Linear algebra: SVD

Statistical Natural Language Processing 1

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Quick recap

So far we reviewed:

- Vectors, matrices
- Operations on vectors and matrices: scalar multiplication, addition, dot product, matrix multiplication
- Matrices as operators (linear functions / transformations)
- Linearity and linear combinations
- Solving systems of linear equations, elimination
- Finding matrix inverse
- Linear regression
- Eigenvalues and eigenvectors

Today's plan

- Singular value decomposition
- Pseudo inverse

Orthogonal matrices

A short detour

- An orthogonal matrix is a square matrix whose columns (and rows) are othonormal (orthogonal unit) vectors
- Some interesting properties:
  - The product of two orthogonal matrices is another orthogonal matrix
  - Orthogonal matrices are invertible
  - Product of an orthogonal matrix with its transpose is the identity matrix

$$Q^T Q = QQ^T = I$$
$$\Rightarrow Q^T = Q^{-1}$$

  - Orthogonal matrices represent length-preserving transformations (rotations and reflections)
  - Determinants of an orthogonal matrix is 1 or -1

Singular Value Decomposition

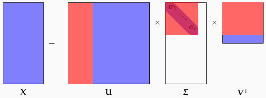
- Singular value decomposition (SVD) of an $n \times m$ matrix $\mathbf{X}$ is

$$\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$$

U is a $n \times n$ orthogonal matrix
Σ is a $n \times m$ diagonal matrix of singular values
V^T is a $m \times m$ orthogonal matrix.

- Singular vectors (columns) in $\mathbf{U}$ are the eigenvectors of $\mathbf{X}\mathbf{X}^T$
- Singular vectors (rows) in $\mathbf{V}^T$ are the eigenvectors of $\mathbf{X}^T\mathbf{X}$

Singular Value Decomposition



- Since $n - r$ rows and $m - r$ rows of $\boldsymbol{\Sigma}$ is 0, the decomposition does need the full matrices

Singular value decomposition and $X^T X$

- Assume $\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$

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

- Columns of $\mathbf{V}$ are eigenvectors of $\mathbf{X}^T\mathbf{X}$
- Values in the diagonal matrix $\boldsymbol{\Sigma}^2$ are the eigenvalues of $\mathbf{X}^T\mathbf{X}$

Singular value decomposition and XX^T

- Assume $\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$

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

- Columns of $\mathbf{U}$ are eigenvectors of $\mathbf{X}\mathbf{X}^T$
- Values in the diagonal matrix $\boldsymbol{\Sigma}^2$ are the eigenvalues of $\mathbf{X}\mathbf{X}^T$
- $\mathbf{X}^T\mathbf{X}$ and $\mathbf{X}\mathbf{X}^T$ share the eigenvalues

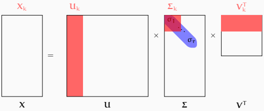
Computing SVD

- Find the eigenvalues and eigenvectors of $\mathbf{X}^T\mathbf{X}$
  - $\mathbf{X}^T\mathbf{X}$ is symmetric (semi) definite, the eigenvectors can be chosen to be orthogonal unit vectors, the eigenvalues are positive
  - $\mathbf{V}$ is the collection of the eigenvectors (of $\mathbf{X}^T\mathbf{X}$)
  - $\sigma_i = \sqrt{\lambda_i}$
- Knowing $\mathbf{V}$ and $\boldsymbol{\Sigma}$,

$$\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$$
$$\mathbf{X}\mathbf{V} = \mathbf{U}\boldsymbol{\Sigma}$$
$$\mathbf{X}\mathbf{V}\boldsymbol{\Sigma}^{-1} = \mathbf{U}$$

- In practice there are more efficient ways to compute SVD

Low rank estimation of a matrix



$\mathbf{X}_k = \mathbf{U}_k\boldsymbol{\Sigma}_k\mathbf{V}_k^T$ is the best rank k estimation of matrix $\mathbf{X}$

SVD: properties and applications

- Singular values are related to matrix norms
- SVD has a wide range of applications from image compression to document indexing to semantics of the words
- It is also a method for dimensionality reduction for visualizations
- A large number of statistical methods also rely on SVD (e.g., PCA, we will discuss later)
- The *condition number* of a matrix, an indication of numerical stability, depends on singular values
- SVD can be computed with good numerical accuracy, as a result it is also used for computing other quantities (e.g., matrix inverse)

Left and right inverses

- For a non-square matrix, or a square matrix with rank lower than n, the inverse is not defined
- From linear regression, we know that $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ acts as a *left inverse*
- Similarly we can define *right inverse* as $\mathbf{X}^T(\mathbf{X}\mathbf{X}^T)^{-1}$
- Remember, however, the existence of $(\mathbf{X}^T\mathbf{X})^{-1}$ requires columns of $\mathbf{X}$ to be independent
- A more general solution falls out of SVD

Computing pseudo inverse

- We want matrix multiplication to get as close to $\mathbf{I}$ as possible. Consider the 3×4 diagonal matrix:

$$\begin{bmatrix} 1/a & 0 & 0 \\ 0 & 1/b & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

- For an $n \times n$ diagonal matrix $\mathbf{\Sigma}$, $\mathbf{\Sigma}^{+} = \mathbf{\Sigma}^{-1}$
- For any invertible $n \times n$ matrix $\mathbf{X}$, $\mathbf{X}^{+} = \mathbf{X}^{-1}$
- In general, if we use singular value decomposition $\mathbf{X}^{+} = \mathbf{V}\mathbf{\Sigma}^{+}\mathbf{U}^{T}$

Summary / next

- We reviewed SVD and pseudo inverse
- SVD is a very important method. We will return to it multiple times during the course

Next:

- A very short introduction to calculus

the SVD song

Further reading

Any of the linear algebra references provided earlier.