

More on sample variance matrix

$$\begin{aligned} \mathbf{S} &= \mathbf{S}_x = [s_{jk}] = (n-1)^{-1} \tilde{\mathbf{X}}' \tilde{\mathbf{X}} \\ &= (n-1)^{-1} \sum_{1 \leq i \leq n} \tilde{\mathbf{x}}_i \tilde{\mathbf{x}}_i', \end{aligned}$$

where $\tilde{\mathbf{X}} = [\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2, \dots, \tilde{\mathbf{x}}_n]'$, $\tilde{\mathbf{x}}_i = \mathbf{x}_i - \bar{\mathbf{x}}$ is the matrix of deviations from the sample mean $\bar{\mathbf{x}}$.

- Diagonal elements:

$$s_{jj} = (n-1)^{-1} \sum_{1 \leq i \leq n} (x_{ij} - \bar{x}_j)^2 = s_j^2,$$

the usual **sample variance**.

$\sqrt{s_{jj}}$ = **sample standard deviation**

- Off-diagonal elements:

$$\begin{aligned} s_{jk} &= (n-1)^{-1} \sum_{1 \leq i \leq n} (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k), \quad j \neq k \\ &= \text{sample covariance of } x_j \text{ and } x_k \end{aligned}$$

- \mathbf{S}_x is *symmetric* ($\mathbf{S}_x' = \mathbf{S}_x$) since

$$\begin{aligned} s_{jk} &= \sum_{1 \leq i \leq n} (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k) \\ &= \sum_{1 \leq i \leq n} (x_{ik} - \bar{x}_k)(x_{ij} - \bar{x}_j) = s_{kj} \end{aligned}$$

Displays for Statistics 5401/8401

Lecture 5

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Christopher Bingham, Instructor

612-625-1024, kb@umn.edu

372 Ford Hall

Class Web Page

<http://www.stat.umn.edu/~kb/classes/5401>

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MacAnova:

```

Cmd> x
(1,1)      2.4      22.9      44
(2,1)     12.3      15.7      32.7
(3,1)     10.6      15.7      35.2
(4,1)     15.1      17.2      33.5
(5,1)     -1.3      22.5      26.7

Cmd> n <- nrow(x)
Cmd> xbar <- sum(x)/n # row vector, 1 by 3
Cmd> xtilde <- x - xbar # deviations from mean, 5 by 3
Cmd> # or xtilde <- x - rep(1/n,n)' %*% x
Cmd> df <- n - 1 # "degrees of freedom"
Cmd> s <- (xtilde' %*% xtilde)/df; s # sample variance matrix
(1,1)     48.337     -22.53      1.562
(2,1)     -22.53      13.07      3.775
(3,1)      1.562      3.775      38.947

```

Black box computation of \mathbf{S} and $\bar{\mathbf{x}}$ using `tabs()`:

```

Cmd> tabs(x,covar:T)
(1,1)     48.337     -22.53      1.562
(2,1)     -22.53      13.07      3.775      S
(3,1)      1.562      3.775      38.947

Cmd> tabs(x,mean:T) # returns plain vector
(1)       7.82      18.8      34.42      Not row vector

Cmd> stats <- covar(x); stats # use pre-defined macro
component: n      sample size
(1)           5
component: mean
(1,1)       7.82      18.8      34.42      xbar, row vec.
component: covariance
(1,1)     48.337     -22.53      1.562
(2,1)     -22.53      13.07      3.775      S
(3,1)      1.562      3.775      38.947

Cmd> stats$covariance # extract S from structure stats
(1,1)     48.337     -22.53      1.562
(2,1)     -22.53      13.07      3.775
(3,1)      1.562      3.775      38.947

```

A matrix of Linear Combinations

Suppose \mathbf{X} is a n by p data matrix and $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_q]$ is a p by q matrix of constants, $\mathbf{a}_j = [a_{1j}, a_{2j}, \dots, a_{pj}]'$. For example, you might have

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 0 & -2 \end{bmatrix}$$

Q. What is the $n \times q$ matrix

$$\mathbf{Y} = [\mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_q] = \mathbf{XA} = [\mathbf{Xa}_1, \mathbf{Xa}_2, \dots, \mathbf{Xa}_q]?$$

A. Each column $\mathbf{Y}_j = \mathbf{Xa}_j$ is a *linear combination* $\sum_{1 \leq \ell \leq p} a_{\ell j} X_{\ell}$ of the columns of \mathbf{X} (e.g. $\mathbf{Y}_1 = \mathbf{X}_1 + \mathbf{X}_2 + \mathbf{X}_3$, $\mathbf{Y}_2 = \mathbf{X}_1 - \mathbf{X}_2$, ...)

Each element $y_{ij} = \mathbf{a}_j' \mathbf{x}_i = \sum_{1 \leq \ell \leq p} a_{\ell j} x_{i\ell}$ is a linear combinations of the x -values for case i .

\mathbf{Y} is a new data matrix derived from the original data matrix \mathbf{X} .

Sample mean and variance matrix of Y

- The sample mean $\bar{y} = \sum_i y_i / n$ of Y is

$$\bar{y} = A' \bar{x} \quad (q \times 1) \text{ column vector}$$

or, as a row vector,

$$\bar{y}' = \bar{x}' A \quad (1 \times q)$$

$$\bar{y}_j = a_j' \bar{x} \quad (\text{univariate mean})$$

- The *variance matrix* S_Y of Y is

$$S_Y = A' S_X A = [a_j' S_X a_k]_{1 \leq j \leq q, 1 \leq k \leq q} \quad (q \times q).$$

Diagonal elements are

$$s_{Y11} = s_{y_1}^2 = a_1' S_X a_1, \dots, s_{Yqq} = s_{y_q}^2 = a_q' S_X a_q$$

This applies when the columns of A define the linear combinations.

Comment: You will find it useful to be able to recognize an expression like $a' S_X a$ as representing the sample variance of a linear combination $a' x$.

MacAnova Example

```

Cmd> x # previously entered data matrix
(1,1)      2.4      22.9      44
(2,1)     12.3     15.7     32.7
(3,1)     10.6     15.7     35.2
(4,1)     15.1     17.2     33.5
(5,1)     -1.3     22.5     26.7

Cmd> a <- matrix(vector(1,1,1,1,-1,0,1,1,-2),3)
Cmd> a # matrix of linear combination coefficients
(1,1)      1      1      1
(2,1)      1     -1      1
(3,1)      1      0     -2

Cmd> y <- x %*% a; y # data matrix of linear combinations
(1,1)     69.3     -20.5     -62.7
(2,1)     60.7     -3.4     -37.4
(3,1)     61.5     -5.1     -44.1
(4,1)     65.8     -2.1     -34.7
(5,1)     47.9     -23.8     -32.2

Cmd> s_x <- tabs(x1, covar:T) # S_x
Cmd> s_y <- tabs(y, covar:T); s_y # S_y
(1,1)     65.968     33.054    -66.884
(2,1)     33.054     106.47     39.693
(3,1)    -66.884     39.693     150.79

Cmd> a' %*% s_x %*% a
(1,1)     65.968     33.054    -66.884
(2,1)     33.054     106.47     39.693
(3,1)    -66.884     39.693     150.79

```

Eigenvalues and Eigenvectors

Let $\mathbf{A} = [a_{ij}]$ be a p by p *square* matrix.

Vocabulary Suppose $\mathbf{u} \neq \mathbf{0}$ is a p by 1 vector that satisfies

$$\mathbf{A}\mathbf{u} = \lambda\mathbf{u} \text{ for some constant } \lambda.$$

Then \mathbf{u} is an **eigenvector** of \mathbf{A} with corresponding **eigenvalue** λ (also called *proper* or *characteristic* value and vector).

```
Cmd> a # note a is symmetric 2 by 2
(1,1)    2.9412    0.23529
(2,1)    0.23529    2.0588
```

Enter vectors \mathbf{u}_1 and \mathbf{u}_2

```
Cmd> u1 <- vector(4, 1); u2 <- vector(-1, 4)
```

```
Cmd> a %*% u1 # a %*% u1 = 3*u1
(1,1)    12      Eigenvalue = 3
(2,1)    3
```

```
Cmd> a %*% u2 # a %*% u2 = 2*u2
(1,1)    -2      Eigenvalue = 2
(2,1)    8
```

$$\mathbf{A}\mathbf{u}_1 = 3 \times \mathbf{u}_1 \text{ and } \mathbf{A}\mathbf{u}_2 = 2 \times \mathbf{u}_2$$

so

- \mathbf{u}_1 is an eigenvector with eigenvalue 3
- \mathbf{u}_2 is an eigenvector with eigenvalue 2

When \mathbf{u} is an eigenvector with eigenvalue λ , so is \mathbf{u}/c where c is a constant

Proof: $\mathbf{A}(\mathbf{u}/c) = \mathbf{A}\mathbf{u}/c = \lambda\mathbf{u}/c = \lambda(\mathbf{u}/c)$.

In particular $\tilde{\mathbf{u}} = \mathbf{u}/\|\mathbf{u}\|$ is an eigenvector such that $\|\tilde{\mathbf{u}}\| = 1$.

```
Cmd> u <- hconcat(u1,u2); sum(u^2) # u is 2 by 2
(1,1)    17      17 squared norms of u1 and u2
```

This shows $\|\mathbf{u}_1\| = \|\mathbf{u}_2\| = \sqrt{17}$

```
Cmd> u / sqrt(17) # columns are eigenvectors
(1,1)    0.97014    -0.24254
(2,1)    0.24254    0.97014
```

MacAnova:

- `eigenvals()` finds eigenvalues
- `eigen()` finds *both* eigenvalues and eigenvectors

```
Cmd> eigenvals(a) # just eigenvalues
(1)    3      2      In decreasing order
```

```
Cmd> eigs <- eigen(a); eigs
component: values
(1)    3      2
component: vectors
(1,1)    -0.97014    0.24254 Normalized columns
(2,1)    -0.24254    -0.97014 norms of columns are 1
```

```
Cmd> eigs$ vectors # or eigs[2] #extract just vectors
(1,1)    -0.97014    0.24254
(2,1)    -0.24254    -0.97014
```

Note that signs are reversed from $\mathbf{u} / \sqrt{17}$. This doesn't matter.

Facts concerning eigenthings

When \mathbf{A} is $p \times p$ *symmetric*, there are

- Exactly p *linearly independent* eigenvectors $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_p$ with *real* elements
- with corresponding *real* eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_p$. The decreasing ordering is conventional.

When \mathbf{A} is non-symmetric, eigenvectors and/or eigenvalues may be *complex*, requiring *imaginary* numbers

For example, you can check

$$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 + i \\ 1 - i \end{bmatrix} = -i \times \begin{bmatrix} 1 + i \\ 1 - i \end{bmatrix}, \quad i = \sqrt{-1}$$

so $\mathbf{u} = \begin{bmatrix} 1 + i \\ 1 - i \end{bmatrix}$ is an eigenvector of

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \text{ eigenvalue } \lambda = -i = -\sqrt{(-1)}$$

Fact: If $\lambda_i \neq 0$, for all eigenvalues λ_i of \mathbf{A} , then \mathbf{A} is non-singular, i.e., \mathbf{A}^{-1} exists.

Vocabulary

A symmetric matrix \mathbf{A} is **positive definite** if $\mathbf{x}'\mathbf{A}\mathbf{x} > 0$ for every $\mathbf{x} \neq \mathbf{0}$

A symmetric matrix \mathbf{A} is **positive semi-definite** if $\mathbf{x}'\mathbf{A}\mathbf{x} \geq 0$ for every $\mathbf{x} \neq \mathbf{0}$

- **Fact:** A symmetric matrix is positive definite if and only if $\lambda_i > 0$, $i = 1, \dots, p$
- **Fact:** A positive definite symmetric matrix is **always invertible** since all eigenvalues $\neq 0$.
- A symmetric matrix is positive semi-definite if and only if $\lambda_i \geq 0$, $i = 1, \dots, p$

Let $\mathbf{A} = \text{diag}[a_{11}, a_{22}, \dots, a_{pp}]$ be diagonal.

Then

- λ_i 's are the a_i 's in decreasing order

Vocabulary: $\mathbf{x}'\mathbf{A}\mathbf{x}$ is an example of a *quadratic form*.

Expanded in full a quadratic form is

$$\begin{aligned}\mathbf{x}'\mathbf{A}\mathbf{x} &= \mathbf{x}'(\mathbf{A}\mathbf{x}) = \sum_{1 \leq i \leq p} x_i \left(\sum_{1 \leq j \leq p} a_{ij} x_j \right) \\ &= \sum_{1 \leq i \leq p} \sum_{1 \leq j \leq p} a_{ij} x_i x_j \\ &= \sum_i a_{ii} x_i^2 + \sum \sum_{i \neq j} a_{ij} x_i x_j \\ &= \sum_i a_{ii} x_i^2 + 2 \sum \sum_{i < j} a_{ij} x_i x_j\end{aligned}$$

The last step is OK because \mathbf{A} is symmetric so $a_{ji} = a_{ij}$.

When $p = 2$,

$$\begin{aligned}\mathbf{x}'\mathbf{A}\mathbf{x} &= a_{11} x_1^2 + a_{22} x_2^2 + a_{12} x_1 x_2 + a_{21} x_2 x_1 \\ &= a_{11} x_1^2 + a_{22} x_2^2 + a_{12} x_1 x_2 + a_{12} x_2 x_1 \\ &= a_{11} x_1^2 + a_{22} x_2^2 + 2a_{12} x_1 x_2\end{aligned}$$

When $p = 3$,

$$\begin{aligned}\mathbf{x}'\mathbf{A}\mathbf{x} &= a_{11} x_1^2 + a_{22} x_2^2 + a_{33} x_3^2 + \\ &\quad 2a_{12} x_1 x_2 + 2a_{13} x_1 x_3 + 2a_{23} x_2 x_3\end{aligned}$$

Suppose \mathbf{S}_x is a $p \times p$ sample variance matrix and suppose $y = \mathbf{a}'\mathbf{x}$ is an arbitrary linear combination with $\mathbf{a} \neq \mathbf{0}$.

Recall that $\mathbf{a}'\mathbf{S}_x\mathbf{a} = s_y^2 \geq 0$. This shows that

\mathbf{S}_x is positive semi-definite

Now suppose \mathbf{S}_x is not *positive* definite.

Then there is at least one $\mathbf{a} \neq \mathbf{0}$, with $\mathbf{a}'\mathbf{S}_x\mathbf{a} = 0$. In other words,

$$s_y^2 = 0, \text{ where } y = \mathbf{a}'\mathbf{x} = \sum_j a_j x_j$$

Also, when \mathbf{S}_x is not positive definite there is at least one 0 eigenvalue and any \mathbf{a} with $\mathbf{a}'\mathbf{S}_x\mathbf{a} = 0$ is an eigenvector with 0 eigenvalue.

Q. When can $s_y^2 = 0$ can happen?

A. Only when

$$y_1 = y_2 = \dots = y_n = \text{constant } c$$

$$\text{Now } y_i = \sum_{1 \leq j \leq p} a_j x_{ij}.$$

This means that for any j with $a_j \neq 0$, the value for the j^{th} x variable is determined by the other variables:

$$x_{ij} = c - (a_1/a_j)x_{i1} - (a_2/a_j)x_{i2} - \dots \\ - (a_{j-1}/a_j)x_{i,j-1} - (a_{j+1}/a_j)x_{i,j+1} - \dots - (a_p/a_j)x_{i,p}$$

so x_j is not really needed.

Vocabulary: In such a case, x_1, x_2, \dots, x_p are **collinear**, there is an exact linear relationship between them.

When the the smallest eigenvalue λ_p of **S** is small relative to the largest λ_1 , that is, $\lambda_p/\lambda_1 \approx 0$, x_1, x_2, \dots, x_p are *nearly collinear*.

Properties of eigenvectors and eigenvalues

Let **A** be $p \times p$ symmetric.

Suppose we want to maximize (find the largest possible value of) the *quadratic form*

$$\mathbf{v}'\mathbf{A}\mathbf{v} = \sum_i a_{ii} v_i^2 + 2\sum_{i < j} a_{ij} v_i v_j$$

over all choices for $p \times 1$ vector **v** such that

$$\|\mathbf{v}\|^2 = \sum_i v_i^2 = 1 \text{ ("unit" vector)}$$

Solution: $\mathbf{v} = \mathbf{u}_1$, the normalized *first* eigenvector.

The maximized value is $\mathbf{u}_1'\mathbf{A}\mathbf{u}_1 = \mathbf{u}_1'(\lambda_1 \mathbf{u}_1) = \lambda_1 \mathbf{u}_1'\mathbf{u}_1 = \lambda_1 \|\mathbf{u}_1\|^2 = \lambda_1$, the largest eigenvalue.

Thus

$$\max_{\|\mathbf{v}\|=1} \mathbf{v}'\mathbf{A}\mathbf{v} = \mathbf{u}_1'\mathbf{A}\mathbf{u}_1 = \lambda_1$$

Similarly, when you want to *minimize* $\mathbf{v}'\mathbf{A}\mathbf{v}$ over all choices for \mathbf{v} such that $\|\mathbf{v}\|^2 = 1$, the **solution** is $\mathbf{v} = \mathbf{u}_p$, the *last* eigenvector with the smallest eigenvalue.

The minimized value is

$$\lambda_p = \mathbf{u}_p' \mathbf{A} \mathbf{u}_p = \text{minimum eigenvalue.}$$

Thus

$$\min_{\|\mathbf{v}\|=1} \mathbf{v}'\mathbf{A}\mathbf{v} = \mathbf{u}_p' \mathbf{A} \mathbf{u}_p = \lambda_p$$

Now, for any \mathbf{w} , $\mathbf{w}'\mathbf{A}\mathbf{w} / \|\mathbf{w}\|^2 = \mathbf{v}'\mathbf{A}\mathbf{v}$, where $\mathbf{v} \equiv \mathbf{w} / \|\mathbf{w}\|$ has $\|\mathbf{v}\| = 1$.

These two results imply that

$$\lambda_1 \geq \mathbf{w}'\mathbf{A}\mathbf{w} / \|\mathbf{w}\|^2 \geq \lambda_p, \text{ for all } \mathbf{w} \neq \mathbf{0}.$$

Or, multiplying by $\|\mathbf{w}\|^2$,

$$\lambda_1 \|\mathbf{w}\|^2 \geq \mathbf{w}'\mathbf{A}\mathbf{w} \geq \lambda_p \|\mathbf{w}\|^2, \text{ for all } \mathbf{w}.$$

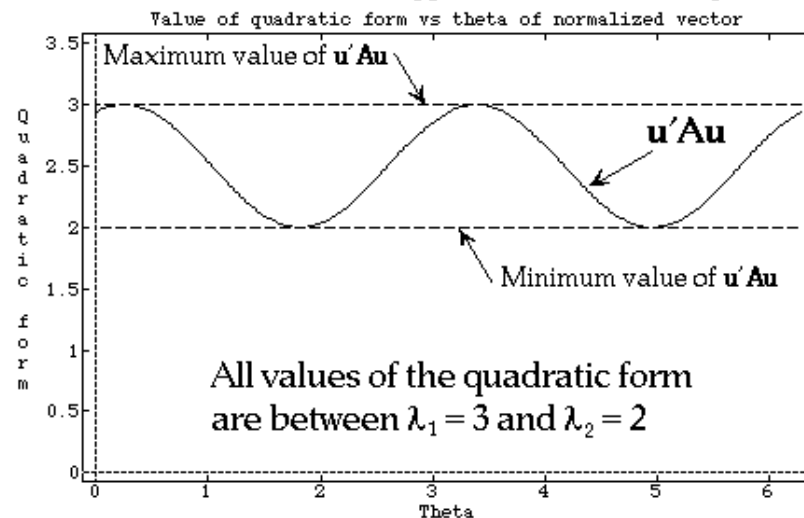
This are bounds on the values of the quadratic form (recall $\lambda_1 = \lambda_{\max}, \lambda_p = \lambda_{\min}$).

For $p = 2$, every unit vectors has the form

$$\mathbf{u} = \begin{bmatrix} \cos \theta \\ \pm \sin \theta \end{bmatrix} \text{ for some } 0 \leq \theta \leq 2\pi$$

Here I computed and graphed $\mathbf{u}'\mathbf{A}\mathbf{u}$ for equally spaced values of θ

```
Cmd> theta <- 2*PI*run(0,250)/250 #equally spaced radian angles
Cmd> qformvals <- 0 * theta # create empty vector
Cmd> for(i,1,length(theta)){
  @u <- vector(cos(theta[i]), sin(theta[i]))
  qformvals[i] <- @u' %*% a %*% @u
};} # compute quadratic form for each angle
Cmd> lineplot(theta,qformvals,xlab:"Theta",\
  title:"Value of quadratic form vs theta of normalized vector",\
  ylab:"Quadratic form",ymin:0,ymax:3.5,show:F)
Cmd> addlines(vector(0,2*PI,?,0,2*PI),\
  vector(2,2,?,3,3),linetype:2)#add lines at y = 2 and 3
```



I gave an example of a *nonsymmetric* matrix whose eigenvectors and eigenvalues were composed of complex numbers rather than real.

There is one important *nonsymmetric* case where eigenvalues and eigenvectors are real:

Fact: Suppose **B** and **C** are *symmetric* $p \times p$ matrices. Then **A** = **BC** is (usually) nonsymmetric but its eigenvectors and eigenvalues are *real*.

You can always assume that the eigenvectors of a symmetric matrix **A** are *normalized*, that is

$$\| \mathbf{u} \| = \sqrt{(\sum_{1 \leq i \leq p} u_i^2)} = 1.$$

MacAnova always produces normalized eigenvectors.

More Facts About Matrices

When **A** is a $p \times p$ square matrix, these five statements are either all true or all false.

1. **A** is non-singular (has an inverse)
2. $\text{rank}(\mathbf{A}) = p$ (**A** has "full rank")
3. $\mathbf{A}\mathbf{b} \neq \mathbf{0}$ for *all* $\mathbf{b} \neq \mathbf{0}$
4. $\det(\mathbf{A}) \neq 0$
5. All eigenvalues $\lambda_i \neq 0$

Here are some ways you might use this equivalence:

- If you have a $\mathbf{b} \neq \mathbf{0}$ but $\mathbf{A}\mathbf{b} = \mathbf{0}$, then **A** is singular, $\det(\mathbf{A}) = 0$ and **A** has at least one eigenvalue = 0 with eigenvector **b**.
- When $\det(\mathbf{A}) = 0$ there is a vector $\mathbf{b} \neq \mathbf{0}$ such that $\mathbf{A}\mathbf{b} = \mathbf{0}$ and **A** has at least one zero eigenvalue

Suppose \mathbf{u} is an eigenvector of $\mathbf{A} = \mathbf{A}'$ with eigenvalue λ . Then, *by definition*, $\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$.

This is the same as

$$\mathbf{A}\mathbf{u} - \lambda\mathbf{u} = (\mathbf{A} - \lambda\mathbf{I}_p)\mathbf{u} = \mathbf{0}.$$

Because $\mathbf{u} \neq \mathbf{0}$, property 4 tells us

$$P(\lambda) \equiv \det(\mathbf{A} - \lambda\mathbf{I}_p) = 0.$$

```
Cmd> write(a) # has eigenvalue 3 and 2
```

```
a:
(1,1)      2.94117647      0.235294118
(2,1)      0.235294118      2.05882353
```

```
Cmd> det(a - 3*dmatrix(2,1))# 3 is eigenvalue of a
```

```
(1) 2.5969e-16
```

Note: write(a) is the simplest way to print a vector or matrix with more significant digits (9) than the default (5).

When $\mathbf{A} = \text{diag}[a_{11}, a_{22}, \dots, a_{pp}]$ is diagonal, its eigenvalues are $a_{11}, a_{22}, \dots, a_{pp}$ and the eigen vectors are $\mathbf{e}_j^p = [0 \dots 0 \underset{1}{1} \underset{j-1}{0} \underset{j}{1} \underset{j+1}{0} \dots \underset{p}{0}]'$,

the columns of \mathbf{I}_p .

$P(\lambda) \equiv \det(\mathbf{A} - \lambda\mathbf{I}_p)$ is actually a polynomial of degree p in λ :

$$P(\lambda) = (-1)^p \lambda^p + d_1 \lambda^{p-1} + \dots + d_{p-1} \lambda + d_p$$

Therefore the eigenvalues λ_i satisfy

$$P(\lambda_i) = 0, i = 1, \dots, p.$$

If you can find the zeros of polynomial, you can compute eigenvalues.

If you like to do such things, for the matrix a in the example which has $\lambda_1 = 3$, $\lambda_2 = 2$, you can check that

$$P(\lambda) = \lambda^2 - 5\lambda + 6$$

For which

$$d_1 = -5 = -(\lambda_1 + \lambda_2), d_2 = 6 = \lambda_1 \times \lambda_2$$

In general,

- $d_1 = (-1)^{p-1} \sum_{1 \leq j \leq p} \lambda_j = (-1)^{p-1} \text{trace}(\mathbf{A})$
- $d_p = \lambda_1 \lambda_2 \dots \lambda_p = \det(\mathbf{A})$

```
Cmd> polyroot(-vector(-trace(a), det(a)))
```

```
(1,1)      2      0      Real and imaginary
(2,1)      3      0      parts of zeros
```