Singular Value Decomposition (SVD)

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

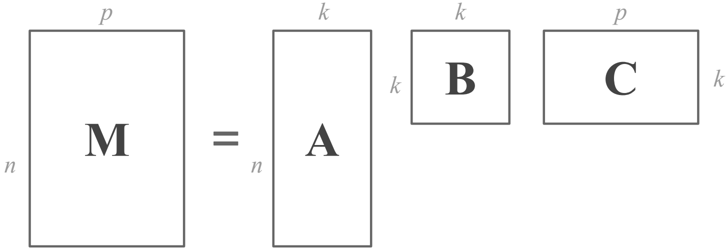
A matrix decomposition can be described by an equation:

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

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

SVD and EVD

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

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

SVD

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

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

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

where

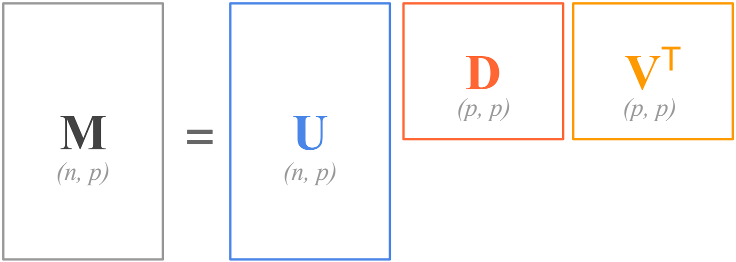
- $\mathbf{U}$ is a $n \times p$ column *orthonormal* matrix containing the **left singular vectors**
- $\mathbf{D}$ is a $p \times p$ **diagonal** matrix containing the **singular values** of $\mathbf{M}$
- $\mathbf{V}$ is a $p \times p$ column **orthonormal** matrix containing the **right singular vectors**

SVD

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

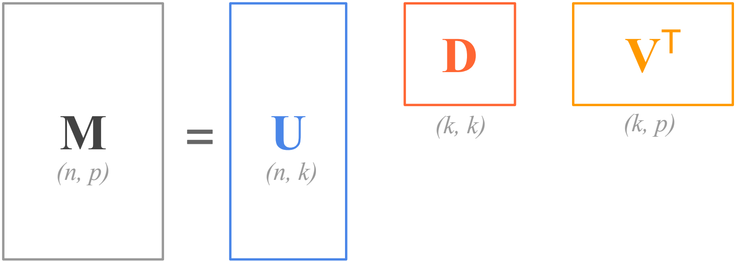
$$\mathbf{M} = \begin{bmatrix} u_{11} & \cdots & u_{1p} \\ u_{21} & \cdots & u_{2p} \\ \vdots & \ddots & \vdots \\ u_{n1} & \cdots & u_{np} \end{bmatrix} \begin{bmatrix} l_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & l_p \end{bmatrix} \begin{bmatrix} v_{11} & \cdots & v_{p1} \\ \vdots & \ddots & \vdots \\ v_{1p} & \cdots & v_{pp} \end{bmatrix}$$

SVD Diagram



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

SVD Diagram



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

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.

SVD

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

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

- $\mathbf{V}$ 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)

```r
# 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
```

```r
# 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)

```
# 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:

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

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 $\mathbf{X}^\mathsf{T}\mathbf{X}$.

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

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

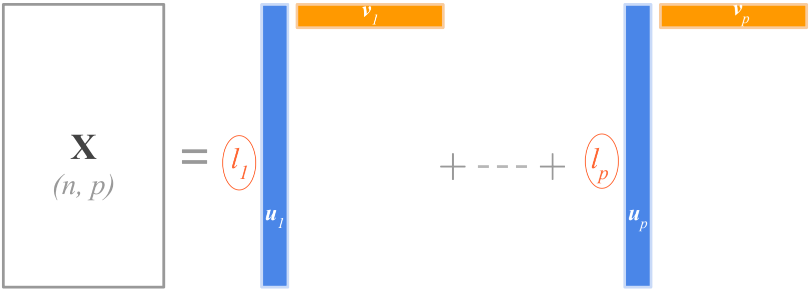
which shows that the matrix $\mathbf{X}$ of rank p is a linear combination of r matrices of rank 1.

SVD Rank-Reduction Theorem

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

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

SVD Diagram



SVD as sum of rank one matrices

SVD Rank-Reduction Theorem

SVD alternative formula:

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

- This expresses the SVD as a sum of p 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 practily any arbitrary rectangular matrix.

SVD Rank-Reduction Theorem

What if you take $r < p$ terms?

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

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

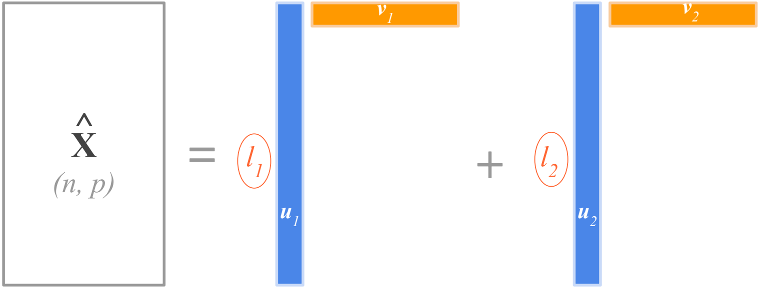
The minimization problem:

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

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

The solution is obtained by taking the first r elements of matrices $\mathbf{U}, \mathbf{D}, \mathbf{V}$ so that $\hat{\mathbf{X}} = \mathbf{U_r}\mathbf{D_r}\mathbf{V_r}^\mathsf{T}$

SVD rank-two approximation



SVD as sum of two rank one matrices

SVD Rank-Reduction Theorem

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

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

The "information" contained in $n \times p$ values is compressed into $n \times 2$ values.