Mathematical Toolkit **Fall 2024**

Lecture 7: October 21, 2024

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1 Singular Value Decomposition for matrices

Using the previous discussion, we can write matrices in convenient form. Let $A \in \mathbb{C}^{m\times n}$, which can be thought of as an operator from $\mathbb{C}^n$ to $\mathbb{C}^m$. Let $\sigma_1, \ldots, \sigma_r$ be the non-zero singular values and let $v_1, \ldots, v_r$ and $w_1, \ldots, w_r$ be the right and left singular vectors respectively. Note that $V = \mathbb{C}^n$ and $W = \mathbb{C}^m$ and $v \in V, w \in W$, we can write the operator $|w\rangle \langle v|$ as the matrix wv^*, where v^* denotes $\overline{v^T}$. This is because for any $u \in V$, $wv^*u = w(v^*u) = \langle v, u\rangle \cdot w$. Thus, we can write

$$A \;=\; \sum_{i=1}^{r} \sigma_i \cdot w_i v_i^* \,.$$

Let $W \in \mathbb{C}^{m\times r}$ be a matrix with $w_1, \ldots, w_r$ as columns, such that i^{th} column equals w_i. Similarly, let $V \in \mathbb{C}^{n\times r}$ be a matrix with $v_1, \ldots, v_r$ as the columns. Let $\Sigma \in \mathbb{C}^{r\times r}$ be a diagonal matrix with $\Sigma_{ii} = \sigma_i$. Then, check that the above expression for A can also be written as

$$A = W\Sigma V^*$$

$$= \begin{pmatrix} \Big| & & \Big| \\ w_1 & \cdots & w_r \\ \Big| & & \Big| \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{pmatrix} \begin{pmatrix} \text{---} \; v_1^* \; \text{---} \\ \vdots \\ \text{---} \; v_r^* \; \text{---} \end{pmatrix}$$

where $V^* = \overline{V^T}$ as before.

We can also complete the bases $\{v_1, \ldots, v_r\}$ and $\{w_1, \ldots, w_r\}$ to bases for $\mathbb{C}^n$ and $\mathbb{C}^m$ respectively and write the above in terms of unitary matrices.

Definition 1.1 *A matrix $U \in \mathbb{C}^{n \times n}$ is known as a* unitary matrix *if the columns of U form an orthonormal basis for $\mathbb{C}^n$.*

Proposition 1.2 *Let $U \in \mathbb{C}^{n \times n}$ be a unitary matrix. Then $UU^* = U^*U = \mathrm{id}$, where* id *denotes the identity matrix.*

Let $\{v_1, \dots, v_n\}$ be a completion of $\{v_1, \dots, v_r\}$ to an orthonormal basis of $\mathbb{C}^n$, and let $V_n \in \mathbb{C}^{n \times n}$ be a unitary matrix with $\{v_1, \dots, v_n\}$ as columns. Similarly, let $W_m \in \mathbb{C}^{m \times m}$ be a unitary matrix with a completion of $\{w_1, \dots, w_r\}$ as columns. Let $\Sigma' \in \mathbb{C}^{m \times n}$ be a matrix with $\Sigma'_{ii} = \sigma_i$ if $i \le r$, and all other entries equal to zero. Then, we can also write

$$
\begin{aligned}
A &= W_m \Sigma' V_n^* \\
&= \begin{pmatrix} w_1 & \cdots & w_r & w_{r+1} & \cdots & w_m \end{pmatrix}
\begin{pmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_r & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix}
\begin{pmatrix} v_1^* \\ \vdots \\ v_r^* \\ v_{r+1}^* \\ \vdots \\ v_n^* \end{pmatrix}
\end{aligned}
$$

2 Low-rank approximation for matrices

Given a matrix $A \in \mathbb{C}^{m \times n}$, we want to find a matrix B of rank at most k which "approximates" A. For now we will consider the notion of approximation in spectral norm i.e., we want to minimize $\|A - B\|_2$, where

$$\|(A - B)\|_2 \;=\; \max_{v \neq 0} \frac{\|(A - B)v\|_2}{\|v\|_2} \,.$$

Here, $\|v\|_2 = \sqrt{\langle v, v \rangle}$ denotes the norm defined by the standard inner product on $\mathbb{C}^n$. The 2 in the notation $\|\cdot\|_2$ comes from the expression we get by expressing v in the orthonormal basis of the coordinate vectors. If $v = (c_1, \dots, c_n)^T$, then $\|v\|_2 = \left(\sum_{i=1}^n |c_i|^2\right)^{1/2}$ which is simply the Euclidean norm we are familiar with [1]. Note that while the norm here seems

[1] In general, one can consider the norm $\|v\|_p := \left(\sum_{i=1}^n |c_i|^p\right)^{1/p}$ for any $p \ge 1$. While these are indeed valid notions of distance satisfying a triangle inequality for any $p \ge 1$, they do not arise as a square root of an inner product when $p \neq 2$.

to be defined in terms of the coefficients, which indeed depend on the choice of the orthonormal basis, the value of the norm is in fact $\sqrt{\langle v, v\rangle}$ *which is just a function of the vector itself and not of the basis we are working with*. The basis and the coefficients merely provide a convenient way of computing the norm.

SVD also gives the optimal solution for another notion of approximation: minimizing the Frobenius norm $\|A - B\|_F$, which equals $(\sum_{ij}(A_{ij} - B_{ij})^2)^{1/2}$. We will see this later. Let $A = \sum_{i=1}^{r} w_i v_i^*$ be the singular value decomposition of A and let $\sigma_1 \geq \cdots \geq \sigma_r > 0$. If $k \geq r$, we can simply use $B = A$ since $\text{rank}(A) = r$. If $k < r$, we claim that $A_k = \sum_{i=1}^{k} \sigma_i w_i v_i^*$ is the optimal solution.

Proposition 2.1 $\|A - A_k\|_2 \;=\; \sigma_{k+1}$.

Proof: Complete $v_1, \ldots, v_k$ to an orthonormal basis $v_1, \ldots, v_n$ for $\mathbb{C}^n$. Given any $v \in \mathbb{C}^n$, we can uniquely express it as $\sum_{i=1}^{n} c_i \cdot v_i$ for appropriate coefficients $c_1, \ldots, c_n$. Thus, we have

$$(A - A_k)v \;=\; \left(\sum_{j=k+1}^{r} \sigma_j \cdot w_j v_j^*\right)\left(\sum_{i=1}^{n} c_i \cdot v_i\right) \;=\; \sum_{j=k+1}^{r}\sum_{i=1}^{n} c_i \sigma_j \cdot \langle v_j, v_i\rangle \cdot w_j \;=\; \sum_{j=k+1}^{r} c_j \sigma_j \cdot w_j\,,$$

where the last equality uses the orthonormality of $\{v_1, \ldots, v_n\}$. We can also complete $w_1, \ldots, w_r$ to an orthonormal basis $w_1, \ldots, w_m$ for $\mathbb{C}^m$. Since $(A - A_k)$ is already expressed in this basis above, we get that

$$\|(A - A_k)v\|_2^2 \;=\; \left\|\sum_{j=k+1}^{r} c_j \sigma_j \cdot w_j\right\|_2^2 \;=\; \left\langle \sum_{j=k+1}^{r} c_j \sigma_j \cdot w_j, \sum_{j=k+1}^{r} c_j \sigma_j \cdot w_j \right\rangle \;=\; \sum_{j=k+1}^{r} \left|c_j\right|^2 \cdot \sigma_j^2\,.$$

Finally, as in the computation with Rayleigh quotients, we have that for any $v \neq 0$ expressed as $v = \sum_{i=1}^{n} c_i \cdot v_i$,

$$\frac{\|(A - A_k)v\|_2^2}{\|v\|_2^2} \;=\; \frac{\sum_{j=k+1}^{r} \left|c_j\right|^2 \cdot \sigma_j^2}{\sum_{i=1}^{n} \left|c_i\right|^2} \;\leq\; \frac{\sum_{j=k+1}^{r} \left|c_j\right|^2 \cdot \sigma_{k+1}^2}{\sum_{i=1}^{n} \left|c_i\right|^2} \;\leq\; \sigma_{k+1}^2\,.$$

This gives that $\|A - A_k\|_2 \leq \sigma_{k+1}$. Check that it is in fact equal to σ_{k+1} (why?) ■

In fact the proof above actually shows the following:

Exercise 2.2 *Let $M \in \mathbb{C}^{m \times n}$ be any matrix with singular values $\sigma_1 \geq \cdots \sigma_r > 0$. Then, $\|M\|_2 = \sigma_1$ i.e., the spectral norm of a matrix is actually equal to its largest singular value.*

Thus, we know that the error of the best approximation B is at most σ_{k+1}. To show the lower bound, we need the following fact.

Exercise 2.3 *Let V be a finite-dimensional vector space and let S_1, S_2 be subspaces of V. Then, $S_1 \cap S_2$ is also a subspace and satisfies*

$$\dim(S_1 \cap S_2) \;\geq\; \dim(S_1) + \dim(S_2) - \dim(V)\,.$$

We can now show the following.

Proposition 2.4 *Let $B \in \mathbb{C}^{m \times n}$ have $\operatorname{rank}(B) \leq k$ and let $k < r$. Then $\|A - B\|_2 \geq \sigma_{k+1}$.*

Proof: By rank-nullity theorem $\dim(\ker(B)) \geq n - k$. Thus, by the fact above

$$\dim\left(\ker(B) \cap \operatorname{Span}\left(v_1, \ldots, v_{k+1}\right)\right) \;\geq\; (n-k) + (k+1) - n \;\geq\; 1\,.$$

Thus, there exists a $z \in \ker(B) \cap \operatorname{Span}\left(v_1, \ldots, v_{k+1}\right) \setminus \{0\}$. Then,

$$\begin{aligned} \|(A-B)z\|_2^2 \;=\; \|Az\|_2^2 \;=\; \langle z, A^*Az \rangle \;&=\; \mathcal{R}_{A^*A}(z) \cdot \|z\|_2^2 \\ &\geq\; \left(\min_{y \in \operatorname{Span}(v_1, \ldots, v_{k+1}) \setminus \{0\}} \mathcal{R}_{A^*A}(y) \right) \cdot \|z\|_2^2 \\ &\geq\; \sigma_{k+1}^2 \cdot \|z\|_2^2\,. \end{aligned}$$

Thus, there exists a $z \neq 0$ such that $\|(A-B)z\|_2 \geq \sigma_{k+1} \cdot \|z\|_2$, which implies $\|A - B\|_2 \geq \sigma_{k+1}$. ■