Matrix Basics II

Matrix Algebra for Data Analysis

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Readme

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Outline

Content of this slides

- Trace
- Rank
- Determinant
- Inverse
- Vector Functions
- Positivity

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Before starting ...

Synopsis

In these slides we will tend to focus on square matrices.

Prerequisite

I'm assuming that you understand the notion of **vector space**

Trace

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Trace

The **trace** of a *square* matrix $\mathbf{X}$ is the sum of its diagonal elements. In R we can use the function `diag()` to extract the elements in the diagonal of a matrix, and then add them with `sum()`

```
# matrix X
set.seed(5)
(X = matrix(sample(1:20, size = 16, replace = TRUE), 4, 4))

##      [,1] [,2] [,3] [,4]
## [1,]    5    3   20    7
## [2,]   14   15    3   12
## [3,]   19   11    6    6
## [4,]    6   17   10    5


# trace of X
sum(diag(X))

## [1] 31
```

Rank

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Rank

Matrix Rank

One of the most important concepts in matrix algebra is that of **rank**. Roughly speaking, the rank of a matrix $\mathbf{X}$ is the dimensionality of the row-column spaces encoded by $\mathbf{X}$.

Nondegenerateness

The **rank** of a matrix $\mathbf{X}$ is a measure of the *nondegenerateness* of the system of linear equations encoded by $\mathbf{X}$.

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Ranks

Column Rank

The **column rank** of a matrix $\mathbf{X}$ is the maximum number of *linearly independent columns* of $\mathbf{X}$. It is the dimension of the column space of $\mathbf{X}$.

Row Rank

The **row rank** of a matrix $\mathbf{X}$ is the maximum number of *linearly independent rows* of $\mathbf{X}$. It is the dimension of the row space of $\mathbf{X}$.

Rank

The column rank is equal to the row rank.

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Rank in R

How to find the rank?

A common approach to find the rank of a matrix is to reduce it to a simpler form. One option in R is to use the `qr()` function which returns the rank (among other results)

```
# matrix X
set.seed(5)
(X = matrix(sample(1:20, size = 16, replace = TRUE), 4, 4))

##      [,1] [,2] [,3] [,4]
## [1,]    5    3   20    7
## [2,]   14   15    3   12
## [3,]   19   11    6    6
## [4,]    6   17   10    5
```

```
# rank of X
Xqr = qr(X)
Xqr$rank

## [1] 4
```

Determinant

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Determinant

Determinant

The determinant is a real number associated with every square matrix. It tells us things about a square matrix that are useful in systems of linear equations, and helps us find the inverse.

Geometric Interpretation

When we regard an $n \times n$ square matrix $\mathbf{X}$ as a linear transformation, the determinant gives the area or volume magnification factor (in the the n-dimensional space) associated to $\mathbf{X}$

Determinant in R

In R, we can use the function `det()` to calculate the determinant of a square matrix:

```
# matrix X
set.seed(5)
(X = matrix(sample(1:20, size = 16, replace = TRUE), 4, 4))

##      [,1] [,2] [,3] [,4]
## [1,]    5    3   20    7
## [2,]   14   15    3   12
## [3,]   19   11    6    6
## [4,]    6   17   10    5


# determinant of X
det(X)

## [1] 35991
```

Inverse

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Matrix Inverse

Inverse

The inverse of a square $n \times n$ matrix $\mathbf{X}$ is that unique $n \times n$ matrix $\mathbf{X^{-1}}$ whose elements are such that:

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

Existance

The inverse of a matrix exists if, and only if, $|\mathbf{X}|$ is non-zero. In other words, if $\mathbf{X}$ is *non-singular*

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Inverse in R

In R, we can use the function `solve()` to calculate the inverse of a square matrix:

```
# matrix X
set.seed(3)
(X = matrix(sample(1:10, size = 9, replace = TRUE), 3, 3))

##      [,1] [,2] [,3]
## [1,]    2    4    2
## [2,]    9    7    3
## [3,]    4    7    6
```

```
# inverse of X
(Xinv = solve(X))

##        [,1]     [,2]     [,3]
## [1,] -0.375  0.17857  0.03571
## [2,]  0.750 -0.07143 -0.21429
## [3,] -0.625 -0.03571  0.39286
```

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Inverse in R (con't)

We can test that $\mathbf{X}\mathbf{X}^{-1} = \mathbf{X}^{-1}\mathbf{X} = \mathbf{I}$

```
# identity
round(Xinv %*% X, 3)

##      [,1] [,2] [,3]
## [1,]    1    0    0
## [2,]    0    1    0
## [3,]    0    0    1
```

```
# identity
round(X %*% Xinv, 3)

##      [,1] [,2] [,3]
## [1,]    1    0    0
## [2,]    0    1    0
## [3,]    0    0    1
```


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Vector Functions

Linear Form

Vector function

A vector function f is a rule which assigns to any vector $\mathbf{x}$ a number $f(\mathbf{x})$.

Forms

There are several types of vector functions. But we will consider just three of them that are fundamental for multivariate statistics

- Linear forms
- Bilinear forms
- Quadratic forms

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Linear Form

Linear form

A vector function of the form

$$f(\mathbf{x}) = \mathbf{x}'\mathbf{A}\mathbf{y}$$

is called a **linear form**, where $\mathbf{A}$ is a constant $n \times p$ matrix, and $\mathbf{y}$ is a constant vector.

Bilinear Form

Bilinear form

A **bilinear form** is a vector function for which the argument is a pair of vectors $\mathbf{x}$ and $\mathbf{y}$, rather than a single vector. Such function is defined as

$$g(\mathbf{x}, \mathbf{y}) = \mathbf{x}'\mathbf{A}\mathbf{y}$$

where $\mathbf{A}$ is a constant $n \times p$ matrix.

Note that

The bilinear function should not be confused with $f^*(\mathbf{x}) = \mathbf{x}'\mathbf{A}\mathbf{y}$, a linear form with $\mathbf{A}$ and $\mathbf{y}$ constant.

Quadratic Form

Quadratic form

A **quadratic form** is a bilinear form defined as:

$$g(\mathbf{x}, \mathbf{x}) = \mathbf{x}'\mathbf{A}\mathbf{x}$$

where $\mathbf{A}$ is a constant square matrix

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Positivity

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Importance of Symmetric Matrices

Symmetric matrices play an important role since they often appear in multivariate statistics:

- in the form of covariance (or correlation) matrices
- in the form of association matrices
- in the form of distance matrices
- in the form of proximity or (dis)similarity matrices

Positivity

Intrinsically related to symmetric matrices (considered as bilinear forms) is the so-called notion of **positivity**

Positivity

Positive Definite

A symmetric **Positive Definite** (P.D.) matrix is a matrix whose eigenvalues are strictly positive.

Positive Semidefinite

A symmetric **Positive Semi-Definite** (P.S.D.) matrix is a matrix whose eigenvalues are nonnegative.

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Negativity

Negative Definite

A symmetric **Negative Definite** (N.D.) matrix is a matrix whose eigenvalues are strictly negative.

Negative Semidefinite

A symmetric **Negative Semi-Definite** (N.S.D.) matrix is a matrix whose eigenvalues are nonpositive.

Indefinite

$\mathbf{X}$ is **indefinite** if it has both positive and negative eigenvalues

Positivity and Negativity

- $\mathbf{X}$ is **positive definite** if $\mathbf{v}'\mathbf{X}\mathbf{v} > \mathbf{0}$ for all $\mathbf{v} \neq \mathbf{0}$
- $\mathbf{X}$ is **positive semidefinite** if $\mathbf{v}'\mathbf{X}\mathbf{v} \geq \mathbf{0}$ for all $\mathbf{v}$
- $\mathbf{X}$ is **negative definite** if $\mathbf{v}'\mathbf{X}\mathbf{v} < \mathbf{0}$ for all $\mathbf{v} \neq \mathbf{0}$
- $\mathbf{X}$ is **negative semidefinite** if $\mathbf{v}'\mathbf{X}\mathbf{v} \leq \mathbf{0}$ for all $\mathbf{v}$

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