Eigenvalue Decomposition

Predictive Modeling & Statistical Learning

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Matrix Decompositions

Decompositions

Matrix decompositions, also known as matrix factorizations

$$\mathbf{M} = \mathbf{AB} \qquad \text{or} \qquad \mathbf{M} = \mathbf{ABC}$$

are a means of expressing a matrix as a product of usually two or three simpler matrices.

Importance of Decompositions

What for?

Matrix decompositions make it easier to study the properties of matrices. Likewise, many computation tasks become easier with decompositions.

They play a relevant role in multivariate data analysis. Often, the solution to many techniques are obtained (or derived) from a matrix decomposition.

Decompositions: What for?

- solving systems of linear equations
- inverting a matrix
- analyzing numerical stability of a system
- understanding the structure of data
- finding basis for column space (or row space) of a matrix

Some Assumptions

Real Matrices

We will assume all matrices to be real matrices, i.e. matrices containing elements in the set of Real numbers.

Dimensions $n \geq p$

Unless otherwise stated, we will also assume matrices with more rows than columns.

Decompositions

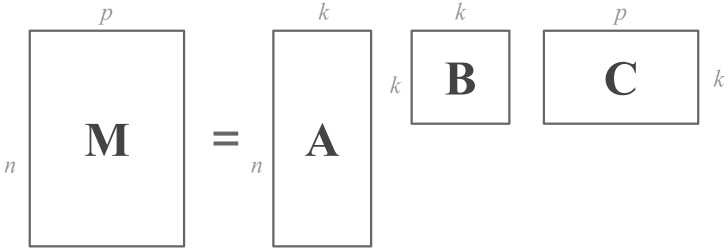
A matrix decomposition can be described by an equation:

$$\mathbf{M} = \mathbf{ABC}$$

where the dimensions of the matrices are as follows:

- $\mathbf{M}$ is $n \times p$ (assume $n > p$)
- $\mathbf{A}$ is $n \times k$ (usually $k < p$)
- $\mathbf{B}$ is $k \times k$ (usually diagonal)
- $\mathbf{C}$ is $k \times p$

Matrix Decomposition



Interpreting Decompositions

The equation that describes a decomposition:

$$\mathbf{M} = \mathbf{A}\mathbf{B}\mathbf{C}$$

- does not explain how to compute one
- does not explain how such decomposition can reveal the structures implicit in a data matrix.
- Seeing how a matrix decomposition reveals structure in a dataset is more complicated
- Each decomposition reveals a different kind of implicit structure

Types of matrices

Two types of matrices

We concentrate on the two types of matrices important in statistics:

- general **rectangular** matrices used to represent data tables.
- **positive semi-definite** matrices used to represent covariance matrices, correlation matrices, and any matrix that results from a crossproduct.

Two Special Decompositions

EVD and SVD

There are many types of matrix decompositions but for now we are going to consider only two:

- Eigen-Value Decomposition (EVD)
- Singular Value Decomposition (SVD)

Eigenvalue Decomposition

- EVD applies to square matrices in general.
- A special type of square matrices are **symmetric** matrices.
- In data analysis methods, these matrices usually appear in the form of cross-product association matrices: e.g. $\mathbf{X}^\mathsf{T}\mathbf{X}$ and $\mathbf{X}\mathbf{X}^\mathsf{T}$
- The attractive thing about EVD is that when applied to symmetric matrices the results have a "simple" nice structure.

Eigenvalue and Eigenvector

Consider the matrix $\mathbf{A}$:

$$\mathbf{A} = \begin{bmatrix} 3 & -2 \\ 1 & 0 \end{bmatrix}$$

associated to the linear transformation $T(\mathbf{x})$ given by:

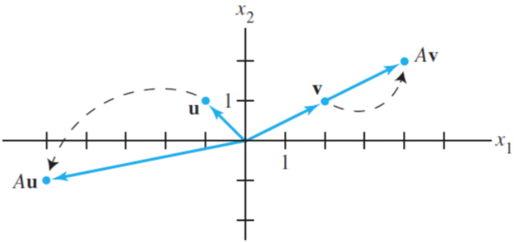
$$T(\mathbf{x}) = \begin{bmatrix} 3 & -2 \\ 1 & 0 \end{bmatrix} \mathbf{x} = \mathbf{A}\mathbf{x}$$

and assume vectors $\mathbf{v} = (2, 1)$ and $\mathbf{u} = (-1, 1)$

Eigenvalue and Eigenvector

$$T(\mathbf{v}) = \begin{bmatrix} 3 & -2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$$

$$T(\mathbf{u}) = \begin{bmatrix} 3 & -2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -5 \\ -1 \end{bmatrix}$$



$\mathbf{u}$ is changing its direction, but not $\mathbf{v}$

Eigenvalue and Eigenvector

Given an $n \times n$ matrix $\mathbf{M}$, λ is an **eigenvalue** of $\mathbf{M}$ if there exists a non-trivial solution $\mathbf{v}$ of the equation:

$$\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$$

The solution $\mathbf{v}$ is the **eigenvector** associated to the eigenvalue λ

Eigen-Value Decomposition

EVD

An $n \times n$ symmetric matrix $\mathbf{M}$ can be decomposed as:

$$\mathbf{M} = \mathbf{A}\mathbf{B}\mathbf{A}^{\mathsf{T}}$$

where

- $\mathbf{A}$ is a $n \times p$ column **orthonormal** matrix containing the eigen-vectors of $\mathbf{M}$
- $\mathbf{B}$ is a $p \times p$ **diagonal** matrix containing the eigen-values of $\mathbf{M}$

Eigen-Value Decomposition

EVD

A more common notation for EVD is:

$$\mathbf{M} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\mathsf{T}}$$

where

- $\mathbf{U}$ is a $n \times p$ column **orthonormal** matrix containing the eigen-vectors of $\mathbf{M}$
- $\mathbf{\Lambda}$ is a $p \times p$ **diagonal** matrix containing the eigen-values of $\mathbf{M}$

EVD

$$\mathbf{M} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\mathsf{T}}$$

$$\mathbf{M} = \begin{bmatrix} u_{11} & \cdots & u_{1p} \\ u_{21} & \cdots & u_{2p} \\ \vdots & \ddots & \vdots \\ u_{n1} & \cdots & u_{np} \end{bmatrix} \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_p \end{bmatrix} \begin{bmatrix} u_{11} & \cdots & u_{n1} \\ u_{12} & \cdots & u_{n2} \\ \vdots & \ddots & \vdots \\ u_{1p} & \cdots & u_{np} \end{bmatrix}$$

Eigenvectors

Vectors, which under a given transformation $\mathbf{M}$ map into themselves or multiples of themselves, are called invariant vectors under that transformation. It follows that such vectors satisfy the relation:

$$\mathbf{M}\mathbf{x} = \lambda\mathbf{x}$$

where λ is a scalar.

Eigenvectors

The matrix equation:

$$\mathbf{Mx} = \lambda \mathbf{x}$$

can be rearranged as follows:

$$\mathbf{Mx} - \lambda \mathbf{x} = \mathbf{0}$$

Eigenvectors

Given

$$\mathbf{Mx} - \lambda\mathbf{x} = \mathbf{0}$$

We can factor out $\mathbf{x}$

$$(\mathbf{M} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}$$

Eigenvectors

Obtaining the eigenstructure of a (square) matrix involves solving the **characteristic equation**

$$det(\mathbf{M} - \lambda_i \mathbf{I}) = 0$$

If $\mathbf{M}$ is of order $n \times n$, then we can obtain n roots of the equation. These roots are called the **eigenvalues**.

EVD in R

`eigen()` in R

`eigen()` function

R provides the function `eigen()` to perform an eigenvalue decomposition of a square matrix.

`eigen()` output

A list with the following components

- `values` a vector containing the eigenvalues
- `vectors` a matrix whose columns contain the eigenvectors

EVD example in R

```
# X'X matrix
set.seed(22)
X <- as.matrix(USArrests)
XtX <- t(X) %*% X

# eigenvalue decomposition
EVD = eigen(XtX)

# elements returned by eigen()
names(EVD)
```

```
## [1] "values"  "vectors"
```

```
# vector of eigenvalues
(lambdas = EVD$values)
```

```
## [1] 2013735.2431   37957.1103    2084.9578     326.5089
```

EVD example in R (con't)

```
# matrix of eigenvectors
(V <- EVD$vectors)

##             [,1]        [,2]        [,3]        [,4]
## [1,] -0.04239181  0.01616262  0.06588426  0.99679535
## [2,] -0.94395706  0.32068580 -0.06655170 -0.04094568
## [3,] -0.30842767 -0.93845891 -0.15496743  0.01234261
## [4,] -0.10963744 -0.12725666  0.98347101 -0.06760284
```

Properties of Matrix Eigenstructures

Properties of Eigenstructures

1. The sum of the eigenvalues of a matrix $\mathbf{A}$ equals the sum of the main diagonal elements (i.e. the trace) of the matrix.

$$\sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} a_{ii}$$

2. The product of the eigenvalues of a matrix $\mathbf{A}$ equals the determinant of $\mathbf{A}$

$$\prod_{i=1}^{n} \lambda_i = |\mathbf{A}|$$

Properties of Eigenstructures

3. If we have the matrix $\mathbf{B} = \mathbf{A} + k\mathbf{I}$, where k is a scalar, then the eigenvectors of $\mathbf{B}$ are the same as those of $\mathbf{A}$, and the i-th eigenvalue of $\mathbf{B}$ is

$$\lambda_i + k$$

where λ_i is the i-th eigenvalue of $\mathbf{A}$

4. If we have the matrix $\mathbf{C} = k\mathbf{A}$, where k is a scalar, then $\mathbf{C}$ has the same eigenvectors as $\mathbf{A}$ and

$$k\lambda_i$$

is the eigenvalue pf $\mathbf{C}$, where λ_i is the i-th eigenvalue of $\mathbf{A}$

Properties of Eigenstructures

5. If we have the matrix $\mathbf{A}^p$, where p is a positive integer, then scalar, then $\mathbf{A}^p$ has the same eigenvectors as $\mathbf{A}$ and

$$\lambda_i^p$$

is the i-th eigenvalue of $\mathbf{A}^p$, where λ_i is the i-th eigenvalue of $\mathbf{A}$

6. If $\mathbf{A}^{-1}$ exists, then $\mathbf{A}^{-p}$ has the same eigenvectors as $\mathbf{A}$ and

$$\lambda_i^{-p}$$

is the i-th eigenvalue of $\mathbf{A}^{-p}$ corresponding to the i-th eigenvalue of $\mathbf{A}$

7. If a symmetric matrix $\mathbf{A}$ can be written as the product

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^{\mathsf{T}}$$

where $\mathbf{D}$ is a diagonal with all entries nonnegative and $\mathbf{U}$ is an orthogonal matrix of eigenvectors, then

$$\mathbf{A}^{1/2} = \mathbf{U}\mathbf{D}^{1/2}\mathbf{U}^{\mathsf{T}}$$

and it is the case that $\mathbf{A}^{1/2}\mathbf{A}^{1/2} = \mathbf{A}$

8. If a symmetric matrix $\mathbf{A}^{-1}$ can be written as the product

$$\mathbf{A}^{-1} = \mathbf{U}\mathbf{D}^{-1}\mathbf{U}^{\mathsf{T}}$$

where $\mathbf{D}^{-1}$ is a diagonal with all entries nonnegative and $\mathbf{U}$ is an orthogonal matrix of eigenvectors, then

$$\mathbf{A}^{-1/2} = \mathbf{U}\mathbf{D}^{-1/2}\mathbf{U}^{\mathsf{T}}$$

and it is the case that $\mathbf{A}^{-1/2}\mathbf{A}^{-1/2} = \mathbf{A}^{-1}$

Power Method

About the Power Method

One of the basic procedures following a successive approximation approach is precisely the Power Method.

In its simplest form, the Power Method (PM) allows us to find **the largest** eigenvector and its corresponding eigenvalue.

About the Power Method

Choose an arbitrary vector $\mathbf{w_0}$ to which we will apply the symmetric matrix $\mathbf{S}$ repeatedly to form the following sequence:

$$\begin{aligned}
\mathbf{w_1} &= \mathbf{S}\mathbf{w_0} \\
\mathbf{w_2} &= \mathbf{S}\mathbf{w_1} = \mathbf{S^2}\mathbf{w_0} \\
\mathbf{w_3} &= \mathbf{S}\mathbf{w_2} = \mathbf{S^3}\mathbf{w_0} \\
&\vdots \\
\mathbf{w_k} &= \mathbf{S}\mathbf{w_{k-1}} = \mathbf{S^k}\mathbf{w_0}
\end{aligned}$$

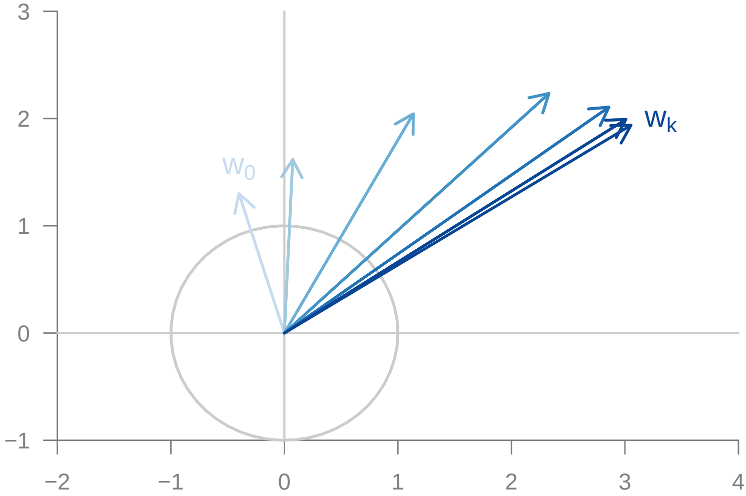
Power Method: Example

Consider a matrix $\mathbf{S}$

$$\mathbf{S} = \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix}$$

and an initial vector $\mathbf{w_0}$

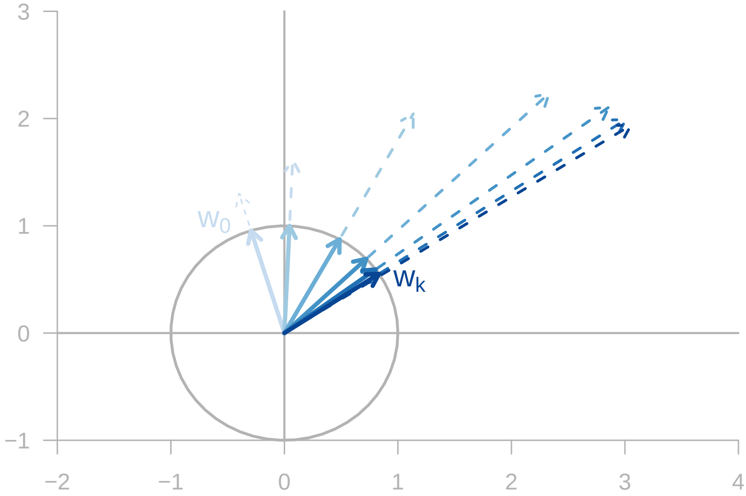
$$\mathbf{w_0} = \begin{bmatrix} -0.4 \\ 1.3 \end{bmatrix}$$



3
2
1
0
−1
−2
−1
0
1
2
3
4
w_0
w_k

About the Power Method

- In practice, we must rescale the obtained vector $\mathbf{w_k}$ at each step.
- The rescaling will allows us to judge whether the sequence is converging.
- After some iterations, the vector $\mathbf{w_{k-1}}$ and $\mathbf{w_k}$ will be very similar
- Assuming a reasonable scaling strategy, the sequence will usually converge to the dominant eigenvector of $\mathbf{S}$.



3
2
1
0
−1
−2
−1
0
1
2
3
4
w_0
w_k

Dominant Eigenvalue

The obtained vector is the dominant eigenvector. To get the corresponding eigenvalue we calculate the so-called **Rayleigh quotient** given by:

$$\lambda = \frac{\mathbf{w_k}^\mathsf{T}\mathbf{S}\mathbf{w_k}}{\mathbf{w_k}^\mathsf{T}\mathbf{w_k}}$$

Remarks

Conditions for the power method to be succesfully used:

- The matrix must have a *dominant* eigenvalue.
- The starting vector $\mathbf{w_0}$ must be nonzero.
- We need to scale each of the vectors $\mathbf{w_k}$
  otherwise the algorithm will "explode"

PM Pseudocode

Let's consider a more detailed version of the PM algorithm:

1. Start with an arbitraty initial vector $\mathbf{w}$
2. Obtain product $\tilde{\mathbf{w}} = \mathbf{S}\mathbf{w}$
3. Normalize $\tilde{\mathbf{w}}$

$$\text{e.g.} \quad \mathbf{w} = \frac{\tilde{\mathbf{w}}}{\left\|\tilde{\mathbf{w}}\right\|_{p=2}}$$

4. Compare $\mathbf{w}$ with its previous version
5. Repeat steps 2 till 4 until convergence

Why does the PM work?

Assume that the matrix $\mathbf{S}$ has p eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_p$, and that they are ordered in decreasing way $|\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_p|$.

Note that the first eigenvalue is strictly greater than the second one. This is a very important assumption.

In the same way, we'll assume that the matrix $\mathbf{S}$ has p linearly independent vectors $\mathbf{u_1}, \ldots, \mathbf{u_p}$ ordered in such a way that $\mathbf{u_j}$ corresponds to λ_j.

Why does the PM work?

The initial vector $\mathbf{w_0}$ may be expressed as a linear combination of $\mathbf{u_1}, \ldots, \mathbf{u_p}$

$$\mathbf{w_0} = a_1\mathbf{u_1} + \cdots + a_p\mathbf{u_p}$$

At every step of the iterative process the vector $\mathbf{w_k}$ is given by:

$$\mathbf{w_k} = a_1\lambda_1^k\mathbf{u_1} + \cdots + a_p\lambda_p^k\mathbf{u_p}$$

Why does the PM work?

Since λ_1 is the dominant eigenvalue, the component in the direction of $\mathbf{u_1}$ becomes relatively greater than the other components as k increases. If we knew λ_1 in advance, we could rescale at each step by dividing by it to get:

$$\left(\frac{1}{\lambda_1^k}\right)\mathbf{w_k} = a_1\mathbf{u_1} + \cdots + a_p\left(\frac{\lambda_p^k}{\lambda_1^k}\right)\mathbf{u_p}$$

which converges to the eigenvector $a_1\mathbf{u_1}$, provided that a_1 is nonzero.

Why does the PM work?

Of course, in real life this scaling strategy is not possible—we don't know λ_1. Consequenlty, the eigenvector is determined only up to a constant multiple, which is not a concern since the really important thing is the *direction* not the length of the vector.

The speed of the convergence depends on how bigger λ_1 is respect with to λ_2, and on the choice of the initial vector $\mathbf{w_0}$. If λ_1 is not much larger than λ_2, then the convergence will be slow.

More Remarks

- The power method is a sequential method.
- We can obtain $\mathbf{w_1}, \mathbf{w_2}$, and so on, step by step.
- If we only need the first k vectors, we can stop the procedure at the desired stage.

Obtaining more eigenvectors?

Once we've obtained the first eigenvector $\mathbf{w_1}$ and eigenvalue λ_1, we can compute the second eigenvector by reducing the matrix $\mathbf{S}$ by the amount explained by the first eigenvector.

This operation of reduction is called **deflation** and the residual matrix is obtained as:

$$\mathbf{S_1} = \mathbf{S} - \lambda_1 \mathbf{w_1} \mathbf{w_1}^\mathsf{T}$$

To get the second eigenvalue and its corresponding eigenvector, we operate on $\mathbf{S_1}$ in the same way as the operations on $\mathbf{S}$.

References

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