College of
EDUCATION

AN INTRODUCTION TO MATRIX ALGEBRA AND THE MULTIVARIATE NORMAL DISTRIBUTION

In This Lecture…

An introduction to matrix algebra

- Scalars, vectors, and matrices
- Basic matrix operations
- Advanced matrix operations

An introduction to matrices in R

- Embedded within the R language

Why Learning a Little Matrix Algebra is Important

Matrix algebra is the alphabet of the language of statistics

- You will most likely encounter formulae with matrices very quickly

For example, imagine you were interested in analyzing some repeated measures data…but things don't go as planned

- From the SAS User's Guide (PROC MIXED):

Formulation of the Mixed Model

The previous general linear model is certainly a useful one (Sea
although you still assume normality.

The mixed model is written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}$$

where everything is the same as in the general linear model exc
Henderson (1990) and Searle, Casella, and McCulloch (1992) fc

A key assumption in the foregoing analysis is that $\boldsymbol{\gamma}$ and $\boldsymbol{\varepsilon}$ are

$$\mathrm{E}\begin{bmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\varepsilon} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

$$\mathrm{Var}\begin{bmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\varepsilon} \end{bmatrix} = \begin{bmatrix} \mathbf{G} & \mathbf{0} \\ \mathbf{0} & \mathbf{R} \end{bmatrix}$$

The variance of $\mathbf{y}$ is, therefore, $\mathbf{V} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}$. You can model

Estimating Covariance Parameters in the Mixed Model

Estimation is more difficult in the mixed model than in the general linear model. Not only do y

$$(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

However, it requires knowledge of $\mathbf{V}$ and, therefore, knowledge of $\mathbf{G}$ and $\mathbf{R}$. Lacking such infc

In many situations, the best approach is to use *likelihood-based* methods, exploiting the ass
(REML). A favorable theoretical property of ML and REML is that they accommodate data tha

PROC MIXED constructs an objective function associated with ML or REML and maximizes i

$$\text{ML:} \quad l(\mathbf{G},\mathbf{R}) = -\frac{1}{2}\log|\mathbf{V}| - \frac{1}{2}\mathbf{r}'\mathbf{V}^{-1}\mathbf{r} - \frac{n}{2}\log(2\pi)$$

$$\text{REML:} \quad l_R(\mathbf{G},\mathbf{R}) = -\frac{1}{2}\log|\mathbf{V}| - \frac{1}{2}\log|\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}| - \frac{1}{2}\mathbf{r}'\mathbf{V}^{-1}\mathbf{r} - \frac{n-p}{2}\log(2\pi)\}$$

where $\mathbf{r} = \mathbf{y} - \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$ and p is the rank of $\mathbf{X}$. PROC MIXED actually minimiz
analytical details for implementing a QR-decomposition approach to the problem. Wolfinger, T

Introduction and Motivation

Nearly all multivariate statistical techniques are described with matrix algebra

When new methods are developed, the first published work typically involves matrices

- It makes technical writing more concise – formulae are smaller

Have you seen:

$$(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$
$$\boldsymbol{\Lambda\Phi\Lambda}^T + \boldsymbol{\Psi}$$

Useful tip: matrix algebra is a great way to get out of boring conversations and other awkward moments

We begin this class with some general definitions (from dictionary.com):

Matrix:

1. A rectangular array of numeric or algebraic quantities subject to mathematical operations
2. The substrate on or within which a fungus grows

Algebra:

1. A branch of mathematics in which symbols, usually **letters** of the alphabet, represent numbers or members of a specified set and are used to represent quantities and to express general relationships that hold for all members of the set

2. A set together with a pair of **binary operations** defined on the set. Usually, the set and the operations include an **identity element**, and the operations are **commutative** or **associative**

Why Learn Matrix Algebra

Matrix algebra can seem very abstract from the purposes of this class (and statistics in general)

Learning matrix algebra is important for:

- Understanding how statistical methods work
  - And when to use them (or not use them)
- Understanding what statistical methods mean
- Reading and writing results from new statistical methods

This is a first lecture of learning the language of multivariate statistics

DATA EXAMPLE AND R

A Guiding Example

To demonstrate matrix algebra, we will make use of data

Imagine that I collected data SAT test scores for both the Math (SATM) and Verbal (SATV) sections of 1,000 students

The descriptive statistics of this data set are given below:

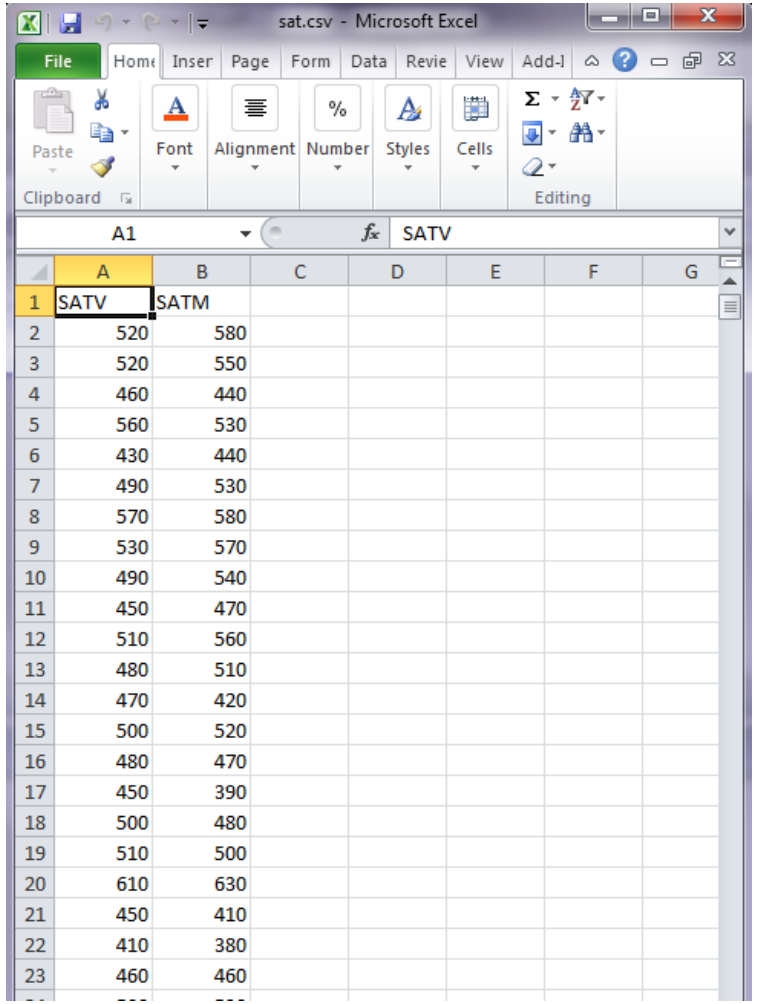
Statistic	SATV	SATM
Mean	499.3	498.3
SD	49.8	81.2

Correlation

SATV	1.00	0.78
SATM	0.78	1.00

The Data…

In Excel:



	A	B	C	D	E	F	G
1	SATV	SATM					
2	520	580					
3	520	550					
4	460	440					
5	560	530					
6	430	440					
7	490	530					
8	570	580					
9	530	570					
10	490	540					
11	450	470					
12	510	560					
13	480	510					
14	470	420					
15	500	520					
16	480	470					
17	450	390					
18	500	480					
19	510	500					
20	610	630					
21	450	410					
22	410	380					
23	460	460					

In R:

	SATV	SATM
1	520	580
2	520	550
3	460	440
4	560	530
5	430	440
6	490	530
7	570	580
8	530	570
9	490	540
10	450	470
11	510	560
12	480	510
13	470	420
14	500	520
15	480	470
16	450	390
17	500	480
18	510	500
19	610	630
20	450	410
21	410	380
22	460	460

DEFINITIONS OF MATRICES, VECTORS, AND SCALARS

Matrices

A matrix is a rectangular array of data

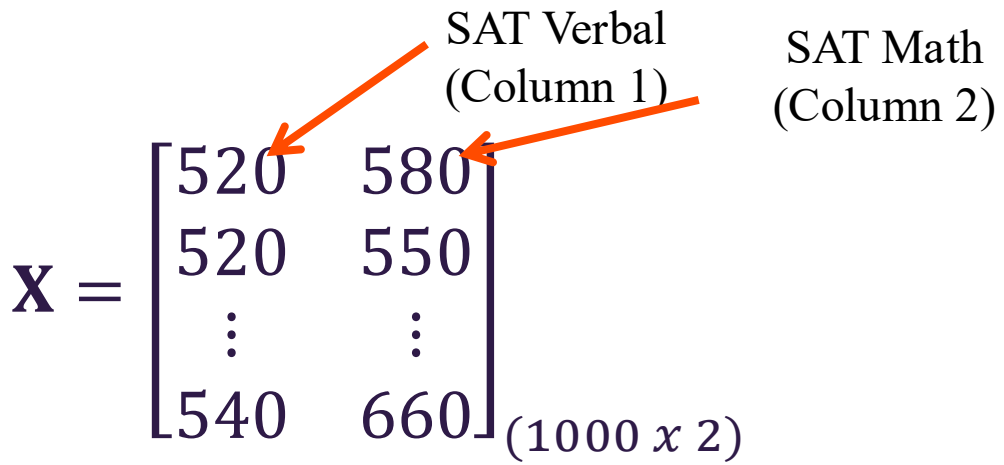
- Used for storing numbers

Matrices can have unlimited dimensions

- For our purposes all matrices will have two dimensions:
  - Row
  - Columns

Matrices are symbolized by **boldface** font in text, typically with capital letters

- Size (r rows x c columns)



Vectors

A vector is a matrix where one dimension is equal to size 1

- Column vector: a matrix of size $r \; x \; 1$

$$\boldsymbol{x}_{\cdot 1} = \begin{bmatrix} 520 \\ 520 \\ \vdots \\ 540 \end{bmatrix}_{1000 \; x \; 1}$$

- Row vector: a matrix of size $1 \; x \; c$

$$\boldsymbol{x}_{1\cdot} = [520 \quad 580]_{1 \; x \; 2}$$

Vectors are typically written in **boldface** font text, usually with lowercase letters

The dots in the subscripts $\boldsymbol{x}_{\cdot 1}$ and $\boldsymbol{x}_{1\cdot}$ represent the dimension aggregated across in the vector

- $\boldsymbol{x}_{1\cdot}$ is the first row and **all** columns of $\mathbf{X}$
- $\boldsymbol{x}_{\cdot 1}$ is the first column and **all** rows of $\mathbf{X}$
- Sometimes the rows and columns are separated by a comma (making it possible to read double-digits in either dimension)

Matrix Elements

A matrix (or vector) is composed of a set of elements

- Each element is denoted by its position in the matrix (row and column)

For our matrix of data $\mathbf{X}$ (size 1000 rows and 2 columns), each element is denoted by:

$$x_{ij}$$

- The first subscript is the index for the rows: i = 1,…,r (= 1000)
- The second subscript is the index for the columns: j = 1,…,c (= 2)

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ \vdots & \vdots \\ x_{1000,1} & x_{1000,2} \end{bmatrix}_{(1000\ x\ 2)}$$

Scalars

A scalar is just a single number

The name scalar is important: the number “scales” a vector –
it can make a vector “longer” or “shorter”

Scalars are typically written without boldface:

$$x_{11} = 520$$

Each element of a matrix is a scalar

Matrix Transpose

The transpose of a matrix is a reorganization of the matrix by switching the indices for the rows and columns

$$\mathbf{X} = \begin{bmatrix} 520 & 580 \\ 520 & 550 \\ \vdots & \vdots \\ 540 & 660 \end{bmatrix}_{(1000\ x\ 2)}$$

$$\mathbf{X}^T = \begin{bmatrix} 520 & 520 & \cdots & 540 \\ 580 & 550 & \cdots & 660 \end{bmatrix}_{(2\ x\ 1000)}$$

An element x_{ij} in the original matrix $\mathbf{X}$ is now x_{ji} in the transposed matrix $\mathbf{X}^T$

Transposes are used to align matrices for operations where the sizes of matrices matter (such as matrix multiplication)

Types of Matrices

Square Matrix: A square matrix has the same number of rows and columns

- Correlation/covariance matrices are square matrices

Diagonal Matrix: A diagonal matrix is a square matrix with non-zero diagonal elements ($x_{ij} \neq 0 \text{ for } i = j$) and zeros on the off-diagonal elements ($x_{ij} = 0 \text{ for } i \neq j$):

$$\mathbf{A} = \begin{bmatrix} 2.759 & 0 & 0 \\ 0 & 1.643 & 0 \\ 0 & 0 & 0.879 \end{bmatrix}$$

- We will use diagonal matrices to form correlation matrices

Symmetric Matrix: A symmetric matrix is a square matrix where all elements are reflected across the diagonal ($a_{ij} = a_{ji}$)

- Correlation and covariance matrices are symmetric matrices

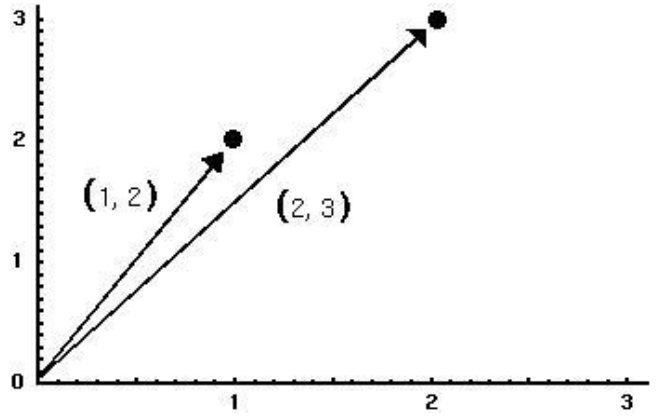
VECTORS

Vectors in Space…

Vectors (row or column) can be represented as lines on a Cartesian coordinate system (a graph)

Consider the vectors: $\mathbf{a} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ and $\mathbf{b} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$

A graph of these vectors would be:



Question: how would a column vector for each of our example variables (SATM and SATV) be plotted?

Vector Length

The length of a vector emanating from the origin is given by the Pythagorean formula

This is also called the Euclidean distance between the endpoint of the vector and the origin

$$L_{\mathbf{x}} = \sqrt{x_{11}^2 + x_{21}^2 + \cdots + x_{r1}^2} = \|\mathbf{x}\|$$

From the last slide: $\|\mathbf{a}\| = \sqrt{5} = 2.24$; $\|\mathbf{b}\| = \sqrt{13} = 3.61$

From our data:

$$\|\mathbf{SATV}\| = 15{,}868.138; \|\mathbf{SATM}\| = 15{,}964.42$$

In data: length is an analog to the standard deviation

In mean-centered variables, the length is the square root of the sum of mean deviations (not quite the SD, but close)

Vector Addition

Vectors can be added together so that a new vector is formed

Vector addition is done element-wise, by adding each of the respective elements together:

- The new vector has the same number of rows and columns

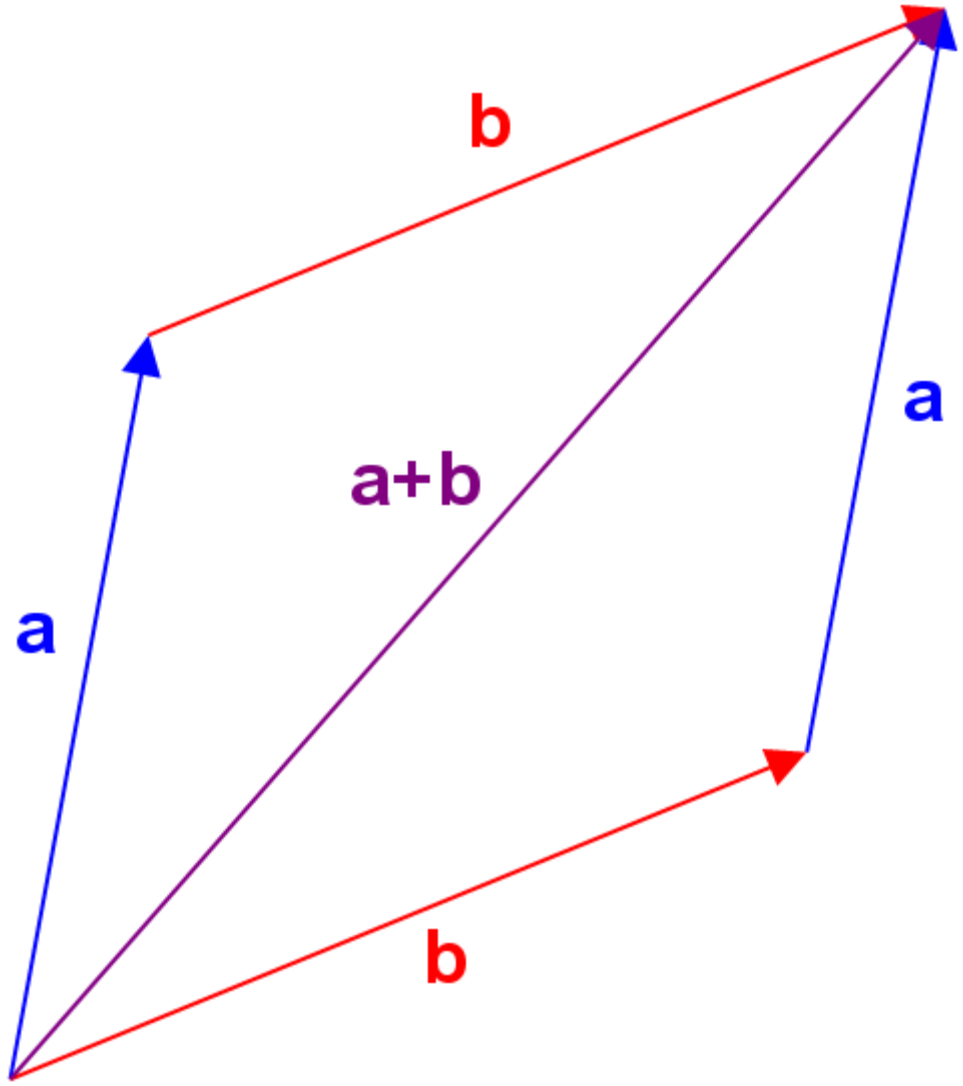
$$\mathbf{c} = \mathbf{a} + \mathbf{b} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} + \begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}$$

- Geometrically, this creates a new vector along either of the previous two
  - Starting at the origin and ending at a new point in space

In Data: a new variable (say, SAT total) is the result of vector addition

$$\boldsymbol{SAT_{TOTAL}} = \boldsymbol{x}_{.1} + \boldsymbol{x}_{.2}$$

Vector Addition: Geometrically



Vector Multiplication by Scalar

Vectors can be multiplied by scalars

- All elements are multiplied by the scalar

$$\mathbf{d} = 2\mathbf{a} = 2\begin{bmatrix}1\\2\end{bmatrix} = \begin{bmatrix}2\\4\end{bmatrix}$$

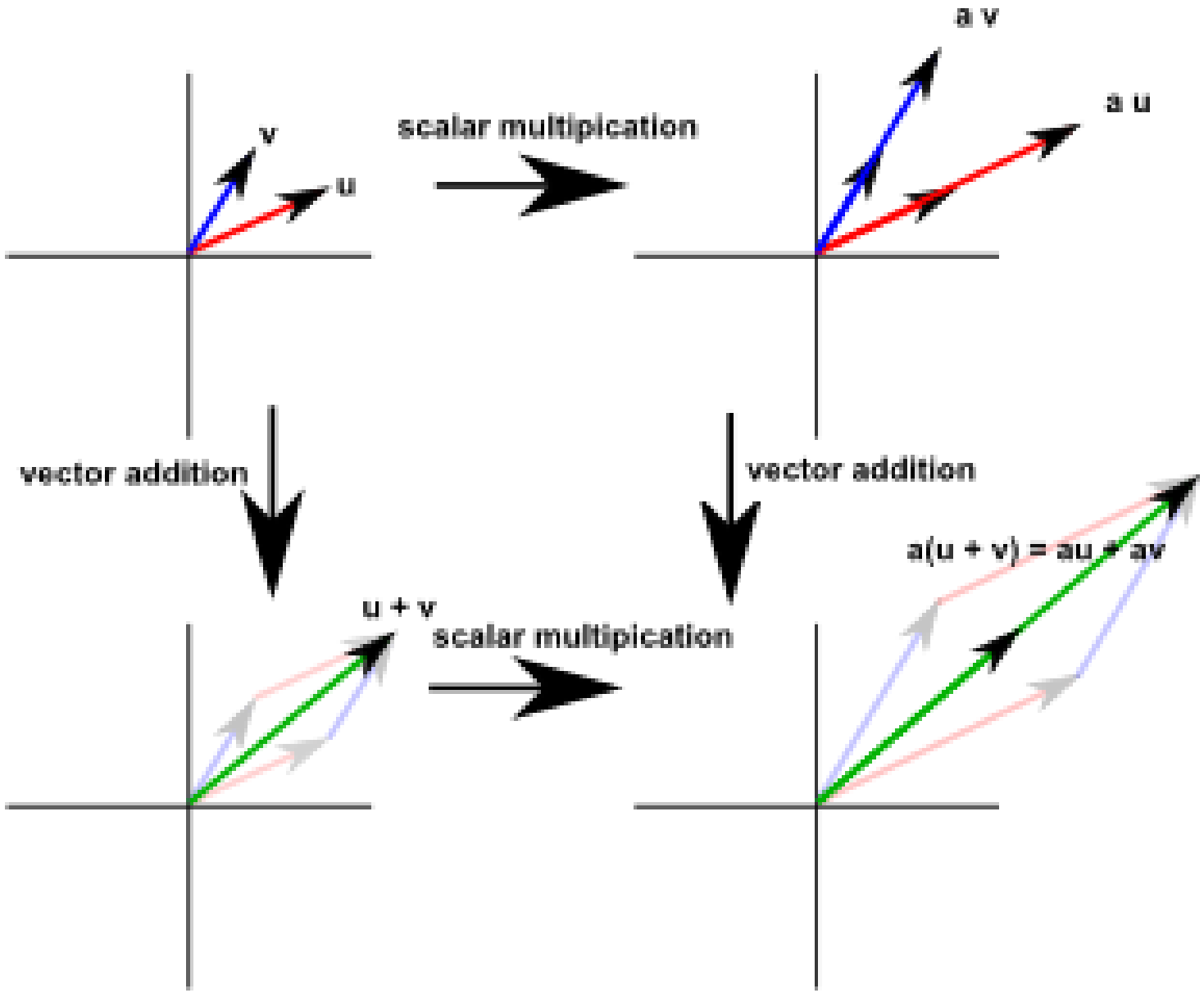
Scalar multiplication changes the length of the vector:

$$\|\mathbf{d}\| = \sqrt{2^2 + 4^2} = \sqrt{20} = 4.47$$

This is where the term scalar comes from: a scalar ends up "rescaling" (resizing) a vector

In Data: the GLM (where **X** is a matrix of data) the fixed effects (slopes) are scalars multiplying the data

Scalar Multiplication: Geometrically



Linear Combinations

Addition of a set of vectors (all multiplied by scalars) is called a linear combination:

$$\mathbf{y} = a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \cdots + a_k\mathbf{x}_k$$

Here, $\mathbf{y}$ is the linear combination

For all *k* vectors, the set of all possible linear combinations is called their span

Typically not thought of in most analyses – but when working with things that don't exist (latent variables) becomes somewhat important

In Data: linear combinations happen frequently:

- Linear models (i.e., Regression and ANOVA)
- Principal components analysis

Linear Dependencies

A set of vectors are said to be linearly dependent if

$$a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \cdots + a_k\mathbf{x}_k = 0$$

-and-

$a_1, a_2, \ldots, a_k$ are all **not** zero

Example: let's make a new variable – SAT Total:

$$\mathbf{SAT_{total}} = 1 * \mathbf{SATV} + 1 * \mathbf{SATM}$$

The new variable is linearly dependent with the others:

$$(1) * \mathbf{SATV} + (1) * \mathbf{SATM} + (-1) * \mathbf{SAT_{total}} = \mathbf{0}$$

In Data: (multi)collinearity is a linear dependency. Linear dependencies are bad for statistical analyses that use matrix inverses

Inner (Dot) Product of Vectors

An important concept in vector geometry is that of the inner product of two vectors

- The inner product is also called the dot product

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^T\mathbf{b} = a_{11}b_{11} + a_{21}b_{21} + \cdots + a_{N1}b_{N1} = \sum_{i=1}^{N} a_{i1}b_{i1}$$

The dot or inner product is related to the angle between vectors and to the projection of one vector onto another

From our example: $\mathbf{a} \cdot \mathbf{b} = 1 * 2 + 2 * 3 = 8$

From our data: $\boldsymbol{x}_{.1} \cdot \boldsymbol{x}_{.2} = 251{,}928{,}400$

- **<u>In data:</u>** the angle between vectors is related to the correlation between variables and the projection is related to regression/ANOVA/linear models

Angle Between Vectors

As vectors are conceptualized geometrically, the angle between two vectors can be calculated

$$\theta_{ab} = \cos^{-1}\left(\frac{\mathbf{a} \cdot \boldsymbol{b}}{\|\mathbf{a}\|\|\mathbf{b}\|}\right)$$

From the example:

$$\theta_{ab} = \cos^{-1}\left(\frac{8}{\sqrt{5}\sqrt{13}}\right) = 0.12$$

From our data:

$$\theta_{SATV,SATM} = \cos^{-1}\left(\frac{251{,}928{,}400}{\sqrt{15{,}868.138}\sqrt{15{,}946.42}}\right) = 0.105$$

In Data: Cosine Angle = Correlation

If you have data that are:

- Placed into vectors
- Centered by the mean (subtract the mean from each observation)

…then the cosine of the angle between those vectors is the correlation between the variables:

$$r_{ab} = cos(\theta_{ab}) = \frac{\mathbf{a} \cdot \boldsymbol{b}}{\|\mathbf{a}\|\|\mathbf{b}\|} = \frac{\sum_{i=1}^{N}(a_{i1} - \bar{a})(b_{i1} - \bar{b})}{\sqrt{\sum_{i=1}^{N}(a_{i1} - \bar{a})^2}\sqrt{\sum_{i=1}^{N}(b_{i1} - \bar{b})^2}}$$

For the SAT example data (using mean centered variables):

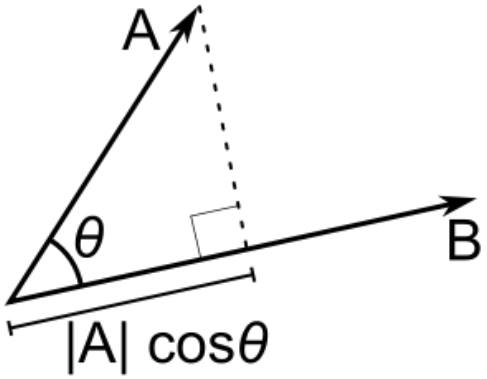
$$r_{SATV,SATM} = \cos(\theta_{SATVc,SATMc}) = \cos\left(\frac{3{,}132{,}223.6}{1{,}573.956 * 2{,}567.0425}\right) = .775$$

Vector Projections

A final vector property that shows up in statistical terms frequently is that of a projection

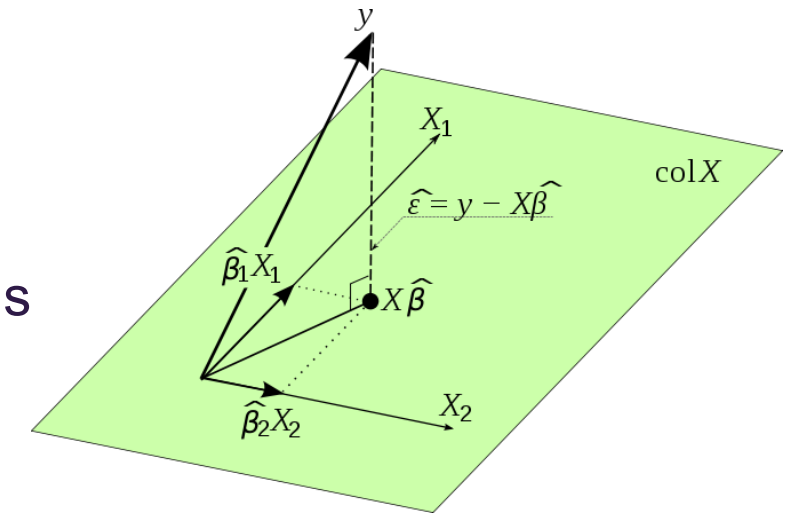
The **projection** of a vector $\mathbf{a}$ onto $\mathbf{b}$ is the orthogonal projection of $\mathbf{a}$ onto the straight line defined by $\mathbf{b}$

- The projection is the "shadow" of one vector onto the other:



$$\mathbf{a}_{\text{proj }\mathbf{b}} = \frac{\mathbf{a}\cdot\mathbf{b}}{\|\mathbf{b}\|^2}\mathbf{b}$$

In data: linear models can be thought of as projections



Vector Projections Example

To provide a bit more context for vector projections, let's consider the projection of mean centered SATV onto SATM:

$$\boldsymbol{SATVc}_{\text{proj } \boldsymbol{SATMc}} = \frac{\boldsymbol{SATVc} \cdot \boldsymbol{SATMc}}{\|\boldsymbol{SATMc}\|^2} \boldsymbol{SATMc}$$

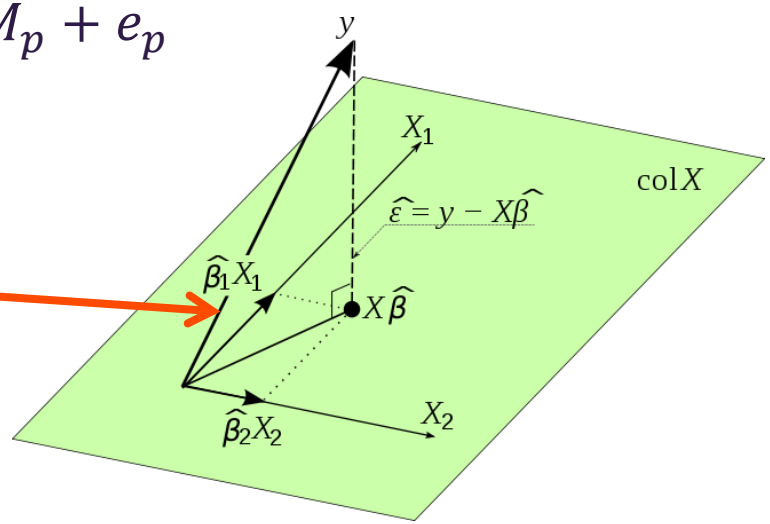
The first portion turns out to be:

$$\frac{\boldsymbol{SATVc} \cdot \boldsymbol{SATMc}}{\|\boldsymbol{SATMc}\|^2} = \frac{3{,}132{,}223.6}{1{,}573.956^2} = .47$$

This is also the regression slope β_1:

$$SATV_p = \beta_0 + \beta_1 SATM_p + e_p$$

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 262.48200    6.18941   42.41   <2e-16 ***
satm          0.47532    0.01226   38.77   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```



MATRIX ALGEBRA

Moving from Vectors to Matrices

A matrix can be thought of as a collection of vectors

- Matrix operations are vector operations on steroids

Matrix algebra defines a set of operations and entities on matrices

- I will present a version meant to mirror your previous algebra experiences

Definitions:

- Identity matrix
- Zero vector
- Ones vector

Basic Operations:

- Addition
- Subtraction
- Multiplication
- "Division"

Matrix Addition and Subtraction

Matrix addition and subtraction are much like vector addition/subtraction

Rules:

- Matrices must be the same size (rows and columns)

Method:

- The new matrix is constructed of element-by-element addition/subtraction of the previous matrices

Order:

- The order of the matrices (pre- and post-) does not matter

Matrix Addition/Subtraction

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \\ a_{41} & a_{42} \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \\ b_{41} & b_{42} \end{bmatrix}$$

$$\mathbf{A} + \mathbf{B} = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} \\ a_{21} + b_{21} & a_{22} + b_{22} \\ a_{31} + b_{31} & a_{32} + b_{32} \\ a_{41} + b_{41} & a_{42} + b_{42} \end{bmatrix} \qquad \mathbf{A} - \mathbf{B} = \begin{bmatrix} a_{11} - b_{11} & a_{12} - b_{12} \\ a_{21} - b_{21} & a_{22} - b_{22} \\ a_{31} - b_{31} & a_{32} - b_{32} \\ a_{41} - b_{41} & a_{42} - b_{42} \end{bmatrix}$$

Matrix Multiplication

Matrix multiplication is a bit more complicated

- The new matrix may be a different size from either of the two multiplying matrices

$$\mathbf{A}_{(r\ x\ c)}\mathbf{B}_{(c\ x\ k)} = \mathbf{C}_{(r\ x\ k)}$$

Rules:

- Pre-multiplying matrix must have number of columns equal to the number of rows of the post-multiplying matrix

Method:

- The elements of the new matrix consist of the inner (dot) product of the row vectors of the pre-multiplying matrix and the column vectors of the post-multiplying matrix

Order:

- The order of the matrices (pre- and post-) matters

Matrix Multiplication

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \\ a_{41} & a_{42} \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix}$$

$$\mathbf{AB} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} & a_{11}b_{13} + a_{12}b_{23} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} & a_{21}b_{13} + a_{22}b_{23} \\ a_{31}b_{11} + a_{32}b_{21} & a_{31}b_{12} + a_{32}b_{22} & a_{31}b_{13} + a_{32}b_{23} \\ a_{41}b_{11} + a_{42}b_{21} & a_{41}b_{12} + a_{42}b_{22} & a_{41}b_{13} + a_{42}b_{23} \end{bmatrix}$$

Multiplication in Statistics

Many statistical formulae with summation can be re-expressed with matrices

A common matrix multiplication form is: $\mathbf{X}^T\mathbf{X}$

- Diagonal elements: $\sum_{i=1}^{N} X_i^2$
- Off-diagonal elements: $\sum_{i=1}^{N} X_{ia}X_{ib}$

For our SAT example:

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} \sum_{i=1}^{N} SATV_i^2 & \sum_{i=1}^{N} SATV_i SATM_i \\ \sum_{i=1}^{N} SATV_i SATM_i & \sum_{i=1}^{N} SATM_i^2 \end{bmatrix} = \begin{bmatrix} 251{,}797{,}800 & 251{,}928{,}400 \\ 251{,}928{,}400 & 254{,}862{,}700 \end{bmatrix}$$

Identity Matrix

The identity matrix is a matrix that, when pre- or post- multiplied by another matrix results in the original matrix:

$$\mathbf{AI} = \mathbf{A}$$
$$\mathbf{IA} = \mathbf{A}$$

The identity matrix is a square matrix that has:

- Diagonal elements = 1
- Off-diagonal elements = 0

$$I_{(3\ x\ 3)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Zero Vector

The zero vector is a column vector of zeros

$$\mathbf{0}_{(3\ x\ 1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

When pre- or post- multiplied the result is the zero vector:

$$\mathbf{A0} = \mathbf{0}$$
$$\mathbf{0A} = \mathbf{0}$$

Ones Vector

A ones vector is a column vector of 1s:

$$\mathbf{1}_{(3\ x\ 1)} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

The ones vector is useful for calculating statistical terms, such as the mean vector and the covariance matrix

Matrix “Division”: The Inverse Matrix

Division from algebra:

First: $\frac{a}{b} = \frac{1}{b}a = b^{-1}a$

Second: $\frac{a}{a} = 1$

“Division” in matrices serves a similar role

- For square and symmetric matrices, an inverse matrix is a matrix that when pre- or post-multiplied with another matrix produces the identity matrix:

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

Calculation of the matrix inverse is complicated

- Even computers have a tough time

Not all matrices can be inverted

- Non-invertible matrices are called singular matrices
  - In statistics, singular matrices are commonly caused by linear dependencies

The Inverse

In data: the inverse shows up constantly in statistics

- Models which assume some type of (multivariate) normality need an inverse covariance matrix

Using our SAT example

- Our data matrix was size (1000 x 2), which is not invertible

- However $\mathbf{X}^T\mathbf{X}$ was size (2 x 2) – square, and symmetric

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 251{,}797{,}800 & 251{,}928{,}400 \\ 251{,}928{,}400 & 254{,}862{,}700 \end{bmatrix}$$

- The inverse is:

$$(\mathbf{X}^T\mathbf{X})^{-1} = \begin{bmatrix} 3.61E-7 & -3.57E-7 \\ -3.57E-7 & 3.56E-7 \end{bmatrix}$$

Matrix Algebra Operations

$$(\mathbf{A}+\mathbf{B})+\mathbf{C}=$$
$$\mathbf{A}+(\mathbf{B}+\mathbf{C})$$
$$\mathbf{A}+\mathbf{B}=\mathbf{B}+\mathbf{A}$$
$$c(\mathbf{A}+\mathbf{B})=c\mathbf{A}+c\mathbf{B}$$
$$(c+d)\mathbf{A}=c\mathbf{A}+d\mathbf{A}$$
$$(\mathbf{A}+\mathbf{B})^T=\mathbf{A}^T+\mathbf{B}^T$$
$$(cd)\mathbf{A}=c(d\mathbf{A})$$
$$(c\mathbf{A})^T=c\mathbf{A}^T$$
$$c(\mathbf{AB})=(c\mathbf{A})\mathbf{B}$$
$$\mathbf{A}(\mathbf{BC})=(\mathbf{AB})\mathbf{C}$$

$$\mathbf{A}(\mathbf{B}+\mathbf{C})=\mathbf{AB}+\mathbf{AC}$$
$$(\mathbf{AB})^T=\mathbf{B}^T\mathbf{A}^T$$

For x_j such that Ax_j exists:

$$\sum_{j=1}^{N}\mathbf{A}\mathbf{x}_j=\mathbf{A}\sum_{j=1}^{N}\mathbf{x}_j$$

$$\sum_{j=1}^{N}(\mathbf{A}\mathbf{x}_j)(\mathbf{A}\mathbf{x}_j)^T=$$

$$\mathbf{A}\left(\sum_{j=1}^{N}\mathbf{x}_j\mathbf{x}_j^T\right)\mathbf{A}^T$$

ADVANCED MATRIX OPERATIONS

Advanced Matrix Functions/Operations

We end our matrix discussion with some advanced topics

- All related to multivariate statistical analysis

To help us throughout, let's consider the correlation matrix of our SAT data:

$$\mathbf{R} = \begin{bmatrix} 1.00 & 0.78 \\ 0.78 & 1.00 \end{bmatrix}$$

Matrix Trace

For a square matrix $\mathbf{A}$ with p rows/columns, the trace is the sum of the diagonal elements:

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

For our data, the trace of the correlation matrix is 2

- For all correlation matrices, the trace is equal to the number of variables because all diagonal elements are 1

The trace is considered the total variance in multivariate statistics

- Used as a target to recover when applying statistical models

Matrix Determinants

A square matrix can be characterized by a scalar value called a determinant:

$$\det \mathbf{A} = |\mathbf{A}|$$

Calculation of the determinant is tedious

- Our determinant was 0.3916

The determinant is useful in statistics:

- Shows up in multivariate statistical distributions
- Is a measure of "generalized" variance of multiple variables

If the determinant is positive, the matrix is called **positive definite → the matrix has an inverse**

If the determinant is not positive, the matrix is called **non-positive definite → the matrix does not have an inverse**

WRAPPING UP

Much Ado About Matrices…

Matrices show up nearly anytime multivariate statistics are used, often in the help/manual pages of the package you intend to use for analysis

You don’t have to do matrix algebra, but please do try to understand the concepts underlying matrices

Your working with multivariate statistics will be better off because of even a small amount of understanding

College of
EDUCATION

AN INTRODUCTION TO THE MULTIVARIATE NORMAL DISTRIBUTION

In This Portion of the Lecture…

Matrices in data

The Multivariate Normal Distribution

DATA EXAMPLE AND R

A Guiding Example

To demonstrate matrix algebra, we will make use of data

Imagine that I collected data SAT test scores for both the Math (SATM) and Verbal (SATV) sections of 1,000 students

The descriptive statistics of this data set are given below:

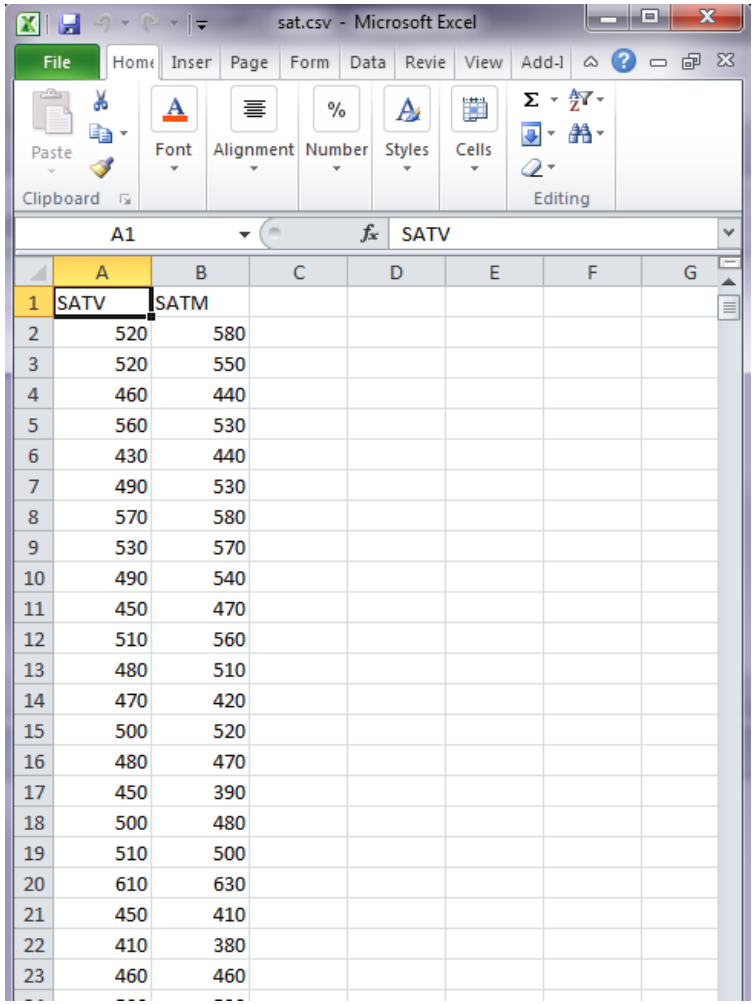
Statistic	SATV	SATM
Mean	499.3	498.3
SD	49.8	81.2

Correlation

SATV	1.00	0.78
SATM	0.78	1.00

The Data…

In Excel:



	A	B	C	D	E	F	G
1	SATV	SATM					
2	520	580					
3	520	550					
4	460	440					
5	560	530					
6	430	440					
7	490	530					
8	570	580					
9	530	570					
10	490	540					
11	450	470					
12	510	560					
13	480	510					
14	470	420					
15	500	520					
16	480	470					
17	450	390					
18	500	480					
19	510	500					
20	610	630					
21	450	410					
22	410	380					
23	460	460					

In R:

	SATV	SATM
1	520	580
2	520	550
3	460	440
4	560	530
5	430	440
6	490	530
7	570	580
8	530	570
9	490	540
10	450	470
11	510	560
12	480	510
13	470	420
14	500	520
15	480	470
16	450	390
17	500	480
18	510	500
19	610	630
20	450	410
21	410	380
22	460	460

MULTIVARIATE STATISTICS AND DISTRIBUTIONS

Multivariate Statistics

Up to this point in this course, we have focused on the prediction (or modeling) of a single variable

- Conditional distributions (aka, generalized linear models)

Multivariate statistics is about exploring **joint distributions**

- How variables relate to each other simultaneously

Therefore, we must adapt our conditional distributions to have multiple variables, simultaneously (later, as multiple outcomes)

We will now look at the joint distributions of two variables $f(x_1, x_2)$ or in matrix form: $f(\mathbf{X})$ (where $\mathbf{X}$ is size N x 2; $f(\mathbf{X})$ gives a scalar/single number)

- Beginning with two, then moving to anything more than two
- We will begin by looking at **multivariate descriptive statistics**
  - **Mean vectors and covariance matrices**

In this lecture, we only consider the **joint distribution** of sets of variables – but next time we will put this into a GLM-like setup

- The **joint distribution** will the be conditional on other variables

Multiple Means: The Mean Vector

We can use a vector to describe the set of means for our data

$$\bar{\mathbf{x}} = \frac{1}{N}\mathbf{X}^T\mathbf{1} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_V \end{bmatrix}$$

- Here $\mathbf{1}$ is a N x 1 vector of 1s
- The resulting mean vector is a *v* x 1 vector of means

For our data: $\bar{\mathbf{x}} = \begin{bmatrix} 499.32 \\ 499.27 \end{bmatrix} = \begin{bmatrix} \bar{x}_{SATV} \\ \bar{x}_{SATM} \end{bmatrix}$

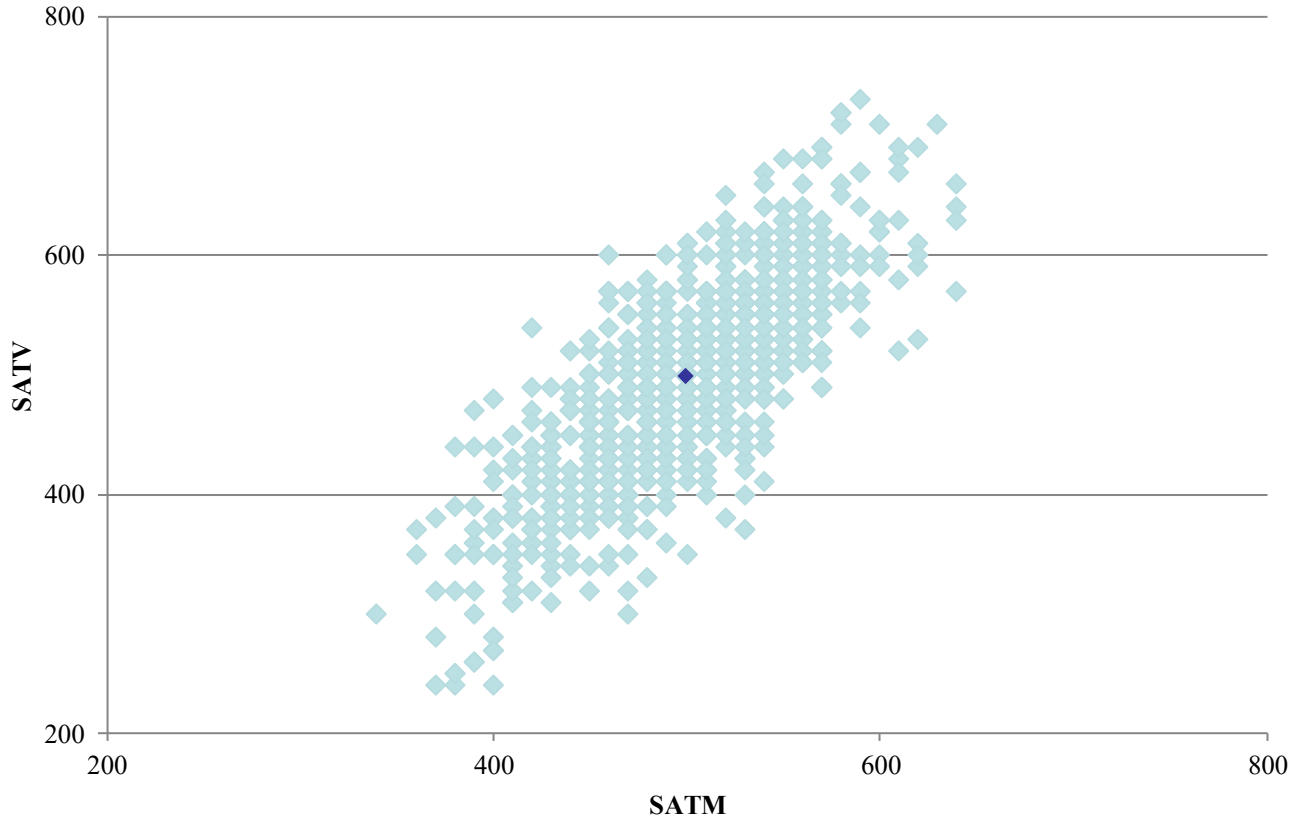
In R:

```
#multivariate statistics ------------------------------
N = (1/length(X[,1]))[1]
ONES = matrix(1,length(X[,1]),1)

XBAR = N*t(X)%*%ONES
XBAR
```

Mean Vector: Graphically

The mean vector is the center of the distribution of both variables



Covariance of a Pair of Variables

The covariance is a measure of the relatedness

- Expressed in the product of the units of the two variables:

$$s_{x_1x_2} = \frac{1}{N}\sum_{p=1}^{N}(x_{p1} - \bar{x}_1)(x_{p2} - \bar{x}_2)$$

- The covariance between SATV and SATM was 3,132.22 (in SAT Verbal-Maths)
- The denominator N is the ML version – unbiased is N-1

Because the units of the covariance are difficult to understand, we more commonly describe association (correlation) between two variables with correlation

- Covariance divided by the product of each variable's standard deviation

Correlation is covariance divided by the product of the standard deviation of each variable:

$$r_{x_1x_2} = \frac{s_{x_1x_2}}{\sqrt{s_{x_1}^2}\sqrt{s_{x_2}^2}}$$

- The correlation between SATM and SATV was 0.78

Correlation is unitless – it only ranges between -1 and 1

- If x_1 **and** x_2 both had variances of 1, the covariance between them would be a correlation
  - Covariance of standardized variables = correlation

Covariance and Correlation in Matrices

The covariance matrix (for any number of variables *v*) is found by:

$$\mathbf{S} = \frac{1}{N}(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}^T)^T(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}^T) = \begin{bmatrix} s_{x_1}^2 & \cdots & s_{x_1x_V} \\ \vdots & \ddots & \vdots \\ s_{x_1x_V} & \cdots & s_{x_V}^2 \end{bmatrix}$$

$$\mathbf{S} = \begin{bmatrix} 2{,}477.34 & 3{,}123.22 \\ 3{,}132.22 & 6{,}589.71 \end{bmatrix}$$

In R:

```
> #calculating the mean vector:
> N = (1/length(X[,1]))[1]
> ONES = matrix(1,length(X[,1]),1)
>
> XBAR = N*t(X)%*%ONES
> XBAR
       [,1]
[1,] 499.32
[2,] 498.27
>
> #calculating the covariance matrix:
> S = N*t(X-ONES%*%t(XBAR))%*%(X-ONES%*%t(XBAR))
> S
         [,1]     [,2]
[1,] 2477.338 3132.224
[2,] 3132.224 6589.707
```

From Covariance to Correlation

If we take the SDs (the square root of the diagonal of the covariance matrix) and put them into a diagonal matrix $\mathbf{D}$, the correlation matrix is found by:

$$\mathbf{R} = \mathbf{D}^{-1}\mathbf{S}\mathbf{D}^{-1} = \begin{bmatrix} \frac{s_{x_1}^2}{\sqrt{s_{x_1}^2}\sqrt{s_{x_1}^2}} & \cdots & \frac{s_{x_1 x_p}}{\sqrt{s_{x_1}^2}\sqrt{s_{x_V}^2}} \\ \vdots & \ddots & \vdots \\ \frac{s_{x_1 x_V}}{\sqrt{s_{x_1}^2}\sqrt{s_{x_V}^2}} & \cdots & \frac{s_{x_V}^2}{\sqrt{s_{x_V}^2}\sqrt{s_{x_V}^2}} \end{bmatrix} = \begin{bmatrix} 1 & \cdots & r_{x_1 x_V} \\ \vdots & \ddots & \vdots \\ r_{x_1 x_V} & \cdots & 1 \end{bmatrix}$$

Example Covariance Matrix

For our data, the covariance matrix was:

$$\mathbf{S} = \begin{bmatrix} 2{,}477.34 & 3{,}123.22 \\ 3{,}132.22 & 6{,}589.71 \end{bmatrix}$$

The diagonal matrix $\mathbf{D}$ was:

$$\mathbf{D} = \begin{bmatrix} \sqrt{2{,}477.34} & 0 \\ 0 & \sqrt{6{,}589.71} \end{bmatrix} = \begin{bmatrix} 49.77 & 0 \\ 0 & 81.18 \end{bmatrix}$$

The correlation matrix $\mathbf{R}$ was:

$$\mathbf{R} = \mathbf{D}^{-1}\mathbf{S}\mathbf{D}^{-1} = \begin{bmatrix} \frac{1}{49.77} & 0 \\ 0 & \frac{1}{81.18} \end{bmatrix} \begin{bmatrix} 2{,}477.34 & 3{,}123.22 \\ 3{,}132.22 & 6{,}589.71 \end{bmatrix} \begin{bmatrix} \frac{1}{49.77} & 0 \\ 0 & \frac{1}{81.18} \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} 1.00 & .78 \\ .78 & 1.00 \end{bmatrix}$$

In R:

```
> D = sqrt(diag(diag(S)))
> D
         [,1]     [,2]
[1,] 49.77286  0.00000
[2,]  0.00000 81.17701
> Dinv = solve(D)
> Dinv
            [,1]       [,2]
[1,] 0.02009127 0.00000000
[2,] 0.00000000 0.01231876
> R2 = Dinv%*%S%*%Dinv
> R2
          [,1]      [,2]
[1,] 1.0000000 0.7752238
[2,] 0.7752238 1.0000000
> R
          [,1]      [,2]
[1,] 1.0000000 0.7752238
[2,] 0.7752238 1.0000000
```

Generalized Variance

The determinant of the covariance matrix is the **generalized variance**

$$\text{Generalized Sample Variance} = |\mathbf{S}|$$

It is a measure of spread across all variables

- Reflecting how much overlap (covariance) in variables occurs in the sample
- Amount of overlap reduces the generalized sample variance
- Generalized variance from our SAT example: 6,514,104.5
- Generalized variance if zero covariance/correlation: 16,324,929

```
> gsv = det(S)
> gsv
[1] 6514104
```

The generalized sample variance is:

- Largest when variables are uncorrelated
- Zero when variables form a linear dependency

In data:

The generalized variance is seldom used descriptively, but shows up more frequently in maximum likelihood functions

Total Sample Variance

The total sample variance is the sum of the variances of each variable in the sample

- The sum of the diagonal elements of the sample covariance matrix
- The trace of the sample covariance matrix

$$Total\ Sample\ Variance = \sum_{v=1}^{V} s_{x_i}^2 = \mathrm{tr}\,\mathbf{S}$$

Total sample variance for our SAT example:

```
> tsv = sum(diag(S))
> tsv
[1] 9067.045
```

The total sample variance does not take into consideration the covariances among the variables

- Will not equal zero if linearly dependency exists

In data:

The total sample variance is commonly used as the denominator (target) when calculating variance accounted for measures

MULTIVARIATE DISTRIBUTIONS (VARIABLES ≥ 2)

Multivariate Normal Distribution

The multivariate normal distribution is the generalization of the univariate normal distribution to multiple variables

- The bivariate normal distribution just shown is part of the MVN

The MVN provides the relative likelihood of observing **all** *V* variables for a subject *p* simultaneously:

$$\mathbf{x}_p = [x_{p1} \quad x_{p2} \quad \cdots \quad x_{pV}]$$

The multivariate normal density function is:

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

The Multivariate Normal Distribution

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

The mean vector is $\boldsymbol{\mu} = \begin{bmatrix} \mu_{x_1} \\ \mu_{x_2} \\ \vdots \\ \mu_{x_V} \end{bmatrix}$

The covariance matrix is $\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{x_1}^2 & \sigma_{x_1x_2} & \cdots & \sigma_{x_1x_V} \\ \sigma_{x_1x_2} & \sigma_{x_2}^2 & \cdots & \sigma_{x_2x_V} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{x_1x_V} & \sigma_{x_2x_V} & \cdots & \sigma_{x_V}^2 \end{bmatrix}$

The covariance matrix must be non-singular (invertible)

Comparing Univariate and Multivariate Normal Distributions

The univariate normal distribution:

$$f(x_p) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$

The univariate normal, rewritten with a little algebra:

$$f(x_p) = \frac{1}{(2\pi)^{\frac{1}{2}}|\sigma^2|^{\frac{1}{2}}} \exp\left[-\frac{(x-\mu)\sigma^{-\frac{1}{2}}(x-\mu)}{2}\right]$$

The multivariate normal distribution

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

- When $V = 1$ (one variable), the MVN is a univariate normal distribution

The Exponent Term

The term in the exponent (without the $-\frac{1}{2}$) is called the **squared Mahalanobis Distance**

$$d^2(\boldsymbol{x}_p) = (\mathbf{x}_p^T - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}_p^T - \boldsymbol{\mu})$$

- Sometimes called the statistical distance
- Describes how far an observation is from its mean vector, in standardized units
- Like a multivariate Z score (but, if data are MVN, is actually distributed as a χ^2variable with DF = number of variables in X)
- Can be used to assess if data follow MVN

Multivariate Normal Notation

Standard notation for the multivariate normal distribution of *v* variables is $N_v(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

- Our SAT example would use a bivariate normal: $N_2(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

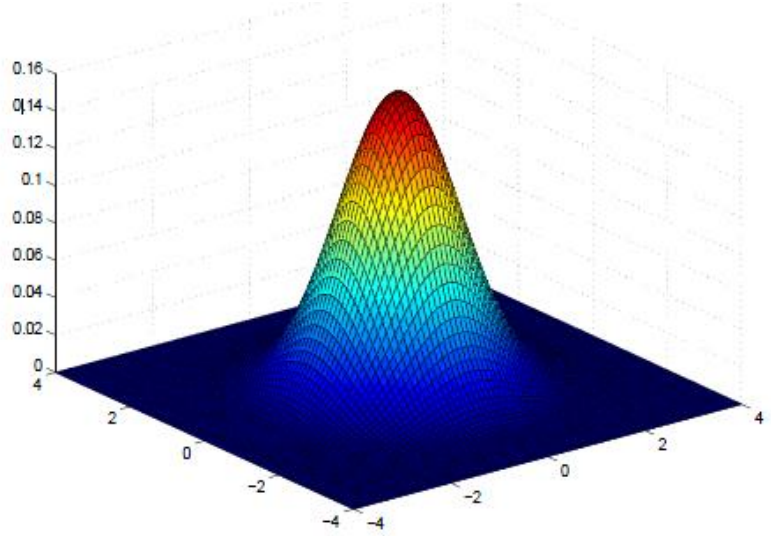
In data:

- The multivariate normal distribution serves as the basis for most every statistical technique commonly used in the social and educational sciences
  - General linear models (ANOVA, regression, MANOVA)
  - General linear mixed models (HLM/multilevel models)
  - Factor and structural equation models (EFA, CFA, SEM, path models)
  - Multiple imputation for missing data

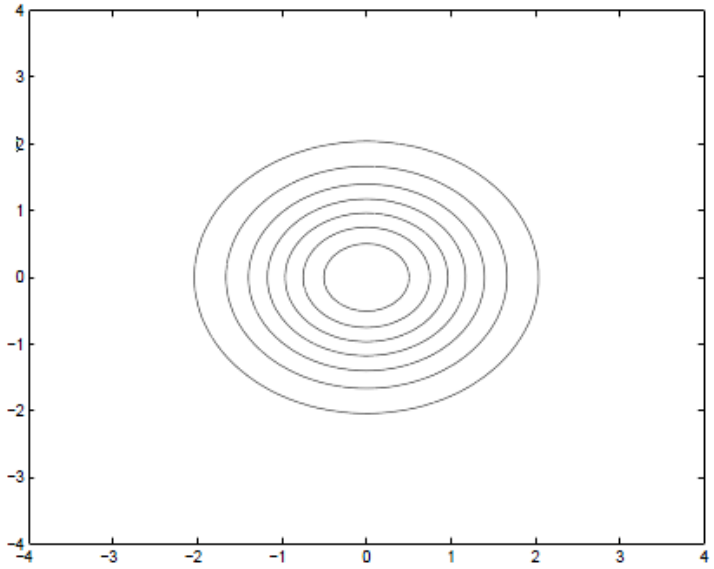
- Simply put, the world of commonly used statistics revolves around the multivariate normal distribution
  - Understanding it is the key to understanding many statistical methods

Bivariate Normal Plot #1

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_{x_1} \\ \mu_{x_2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{x_1}^2 & \sigma_{x_1 x_2} \\ \sigma_{x_1 x_2} & \sigma_{x_2}^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



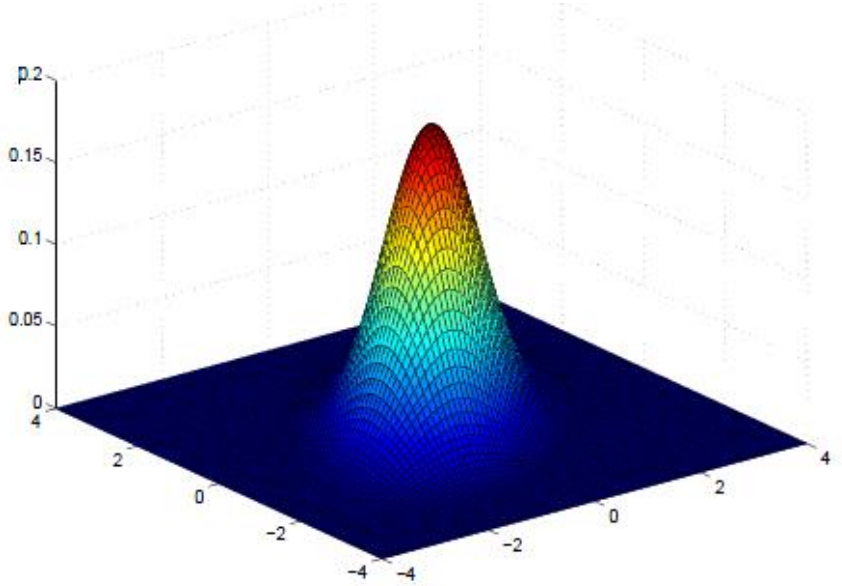
Density Surface (3D)



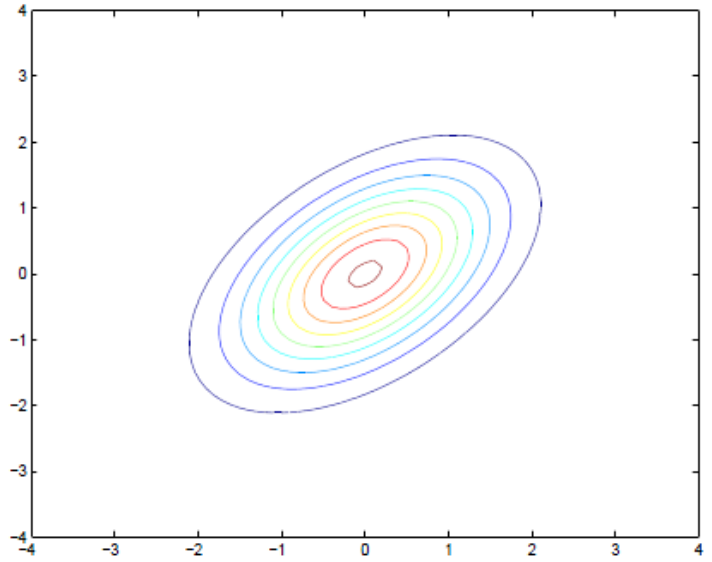
Density Surface (2D):
Contour Plot

Bivariate Normal Plot #2 (Multivariate Normal)

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_{x_1} \\ \mu_{x_2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{x_1}^2 & \sigma_{x_1 x_2} \\ \sigma_{x_1 x_2} & \sigma_{x_2}^2 \end{bmatrix} = \begin{bmatrix} 1 & .5 \\ .5 & 1 \end{bmatrix}$$



Density Surface (3D)



Density Surface (2D):
Contour Plot

Multivariate Normal Properties

The multivariate normal distribution has some useful properties

If $\mathbf{X}$ is distributed multivariate normally:

1. Linear combinations of $\mathbf{X}$ are normally distributed

2. All subsets of $\mathbf{X}$ are multivariate normally distributed

3. A zero covariance between a pair of variables of $\mathbf{X}$ implies that the variables are independent

4. Conditional distributions of $\mathbf{X}$ are multivariate normal

Multivariate Normal Distribution in PROC IML

To demonstrate how the MVN works, we will now investigate how the PDF provides the likelihood (height) for a given observation:

- Here we will use the SAT data and assume the sample mean vector and covariance matrix are known to be the true:

$$\boldsymbol{\mu} = \begin{bmatrix} 499.32 \\ 498.27 \end{bmatrix}; \mathbf{S} = \begin{bmatrix} 2{,}477.34 & 3{,}123.22 \\ 3{,}132.22 & 6{,}589.71 \end{bmatrix}$$

We will compute the likelihood value for several observations (SEE EXAMPLE R SYNTAX FOR HOW THIS WORKS):

$$\boldsymbol{x}_{631,\cdot} = [590 \quad 730]; f(\boldsymbol{x}) = 0.0000001393048$$
$$\boldsymbol{x}_{717,\cdot} = [340 \quad 300]; f(\boldsymbol{x}) = 0.0000005901861$$
$$\boldsymbol{x} = \bar{\boldsymbol{x}} = [499.32 \quad 498.27]; f(\boldsymbol{x}) = 0.000009924598$$

Note: this is the height for these observations, not the joint likelihood across all the data

- We will use the R package lavaan to find estimates of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ using maximum likelihood

WRAPPING UP

Wrapping Up

We are now ready to discuss multivariate models and the art/science of multivariate modeling

Many of the concepts of univariate models carry over

- Maximum likelihood
- Model building via nested models

All of the concepts involve multivariate distributions

Wrapping Up

- This lecture sets the stage to discuss multivariate statistical methods that use maximum likelihood
- Matrix algebra was necessary to concisely talk about our distributions (which will soon become our statistical models)
- The multivariate normal distribution will be necessary to understand as it is the most used distribution for estimation of multivariate models