Multivariate Statistical Analysis

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Lecture 4 for Applied Multivariate Analysis

Outline

Matrix decompositions, there are many: singular value, cholesky, etc.

Eigen values and eigen vectors of matrices are needed for some of the methods to be discussed, including principal components analysis, principal component regression. Determining the eigen values and eigen vectors of a matrix is a very difficult computational problem for all except the simplest cases. We will look at the `eigen()` function in R to do these.

- These decompositions will form the core of at least half our multivariate methods (although we need to mention at some point that we actually tend to use the singular value decomposition as a means of getting to these values).
- If **A** is a square $p \times p$ matrix, the eigenvalues (latent roots, characteristic roots) are the roots of the equation:

$$|\mathbf{A} - \lambda \mathbf{I}| = \mathbf{0}$$

This (characteristic) equation is a polynomial of degree p in λ. The roots, the eigenvalues of $\mathbf{A}$ are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_p$. For each eigen value λ_i there is a corresponding eigen vector $\mathbf{e}_i$ which can be found by solving:

$$(\mathbf{A} - \lambda_i \mathbf{I})\mathbf{e_i} = \mathbf{0}$$

There are many solutions for $\mathbf{e_i}$. For our (statistical) purposes, we usually set it to have length 1, i.e. we obtain a normalised eigenvector for λ_i by $\mathbf{a_i} = \frac{\mathbf{e_i}}{\sqrt{\mathbf{e_i}^T \mathbf{e_i}}}$.

Some properties of eigendecompositions

(a) $trace(\mathbf{A}) = \Sigma_{i=1}^{p} \lambda_i$

(b) $|\mathbf{A}| = \prod_{i=1}^{p} \lambda_i$

Also, if **A** is symmetric:

(c) The normalised eigenvectors corresponding to unequal eigenvalues are orthonormal (this is a bit of circular definition, if the eigenvalues are equal the corresponding eigenvectors are not unique, and one "fix" is to choose orthonormal eigenvectors).

(d) Correlation and covariance matrices: are symmetric positive definite (or semi-definite). If such a matrix is of full rank p then all the eigen values are positive. If the matrix is of rank $m < p$ then there will be m positive eigenvalues and $p - m$ zero eigenvalues.

Eigenanalysis

Consider the following matrix: $\mathbf{A} = \begin{pmatrix} 1 & 4 \\ 2 & 3 \end{pmatrix}$

Find the eigenvalues:

$$
\begin{aligned}
\begin{vmatrix} 1-\lambda & 4 \\ 2 & 3-\lambda \end{vmatrix} &= (1-\lambda)(3-\lambda) - 8 = 0 \\
&= 3 - \lambda - 3\lambda + \lambda^2 - 8 = 0 \\
&= \lambda^2 - 4\lambda - 5 = 0 \\
&= (\lambda - 5)(\lambda + 1) = 0 \\
&= \lambda = -1, 5
\end{aligned}
$$

Now, assuming $\lambda = -1$:

$$\mathbf{A} - \lambda \mathbf{I} = \mathbf{A} + \mathbf{I} = \begin{pmatrix} 1 & 4 \\ 2 & 3 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 4 \\ 2 & 4 \end{pmatrix}$$

So that:

$$(\mathbf{A} + \mathbf{I})\mathbf{e} = 0 = \begin{pmatrix} 2 & 4 \\ 2 & 4 \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

So two solutions are given by:

$$2e_1 + 4e_2 = 0$$
$$2e_1 + 4e_2 = 0$$

which are the same(!) and have *a* solution $e_1 = 2, e_2 = -1$, so $\begin{pmatrix} 2 \\ -1 \end{pmatrix}$ is an eigenvector. Given the length of this vector ($\sqrt{2^2 + -1^2}$), we have a normalised eigenvector as:

$$\begin{pmatrix} 2/\sqrt{5} \\ -1/\sqrt{5} \end{pmatrix}$$

- A *normalised* vector is one scaled to have unit length,
- For the vector **x** this can be found by taking $\frac{\mathbf{e_i}}{\sqrt{\mathbf{x'x}}}$
- Trivial in R:

```
> x<-c(2,-1)
> z<-x/sqrt(t(x)%*%x)
> z
[1]  0.8944272 -0.4472136
> t(z) %*% z ## check the length
     [,1]
[1,]    1
```

Also, we might like to consider the case where $\lambda = 5$:

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

So that:

$$(\mathbf{A} - 5\mathbf{I})\mathbf{e} = 0 = \begin{pmatrix} -4 & 4 \\ 2 & -2 \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

So two solutions are given by:

$$-4e_1 + 4e_2 = 0$$
$$2e_1 - 2e_2 = 0$$

which are the same(!) and have *a* solution $e_1 = 1, e_2 = 1$, so $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is an eigenvector. Given the length of this vector $(\sqrt{1^2 + 1^2})$, we have a normalised eigenvector as:

$$\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

Side note: Orthonormality

We have already discussed that two vectors $\mathbf{x}$ and $\mathbf{y}$, of order $k \times 1$ are orthogonal if $\mathbf{x}'\mathbf{y} = 0$. but we can further say that if two vectors $\mathbf{x}$ and $\mathbf{y}$ are orthogonal *and* of unit length, i.e. if $\mathbf{x}'\mathbf{y} = 0$, $\mathbf{x}'\mathbf{x} = 1$ and $\mathbf{y}'\mathbf{y} = 1$ then they are orthonormal.

Outline

Orthonormality

Consider these three vectors. Which of these are orthogonal ?

$$\mathbf{x} = \begin{pmatrix} 1 \\ -2 \\ 3 \\ -4 \end{pmatrix} \mathbf{y} = \begin{pmatrix} 6 \\ 7 \\ 1 \\ -2 \end{pmatrix} \mathbf{z} = \begin{pmatrix} 5 \\ -4 \\ 5 \\ 7 \end{pmatrix}$$

Normalise the two orthogonal vectors, so that we have two orthonormal vectors.

Now identify the two orthonormal vectors:

$$\mathbf{x}_{norm} = \begin{pmatrix} 1/\sqrt{30} \\ -2/\sqrt{30} \\ 3/\sqrt{30} \\ -4/\sqrt{30} \end{pmatrix}$$

$$\mathbf{y}_{norm} = \begin{pmatrix} 6/\sqrt{90} \\ 7/\sqrt{90} \\ 1/\sqrt{90} \\ 2/\sqrt{90} \end{pmatrix}$$

$$\mathbf{z}_{norm} = \begin{pmatrix} 5/\sqrt{115} \\ -4/\sqrt{115} \\ 5/\sqrt{115} \\ 7/\sqrt{115} \end{pmatrix}$$

Further practice
Orthogonality

- Find a vector which is orthogonal to

$$\mathbf{u} = \begin{pmatrix} 1 \\ 3 \end{pmatrix}$$

- $\begin{pmatrix} 3 \\ 1 \end{pmatrix}$
- $\begin{pmatrix} 1 \\ 3 \end{pmatrix}$
- $\begin{pmatrix} 3 \\ -1 \end{pmatrix}$
- $\begin{pmatrix} -3 \\ -1 \end{pmatrix}$

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Orthogonality

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Further practice

Orthogonality

- *A* vector which is orthogonal to

$$\mathbf{u} = \begin{pmatrix} 1 \\ 3 \end{pmatrix}$$

- $\begin{pmatrix} 3 \\ -1 \end{pmatrix}$

Further practice
Orthogonality

- *A* vector which is orthogonal to

$$\mathbf{u} = \begin{pmatrix} 1 \\ 3 \end{pmatrix}$$

- $\begin{pmatrix} 3 \\ -1 \end{pmatrix}$

Do please note carefully that this is not a unique solution. Any w_1 and w_2 that satisfies $w_1 + 3w_2 = 0$ will be orthogonal to $\mathbf{u}$. Did you find any others?

- And a vector which is orthogonal to:

$$\mathbf{v} = \begin{pmatrix} 2 \\ 4 \\ -1 \\ 2 \end{pmatrix}$$

$$\begin{pmatrix} 4 \\ 0 \\ 2 \\ 1 \end{pmatrix} \quad \begin{pmatrix} 0 \\ 0 \\ 2 \\ 1 \end{pmatrix} \quad \begin{pmatrix} 0 \\ -4 \\ 2 \\ 1 \end{pmatrix} \quad \begin{pmatrix} -2 \\ 0 \\ 2 \\ 1 \end{pmatrix}$$

- And a vector which is orthogonal to:

$$\mathbf{v} = \begin{pmatrix} 2 \\ 4 \\ -1 \\ 2 \end{pmatrix}$$

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

If you are really comfortable with eigenanalysis of 2×2 matrices have a go at these 3×3 matrices.

$$\mathbf{e} = \begin{pmatrix} 1 & 4 & 0 \\ 4 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{f} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 9 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{g} = \begin{pmatrix} 13 & -4 & 2 \\ -4 & 13 & -2 \\ 2 & -2 & 10 \end{pmatrix}$$

Outline

Transposing matrices

Turns the first column into the first row etc.. A transposed matrix is denoted by a superscripted ′, in other words $\mathbf{A}^\mathbf{T}$ is the transpose of **A**.

$$\textit{If } \mathbf{A} = \begin{pmatrix} 3 & 1 \\ 5 & 6 \\ 4 & 4 \end{pmatrix} \text{ then } \mathbf{A}^\mathbf{T} = \begin{pmatrix} 3 & 5 & 4 \\ 1 & 6 & 4 \end{pmatrix}$$

As with vectors, transposing matrices in **R** simply requires a call to `t()`, the dimensions can be checked with `dim()`.

Outline

Symmetric matrices

- Symmetric around the diagonal $i = j$.
- For matrix **A**, it is symmetric whenever $a_{ij} = a_{ji}$.
- The correlation matrix and the variance-covariance matrix are the most common symmetric matrices we will encounter,

Outline

Diagonal matrix

Elements on the diagonal (where $i = j$) and zero elsewhere (where $i \neq j$). For example, the matrix **A** given as follows:

$$\mathbf{A} = \begin{pmatrix} 13 & 0 & 0 \\ 0 & 27 & 0 \\ 0 & 0 & 16 \end{pmatrix}$$

is a diagonal matrix. To save paper and ink, **A** can also be written as:

$$\mathbf{A} = diag \begin{pmatrix} 13 & 27 & 16 \end{pmatrix}$$

Outline

Finally, note that we can partition a large matrix into smaller ones:

$$\left(\begin{array}{cc|c} 2 & 5 & 4 \\ \hline 0 & 7 & 8 \\ 4 & 3 & 4 \end{array}\right)$$

So we could work with submatrices such as $\begin{pmatrix} 0 & 7 \\ 4 & 3 \end{pmatrix}$.

e.g. If $\mathbf{X}$ was partitioned as $\begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix}$ and $\begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \mathbf{Y}_3 \end{pmatrix}$ then:

$$\mathbf{XY} = \begin{pmatrix} \mathbf{X}_1\mathbf{Y}_1 & \mathbf{X}_1\mathbf{Y}_2 & \mathbf{X}_1\mathbf{Y}_3 \\ \mathbf{X}_2\mathbf{Y}_1 & \mathbf{X}_2\mathbf{Y}_2 & \mathbf{X}_2\mathbf{Y}_3 \end{pmatrix}$$