Singular Value Decomposition (SVD)

Matrix Algebra 4 Statistical Learning

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Introduction

Two Special Decompositions

Last time we talked about the Eigen Value Decomposition (EVD).

In these slides, we'll talk about a closely related decomposition of EVD: the so-called Singular Value Decomposition (SVD)

Recap

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.

Types of matrices

Two types of matrices

We said that in data analysis we typically concentrate on two types of matrices:

- 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.

Singular Value Decomposition

- One of the most important decompositions in matrix algebra
- Can be applied to **any** rectangular matrix
- ANY: rectangular or square, singular or nonsigular.

Singular Value Decomposition

Let $\mathbf{M}$ be an $n \times p$ matrix.

For convenience, let's also assume that $\mathbf{M}$ is a "tall" matrix with $n > p$, although this is not essential.

Likewise, let's assume for the moment that the rank of $\mathbf{M}$ is $r \leq p < n$

Singular Value Decomposition

We can represent $\mathbf{M}$ as a triple product given by:

$$\mathbf{M} = \mathbf{U}\mathbf{D}\mathbf{V}^{\mathsf{T}}$$

where

- $\mathbf{U}$ is a $n \times r$ matrix which is **orthonormal** by columns: $\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I}_r$
- $\mathbf{D}$ is a $r \times r$ **diagonal** matrix consisting of r positive diagonal entries.
- $\mathbf{V}$ is a $p \times r$ matrix which is **orthonormal** by columns: $\mathbf{V}^{\mathsf{T}}\mathbf{V} = \mathbf{I}_r$

Singular Value Decomposition

The representation of $\mathbf{M}$ as the triple product $\mathbf{UDV}^\mathsf{T}$ is called its *singular value decomposition*, occasionally referred to as "basic structure".

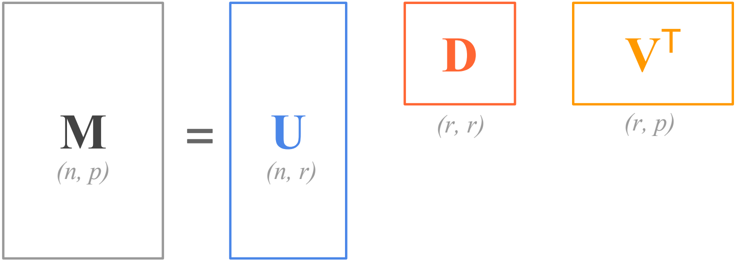
- $\mathbf{U}$ is the matrix of **left singular vectors** of $\mathbf{M}$
- $\mathbf{D}$ is the matrix of **singular values** of $\mathbf{M}$
- $\mathbf{V}$ is the matrix of **right singular vectors** of $\mathbf{M}$

SVD

$$\mathbf{M} = \mathbf{U}\mathbf{D}\mathbf{V}^{\mathsf{T}}$$

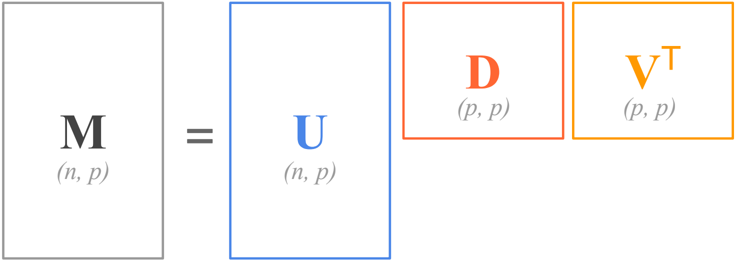
$$\mathbf{M} = \begin{bmatrix} u_{11} & \cdots & u_{1r} \\ u_{21} & \cdots & u_{2r} \\ \vdots & \ddots & \vdots \\ u_{n1} & \cdots & u_{nr} \end{bmatrix} \begin{bmatrix} l_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & l_r \end{bmatrix} \begin{bmatrix} v_{11} & \cdots & v_{p1} \\ \vdots & \ddots & \vdots \\ v_{1r} & \cdots & v_{pr} \end{bmatrix}$$

SVD Diagram



When $\mathbf{M}$ is of rank $r < p$

SVD Diagram



When $\mathbf{M}$ is of full rank p

About SVD

Singular Value Decomposition

We can think of the SVD structure as *the basic structure of a matrix*. What do we mean by "basic"? Well, this has to do with what each of the matrices $\mathbf{UDV}^{\mathsf{T}}$ represent.

- $\mathbf{U}$ is the orthonormalized matrix which is the most basic component. It's like the skeleton of the matrix.
- $\mathbf{D}$ is referred to as the *spectrum* and it is a scale component.
- $\mathbf{V}$ is an orientation component, also referred to as the *rotation* matrix.

About SVD

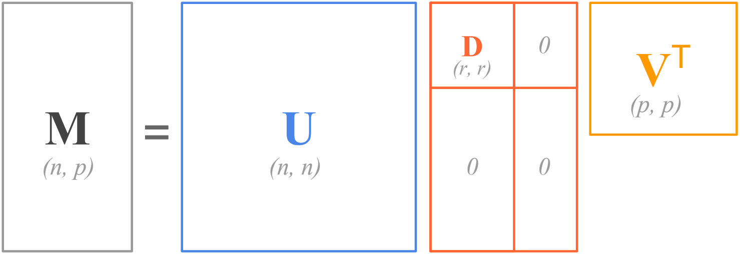
Note that:

- $\mathbf{U}$ cannot be orthogonal $(\mathbf{U}\mathbf{U}^\mathsf{T} = \mathbf{I_n})$ unless $r = p$
- $\mathbf{V}$ cannot be orthogonal $(\mathbf{V}\mathbf{V}^\mathsf{T} = \mathbf{I_p})$ unless $r = p = m$
- All elements of $\mathbf{D}$ can be taken to be positive, ordered from large to small (with ties allowed)

Full SVD

If we let $\mathbf{D}$ be the first r rows and r columns embedded in a (larger) $n \times p$ *rectangular* matrix, with $n - r$ rows and $p - r$ columns of zeros elsewhere, both $\mathbf{U}$ and $\mathbf{V}^{\mathsf{T}}$ could be made fully orthogonal and, in this sense, properly constitute rotation matrices of order $n \times n$ and $p \times p$, respectively. This generalization can be called the full SVD of a matrix.

"Full" SVD Diagram



When $\mathbf{M}$ is of rank $r \leq p$

About SVD

The preceding generalization is a significant one. It tells us that ANY matrix with real-valued entries can be represented as the product of:

- a rotation (possibly followed by a reflection), followed by
- a stretch, followed by
- a rotation

SVD

- $\mathbf{U}$ is unitary, and its columns form a basis for the space spanned by the columns of $\mathbf{M}$.

$$\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I}_p$$

- $\mathbf{V}$ is unitary, and its columns form a basis for the space spanned by the rows of $\mathbf{M}$.

$$\mathbf{V}^{\mathsf{T}}\mathbf{V} = \mathbf{I}_p$$

- $\mathbf{D}$ has non-negative real numbers on the diagonal (assuming $\mathbf{M}$ is real).

SVD in R

`svd()` in R

`svd()` function

R provides the function `svd()` to perform a singular value decomposition of a given matrix

`svd()` output

A list with the following components

- `d` a vector containing the singular values
- `u` a matrix whose columns contain the left singular vectors
- `v` a matrix whose columns contain the right singular vectors

SVD example in R

```
# X matrix
set.seed(22)
X = matrix(rnorm(20), 5, 4)

# singular value decomposition
SVD = svd(X)

# elements returned by svd()
names(SVD)

## [1] "d" "u" "v"

# vector of singular values
(d = SVD$d)

## [1] 3.9516353 2.0223602 1.4748193 0.4324292
```

SVD example in R (con't)

```
# matrix of left singular vectors
(U = SVD$u)

##            [,1]        [,2]       [,3]        [,4]
## [1,] -0.4251177 -0.53913435 -0.7232572  0.00979433
## [2,]  0.5268694 -0.76862769  0.2860048  0.05610045
## [3,]  0.5752546  0.04999546 -0.4421464  0.13107213
## [4,]  0.2215220  0.05272644 -0.1702161 -0.95123359
## [5,] -0.4021114 -0.33655016  0.4130778 -0.27337073

# matrix of right singular vectors
(V = SVD$v)

##            [,1]       [,2]        [,3]       [,4]
## [1,]  0.5708354 -0.7406782  0.33862988  0.1042716
## [2,] -0.2741800 -0.5295008 -0.76797328  0.2338189
## [3,]  0.2772481  0.3206239 -0.04462207  0.9046229
## [4,]  0.7225689  0.2611992 -0.54180782 -0.3407543
```

SVD example in R (con't)

```
# U orthonormal  (U'U = I)
t(U) %*% U

##               [,1]          [,2]          [,3]          [,4]
## [1,] 1.000000e+00  1.387779e-16  2.775558e-17  0.000000e+00
## [2,] 1.387779e-16  1.000000e+00 -2.775558e-17 -8.326673e-17
## [3,] 2.775558e-17 -2.775558e-17  1.000000e+00  5.551115e-17
## [4,] 0.000000e+00 -8.326673e-17  5.551115e-17  1.000000e+00

# V orthonormal  (V'V = I)
t(V) %*% V

##                [,1]          [,2]          [,3]          [,4]
## [1,]  1.000000e+00 -1.110223e-16 -5.551115e-17  1.110223e-16
## [2,] -1.110223e-16  1.000000e+00  8.326673e-17  1.942890e-16
## [3,] -5.551115e-17  8.326673e-17  1.000000e+00 -8.326673e-17
## [4,]  1.110223e-16  1.942890e-16 -8.326673e-17  1.000000e+00
```

SVD example in R (con't)

```r
# X equals U D V'
U %*% diag(d) %*% t(V)

##            [,1]        [,2]        [,3]       [,4]
## [1,] -0.5121391  1.85809239 -0.76390728 -0.9221536
## [2,]  2.4851837 -0.06602641  0.08196190  0.8615624
## [3,]  1.0078262 -0.16276495  0.74302828  2.0029422
## [4,]  0.2928146 -0.19986068 -0.08402219  0.9365510
## [5,] -0.2089594  0.30056173 -0.79289452 -1.6157349

# compare to X
X

##            [,1]        [,2]        [,3]       [,4]
## [1,] -0.5121391  1.85809239 -0.76390728 -0.9221536
## [2,]  2.4851837 -0.06602641  0.08196190  0.8615624
## [3,]  1.0078262 -0.16276495  0.74302828  2.0029422
## [4,]  0.2928146 -0.19986068 -0.08402219  0.9365510
## [5,] -0.2089594  0.30056173 -0.79289452 -1.6157349
```

SVD and Cross-products

Data Matrix

Data

The analyzed data can be expressed in matrix format $\mathbf{X}$:

$$\underset{n\times p}{\mathbf{X}} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

- n objects in the rows
- p variables in the columns

Relation of SVD and Cross-Product Matrices

The cross-product matrix of columns of $\mathbf{X}$ can be expressed as:

$$\mathbf{X}^\mathsf{T}\mathbf{X} = \mathbf{V}\mathbf{D}^2\mathbf{V}^\mathsf{T}$$

Relation of SVD and Cross-Product Matrices

The cross-product matrix of columns can be expressed as:

$$\begin{aligned}\mathbf{X}^\mathsf{T}\mathbf{X} &= (\mathbf{UDV}^\mathsf{T})^\mathsf{T}(\mathbf{UDV}^\mathsf{T}) \\ &= (\mathbf{VDU}^\mathsf{T})(\mathbf{UDV}^\mathsf{T}) \\ &= \mathbf{VD}(\mathrm{U}^\mathsf{T}\mathrm{U})\mathbf{DV}^\mathsf{T} \\ &= \mathbf{VD^2V}^\mathsf{T}\end{aligned}$$

Relation of SVD and Cross-Product Matrices

The cross-product matrix of rows of $\mathbf{X}$ can be expressed as:

$$\mathbf{X}\mathbf{X}^{\mathsf{T}} = \mathbf{U}\mathbf{D}^{\mathbf{2}}\mathbf{U}^{\mathsf{T}}$$

Relation of SVD and Cross-Product Matrices

The cross-product matrix of rows can be expressed as:

$$\begin{aligned}
\mathbf{X}\mathbf{X}^\mathsf{T} &= (\mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T})(\mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T})^\mathsf{T} \\
&= (\mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T})(\mathbf{V}\mathbf{D}\mathbf{U}^\mathsf{T}) \\
&= \mathbf{U}\mathbf{D}(\mathbf{V}^\mathsf{T}\mathbf{V})\mathbf{D}\mathbf{U}^\mathsf{T} \\
&= \mathbf{U}\mathbf{D}^\mathbf{2}\mathbf{U}^\mathsf{T}
\end{aligned}$$

Relation of SVD and Cross-Product Matrices

One of the interesting things about SVD is that $\mathbf{U}$ and $\mathbf{V}$ are matrices whose columns are eigenvectors of product moment matrices that are *derived* from $\mathbf{X}$. Specifically,

- $\mathbf{U}$ is the matrix of eigenvectors of (symmetric) $\mathbf{X}\mathbf{X}^\mathsf{T}$ of order $n \times n$
- $\mathbf{V}$ is the matrix of eigenvectors of (symmetric) $\mathbf{X}^\mathsf{T}\mathbf{X}$ of oreder $p \times p$

Of additional interest is the fact that $\mathbf{D}$ is a diagonal matrix whose main diagonal entries are the square roots of $\mathbf{\Lambda}$, the *common* matrix of eigenvalues of $\mathbf{X}\mathbf{X}^\mathsf{T}$ and $\mathbf{X}^\mathsf{T}\mathbf{X}$.

Relation between EVD and SVD

The EVD of the cross-product matrix of columns (or minor product moment) $\mathbf{X}^\mathsf{T}\mathbf{X}$ can be expressed as:

$$\mathbf{X}^\mathsf{T}\mathbf{X} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^\mathsf{T}$$

in terms of the SVD factorization of $\mathbf{X}$:

$$\mathbf{X}^\mathsf{T}\mathbf{X} = \mathbf{V}\mathbf{D}^\mathbf{2}\mathbf{V}^\mathsf{T}$$

Relation between EVD and SVD

The EVD of the cross-product matrix of rows (or major product moment) $\mathbf{X}\mathbf{X}^\mathsf{T}$ can be expressed as:

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in terms of the SVD factorization of $\mathbf{X}$:

$$\mathbf{X}\mathbf{X}^\mathsf{T} = \mathbf{U}\mathbf{D^2}\mathbf{U}^\mathsf{T}$$

Rank Reduction

SVD Rank-Reduction Theorem

In terms of the diagonal elements $l_1, l_2, \ldots, l_r$ of $\mathbf{D}$, the columns $\mathbf{u_1}, \ldots, \mathbf{u_r}$ of $\mathbf{U}$, and the columns $\mathbf{v_1}, \ldots, \mathbf{v_r}$ of $\mathbf{V}$, the basic structure of $\mathbf{X}$ may be written as

$$\mathbf{X} = l_1 \mathbf{u_1} \mathbf{v_1}^\mathsf{T} + l_2 \mathbf{u_2} \mathbf{v_2}^\mathsf{T} + \cdots + l_p \mathbf{u_r} \mathbf{v_r}^\mathsf{T}$$

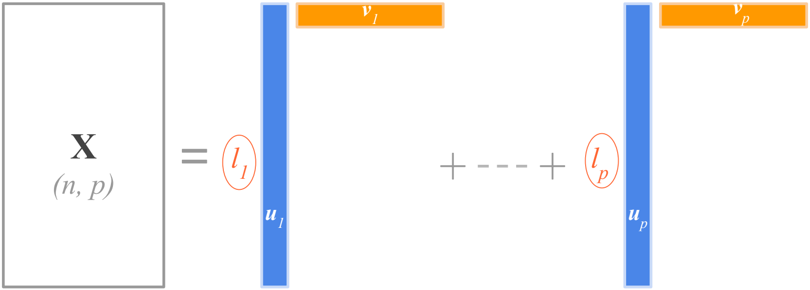
which shows that the matrix $\mathbf{X}$ of rank p is a linear combination of r matrices of rank 1.

SVD Rank-Reduction Theorem

A very interesting and alternative way to represent the SVD is with the following formula:

$$\mathbf{X} = \sum_{k=1}^{r} l_k \mathbf{u_k} \mathbf{v_k}^\mathsf{T}$$

SVD Diagram



SVD as sum of rank one matrices (assuming $r = p$)

SVD Rank-Reduction Theorem

SVD alternative formula:

$$\mathbf{X} = \sum_{k=1}^{r} l_k \mathbf{u_k} \mathbf{v_k}^\mathsf{T}$$

- This expresses the SVD as a sum of r rank-1 matrices.
- This result is formalized in what is known as the **SVD theorem** described by Carl Eckart and Gale Young in 1936, and it is often referred to as the *Eckart-Young theorem*.
- This theorem applies to practically any arbitrary rectangular matrix.

SVD Rank-Reduction Theorem

What if you take $m < r$ terms?

$$\hat{\mathbf{X}} = \sum_{k=1}^{m} l_k \mathbf{u_k} \mathbf{v_k}^\top$$

How would $\hat{\mathbf{X}}$ compare to $\mathbf{X}$?

SVD Rank-Reduction Theorem

The SVD theorem of Eckart and Young is related to the important problem of approximating a matrix.

The basic result says that if $\mathbf{X}$ is an $n \times p$ rectangular matrix, then the best r-dimensional approximation $\hat{\mathbf{X}}$ to $\mathbf{X}$ is obtained by minimizing:

$$min \quad \|\mathbf{X} - \hat{\mathbf{X}}\|^2$$

SVD Rank-Reduction Theorem

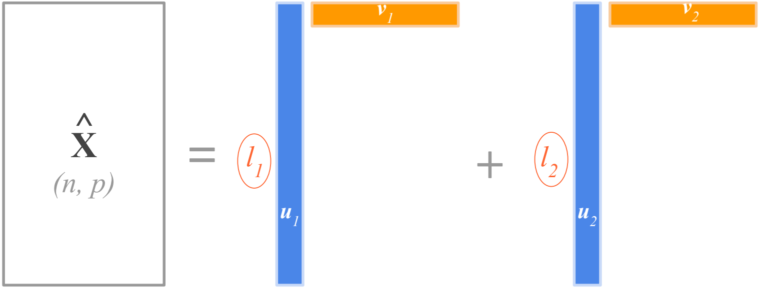
The minimization problem:

$$min \quad \|\mathbf{X} - \hat{\mathbf{X}}\|^2$$

is a special type of approximation: a least squares approximation.

The solution is obtained by taking the first m elements of matrices $\mathbf{U}, \mathbf{D}, \mathbf{V}$ so that $\hat{\mathbf{X}} = \mathbf{U_m D_m V_m^\mathsf{T}}$

SVD rank-two approximation



SVD as sum of two rank one matrices

SVD Rank-Reduction Theorem

The best 2-rank approximation $\hat{\mathbf{X}}$ of $\mathbf{X}$ is given by:

$$\hat{\mathbf{X}} = l_1 \mathbf{u_1} \mathbf{v_1}^\mathsf{T} + l_2 \mathbf{u_2} \mathbf{v_2}^\mathsf{T}$$

We can say that the "information" contained in $n \times p$ values is compressed into $n \times 2$ values.

Bibliography

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