Advanced Algorithms

Lecture 18: Low Rank Approximation

Lecturer: Nathan Klein

1 Singular Value Decomposition

Remember that that *rank* of a matrix $A \in \mathbb{R}^{m \times n}$ is equal to to any of the following equivalent things:

1. The number of linearly independent rows of A.
2. The number of linearly independent columns of A.
3. The number of non-zero eigenvalues of A if $m = n$, or the number of non-zero singular values of A if $m \neq n$.

If a matrix is rank ℓ, then it can be written as a sum of ℓ rank 1 matrices. For any rank 1 matrix $A \in \mathbb{R}^{m \times n}$, we can write $A = uv^T$ for $u \in \mathbb{R}^m, v \in \mathbb{R}^n$.

Notice that eigenvalues are only defined for matrices $A \in \mathbb{R}^{n \times n}$. If $A \in \mathbb{R}^{m \times n}$ for $m \neq n$, then Ax cannot possibly equal λx because $Ax \in \mathbb{R}^m$ and $x \in \mathbb{R}^n$. For matrices with $m \neq n$, the analog of an eigenvalue is a *singular value*.

Before we talk more about singular values, recall the spectral theorem for symmetric matrices we introduced earlier in the course:

Theorem 1.1 (Spectral Theorem)**.** *Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Then, there are n eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ with corresponding orthonormal eigenvectors $v_1, \ldots, v_n$ so that*

$$A = \sum_{i=1}^{n} \lambda_i v_i v_i^T = V \Lambda V^T$$

where V has columns $v_1, \ldots, v_n$ (so $V^T V = I$) and Λ is the diagonal matrix with $\Lambda_{ii} = \lambda_i$.

A natural question is: what about for general matrices $A \in \mathbb{R}^{m \times n}$, or for matrices in $\mathbb{R}^{n \times n}$ which are not symmetric? It turns out all you need to do is turn A into a symmetric matrix using $A^T A$, and then apply the spectral theorem.

Theorem 1.2 (Singular Value Decomposition (SVD))**.** *Let $A \in \mathbb{R}^{m \times n}$. Then there are orthonormal vectors $u_1, \ldots, u_\ell$, orthonormal vectors $v_1, \ldots, v_\ell$, and singular values $\sigma_1 \geq \sigma_2 \geq \ldots, \geq \sigma_\ell$ such that:*

$$A = \sum_{i=1}^{\ell} \sigma_i u_i v_i^T = U \Sigma V^T$$

In addition, we have $\ell \leq \min\{m, n\}$ and $\sigma_i \in \mathbb{R}_{>0}$ for all i. (And here U is the matrix with columns $u_1, \ldots, u_\ell$ and V the matrix with columns $v_1, \ldots, v_\ell$.)

The u_i are called the left singular vectors and the v_i the right singular vectors. There are a few differences in this statement compared to the spectral theorem. The most important difference is that instead of $v_i v_i^T$, we have $u_i v_i^T$, i.e., these vectors can differ. Second, we typically list the singular values in decreasing order, whereas eigenvalues are in increasing order. Finally, singular values are all positive: we can negate u_i to flip the sign of the singular value, and then by convention we just delete the singular values of value 0.

To get a handle on why things are a bit different, consider the following matrix:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

This is a rank 1 matrix. But it's clear you can't write it in the form $\lambda v v^T$. So, we need to relax the criteria: we need to write it in the form $\lambda u v^T$, which is easy: just pick $u = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ and $v = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$.

Now that we have a handle on it, let's prove the SVD. The nice thing about the SVD is that it gives us an ordering of how important each rank 1 matrix is: the bigger the value σ_i, the higher the contribution.

Proof of SVD. $A^T A \in \mathbb{R}^{n \times n}$ is PSD since by definition it has a square root. Since it is symmetric, we can apply the spectral theorem, so there are non-negative eigenvalues $\lambda_1, \dots, \lambda_n$ and orthonormal $v_1, \dots, v_n$ such that $A^T A = \sum_{i=1}^n \lambda_i v_i v_i^T$. First, throw away all λ_i which are 0 so that $A^T A = \sum_{i=1}^{\ell} \lambda_i v_i v_i^T$ after re-indexing for some $\ell \leq \min\{n, m\}$ since the rank of the matrix is at most $\min\{m, n\}$. Let $v_1, \dots, v_\ell$ be the orthonormal set above. First, notice that

$$\|Av_i\|_2^2 = v_i^T A^T A v_i = v_i^T \lambda v_i = \lambda$$

since v_i is an eigenvector of $A^T A$. So, $\|Av_i\|_2 = \sqrt{\lambda}$. Now, define for all i:

$$u_i = \frac{Av_i}{\|Av_i\|_2} = \frac{Av_i}{\sqrt{\lambda_i}} = \frac{Av_i}{\sigma_i}$$

In other words, set $\sigma_i = \sqrt{\lambda_i}$. By definition, these vectors have norm 1. Furthermore, they are orthonormal, because when $i \neq j$ we have:

$$u_i^T u_j = \frac{(Av_i)^T}{\sigma_i} \frac{Av_j}{\sigma_j} = \frac{v_i^T A^T A v_j}{\sigma_i \sigma_j} = \frac{v_i^T \lambda_j v_j}{\sigma_i \sigma_j} = 0$$

where we used that the v_i are orthonormal. So, the only thing remaining to prove is that $A = \sum_{i=1}^{\ell} \sigma_i u_i v_i^T$. It suffices to prove that $Av_j = (\sum_{i=1}^{\ell} \sigma_i u_i v_i^T) v_j$ for all $1 \leq j \leq n$ for the basis $v_1, \dots, v_n$. This is enough, because then:

$$Ax = A(\sum_{j=1}^n v_j \langle x, v_j \rangle) = \sum_{j=1}^n Av_j \langle x, v_j \rangle = \sum_{j=1}^n \sum_{i=1}^{\ell} (\sigma_i u_i v_i^T) v_j \langle x, v_j \rangle = \sum_{i=1}^{\ell} \sigma_i u_i v_i^T \sum_{j=1}^n v_j \langle x, v_j \rangle$$

and this is $(\sum_{i=1}^{\ell}\sigma_i u_i v_i^T)x$. So, since they have the same product with every vector, they are the same matrix. So let's prove that $Av_j = (\sum_{i=1}^{\ell}\sigma_i u_i v_i^T)v_i$ for all $1 \le j \le n$ for the basis $v_1, \ldots, v_n$.

$$(\sum_{i=1}^{\ell}\sigma_i u_i v_i^T)v_j = \sum_{i=1}^{\ell}\sigma_i u_i\langle v_i, v_j\rangle = \sigma_j u_j v_j^T v_j = \sigma_j u_j = \sigma_j\frac{Av_j}{\sigma_j} = Av_j \qquad \square$$

2 Low Rank Approximation

A common task is to take a matrix $A \in \mathbb{R}^{m\times n}$ and find a new *low rank* matrix that approximates A. This has many applications:

1. The most tangible application is image compression. Given a matrix of pixels, we can use a low-rank approximation to compress the image.
2. In recommendation systems, we have a matrix encoding user ratings. For example, suppose each row is a user, and each column is a movie. The entry is 0 if the user has not rated the movie, and otherwise is some integer rating, perhaps 1 if they liked it and -1 otherwise. Now, we want to figure out what movies a particular user will like. It turns out a pretty good approach here is to find a low rank approximation of this matrix. For example, if everyone likes exactly the same movies (all movies are just good or bad), that's a rank 1 matrix since every row is the same. If that is the ground truth, then a rank 1 approximation is likely to figure this out.

Unsurprisingly, the best way to approximate a matrix A with a matrix of rank k is to use the top k singular values. There is even a theorem:

Theorem 2.1. *Let $A \in \mathbb{R}^{m\times n}$. Then, an optimal rank k approximation of A can be obtained by taking the top k singular values of A, i.e., $\tilde{A} = \sum_{i=1}^{k}\sigma_i u_i v_i^T$. Formally:*

$$\inf_{rank \tilde{A}=k}\|A-\tilde{A}\|_2 = \sigma_{k+1}$$

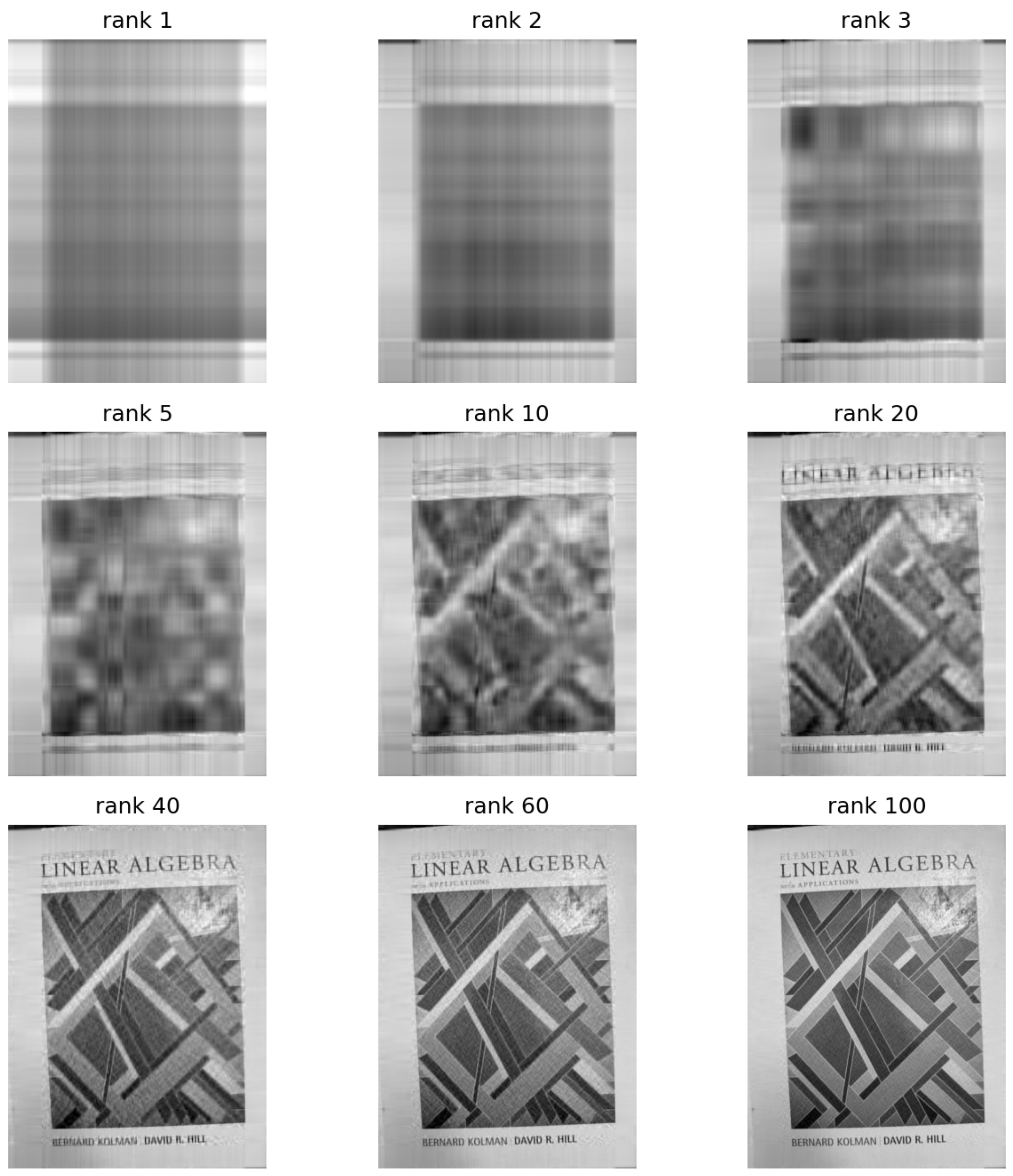
where recall $\|A\|_2$ for a matrix A is the spectral norm, or its largest singular value.

We will prove that $\|A-\tilde{A}\| \le \sigma_{k+1}$ by showing $\tilde{A} = \sum_{i=1}^{k}\sigma_i u_i v_i^T$ achieves this. We will leave the other direction as an exercise. Notice that:

$$A - \tilde{A} = \sum_{i=k+1}^{\ell}\sigma_i u_i v_i^T$$

So, $\|A-\tilde{A}\|_2 = \sigma_{max}\sum_{i=k+1}^{\ell}\sigma_i u_i v_i^T = \sigma_{k+1}$.

On your homework, you will visualize the effects of low rank approximation on images to produce something like the below. Naïvely, this is an image of about 1000×1000 pixels, which would require about half a megabyte if every pixel has 32 different possible values. To store a rank 60 version would require about a tenth of that.


rank 1
rank 2
rank 3
rank 5
rank 10
rank 20
rank 40
rank 60
rank 100