Matrix methods – Singular value decomposition

MATH 2740 – Mathematics of Data Science – Lecture 09

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Fall 202X

The University of Manitoba campuses are located on original lands of Anishinaabeg, Ininew, Anisininew, Dakota and Dene peoples, and on the National Homeland of the Red River Métis. We respect the Treaties that were made on these territories, we acknowledge the harms and mistakes of the past, and we dedicate ourselves to move forward in partnership with Indigenous communities in a spirit of Reconciliation and collaboration.

Outline

Computing the SVD

Applications of the SVD – Least squares

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Computing the SVD (case of $\neq$ eigenvalues)

To compute the SVD, we use the following result

Theorem 7

Let $A \in \mathcal{M}_n$ symmetric, $(\lambda_1, \boldsymbol{u}_1)$ and $(\lambda_2, \boldsymbol{u}_2)$ be eigenpairs, $\lambda_1 \neq \lambda_2$. Then $\boldsymbol{u}_1 \bullet \boldsymbol{u}_2 = 0$

Proof of Theorem 7

$A \in \mathcal{M}_n$ symmetric, $(\lambda_1, \boldsymbol{u}_1)$ and $(\lambda_2, \boldsymbol{u}_2)$ eigenpairs with $\lambda_1 \neq \lambda_2$

$$\begin{aligned}
\lambda_1(\boldsymbol{v}_1 \bullet \boldsymbol{v}_2) &= (\lambda_1 \boldsymbol{v}_1) \bullet \boldsymbol{v}_2 \\
&= A\boldsymbol{v}_1 \bullet \boldsymbol{v}_2 \\
&= (A\boldsymbol{v}_1)^T \boldsymbol{v}_2 \\
&= \boldsymbol{v}_1^T A^T \boldsymbol{v}_2 \\
&= \boldsymbol{v}_1^T (A\boldsymbol{v}_2) \qquad [A \text{ symmetric so } A^T = A] \\
&= \boldsymbol{v}_1^T (\lambda_2 \boldsymbol{v}_2) \\
&= \lambda_2(\boldsymbol{v}_1^T \boldsymbol{v}_2) \\
&= \lambda_2(\boldsymbol{v}_1 \bullet \boldsymbol{v}_2)
\end{aligned}$$

So $(\lambda_1 - \lambda_2)(\boldsymbol{v}_1 \bullet \boldsymbol{v}_2) = 0$. But $\lambda_1 \neq \lambda_2$, so $\boldsymbol{v}_1 \bullet \boldsymbol{v}_2 = 0$ $\square$

Computing the SVD (case of $\neq$ eigenvalues)

If all eigenvalues of A^TA (or AA^T) are distinct, we can use Theorem 7

1. Compute $A^TA \in \mathcal{M}_n$
2. Compute eigenvalues $\lambda_1, \ldots, \lambda_n$ of A^TA; order them as $\lambda_1 > \cdots > \lambda_n \geq 0$ ($>$ not $\geq$ since $\neq$)
3. Compute singular values $\sigma_1 = \sqrt{\lambda_1}, \ldots, \sigma_n = \sqrt{\lambda_n}$
4. Diagonal matrix D in Σ is either in $\mathcal{M}_n$ (if $\sigma_n > 0$) or in $\mathcal{M}_{n-1}$ (if $\sigma_n = 0$)

5. Since eigenvalues are distinct, Theorem 7 $\implies$ eigenvectors are orthogonal set. Compute these eigenvectors in the same order as the eigenvalues
6. Normalise them and use them to make the matrix V, i.e., $V = [\boldsymbol{v}_1 \cdots \boldsymbol{v}_n]$
7. To find the $\boldsymbol{u}_i$, compute, for $i = 1, \ldots, r$,

$$\boldsymbol{u}_i = \frac{1}{\sigma_i} A \boldsymbol{v}_i$$

and ensure that $\|\boldsymbol{u}_i\| = 1$

Computing the SVD (case where some eigenvalues are $=$)

1. Compute $A^T A \in \mathcal{M}_n$
2. Compute eigenvalues $\lambda_1, \ldots, \lambda_n$ of $A^T A$; order them as $\lambda_1 \geq \cdots \geq \lambda_n \geq 0$
3. Compute singular values $\sigma_1 = \sqrt{\lambda_1}, \ldots, \sigma_n = \sqrt{\lambda_n}$, with $r \leq n$ the index of the last positive singular value
4. For eigenvalues that are distinct, proceed as before
5. For eigenvalues with multiplicity > 1, we need to ensure that the resulting eigenvectors are LI *and* orthogonal

Dealing with eigenvalues with multiplicity > 1

When an eigenvalue has (algebraic) multiplicity > 1, e.g., characteristic polynomial contains a factor like $(\lambda - 2)^2$, things can become a little bit more complicated

The proper way to deal with this involves the so-called Jordan Normal Form (another matrix decomposition)

In short: not all square matrices are diagonalisable, but all square matrices admit a JNF

Sometimes, we can find several LI eigenvectors associated to the same eigenvalue. Check this. If not, need to use the following

Definition 8 (Generalised eigenvectors)

The vector $\boldsymbol{x} \neq \mathbf{0}$ is a **generalized eigenvector** of rank m of $A \in \mathcal{M}_n$ corresponding to eigenvalue λ if

$$(A - \lambda\mathbb{I})^m \boldsymbol{x} = \mathbf{0}$$

but

$$(A - \lambda\mathbb{I})^{m-1} \boldsymbol{x} \neq \mathbf{0}$$

Procedure for generalised eigenvectors

$A \in \mathcal{M}_n$ and assume λ eigenvalue with algebraic multiplicity k

Find $\boldsymbol{v}_1$, "classic" eigenvector, i.e., $\boldsymbol{v}_1 \neq \mathbf{0}$ s.t. $(A - \lambda\mathbb{I})\boldsymbol{v}_1 = \mathbf{0}$

Find generalised eigenvector $\boldsymbol{v}_2$ of rank 2 by solving for $\boldsymbol{v}_2 \neq \mathbf{0}$,

$$(A - \lambda\mathbb{I})\boldsymbol{v}_2 = \boldsymbol{v}_1$$

...

Find generalised eigenvector $\boldsymbol{v}_k$ of rank k by solving for $\boldsymbol{v}_k \neq \mathbf{0}$,

$$(A - \lambda\mathbb{I})\boldsymbol{v}_k = \boldsymbol{v}_{k-1}$$

Then $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$ LI

Back to the normal procedure

With the LI eigenvectors $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ corresponding to λ

Apply Gram-Schmidt to get orthogonal set

For all eigenvalues with multiplicity > 1, check that you either have LI eigenvectors or do what we just did

When you are done, be back on your merry way to step 6 in the case where eigenvalues are all $\neq$

I am caricaturing a little here: there can be cases that do not work exactly like this, but this is general enough..

Computing the SVD

Applications of the SVD – Least squares

Least squares revisited

Theorem 9

Let $A \in \mathcal{M}_{mn}$, $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{b} \in \mathbb{R}^m$. The least squares problem $A\boldsymbol{x} = \boldsymbol{b}$ has a unique least squares solution $\tilde{\boldsymbol{x}}$ of minimal length (closest to the origin) given by

$$\tilde{\boldsymbol{x}} = A^+ \boldsymbol{b}$$

where A^+ is the pseudoinverse of A

Definition 10 (Pseudoinverse)

$A = U\Sigma V^T$ an SVD for $A \in \mathcal{M}_{mn}$, where

$$\Sigma = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix}, \text{ with } D = \mathrm{diag}(\sigma_1, \ldots, \sigma_r)$$

(D contains the nonzero singular values of A ordered as usual)

The **pseudoinverse** (or **Moore-Penrose inverse**) of A is $A^+ \in \mathcal{M}_{nm}$ given by

$$A^+ = V\Sigma^+ U^T$$

with

$$\Sigma^+ = \begin{pmatrix} D^{-1} & 0 \\ 0 & 0 \end{pmatrix} \in \mathcal{M}_{nm}$$