More Linear Algebra[1]

STA 302: Fall 2013

[1] See Chapter 2 of *Linear models in statistics* for more detail. This slide show is an open-source document. See last slide for copyright information.

Overview

1. Things you already know
2. Spectral decomposition
3. Positive definite matrices
4. Square root matrices
5. R

You already know about

- Matrices $\mathbf{A} = [a_{ij}]$
- Matrix addition and subtraction $\mathbf{A} + \mathbf{B} = [a_{ij} + b_{ij}]$
- Scalar multiplication $a\mathbf{B} = [a\, b_{ij}]$
- Matrix multiplication $\mathbf{AB} = \left[\sum_k a_{ik} b_{kj}\right]$
- Inverse $\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$
- Transpose $\mathbf{A}' = [a_{ji}]$
- Symmetric matrices $\mathbf{A} = \mathbf{A}'$
- Determinants
- Linear independence

Linear independence

$\mathbf{X}$ be an $n \times p$ matrix of constants.The columns of $\mathbf{X}$ are said to be *linearly dependent* if there exists $\mathbf{v} \neq \mathbf{0}$ with $\mathbf{X}\mathbf{v} = \mathbf{0}$. We will say that the columns of $\mathbf{X}$ are linearly *independent* if $\mathbf{X}\mathbf{v} = \mathbf{0}$ implies $\mathbf{v} = \mathbf{0}$.

For example, show that $\mathbf{A}^{-1}$ exists implies that the columns of $\mathbf{A}$ are linearly independent.

$$\mathbf{A}\mathbf{v} = \mathbf{0} \Rightarrow \mathbf{A}^{-1}\mathbf{A}\mathbf{v} = \mathbf{A}^{-1}\mathbf{0} \Rightarrow \mathbf{v} = \mathbf{0}$$

How to show $\mathbf{A}^{-1\prime} = \mathbf{A}^{\prime -1}$

Suppose $\mathbf{B} = \mathbf{A}^{-1}$, meaning $\mathbf{AB} = \mathbf{BA} = \mathbf{I}$. Must show two things: $\mathbf{B}'\mathbf{A}' = \mathbf{I}$ and $\mathbf{A}'\mathbf{B}' = \mathbf{I}$.

$$\begin{aligned} \mathbf{AB} = \mathbf{I} \quad &\Rightarrow \quad \mathbf{B}'\mathbf{A}' = \mathbf{I}' = \mathbf{I} \\ \mathbf{BA} = \mathbf{I} \quad &\Rightarrow \quad \mathbf{A}'\mathbf{B}' = \mathbf{I}' = \mathbf{I} \end{aligned}$$

■

Extras

You may not know about these, but we may use them occasionally

- Trace
- Rank
- Partitioned matrices

Trace of a square matrix

- Sum of diagonal elements
- Obvious: $tr(\mathbf{A}+\mathbf{B}) = tr(\mathbf{A}) + tr(\mathbf{B})$
- Not obvious: $tr(\mathbf{AB}) = tr(\mathbf{BA})$

Rank

- Row rank is the number of linearly independent rows
- Column rank is the number of linearly independent columns
- Rank of a matrix is the minimum of row rank and column rank
- $rank(\mathbf{AB}) = \min\left(rank(\mathbf{A}), rank(\mathbf{B})\right)$

Partitioned matrix

- A matrix of matrices

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{B} \\ \hline \mathbf{C} & \mathbf{D} \end{array}\right]$$

- Row by column (matrix) multiplication works, provided the matrices are the right sizes.

Eigenvalues and eigenvectors

Let $\mathbf{A} = [a_{i,j}]$ be an $n \times n$ matrix, so that the following applies to square matrices. $\mathbf{A}$ is said to have an *eigenvalue* λ and (non-zero) *eigenvector* $\mathbf{x}$ corresponding to λ if

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}.$$

- Eigenvalues are the λ values that solve the determinantal equation $|\mathbf{A} - \lambda\mathbf{I}| = 0$.
- The determinant is the product of the eigenvalues: $|\mathbf{A}| = \prod_{i=1}^{n} \lambda_i$

Spectral decomposition of symmetric matrices

The *Spectral decomposition theorem* says that every square and symmetric matrix $\mathbf{A} = [a_{i,j}]$ may be written

$$\mathbf{A} = \mathbf{C}\mathbf{D}\mathbf{C}',$$

where the columns of $\mathbf{C}$ (which may also be denoted $\mathbf{x}_1, \ldots, \mathbf{x}_n$) are the eigenvectors of $\mathbf{A}$, and the diagonal matrix $\mathbf{D}$ contains the corresponding eigenvalues.

$$\mathbf{D} = \left[\begin{array}{cccc} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{array} \right]$$

The eigenvectors may be chosen to be orthonormal, so that $\mathbf{C}$ is an orthogonal matrix. That is, $\mathbf{C}\mathbf{C}' = \mathbf{C}'\mathbf{C} = \mathbf{I}$.

Positive definite matrices

The $n \times n$ matrix $\mathbf{A}$ is said to be *positive definite* if

$$\mathbf{y}'\mathbf{A}\mathbf{y} > 0$$

for *all* $n \times 1$ vectors $\mathbf{y} \neq \mathbf{0}$. It is called *non-negative definite* (or sometimes positive semi-definite) if $\mathbf{y}'\mathbf{A}\mathbf{y} \geq 0$.

Example: Show $\mathbf{X}'\mathbf{X}$ non-negative definite

Let $\mathbf{X}$ be an $n \times p$ matrix of real constants and $\mathbf{y}$ be $p \times 1$. Then $\mathbf{Z} = \mathbf{X}\mathbf{y}$ is $n \times 1$, and

$$\begin{aligned} & \mathbf{y}' \left(\mathbf{X}'\mathbf{X}\right) \mathbf{y} \\ = & (\mathbf{X}\mathbf{y})'(\mathbf{X}\mathbf{y}) \\ = & \mathbf{Z}'\mathbf{Z} \\ = & \sum_{i=1}^{n} Z_i^2 \geq 0 \end{aligned}$$

Some properties of symmetric positive definite matrices

Variance-covariance matrices are often assumed positive definite.

For a symmetric matrix,

Positive definite

$\Downarrow$

All eigenvalues positive

$\Downarrow$

Inverse exists $\Leftrightarrow$ Columns (rows) linearly independent

If a real symmetric matrix is also non-negative definite, as a variance-covariance matrix *must* be, Inverse exists $\Rightarrow$ Positive definite

Showing Positive definite $\Rightarrow$ Eigenvalues positive

For example

Let $\mathbf{A}$ be square and symmetric as well as positive definite.

- Spectral decomposition says $\mathbf{A} = \mathbf{CDC}'$.
- Using $\mathbf{y}'\mathbf{A}\mathbf{y} > 0$, let $\mathbf{y}$ be an eigenvector, say the third one.
- Because eigenvectors are orthonormal,

$$
\begin{aligned}
\mathbf{y}'\mathbf{A}\mathbf{y} &= \mathbf{y}'\mathbf{CDC}'\mathbf{y} \\
&= \begin{pmatrix} 0 & 0 & 1 & \cdots & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} \\
&= \lambda_3 \\
&> 0
\end{aligned}
$$

Inverse of a diagonal matrix

Suppose $\mathbf{D} = [d_{i,j}]$ is a diagonal matrix with non-zero diagonal elements. It is easy to verify that

$$\begin{pmatrix} d_{1,1} & 0 & \cdots & 0 \\ 0 & d_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_{n,n} \end{pmatrix} \begin{pmatrix} 1/d_{1,1} & 0 & \cdots & 0 \\ 0 & 1/d_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/d_{n,n} \end{pmatrix} = \mathbf{I}$$

And

$$\begin{pmatrix} 1/d_{1,1} & 0 & \cdots & 0 \\ 0 & 1/d_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/d_{n,n} \end{pmatrix} \begin{pmatrix} d_{1,1} & 0 & \cdots & 0 \\ 0 & d_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_{n,n} \end{pmatrix} = \mathbf{I}$$

Showing Eigenvalues positive $\Rightarrow$ Inverse exists

For a symmetric, positive definite matrix

Let $\mathbf{A}$ be symmetric and positive definite. Then $\mathbf{A} = \mathbf{CDC}'$ and its eigenvalues are positive.

Let $\mathbf{B} = \mathbf{CD}^{-1}\mathbf{C}'$

Showing $\mathbf{B} = \mathbf{A}^{-1}$:

$$\begin{aligned} \mathbf{AB} &= \mathbf{CDC}'\,\mathbf{CD}^{-1}\mathbf{C}' = \mathbf{I} \\ \mathbf{BA} &= \mathbf{CD}^{-1}\mathbf{C}'\,\mathbf{CDC}' = \mathbf{I} \end{aligned}$$

So

$$\mathbf{A}^{-1} = \mathbf{CD}^{-1}\mathbf{C}'$$

Square root matrices

For symmetric, non-negative definite matrices

Define

$$\mathbf{D}^{1/2} = \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_n} \end{pmatrix}$$

So that

$$\begin{aligned} \mathbf{D}^{1/2}\mathbf{D}^{1/2} &= \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_n} \end{pmatrix} \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_n} \end{pmatrix} \\ &= \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} = \mathbf{D} \end{aligned}$$

For a non-negative definite, symmetric matrix $\mathbf{A}$

Define

$$\mathbf{A}^{1/2} = \mathbf{C}\mathbf{D}^{1/2}\mathbf{C}'$$

So that

$$\begin{aligned}
\mathbf{A}^{1/2}\mathbf{A}^{1/2} &= \mathbf{C}\mathbf{D}^{1/2}\mathbf{C}'\mathbf{C}\mathbf{D}^{1/2}\mathbf{C}' \\
&= \mathbf{C}\mathbf{D}^{1/2}\,\mathbf{I}\,\mathbf{D}^{1/2}\mathbf{C}' \\
&= \mathbf{C}\mathbf{D}^{1/2}\mathbf{D}^{1/2}\mathbf{C}' \\
&= \mathbf{C}\mathbf{D}\mathbf{C}' \\
&= \mathbf{A}
\end{aligned}$$

The square root of the inverse is the inverse of the square root

Let $\mathbf{A}$ be symmetric and positive definite, with $\mathbf{A} = \mathbf{CDC}'$.

Let $\mathbf{B} = \mathbf{CD}^{-1/2}\mathbf{C}'$. What is $\mathbf{D}^{-1/2}$?

Show $\mathbf{B} = \left(\mathbf{A}^{-1}\right)^{1/2}$

$$\begin{aligned} \mathbf{BB} &= \mathbf{CD}^{-1/2}\mathbf{C}'\mathbf{CD}^{-1/2}\mathbf{C}' \\ &= \mathbf{CD}^{-1}\mathbf{C}' = \mathbf{A}^{-1} \end{aligned}$$

Show $\mathbf{B} = \left(\mathbf{A}^{1/2}\right)^{-1}$

$$\begin{aligned} \mathbf{A}^{1/2}\mathbf{B} &= \mathbf{CD}^{1/2}\mathbf{C}'\mathbf{CD}^{-1/2}\mathbf{C}' = \mathbf{I} \\ \mathbf{BA}^{1/2} &= \mathbf{CD}^{-1/2}\mathbf{C}'\mathbf{CD}^{1/2}\mathbf{C}' = \mathbf{I} \end{aligned}$$

Just write $$\mathbf{A}^{-1/2} = \mathbf{CD}^{-1/2}\mathbf{C}'$$

Matrix calculation with R

```
> is.matrix(3)  # Is the number 3 a 1x1 matrix?
```

```
[1] FALSE
```

```
> treecorr = cor(trees); treecorr
```

```
           Girth    Height    Volume
Girth  1.0000000 0.5192801 0.9671194
Height 0.5192801 1.0000000 0.5982497
Volume 0.9671194 0.5982497 1.0000000
```

```
> is.matrix(treecorr)
```

```
[1] TRUE
```

Creating matrices

Bind rows into a matrix

```
> # Bind rows of a matrix together
> A = rbind(  c(3, 2, 6,8),
+             c(2,10,-7,4),
+             c(6, 6, 9,1)   ); A

     [,1] [,2] [,3] [,4]
[1,]    3    2    6    8
[2,]    2   10   -7    4
[3,]    6    6    9    1


> # Transpose
> t(A)

     [,1] [,2] [,3]
[1,]    3    2    6
[2,]    2   10    6
[3,]    6   -7    9
[4,]    8    4    1
```

Matrix multiplication

Remember, $\mathbf{A}$ is 3×4

```
> # U = AA' (3x3), V = A'A (4x4)
> U = A %*% t(A)
> V = t(A) %*% A; V

     [,1] [,2] [,3] [,4]
[1,]   49   62   58   38
[2,]   62  140   -4   62
[3,]   58   -4  166   29
[4,]   38   62   29   81
```

Determinants

```
> # U = AA' (3x3), V = A'A (4x4)
> # So rank(V) cannot exceed 3 and det(V)=0
> det(U); det(V)

[1] 1490273
[1] -3.622862e-09
```

Inverse of **U** exists, but inverse of **V** does not.

Inverses

- The `solve` function is for solving systems of linear equations like $\mathbf{Mx} = \mathbf{b}$.
- Just typing `solve(M)` gives $\mathbf{M}^{-1}$.

```
> solve(U)

              [,1]          [,2]          [,3]
[1,]  0.0173505123 -8.508508e-04 -1.029342e-02
[2,] -0.0008508508  5.997559e-03  2.013054e-06
[3,] -0.0102934160  2.013054e-06  1.264265e-02


> solve(V)


Error in solve.default(V) :
  system is computationally singular: reciprocal condition
  number = 6.64193e-18
```

Eigenvalues and eigenvectors

```
> eigen(U)

$values
[1] 234.01162 162.89294  39.09544

$vectors
           [,1]       [,2]        [,3]
[1,] -0.6025375  0.1592598  0.78203893
[2,] -0.2964610 -0.9544379 -0.03404605
[3,] -0.7409854  0.2523581 -0.62229894
```

V should have at least one zero eigenvalue

```
> eigen(V)

$values
[1]  2.340116e+02  1.628929e+02  3.909544e+01 -1.012719e-14

$vectors
           [,1]         [,2]       [,3]         [,4]
[1,] -0.4475551  0.006507269 -0.2328249  0.863391352
[2,] -0.5632053 -0.604226296 -0.4014589 -0.395652773
[3,] -0.5366171  0.776297432 -0.1071763 -0.312917928
[4,] -0.4410627 -0.179528649  0.8792818  0.009829883
```

Spectral decomposition $\mathbf{V} = \mathbf{CDC}'$

```
> eigenV = eigen(V)
> C = eigenV$vectors; D = diag(eigenV$values); D

         [,1]     [,2]     [,3]          [,4]
[1,] 234.0116   0.0000  0.00000  0.000000e+00
[2,]   0.0000 162.8929  0.00000  0.000000e+00
[3,]   0.0000   0.0000 39.09544  0.000000e+00
[4,]   0.0000   0.0000  0.00000 -1.012719e-14
```

```
> # C is an orthoganal matrix
> C %*% t(C)

              [,1]         [,2]         [,3]          [,4]
[1,]  1.000000e+00 5.551115e-17 0.000000e+00 -3.989864e-17
[2,]  5.551115e-17 1.000000e+00 2.636780e-16  3.556183e-17
[3,]  0.000000e+00 2.636780e-16 1.000000e+00  2.558717e-16
[4,] -3.989864e-17 3.556183e-17 2.558717e-16  1.000000e+00
```

Verify $\mathbf{V} = \mathbf{CDC}'$

```
> V;   C %*% D %*% t(C)

     [,1] [,2] [,3] [,4]
[1,]   49   62   58   38
[2,]   62  140   -4   62
[3,]   58   -4  166   29
[4,]   38   62   29   81

     [,1] [,2] [,3] [,4]
[1,]   49   62   58   38
[2,]   62  140   -4   62
[3,]   58   -4  166   29
[4,]   38   62   29   81
```

Square root matrix $\mathbf{V}^{1/2} = \mathbf{C}\mathbf{D}^{1/2}\mathbf{C}'$

```
> sqrtV = C %*% sqrt(D) %*% t(C)

Warning message:
In sqrt(D) : NaNs produced

> # Multiply to get V
> sqrtV %*% sqrtV;  V

     [,1] [,2] [,3] [,4]
[1,]  NaN  NaN  NaN  NaN
[2,]  NaN  NaN  NaN  NaN
[3,]  NaN  NaN  NaN  NaN
[4,]  NaN  NaN  NaN  NaN
     [,1] [,2] [,3] [,4]
[1,]   49   62   58   38
[2,]   62  140   -4   62
[3,]   58   -4  166   29
[4,]   38   62   29   81
```

What happened?

```
> D; sqrt(D)

         [,1]     [,2]     [,3]          [,4]
[1,] 234.0116   0.0000  0.00000  0.000000e+00
[2,]   0.0000 162.8929  0.00000  0.000000e+00
[3,]   0.0000   0.0000 39.09544  0.000000e+00
[4,]   0.0000   0.0000  0.00000 -1.012719e-14

         [,1]     [,2]     [,3] [,4]
[1,] 15.29744  0.00000 0.000000    0
[2,]  0.00000 12.76295 0.000000    0
[3,]  0.00000  0.00000 6.252635    0
[4,]  0.00000  0.00000 0.000000  NaN

Warning message:
In sqrt(D) : NaNs produced
```

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