Recitation 11

October 17, 2024

1 Recap

1.1 The SVD

For an $m \times n$ matrix A of rank r, the SVD of A is the decomposition:

$$
\begin{aligned}
A &= \underbrace{\begin{pmatrix} u_1 & \cdots & u_r \end{pmatrix}}_{m\times r\ \hat{U}} \underbrace{\begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{pmatrix}}_{r\times r\ \hat{\Sigma}} \underbrace{\begin{pmatrix} v_1 & \cdots & v_r \end{pmatrix}^T}_{(n\times r)^T\ \hat{V}^T} \\
&= \underbrace{\begin{pmatrix} u_1 & \cdots & u_m \end{pmatrix}}_{m\times m\ U} \underbrace{\begin{pmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_r & 0 & \cdots \\ & & 0 & 0 & \cdots \\ & & \vdots & \vdots & \ddots \end{pmatrix}}_{m\times n\ \Sigma} \underbrace{\begin{pmatrix} v_1 & \cdots & v_n \end{pmatrix}^T}_{n\times n\ V^T} \\
&= \sigma_1 u_1 v_1^T + \sigma_r u_r v_r^T + \cdots + \sigma_r u_r v_r^T
\end{aligned}
$$

where $\hat{U}\hat{\Sigma}\hat{V}^T$ is the "compact" SVD and $U\Sigma V^T$ is the "full" SVD; the two versions encapsulate nearly the same information in different formats. Here,

- **Singular values**: $\sigma_1, \sigma_2, \cdots, \sigma_r > 0$, the positive scaling factors on the diagonal of Σ, usually sorted in a non-increasing order $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$.
- **Left singular vectors**: $u_1, \ldots, u_r$, which form an orthonormal basis for $C(A)$. The remaining $m - r$ vectors $u_{r+1}, \ldots, u_m$ in U (in the full SVD) form a basis for $C(A)^\perp = N(A^T)$, so that U is an orthogonal matrix.
- **Right singular vectors**: $v_1, \ldots, v_r$, which form an orthonormal basis for $C(A^T)$. The remaining $n - r$ vectors $v_{r+1}, \ldots, v_n$ in V (in the full SVD) form a basis for $C(A^T)^\perp = N(A)$, so that V is an orthogonal matrix.

We can't (yet) prove why this factorization exists or explain how to compute it, but we will focus for now on how to *use* the SVD. It is one of most powerful tools of applied linear algebra.

1.2 Induced Norm

The **induced L2 norm** of a matrix, denoted $\|A\|$ (or $\|A\|_2$), is defined as:

$$\|A\| = \max_{x \neq 0} \frac{\|Ax\|}{\|x\|} = \sigma_{\max}(A) \quad (\text{or } 0 \text{ if } A = 0),$$

where $\sigma_{\max}(A)$ is the largest singular value of A. This norm is commonly used in linear algebra, for instance, in the Eckart–Young theorem for low-rank approximations, which states that the truncated SVD of rank k is the closest rank-k matrix to A in both the induced norm and the Frobenius norm.

1.3 Condition Number

The **condition number** $\kappa(A)$ of an invertible square matrix A is defined as:

$$\kappa(A) = \|A\| \cdot \|A^{-1}\| = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)},$$

where $\sigma_{\min}(A)$ is the smallest singular value of A.

As we discussed in class, the condition number is crucial for analyzing the **sensitivity to perturbations**. When solving $Ax = b$, a small perturbation Δb in the right-hand side results in a perturbation $\Delta x = A^{-1}\Delta b$ in the solution, with the relative error bounded by:

$$\frac{\|\Delta x\|/\|x\|}{\|\Delta b\|/\|b\|} \leq \kappa(A).$$

For an **ill-conditioned** matrix ($\kappa(A) \gg 1$), which is nearly singular, a small error in b can lead to a large error in x. In such cases, regularization may be necessary to obtain a stable and meaningful solution.

In contrast, if A is an orthogonal matrix Q (or any scalar multiple αQ), the condition number is $\kappa(A) = \kappa(\alpha Q) = \kappa(Q) = 1$. This is the smallest possible condition number, as such matrices are as "far from singular" as possible.

2 Exercises

1. Show, using the SVD, that $A^T A$ is invertible if A has full column rank. Additionally, prove that $C(A^T) = C(A^T A)$ always holds.

   Note: this result was previously proven in recitation 7 using another approach.

2. If A is a 1-column matrix, whose column is the vector $a \in \mathbb{R}^n$, write the induced norm $\|A\|$ in terms of a.

3. Show that the induced norm satisfies the inequality $\|AB\| \leq \|A\| \cdot \|B\|$ for any matrices A and B of compatible sizes. (Hint: Use the definition of the induced norm in terms of $\max_{x\neq 0}$, not the SVD.)

   Based on this result and the previous exercise, what does this imply for $\|Ay\|$ where y is a vector?

4. From the previous result, how does $\kappa(AB)$ compare to $\kappa(A)\cdot\kappa(B)$ for square matrices A and B?

5. Suppose that instead of an error in b, we make an error ΔA in A, i.e. we solve $(A + \Delta A)(x + \Delta x) = b$ instead of $Ax = b$.

   (a) Assuming that the errors are small so that we can neglect the second-order term $\Delta A \Delta x$, find an approximate formula for Δx in terms of A (or A^{-1}), x, ΔA, and/or b.

   (b) Using the approximate Δx from the previous part, show that $\frac{\|\Delta x\|/\|x\|}{\|\Delta A\|/\|A\|} \leq \kappa(A)$. where $\|A\|$ is the induced norm. That is, the same condition-number bound applies to error in b or errors in A!

6. (a) Show that $\kappa(A^T A) = \kappa(A)^2$.

   (b) Explain why this holds even for non-square $m \times n$ matrices, if we generalize the condition number as $\kappa(A) = \|A\| \cdot \|A^+\| = \sigma_{\max}/\sigma_{\min}$ in that case.

Solutions

1. Let $A = \hat{U}\hat{\Sigma}\hat{V}^T$ be the compact SVD of A, where $\hat{U}$ is an $m \times r$ orthogonal matrix, $\hat{V}$ is an $n \times r$ orthogonal matrix, and $\hat{\Sigma}$ is a diagonal $r \times r$ matrix with singular values of A on the diagonal. Then,

$$A^T A = (\hat{U}\hat{\Sigma}\hat{V}^T)^T(\hat{U}\hat{\Sigma}\hat{V}^T) = \hat{V}\hat{\Sigma}^T\hat{U}^T\hat{U}\hat{\Sigma}\hat{V}^T.$$

Since $\hat{U}$ has orthonormal columns, we have $\hat{U}^T\hat{U} = I_r$, and thus:

$$A^T A = \hat{V}(\hat{\Sigma}^T\hat{\Sigma})\hat{V}^T.$$

Here, $\hat{\Sigma}^T\hat{\Sigma}$ is a diagonal matrix where each diagonal element is σ_i^2, with σ_i being the singular values of A. This gives us:

$$\Sigma^T\Sigma = \underbrace{\begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_r^2 \end{pmatrix}}_{r\times r}.$$

Therefore, $\hat{V}(\hat{\Sigma}^T\hat{\Sigma})\hat{V}^T$ is the compact SVD of $A^T A$. This implies the following:

(a) The ranks of A and $A^T A$ are the same, and the singular values of $A^T A$ are the squares of the singular values of A.

(b) $A^T A$ is invertible if and only if A has full column rank, i.e., $r = n$, so that the $n \times n$ matrix $A^T A$ also has rank n.

(c) The column space of $A^T A$, $C(A^T A)$, is spanned by the columns of $\hat{V}$. Similarly, since $A^T = \hat{V}\hat{\Sigma}^T\hat{U}^T$, we have $C(A^T)$ also spanned by the columns of $\hat{V}$. Therefore, $C(A^T A) = C(A^T)$.

2. Let A be a 1-column matrix with column a. The induced norm of A is given by:

$$\|A\| = \max_{x\neq 0} \frac{\|Ax\|}{\|x\|}$$

Since x is a 1-component vector $x = (\chi)$ with a single scalar component χ, this reduces to scalar operations: $Ax = a\chi$ and $\|x\| = |\chi|$, so that the x terms cancel out:

$$\|A\| = \max_{\chi\neq 0} \frac{\|a\| \cdot |\chi|}{|\chi|} = \|a\|.$$

Alternatively, we can use the compact SVD of A, which has rank 1. The SVD is

$$A = \underbrace{\frac{a}{\|a\|}}_{n\times 1} \underbrace{\left(\|a\|\right)}_{1\times 1} \underbrace{\left(1\right)}_{1\times 1},$$

Thus, $\|a\|$ is the largest (and the only) singular value for A, so $\|A\| = \|a\|$.

3. By the definition of the induced norm:

$$\|AB\| = \max_{x\neq 0} \frac{\|ABx\|}{\|x\|} = \max_{x\neq 0} \frac{\|A(Bx)\|}{\|x\|} = \max_{x\neq 0} \left(\frac{\|A(Bx)\|}{\|Bx\|}\right)\left(\frac{\|Bx\|}{\|x\|}\right).$$

   Since the maximum of a product is bounded by the product of the maxima, we have:

$$\|AB\| \leq \max_{y\neq 0} \frac{\|Ay\|}{\|y\|} \cdot \max_{x\neq 0} \frac{\|Bx\|}{\|x\|} = \|A\| \cdot \|B\|,$$

   where $y = Bx$. Thus, $\|AB\| \leq \|A\| \cdot \|B\|$.

   Additionally, for any vector y, this implies that $\|Ay\| \leq \|A\| \cdot \|y\|$, treating y as a 1-column matrix (as in problem 2).

4. We showed that $\|AB\| \leq \|A\| \cdot \|B\|$. Since $(AB)^{-1} = B^{-1}A^{-1}$, it follows that:

$$\|(AB)^{-1}\| \leq \|B^{-1}\| \cdot \|A^{-1}\|.$$

   Therefore,

$$\begin{aligned} \kappa(AB) &= \|AB\| \cdot \|(AB)^{-1}\| \\ &\leq (\|A\| \cdot \|B\|) \cdot (\|B^{-1}\| \cdot \|A^{-1}\|) \\ &= \kappa(A) \cdot \kappa(B). \end{aligned}$$

   Thus, $\kappa(AB) \leq \kappa(A) \cdot \kappa(B)$.

5. (a) Starting from $(A + \Delta A)(x + \Delta x) = b$ and neglecting the second-order term $\Delta A \Delta x$, we have:

$$\begin{aligned} b &= (A + \Delta A)(x + \Delta x) \\ &= \cancelto{b}{Ax} + \Delta A x + A\Delta x + \cancelto{\approx 0}{\Delta A \Delta x} \\ &\approx b + A\Delta x + \Delta A x. \end{aligned}$$

   After canceling $Ax = b$, we get:

$$A\Delta x \approx -\Delta A x.$$

   Thus, the approximate formula for Δx is:

$$\Delta x \approx -A^{-1}\Delta A x,$$

   which approaches zero proportionally to ΔA.

   (b) The relative error in x can be approximated using part (a):

$$\frac{\|\Delta x\|}{\|x\|} \approx \frac{\|A^{-1}(\Delta A)x\|}{\|x\|}.$$

   Using the inequality from problem (3):

$$\frac{\|A^{-1}(\Delta A)x\|}{\|x\|} \leq \|A^{-1}\Delta A\| \leq \|A^{-1}\| \cdot \|\Delta A\|.$$

Therefore, we get:

$$
\begin{aligned}
\frac{\|\Delta x\|/\|x\|}{\|\Delta A\|/\|A\|} &\approx \frac{\|A^{-1}(\Delta A)x\|}{\|x\|} \cdot \frac{\|A\|}{\|\Delta A\|} \\
&\leq (\|A^{-1}\| \cdot \cancel{\|\Delta A\|}) \frac{\|A\|}{\cancel{\|\Delta A\|}} \\
&= \|A^{-1}\| \cdot \|A\| = \kappa(A).
\end{aligned}
$$

Remark: The condition number $\kappa(A)$ is related to error growth for any type of error, including errors in b, A as we have shown. A similar analysis can be applied to roundoff errors (with the help of some numerical-analysis knowledge, beyond 18.C06, of "backwards stable" algorithms).

6. (a) From problem (1), we know that the singular values of $A^T A$ are the squares of the singular values of A. Therefore, the condition number of $A^T A$ is:

$$
\kappa(A^T A) = \frac{\sigma_{\max}(A^T A)}{\sigma_{\min}(A^T A)} = \left(\frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}\right)^2 = \kappa(A)^2.
$$

(b) Nothing changes in the generalized case, since it is still true that the singular values of $A^T A$ are the squares of the singular values of A, and the pseudo-inverse inverts these singular values (exactly as the inverse does in the invertible case).

Remark: Because of this, numerical linear algebra (beyond the scope of 18.C06) typically does *not* solve least-squares problems by solving the normal equations $A^T A\hat{x} = A^T b$, since that squares the sensitivity to errors (e.g., roundoff errors). Instead, one prefers other algorithms based on QR factorization or the SVD.