of } x = Lx = \sqrt{x'x}$$

$$\cos(\theta) = \frac{x'y}{LxLy} = \frac{x'y}{\sqrt{x'x}\sqrt{y'y}}$$

$$x'y = 0 \quad \text{if and only if} \quad x \quad \& \quad y \quad \text{are perpendicular}$$

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Linear Dependence

Linearly Dependent: A set of vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k$ is said to be linearly dependent if there exists constants c_1, c_2, \dots, c_k not all equal to zero such that

$$c_1 \mathbf{x}_1 + c_2 \mathbf{x}_2 + \dots + c_k \mathbf{x}_k = \mathbf{0}$$

If vectors are linearly dependent, then one vector in the set can be written as a function (linear combination) of the others; that is,

$$\mathbf{x}_i = -\frac{1}{c_i} \left(\sum_{k \neq i} c_k \mathbf{x}_k \right)$$

e.g.,

$$\mathbf{x}_1 = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \quad \mathbf{x}_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \mathbf{x}_3 = \begin{pmatrix} -4 \\ 2 \\ -2 \\ 4 \end{pmatrix}$$

If $c_1 = 1$, $c_2 = -5$ and $c_3 = -1$, then $1\mathbf{x}_1 - 5\mathbf{x}_2 - 1\mathbf{x}_3 = \mathbf{0}$

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Linear Independence

If there are **no** constants c_1, c_2, \dots, c_k not all equal to zero such that

$$c_1 \mathbf{x}_1 + c_2 \mathbf{x}_2 + \dots + c_k \mathbf{x}_k = \mathbf{0}$$

Then the vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k$ are linearly independent.

Vectors are linearly independent if you **cannot** write one as a linear combination of the others

Example

$$\mathbf{x}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{x}_2 = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{x}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

The only constants that make the condition true is

$$c_1 = c_2 = c_k = 0$$

If all vectors in a set are $(k \times 1)$, at most how many vectors could possibly be in a set of linearly independent vectors?

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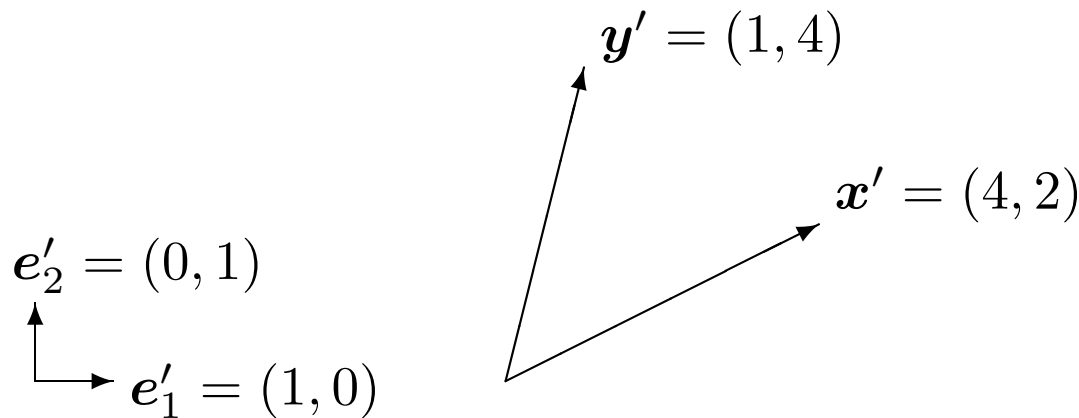
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Geometry of Linear (In)Dependence

A basis is a set of linearly independent vectors and a basis defines a space.

- For example, $e'_1 = (1, 0)$ and $e'_2 = (0, 1)$ define the space in a plane — these are special ones, a “**standard basis**”.
- The dimension of the space defined by a set of vectors equals the number of linearly independent vectors in the set.



Any third vector in either of these spaces must be a linear combination of the other two? Try $z' = (6, 2)$

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More about Basis

- An example of a standard basis is the set of vectors e_1, e_2, \dots, e_p where e_k equals a $(p \times 1)$ vector with all 0 except for a 1 in the k^{th} position.

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad e_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \dots, \quad e_p = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

- These vectors are all orthogonal: $e'_k e_l = 0$
- They all have length equal to 1: $L e_k = \sqrt{e'_k e_k} = 1$
- Any basis can always be transformed to an orthogonal one (This can be done using the Gram-Schmidt orthogonalization process).

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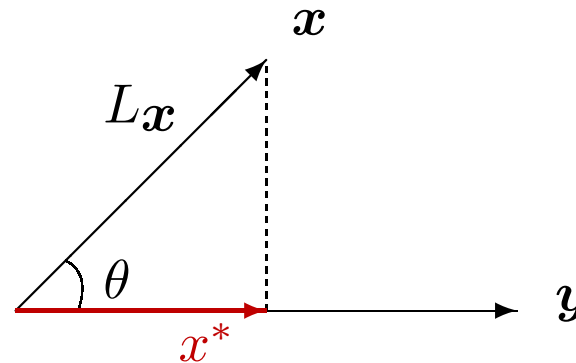
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Projection of a Vector

Projection of x onto y :



The projection of x onto y is in the same direction as y , but has a different length.

■ Length of projection:

- ◆ We know that $\cos(\theta) = L_{x^*} / L_x$.
- ◆ We also know that $\cos(\theta) = (x'y) / (L_x L_y)$
- ◆ So the length of the projection is

$$L_{x^*} = L_x \cos(\theta) = L_x \left(\frac{x'y}{L_x L_y} \right) = \frac{x'y}{L_y}$$

■ For the direction, find a unit vector in the direction of y ,

$$\frac{1}{L_y} y$$

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Projection of a Vector (continued)

- Multiply the length of the projection Lx^* (a scalar) times the unit vector in the direction of y (recall what happens when you multiply a vector by a scalar).

- The projection of x on y is

$$x^* = \underbrace{\left(\frac{x'y}{Ly} \right)}_{\text{scalar}} \underbrace{\left(\frac{y}{Ly} \right)}_{\text{unit vector in same direction as } y}$$

$$= \underbrace{\frac{x'y}{y'y}}_{\text{scalar}} \underbrace{y}_{\text{vector}}$$

- One use of this concept: observations (e.g., x) can be broken down into the sum of mean (projection) plus deviation or residual (vertical distance from x to end of x^*).

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Zero and One Vector

The **null vector** contains all 0's,

$$\mathbf{0} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

One use: null hypothesis values when testing multiple means.

Vector of One's

$$\mathbf{1}_n = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

Some of the many uses:

- Sum up elements of a vector or sum rows or columns of a matrix.
- Important when we talk about geometry of the mean.

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Matrices

- A Matrix is any rectangular array of real numbers. We'll use upper case bold Roman letters to represent them.

- An arbitrary matrix with n rows and p columns

$$\mathbf{A}_{(n \times p)} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1p} \\ a_{21} & a_{22} & \dots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{np} \end{pmatrix}$$

- The first subscript indicates the row and second indicates a column.

- A matrix with n rows and p columns is said to have order $(n \times p)$.

- Another way to indicate a matrix (and it's order) is

$$\mathbf{A} = \{a_{ij}\}_{n \times p}$$

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Matrix Operations & Definitions of Special Ones

- Transpose operation is indicated by ' (e.g., A').

$$A' = B \iff b_{ij} = a_{ji}$$

Transpose changes the rows to columns and columns to rows

- Sometimes the letter \mathbb{T} is used to indicate transpose, e.g., $A^{\mathbb{T}}$,

Example:

$$A_{(4 \times 2)} = \begin{pmatrix} 1 & 2 \\ 5 & 1 \\ 3 & 5 \\ 3 & 0 \end{pmatrix} \quad \text{and} \quad A'_{(2 \times 4)} =$$

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Equal Matrices

Suppose we have two matrices \mathbf{A} and \mathbf{B} of the same $n \times p$ order:

$$\mathbf{A} = \begin{pmatrix} a_{11} & \cdots & a_{1p} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{np} \end{pmatrix}_{n \times p} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} b_{11} & \cdots & b_{1p} \\ \vdots & \ddots & \vdots \\ b_{n1} & \cdots & b_{np} \end{pmatrix}_{n \times p}$$

As a definition for equality of two matrices of the same order (and for which it only makes sense to talk about equality), we have:

$$\mathbf{A} = \mathbf{B} \quad \text{if and only if} \quad a_{ij} = b_{ij} \quad \text{for all } i \text{ and } j.$$

“if and only if” statement (sometimes abbreviated as “iff”) implies two conditions:

1. If $\mathbf{A} = \mathbf{B}$, then $a_{ij} = b_{ij}$ for all i and j , and
2. if $a_{ij} = b_{ij}$ for all i and j , then $\mathbf{A} = \mathbf{B}$.

Any definition by its very nature implies an “if and only if” statement.

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Scalar Multiplication

- $c\mathbf{A}$ where c is a scalar (constant) and \mathbf{A} is an arbitrary matrix of any size.

- Multiply each element of \mathbf{A} by the scalar c .

$$c\mathbf{A} = \begin{pmatrix} ca_{11} & \cdots & ca_{1p} \\ \vdots & \ddots & \vdots \\ ca_{n1} & \cdots & ca_{np} \end{pmatrix} = c \begin{pmatrix} a_{11} & \cdots & a_{1p} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{np} \end{pmatrix}$$

- $\mathbf{B} = c\mathbf{A} \implies ca_{ij}$.

- Example where $c = 3$:

$$\mathbf{B} = 3\mathbf{A} = 3 \begin{pmatrix} 1 & 2 \\ 5 & 1 \\ 3 & 5 \\ 3 & 0 \end{pmatrix}$$

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Matrix Addition

- Addition is **element-by-element**.

$$C = A + B \implies c_{ij} = a_{ij} + b_{ij}$$

- Two matrices must have the **same order** (referred to as conformal for addition).

- Example:

$$C = A + B = \begin{pmatrix} 1 & 2 \\ 5 & 1 \\ 3 & 5 \\ 3 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -6 \\ 3 & 1 \\ 3 & -2 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -4 \\ 8 & 2 \\ 6 & 3 \\ 4 & 0 \end{pmatrix}$$

- Matrix addition is **commutative** (i.e., order does not matter):
 $A + B = B + A$.

- Matrix addition is **associative**: $(A + B) + C = A + (B + C)$

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Matrix Multiplication

■ Let $A_{(n \times k)}$ and $B_{(k \times p)}$.

■ For $C = AB$,

$$c_{ij} = \sum_{l=1}^k a_{il} b_{lj}$$

$$= a'_i b_j$$

= the inner product between the i^{th} row of A and the j^{th} column of B

$$= \begin{bmatrix} a_{i1} & a_{i2} & \dots & a_{ik} \end{bmatrix} \begin{bmatrix} b_{1j} \\ b_{2j} \\ \vdots \\ b_{kj} \end{bmatrix}$$

■ The number of columns of A must equal the number of rows of B .

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Matrix Multiplication

Example: $A_{(2 \times 3)} B_{(3 \times 2)}$

$$\begin{pmatrix} 1 & 2 & 3 \\ 5 & 1 & 2 \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 4 & 3 \\ -2 & 1 \end{pmatrix} =$$

=

=

■ In General, matrix multiplication is not commutative; it may not even be possible to calculate both AB and BA . e.g.,

$$B_{(3 \times 2)} A_{(2 \times 3)} = \begin{pmatrix} 2 & 4 & 6 \\ 19 & 11 & 18 \\ 3 & -3 & -4 \end{pmatrix} \neq A_{(2 \times 3)} B_{(3 \times 2)}$$

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Matrix Multiplication is Associative

Matrix multiplication is **associative**:

$$ABC = (AB)C = A(BC)$$

Using A and B from the previous slide and C ,

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 5 & 1 & 2 \end{pmatrix}, \quad B = \begin{pmatrix} 2 & 0 \\ 4 & 3 \\ -2 & 1 \end{pmatrix}, \quad C = \begin{pmatrix} 5 & 2 \\ 3 & 10 \end{pmatrix}$$

$$(AB)C = \begin{pmatrix} 4 & 9 \\ 10 & 5 \end{pmatrix} \begin{pmatrix} 5 & 2 \\ 3 & 10 \end{pmatrix} = \begin{pmatrix} 47 & 98 \\ 65 & 70 \end{pmatrix}$$

$$A(BC) = \begin{pmatrix} 1 & 2 & 3 \\ 5 & 1 & 2 \end{pmatrix} \begin{pmatrix} 10 & 4 \\ 29 & 38 \\ -7 & 6 \end{pmatrix} = \begin{pmatrix} 47 & 98 \\ 65 & 70 \end{pmatrix}$$

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More Properties of Matrix Operations

■ Matrix multiplication is Distributive

◆ Left distributive:

$$AB + AC = A(B + C)$$

◆ Right distributive:

$$AC + BC = (A + B)C$$

■ Properties of transposes:

◆ Product of transposes

$$(AB)' = B' A' \quad \text{and} \quad (ABC)' = C' B' A'$$

etc.

◆ Transpose of a transpose equals the un-transposed matrix:

$$(A')' = A$$

◆ Transpose of a sum equals the sum of the transposes:

$$(A + B)' = A' + B'$$

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Square and Symmetric Matrices

A Square Matrix has the same number of rows as columns.
e.g.,

$$\mathbf{A}_{(2 \times 2)} = \begin{pmatrix} 1 & 2 \\ 5 & 7 \end{pmatrix}$$

A Symmetric Matrix is a square matrix where the rows equal the columns

$$\mathbf{A} = \mathbf{A}' \quad \text{i.e., } a_{ij} = a_{ji}$$

Alternatively, the upper triangle equals the transpose of the lower triangle (and visa versa).

e.g.,

$$\mathbf{A} = \mathbf{A}' = \begin{pmatrix} 9 & 1 & 3 \\ 1 & 3 & 4 \\ 3 & 4 & 10 \end{pmatrix}$$

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$$\mathbf{A} = \mathbf{A}' = \begin{pmatrix} 1 & 4 & 3 \\ 4 & 7 & -1 \\ 3 & -1 & 3 \end{pmatrix}$$

- The “main” or “principal diagonal” entries are in red.
- The sum of main diagonal entries of a square matrix is called the trace; thus,

$$\text{trace}(\mathbf{A}_{(p \times p)}) \equiv \text{tr}(\mathbf{A}) = a_{11} + \cdots + a_{pp}$$

- Our example,

$$\text{tr}(\mathbf{A}) = 1 + 7 + 3 = 11$$



Null and Diagonal Matrices

A Null Matrix has all elements equal to 0.

$$\mathbf{0}_{(n \times p)} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix}$$

A Diagonal Matrix is a square matrix where the only non-zero elements are on the diagonal, e.g.,

$$\mathbf{D}_{(p \times p)} = \begin{pmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{pp} \end{pmatrix}$$

Sometimes it's written as $\text{diag}(a_{11}, a_{22}, \dots, a_{pp})$

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Pre-Multiplication by a Diagonal Matrix

When you “pre-multiply” a matrix by a diagonal matrix it has the effect of multiplying each row by the corresponding diagonal, e.g.,

$$\begin{pmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{pp} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1p} \\ b_{21} & b_{22} & \dots & b_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ b_{p1} & b_{p2} & \dots & b_{pp} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & \dots & a_{11}b_{1p} \\ a_{22}b_{21} & a_{22}b_{22} & \dots & a_{22}b_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{pp}b_{p1} & a_{pp}b_{p2} & \dots & a_{pp}b_{pp} \end{pmatrix} = \begin{pmatrix} a_{11}b'_1 \\ a_{22}b'_2 \\ \vdots \\ a_{pp}b'_p \end{pmatrix}$$

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Post-Multiplication by a Diagonal Matrix

When you “post-multiply” a matrix by a diagonal matrix it has the effect of multiplying each column by the corresponding diagonal, e.g.,

$$\begin{pmatrix} b_{11} & b_{12} & \dots & b_{1p} \\ b_{21} & b_{22} & \dots & b_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ b_{p1} & b_{p2} & \dots & b_{pp} \end{pmatrix} \begin{pmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{pp} \end{pmatrix}$$

$$= \begin{pmatrix} a_{11}b_{11} & a_{22}b_{12} & \dots & a_{pp}b_{1p} \\ a_{11}b_{21} & a_{22}b_{22} & \dots & a_{pp}b_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{11}b_{p1} & a_{22}b_{p2} & \dots & a_{pp}b_{pp} \end{pmatrix} = (a_{11}\mathbf{b}_1, a_{22}\mathbf{b}_2, \dots, a_{pp}\mathbf{b}_p)$$

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Identity Matrix

The Identity Matrix is a diagonal matrix with all entries equal to 1, e.g.,

$$\mathbf{I}_p = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix}$$

\mathbf{I}_p is called the identity matrix because

$$\mathbf{I}_p \mathbf{A}_{(p \times p)} = \mathbf{A}_{(p \times p)} \mathbf{I}_p = \mathbf{A}_{(p \times p)}$$

e.g.,

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ 3 & 5 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ 3 & 5 & 2 \end{pmatrix}$$

Often see $\sigma^2 \mathbf{I}$ or $\mathbf{A} \mathbf{A}^{-1} = \mathbf{I}$.

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Determinant of a Matrix

The determinant of a square matrix, $A_{p \times p}$, is a scalar that is associated with that matrix. Determinants are denoted by $|A|$ or $\det(A)$.

How to compute the determinant of

■ A 1×1 matrix:

$$|a| = a$$

■ A 2×2 matrix:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \longrightarrow |A| = ad - bc$$

■ A 3×3 matrix:

$$A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \longrightarrow |A| = aei + dhc + gfb - (ceg + fha + idb)$$

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Determinant of a $(p \times p)$ Matrix

For $p > 3$, this requires the use a recursive process, but first need some definitions:

- Let A_{uv} is be the $(p - 1) \times (p - 1)$ submatrix of A constructed by deleting the u^{th} row and v^{th} column of A
- Minor entry of a_{uv} is the $\det(A_{uv})$
- The signed minor of $(-1)^{u+v} \det(A_{uv})$ is the cofactor of a_{uv} .

The recursive algorithm:

- (1) Chose some row (or column) either arbitrarily or for convenience.
- (2) Find the cofactors for the entries in it.
- (3) The cofactors would then be weighted by the relevant entries and summed. i.e.,

$$\det(\mathbf{A}) = \sum_{u=1}^p a_{uv} (-1)^{u+v} \det(\mathbf{A}_{uv})$$

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Example: Determinant of a (4×4) matrix

$$A = \begin{pmatrix} 4 & 3 & 2 & 1 \\ 2 & 5 & 1 & 0 \\ 1 & 3 & 2 & 1 \\ 3 & 2 & 1 & 4 \end{pmatrix}$$

I'll use the 2nd row, which I highlighted in red:

$$\begin{aligned} \det(A) &= 2(-1)^{1+2} \begin{vmatrix} 3 & 2 & 1 \\ 3 & 2 & 1 \\ 2 & 1 & 4 \end{vmatrix} + 5(-1)^{2+2} \begin{vmatrix} 4 & 2 & 1 \\ 1 & 2 & 1 \\ 3 & 1 & 4 \end{vmatrix} \\ &\quad + 1(-1)^{2+3} \begin{vmatrix} 4 & 3 & 1 \\ 1 & 3 & 1 \\ 3 & 2 & 4 \end{vmatrix} + 0(-1)^{2+4} \begin{vmatrix} 4 & 3 & 2 \\ 1 & 3 & 2 \\ 3 & 2 & 1 \end{vmatrix} \\ &= -2(0) + 5(21) - 1(30) + 0 \\ &= 75 \end{aligned}$$

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More About Determinants

- The determinant of a diagonal matrix is equal to the product of the diagonal elements:

$$\mathbf{A} = \begin{pmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & a_{pp} \end{pmatrix} \longrightarrow \det(\mathbf{A}) = \prod_{j=1}^p a_{jj}$$

- The determinant of an upper– (or lower–) triangular matrix equals the product of the diagonal elements:

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1p} \\ 0 & a_{22} & \dots & a_{2p} \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & a_{pp} \end{pmatrix} \longrightarrow \det(\mathbf{A}) = \prod_{j=1}^p a_{jj}$$

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Properties of Determinants

- If one row (or column) of A is multiplied by a constant c , the new determinant is $c \det(A)$.
- If two rows or two columns of a matrix are interchanged, the sign of the determinant is changed.
- If two rows or two columns of a matrix are equal, then the determinant is zero... (see example on previous page).
- The determinant is unchanged by adding a multiple of some row to another row (the same is true for columns).
- A zero row or column implies a zero determinant.
- $\det(AB) = \det(A) \det(B)$

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Inverse of a Matrix

- Let A be a square ($k \times k$) matrix.
- The inverse of a matrix is the analog to scalar

$$a^{-1} = \frac{1}{a} \quad \text{so} \quad a^{-1}a = 1$$

- There may exist a matrix $B_{(k \times k)}$ such that

$$AB = BA = I_k$$

- B is called the Inverse of A and is denoted as $B = A^{-1}$.
- The inverse exists *if and only if* the k columns (or rows) of A are linearly independent. i.e.,

$$c_1 \mathbf{a}_1 + c_2 \mathbf{a}_2 + \dots + c_k \mathbf{a}_k = \mathbf{0}$$

where $c_1 = c_2 = \dots = c_k = 0$.

- If A^{-1} exists, A is nonsingular.
- If A^{-1} does not exist, then A is singular.

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Inverse of a Matrix

■ A little example

$$\mathbf{A} = \begin{pmatrix} 3 & 2 \\ 4 & 1 \end{pmatrix}, \quad \mathbf{A}^{-1} = \frac{1}{10} \begin{pmatrix} -2 & 4 \\ 8 & -6 \end{pmatrix}$$

$$\mathbf{A}\mathbf{A}^{-1} = \frac{1}{10} \begin{pmatrix} (-6 + 16) & (12 - 12) \\ (-8 + 8) & (16 - 6) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

■ Steps for computing the inverse of a matrix:

- ◆ (1) Form a matrix of the same size as \mathbf{A} containing the minors for all entries of \mathbf{A} (i.e., for the $(i, j)^{th}$ entry, the minor is $\det(\mathbf{A}_{ij})$).
- ◆ (2) Multiply the matrix of minors by $(-1)^{i+j}$ to produce the matrix of cofactors.
- ◆ (3) Divide all entries in the cofactors matrix by $\det(\mathbf{A})$.
- ◆ (4) The transpose of the matrix found in (3) gives \mathbf{A}^{-1} .

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Example: Computing the Inverse

- The matrix A and its determinant:

$$A = \begin{pmatrix} 1 & 3 & 2 \\ 0 & 1 & 1 \\ 0 & 2 & 1 \end{pmatrix} \quad \text{and} \quad \det(A) = -1$$

- (1) Matrix of minors:

$$\begin{pmatrix} -1 & 0 & 0 \\ -1 & 1 & 2 \\ 1 & 1 & 1 \end{pmatrix}$$

- (2) Matrix of cofactors (i.e., $(-1)^{i+j}$)

$$\begin{pmatrix} -1 & 0 & 0 \\ 1 & 1 & -2 \\ 1 & -1 & 1 \end{pmatrix}$$

- (3) Divide cofactors by $\det(A) = -1$:

$$\begin{pmatrix} 1 & 0 & 0 \\ -1 & -1 & 2 \\ -1 & 1 & -1 \end{pmatrix}$$

- (4) Transpose gives A^{-1}

$$A^{-1} = \begin{pmatrix} 1 & -1 & -1 \\ 0 & -1 & 1 \\ 0 & 2 & -1 \end{pmatrix}$$

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Inverse of a Matrix

- Check that answer is correct:

$$\begin{pmatrix} 1 & 3 & 2 \\ 0 & 1 & 1 \\ 0 & 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & -1 & -1 \\ 0 & -1 & 1 \\ 0 & 2 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- Computing inverse for 2×2 is easy:

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

- Except for small matrices ($k = 2$ or 3), calculating the matrix inverse is (usually) difficult, so we'll let the computer do it for use.
- The exceptions are for diagonal and triangular matrices....

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Inverse of a Diagonal and Triangular Matrices

Inverse of a Diagonal Matrix:

$$\mathbf{A} = \begin{pmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{pp} \end{pmatrix} \quad \mathbf{A}^{-1} = \begin{pmatrix} 1/a_{11} & 0 & \dots & 0 \\ 0 & 1/a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1/a_{pp} \end{pmatrix}$$

Inverse of a Triangular matrix is a triangular matrix:

$$\mathbf{A} = \begin{pmatrix} a_{11} & 0 & \dots & 0 \\ a_{21} & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1} & a_{p2} & \dots & a_{pp} \end{pmatrix} \quad \mathbf{A}^{-1} = \begin{pmatrix} 1/a_{11} & 0 & \dots & 0 \\ b_{21} & 1/a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ b_{p1} & b_{p2} & \dots & 1/a_{pp} \end{pmatrix}$$

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Orthogonal Matrices

- $A_{p \times p}$ is an **orthogonal** matrix if for all pairs of columns (rows)

$$\mathbf{a}'_i \mathbf{a}_k = \begin{cases} 0 & \text{for } i \neq k \\ 1 & \text{for } i = k \end{cases}$$

- If A is orthogonal, then $A' = A^{-1}$; that is, $AA^{-1} = I = AA'$ and $A^{-1}A = I = A'A$.

- Because

- ◆ $A'A = I \implies$ Each column of A has length equal to 1 and all pairs of columns are orthogonal (i.e., perpendicular).
- ◆ $AA' = I \implies$ Each row of A has length equal to 1 and all pairs of rows are orthogonal.

- If A is orthogonal, then $\det(A) = \pm 1$.

- If A and B are both orthogonal, the AB is also orthogonal.

- Lengths of vectors don't change under orthogonal transformations; that is, let $\mathbf{y} = A\mathbf{x}$; then

$$L^2_{\mathbf{y}} = \mathbf{y}'\mathbf{y} = (A\mathbf{x})'(A\mathbf{x}) = \mathbf{x}'A'A\mathbf{x} = \mathbf{x}'I\mathbf{x} = \mathbf{x}'\mathbf{x} = L^2_{\mathbf{x}}$$

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Rank of a Matrix

- We can consider a matrix $A_{n \times p}$ as a collection of column vectors and/or a collection of row vectors:

$$A = \begin{pmatrix} \mathbf{r}'_1 \\ \mathbf{r}'_2 \\ \vdots \\ \mathbf{r}'_n \end{pmatrix} = (\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_p)$$

where $\mathbf{r}'_i = (a_{i1}, a_{i2}, \dots, a_{ip})$ and $\mathbf{c}'_j = (a_{1j}, a_{2j}, \dots, a_{nj})$.

- The **Rank** of a matrix is the maximum number of independent rows or columns in a matrix (row rank equals column rank).
- The rank of a matrix must be less than or equal to the smaller of n and p .
- **Full Rank** of a matrix means that the rank of the matrix equals the smaller of n or p .

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$$A = \begin{pmatrix} 1 & 1 & 1 \\ 2 & 5 & -1 \\ 0 & 1 & -1 \end{pmatrix}$$

Rows as vectors:

$$2 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 2 \\ 5 \\ -1 \end{pmatrix} + 3 \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Linearly independent or dependent? What's the row rank?

Columns as vectors

$$-2 \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 5 \\ 1 \end{pmatrix} + \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Linearly independent or dependent? What's the column rank?



Usefulness Properties of Rank

- A and A' have the same rank.
- $A'A$, AA' , and A have the same rank.
- The rank of a matrix is unchanged by a pre- or postmultiplication by a nonsingular matrix.
- The rank of a matrix is unchanged by what are called elementary row and column operations:
 - ◆ Interchange of two rows or two columns.
 - ◆ Multiplication of a row or a column by a scalar.
 - ◆ Addition of a row (or column) to another row (or column).

This is true because any elementary operation can be represented by a premultiplication (if the operation is to be on rows) or a postmultiplication (if the operation is to be on columns) of a nonsingular matrix.

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Quadratic Forms

- Suppose $A_{n \times n}$ is symmetric and let $\mathbf{x}' = (x_1, \dots, x_n)$. A quadratic form is defined by

$$\begin{aligned} \mathbf{x}' A \mathbf{x} &= \sum_{j=1}^n \sum_{k=1}^n a_{jk} x_j x_k \\ &= a_{11}x_1^2 + a_{22}x_2^2 + \dots + a_{pp}x_n^2 \\ &\quad + 2a_{12}x_1x_2 + \dots + 2a_{1n}x_1x_n + \dots + 2a_{(n-1)n}x_{n-1}x_n \end{aligned}$$

- Why are quadratic forms important? One example, ... What does this equal?

$$(x_1, x_2, \dots, x_n) \begin{pmatrix} n/(1-n) & -1/n & \dots & -1/n \\ -1/n & n/(1-n) & \dots & -1/n \\ \vdots & \vdots & \ddots & \vdots \\ -1/n & -1/n & \dots & n/(1-n) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

$$\sum_{j=1}^n (x_j - \bar{x})^2$$

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More about Quadratic Forms

- A symmetric matrix A (and associated quadratic form) is
 - ◆ positive definite (p.d.) if $x'Ax > 0$ for all $x \neq 0$.
 - ◆ positive semi-definite (p.s.d) if $x'Ax \geq 0$ for all x .

- Negative definite, negative semi-definite, and indefinite forms exist as well; however, **correlation and covariance matrices (and W)**
 - ◆ Are at least positive semi-definite.
 - ◆ Satisfies the stronger condition of being positive definite if the vectors of the variables on which the correlation and covariance matrices is based, are linearly independent.

- Matrices that are positive definite have inverses (i.e., nonsingular).

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First Pass at Eigenvalues and Eigenvectors

- A square matrix $A_{p \times p}$ has an **eigenvalue** λ (a scalar) and a corresponding **eigenvector** x ($\neq 0$) if

$$Ax = \lambda x \quad \text{or equivalently} \quad (A - \lambda I)x = 0$$

- Note:

$$Ax = \lambda x$$

$$Ax - \lambda x = 0$$

$$Ax - \lambda Ix = 0$$

$$(Ax - \lambda I)x = 0$$

- Usually we divide x by its length Lx so that we get a normalized eigenvector; eigenvectors with length = 1,

$$e = \frac{x}{Lx} \quad \longrightarrow \quad e'e = \left(\frac{x'}{Lx} \right) \left(\frac{x}{Lx} \right) = \frac{x'x}{x'x} = 1$$

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- If $A_{p \times p}$ is **symmetric**, then A has p pairs of eigenvalues and eigenvectors

$$\lambda_1, e_1 \quad \lambda_2, e_2 \quad \dots \quad \lambda_p, e_p$$

- Matrix decomposition (very important)

$$A = \lambda_1 e_1 e_1' + \lambda_2 e_2 e_2' + \dots + \lambda_p e_p e_p'$$

- We'll cover this in more detail later, as well as some other topics (including SVD of rectangular matrices).



Random Vectors and Matrices

Mean Vectors, Covariance Matrices and Correlation Matrices

- **Random vector** is a vector whose elements are random variables.
- **Random matrix** is a matrix whose elements are random variables.
- Let $\mathbf{X} = \{X_{jk}\}_{n \times p}$ be a random matrix (i.e., data matrix).

The expected value of \mathbf{X} equals the expected values of its entries (the random variables):

$$E(\mathbf{X}) = \begin{pmatrix} E(X_{11}) & E(X_{12}) & \cdots & E(X_{1p}) \\ E(X_{21}) & E(X_{22}) & \cdots & E(X_{2p}) \\ \vdots & \vdots & \ddots & \vdots \\ E(X_{n1}) & E(X_{n2}) & \cdots & E(X_{np}) \end{pmatrix}$$

assuming $E(X_{jk})$ exists for all (j, k) .

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Expected Values

- $E(X_{jk})$ equals the expected value or mean of random variable X_{jk} .

- If X_{jk} is **discrete**, then

$$E(X_{jk}) = \sum_{\text{all } x} x_{jk} p_{jk}(x_{jk})$$

where $p_{jk}(x_{jk})$ is the probability **mass** function of X_{jk} .

- If X_{jk} is **continuous**, then

$$E(X_{jk}) = \int_{-\infty}^{+\infty} x_{jk} f_{jk}(x_{jk}) dx_{jk}$$

where $f_{jk}(x_{jk})$ is the probability **density** function of X_{jk} .

In this class, our “dependent” variables will be continuous and we’ll use the multivariate normal distribution.

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Expected Values (continued)

■ Little example using a discrete variable

- ◆ Let X_{11} be a Bernoulli random variable.
- ◆ The probability mass function is

$$X_{11} = \begin{cases} 0 & \text{with probability} = 1 - \pi_{11} \\ 1 & \text{with probability} = \pi_{11} \end{cases}$$

- ◆ The mean of X_{11} is

$$E(X_{11}) = 0(1 - \pi_{11}) + 1\pi_{11} = \pi_{11}$$

Here “all x ” = $\{0, 1\}$.

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Expected Values for Matrices

- Let $X_{n \times p}$ and $Y_{n \times p}$ be random matrices, then

$$E(X + Y) = E(X) + E(Y)$$

- Also let $A_{m \times n}$ and $B_{p \times k}$ be matrices of constants, then

$$E(AXB) = AE(X)B$$

- Preliminaries: Let $X_{n \times 1}$ be a random vector where each element X_i is a random variable with

$$\mu_i = E(X_i) \quad \text{and} \quad \sigma_{ii} = E((X_i - \mu_i)^2)$$

for all $i = 1, \dots, p$, and $\sqrt{\sigma_{ii}}$ equals the standard deviation.

- The covariance between X_i and X_k is

$$\sigma_{ik} = E((X_i - \mu_i)(X_k - \mu_k))$$

These expected values are computed using the **joint** probability mass function (if discrete) or the probability density function (if continuous) for X_i and X_k ,

$$f_{ik}(x_i, x_k) \quad \text{or} \quad p_{ik}(x_i, x_k)$$

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Implications of Statistical Independence

- Let's consider all p random variables simultaneously (i.e., the random vector)

$$\mathbf{X}' = (X_1, X_2, \dots, X_p)$$

- Let $f(\mathbf{x})$ be the joint probability density (mass) function,

$$f(\mathbf{x}) = f(x_1, x_2, \dots, x_p)$$

In this class, $f(\mathbf{x})$ is the **multivariate normal distribution**.

- If X_i and X_k are statistically independent, then the joint probability function factors, e.g.,

$$f_{ik}(x_i, x_k) = f_i(x_i)f_k(x_k) \implies \sigma_{ik} = 0$$

Statistical independence implies $\sigma_{ik} = 0$.

- If all $\binom{p}{2}$ pairs of variables are statistically independent, then

$$f(\mathbf{x}) = f(x_1, x_2, \dots, x_p) = f_1(x_1)f_2(x_2) \cdots f_p(x_p) \implies \sigma_{ik} = 0 \quad \forall i, k$$

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- In general, the reverse is not true; that is, a 0 covariance does not necessarily imply statistical independence.

The exception is when $f(x)$ is multivariate normal.

- In sum,
 - ◆ Statistical independence implies 0 covariance.
 - ◆ 0 covariance does not imply statistical independence.
 - ◆ 0 covariance and multivariate normal implies statistical independence.

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$$E(\mathbf{X}) = \boldsymbol{\mu} = \begin{pmatrix} E(X_1) \\ E(X_2) \\ \vdots \\ E(X_p) \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_p \end{pmatrix}$$

and

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p1} & \sigma_{p2} & \cdots & \sigma_{pp} \end{pmatrix}$$

where $\sigma_{ik} = \sigma_{ki}$.

In sum, $\boldsymbol{\Sigma}$ is $p \times p$ symmetric matrix with variances along the diagonal and covariances on the off-diagonal.

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Definition of Covariance Matrix

$$\begin{aligned} \Sigma &= E((\mathbf{X} - \boldsymbol{\mu})(\mathbf{X} - \boldsymbol{\mu})') \\ &= E \left(\begin{pmatrix} (X_1 - \mu_1) \\ (X_2 - \mu_2) \\ \vdots \\ (X_p - \mu_p) \end{pmatrix} \left((X_1 - \mu_1), (X_2 - \mu_2), \dots, (X_p - \mu_p) \right) \right) \\ &= \begin{pmatrix} E((X_1 - \mu_1)^2) & E((X_1 - \mu_1)(X_2 - \mu_2)) & \cdots & E((X_1 - \mu_1)(X_p - \mu_p)) \\ E((X_2 - \mu_1)(X_1 - \mu_1)) & E((X_2 - \mu_2)^2) & \cdots & E((X_2 - \mu_2)(X_p - \mu_p)) \\ \vdots & \vdots & \ddots & \vdots \\ E((X_p - \mu_p)(X_1 - \mu_1)) & E((X_p - \mu_p)(X_2 - \mu_2)) & \cdots & E((X_p - \mu_p)^2) \end{pmatrix} \end{aligned}$$

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Estimation of Population Quantities

The sample mean vector $\bar{\mathbf{x}}$ is an estimator of $\boldsymbol{\mu}$:

$$\bar{\mathbf{x}} = \begin{pmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_p \end{pmatrix}$$

The matrix of sample variances and covariances S is an estimator of Σ :

$$S = \begin{pmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ s_{21} & s_{22} & \cdots & s_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{p1} & s_{p2} & \cdots & s_{pp} \end{pmatrix}$$

where

$$s_{ik} = \frac{1}{n} \sum_{j=1}^n (x_{ij} - \bar{x}_i)(x_{kj} - \bar{x}_k),$$

so $s_{ik} = s_{ki}$

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- \bar{x} is the maximum likelihood estimator of μ .
- S is the maximum likelihood estimator of Σ .
- Maximum likelihood estimators are denoted by $\hat{\cdot}$, i.e., $\hat{\mu}$ and $\hat{\Sigma}$.
- $\hat{\Sigma} = S$ is a biased estimator of Σ . For an unbiased one, divide sum of squared deviations by $(n - 1)$.
- The sum of squared deviations and sum of cross-product deviations

$$W = \{w_{ik}\}_{p \times p}$$

where $w_{ik} = \sum_{j=1}^n (x_{ji} - \bar{x}_i)(x_{jk} - \bar{x}_k)$, which are the numerators of the variances and covariances.



Correlation Matrices

The population (Pearson product-moment) correlation coefficient is

$$\rho_{ik} = \frac{\sigma_{ik}}{\sqrt{\sigma_{ii}}\sqrt{\sigma_{kk}}}$$

which measures the amount of linear association between the random variables X_i and X_k .

The population correlation matrix:

$P =$

$$\begin{pmatrix} 1 & \rho_{12} & \cdots & \rho_{1p} \\ \rho_{21} & 1 & \cdots & \rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{p1} & \rho_{p2} & \cdots & 1 \end{pmatrix} = \begin{pmatrix} \sigma_{11}/\sqrt{\sigma_{11}\sigma_{11}} & \sigma_{12}/\sqrt{\sigma_{11}\sigma_{22}} & \cdots & \sigma_{1p}/\sqrt{\sigma_{11}\sigma_{pp}} \\ \sigma_{21}/\sqrt{\sigma_{22}\sigma_{11}} & \sigma_{22}/\sqrt{\sigma_{22}\sigma_{22}} & \cdots & \sigma_{2p}/\sqrt{\sigma_{22}\sigma_{pp}} \\ \vdots & \vdots & \cdots & \vdots \\ \sigma_{p1}/\sqrt{\sigma_{pp}\sigma_{11}} & \sigma_{p2}/\sqrt{\sigma_{pp}\sigma_{22}} & \cdots & \sigma_{pp}/\sqrt{\sigma_{pp}\sigma_{pp}} \end{pmatrix}$$

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Correlation/Covariance Matrix Relationship

in matrix terms...

Define

$$D_{p \times p}^{-1/2} = \begin{pmatrix} 1/\sqrt{\sigma_{11}} & 0 & \cdots & 0 \\ 0 & 1/\sqrt{\sigma_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/\sqrt{\sigma_{pp}} \end{pmatrix}$$

Recall:

- Pre-multiplication of a matrix by a diagonal matrix \longrightarrow multiply the j^{th} row of the matrix by the d_{jj} (j^{th} diagonal elements).
- Post-multiplication of a matrix by a diagonal matrix \longrightarrow multiply the k^{th} column of the matrix by the k^{th} diagonal element, d_{kk} .

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Correlation/Covariance Matrix Relationship

So

$$P = D^{-1/2} \Sigma D^{-1/2} \quad \text{and} \quad \Sigma = D^{1/2} P D^{1/2}$$

where $D^{1/2} = \text{diag}(\sqrt{\sigma_{ii}})$.

e.g.,

$$\Sigma = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 4 & 3 \\ 2 & 3 & 9 \end{pmatrix} \quad D^{-1/2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/3 \end{pmatrix}$$

$$P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/3 \end{pmatrix} \begin{pmatrix} 1 & 1 & 2 \\ 1 & 4 & 3 \\ 2 & 3 & 9 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/3 \end{pmatrix} \\ = \begin{pmatrix} 1 & 1/2 & 2/6 \\ 1/2 & 1 & 1/2 \\ 2/3 & 1/5 & 1 \end{pmatrix}$$

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Estimation of Correlation Matrix

The sample correlation matrix R estimates P ,

$$R = \begin{pmatrix} 1 & r_{12} & \cdots & r_{1p} \\ r_{21} & 1 & \cdots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{p1} & r_{p2} & \cdots & 1 \end{pmatrix}$$

where $r_{ik} = s_{ik} / (\sqrt{s_{ii}}\sqrt{s_{kk}})$.

The relationship between S and R is the same as the one between Σ and P .

Let $D_s^{-1/2} = \text{diag}(\sqrt{s_{ii}})$, then

$$S = D_s^{1/2} R D_s^{1/2} \quad \text{and} \quad R = D_s^{-1/2} S D_s^{-1/2}$$

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Useful Matrix Formulas: Mean vector

$(n \times p)$ Data Matrix \mathbf{X}

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix}$$

$(p \times 1)$ Mean vector $\bar{\mathbf{x}}$

$$\bar{\mathbf{x}} = \frac{1}{n} \mathbf{X}' \mathbf{1}_n = \begin{pmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_p \end{pmatrix} = \frac{1}{n} \begin{pmatrix} x_{11} & x_{21} & \dots & x_{n1} \\ x_{12} & x_{22} & \dots & x_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1p} & x_{2p} & \dots & x_{np} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

or as a row vector

$$\bar{\mathbf{x}}' = \frac{1}{n} \mathbf{1}_n' \mathbf{X}$$

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Matrix of Deviations from Means

Note:

$$\mathbf{1}_n \bar{\mathbf{x}}' = \frac{1}{n} \mathbf{1}_n \mathbf{1}_n' \mathbf{X} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} (\bar{x}_1, \bar{x}_2, \dots, \bar{x}_p) = \begin{pmatrix} \bar{x}_1 & \bar{x}_2 & \dots & \bar{x}_p \\ \bar{x}_1 & \bar{x}_2 & \dots & \bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ \bar{x}_1 & \bar{x}_2 & \dots & \bar{x}_p \end{pmatrix}$$

So,

$$\mathbf{X} - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n' \mathbf{X} = \begin{pmatrix} x_{11} - \bar{x}_1 & x_{12} - \bar{x}_2 & \dots & x_{1p} - \bar{x}_p \\ x_{21} - \bar{x}_1 & x_{22} - \bar{x}_2 & \dots & x_{2p} - \bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} - \bar{x}_1 & x_{n2} - \bar{x}_2 & \dots & x_{np} - \bar{x}_p \end{pmatrix}$$

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Covariance Matrix

$(p \times p)$ Variance/Covariance Matrix S

$$\begin{aligned} S &= \left(\frac{1}{n-1} \right) \left(X - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n X \right)' \left(X - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n X \right) \\ &= \left(\frac{1}{n-1} \right) X' \left(I - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n \right)' \left(I - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n \right) X \\ &= \left(\frac{1}{n-1} \right) X' \left(I - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n \right) X \end{aligned}$$

Since

$$\left(I - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n \right)' \left(I - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n \right) = \left(I - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n \right)$$

Also,

$$W = (n-1)S = X' \left(I - \frac{1}{n} \mathbf{1}_n \mathbf{1}'_n \right) X$$

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Correlation Matrix

Define:

$$D_{p \times p} = \begin{pmatrix} s_{11} & 0 & \dots & 0 \\ 0 & s_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & s_{pp} \end{pmatrix}$$

and

$$D_{p \times p}^{-1/2} = \begin{pmatrix} 1/\sqrt{s_{11}} & 0 & \dots & 0 \\ 0 & 1/\sqrt{s_{22}} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1/\sqrt{s_{pp}} \end{pmatrix}$$

$(p \times p)$ Correlation Matrix R

$$\begin{aligned} R &= D^{-1/2} S D^{-1/2} \\ &= \left(\frac{1}{n-1} \right) D^{-1/2} X' \left(I - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n' \right) X D^{-1/2} \end{aligned}$$

And

$$S = D^{1/2} R D^{1/2}$$

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Useful Matrix Formulas

● Useful Matrix Formulas:

Mean vector

● Matrix of Deviations from Means

● Covariance Matrix

● Correlation Matrix

Matrix Software



Matrix Software: SAS/IML

● Outline

Motivation

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Matrix Software

- Matrix Software: SAS/IML
- SAS/IML (continued)
- MATLAB
- R (SPlus)
- R (continued)

```
proc iml;
```

```
* Create matrices;
```

```
A = {1 2 3,  
      5 1 2};
```

```
B = {2 0,  
      4 3,  
     -2 1};
```

```
* Matrix addition;
```

```
E = A + B;
```

```
print E;
```

```
* Matrix Multiplication;
```

```
AB=A*B;
```

```
BA=B*A;
```

```
print 'Multiplication is (usually) not commutative',
```

```
      'AB= ' AB,
```

```
      'BA= ' BA;
```



SAS/IML (continued)

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* Determinant of a matrix;

$$A = \begin{Bmatrix} 4 & 3 & 2 & 1, \\ 2 & 5 & 1 & 0, \\ 1 & 3 & 2 & 1, \\ 3 & 2 & 1 & 4 \end{Bmatrix};$$

```
detA = det(A);
```

```
print detA;
```

* Inverse of a matrix;

```
invA = inv(A);
```

```
check1 = invA*A;
```

```
check2 = A*invA;
```

* Trace of a matrix;

```
trA = trace(A);
```

```
print invA, check1, check2, trA;
```



MATLAB

$$A = \begin{bmatrix} 1 & 2 & 3; \\ 5 & 1 & 2 \end{bmatrix}$$

$$B = \begin{bmatrix} 2 & 0; \\ 4 & 3; \\ -2 & 1 \end{bmatrix}$$

$$E = A + B'$$

$$AB = A * B$$

$$BA = B * A$$

$$A = \begin{bmatrix} 4 & 3 & 2 & 1; \\ 2 & 5 & 1 & 0; \\ 1 & 3 & 2 & 1; \\ 3 & 2 & 1 & 4 \end{bmatrix}$$

$$\det A = \det(A)$$

$$\text{inv}A = \text{inv}(A)$$

$$\text{inv}A * A;$$

$$A * \text{inv}A;$$

$$\text{trace}(A)$$

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R (SPlus)

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```
# Example of R code for simple matrix operations
```

```
#
```

```
# Create matrices
```

```
A <- matrix(c(1,5, 2,1, 3,2), nrow=2, ncol=3)
```

```
B <- matrix(c(2, 4, -2, 0, 3, 1), nrow=3, ncol=2)
```

```
# Matrix addition (A plus transpose of B)
```

```
# Matrix multiplication
```

```
AB <- A %*% B
```

```
BA <- B %*% A
```

```
# Note that the following does element by
```

```
# element multiplication
```

```
AtB <- A * t(B)
```



R (continued)

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- R (continued)

```
# Determinant of a matrix
```

```
A <- matrix(c(4, 2, 1, 3,  
              3, 5, 3, 2,  
              2, 1, 2, 1,  
              1, 0, 1, 4),  
            nrow=4, ncol=4)
```

```
det <- det(A)
```

```
# inverse of a matrix
```

```
invA <- solve(A)
```

```
# Check
```

```
AinvA <- A %*% invA
```

```
invAA <- invA %*% A
```