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## Numerical Analysis Hilary Term 2024

### Lecture 5: Singular Value Decomposition

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We now introduce the Singular Value Decomposition (SVD), an extremely important matrix decomposition applicable to any matrix, including nonsymmetric and rectangular ones.

**Theorem.** (SVD) Every matrix  $A \in \mathbb{R}^{m \times n}$  with  $m \geq n$  can be written as

$$A = U\Sigma V^T, \quad (1)$$

where  $U \in \mathbb{R}^{m \times n}$  and  $V \in \mathbb{R}^{n \times n}$  are matrices with orthonormal columns, i.e.,  $U^T U = I_n$  and  $V^T V = I_n = V V^T$  ( $V$  is square orthogonal; note that  $U U^T \neq I_m$ ), and

$$\Sigma = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{bmatrix} \quad (= \text{diag}(\sigma_1, \dots, \sigma_n))$$

is a diagonal matrix with nonnegative diagonal entries. In short, the SVD is a decomposition of  $A$  into a product of 'orthonormal-diagonal-orthogonal' matrices; when  $A$  is square  $m = n$ , 'orthogonal-diagonal-orthogonal'.

One can think of orthogonal matrices as a length-preserving rotation, so the SVD indicates that applying a matrix performs a rotation, followed by shrinkage or amplification of the elements, followed by another (different) rotation.

$\sigma_i$  are called the *singular values* and usually arranged in decreasing order  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$ . The columns of  $U, V$  are called the (left and right) *singular vectors* of  $A$ . The *rank* of a matrix  $A$  is the number of its positive singular values (this is equivalent e.g. to the number of linearly independent columns or rows).

**Proof.** Let's prove the existence of the SVD (1) by the following steps.

1. The matrix  $A^T A \in \mathbb{R}^{n \times n}$  is symmetric. This is straightforward to verify, either by direct calculations or from the general identity  $(XY)^T = Y^T X^T$ .
2. The eigenvalues of  $A^T A$  are all real and nonnegative (such matrices are called symmetric positive definite). To see this, suppose  $A^T A x = \lambda x$ ,  $x \neq 0$ . Then  $x^T A^T A x = \lambda x^T x$ , so  $\lambda = \frac{x^T A^T A x}{x^T x} = \frac{y^T y}{x^T x} \geq 0$ , where  $y = Ax$ .
3. Let  $A^T A = V D^2 V^T$  be the symmetric eigenvalue decomposition, with  $V \in \mathbb{R}^{n \times n}$  orthogonal and  $D$  diagonal. Then let  $B = AV$ . Now  $B^T B = D^2$  is a diagonal matrix, implying that the columns of  $B$  are pairwise orthogonal.
4. Let's write  $B^T B = D^2 = \text{diag}(\lambda_1, \dots, \lambda_\ell, 0, \dots, 0)$ , where  $\lambda_\ell > 0$ .
  - (a) It is possible that  $\ell = n$ , and this is an important case (happens iff  $\text{rank}(A) = n$ , more generally  $\ell$  is equal to  $\text{rank}(A)$ ) where there is no 0 diagonal entry in  $D^2$ . We then have  $D^{-1} = \text{diag}(1/\sqrt{\lambda_1}, \dots, 1/\sqrt{\lambda_\ell})$ . Take  $U := B D^{-1} = A V D^{-1}$ , which has orthonormal columns  $U^T U = I_n$ . We are then done, as taking  $\Sigma = D$ ,  $A = U \Sigma V^T$ .

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- (b) When  $\ell < n$  (the rank-deficient case),  $B$  has columns that are 0. Let  $D_\ell = \text{diag}(\lambda_1, \dots, \lambda_\ell)$ . We still have  $B \begin{bmatrix} D_\ell^{-1} & \\ & I_{n-\ell} \end{bmatrix} = [U_1, 0]$ , and so

$$A = [U_1, 0] \begin{bmatrix} D_r & \\ & I_{n-\ell} \end{bmatrix} V^T = [U_1, U_2] \begin{bmatrix} D_\ell & \\ & 0 \end{bmatrix} V^T$$

for any  $U_2$ ; we take it to be orthonormal  $U_2^T U_2 = I_{n-\ell}$  and  $U_2^T U_1 = 0$  ( $U_2$  is any orthonormal matrix in the orthogonal complement of  $U_1$ ; its existence can be verified e.g. using Householder reflectors). Taking  $U = [U_1, U_2]$  completes the proof, again with  $\Sigma = D$ .

□

Some comments:

- Analogous to the full QR factorisation, there is a 'full SVD'  $A = \tilde{U} \tilde{\Sigma} \tilde{V}^T$ , where  $\tilde{U} = [U \ U_\perp] \in \mathbb{R}^{m \times m}$  is orthogonal and  $\tilde{\Sigma} \in \mathbb{R}^{m \times n} = \begin{bmatrix} \Sigma & \\ 0_{(m-n) \times n} \end{bmatrix}$  and  $\tilde{V} = V$ . This can be obtained by starting from (1) and finding an orthogonal complement  $U_\perp$  of  $U$ .
- Fat matrices: the assumption  $m \geq n$  is just for convenience; if  $m < n$ , one still has  $A = U \Sigma V^T$  where  $\Sigma \in \mathbb{R}^{m \times m}$  is diagonal,  $U \in \mathbb{R}^{m \times m}$  is orthogonal, and  $V \in \mathbb{R}^{n \times m}$  has orthonormal columns. Below we continue with the assumption  $m \geq n$ .
- The SVD extends directly to matrices with nonreal entries:  $A = U \Sigma V^*$ , where  $U, V$  are unitary matrices and  $*$  denotes the conjugate transpose.

**Matrix spectral norm** Let us briefly introduce the *spectral norm*<sup>1</sup> for matrices  $A \in \mathbb{R}^{m \times n}$ :  $\|A\|_2 = \sigma_1(A)$ , i.e., the largest singular value. It is a nonnegative scalar that measures 'how large' the matrix is. It has the equivalent characterisation  $\|A\|_2 = \max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}$ , where the norms in the right-hand side are the standard Euclidean norm (length) for vectors  $\|x\|_2 = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$ .

**Low-rank approximation** The SVD is useful for theoretical purposes, as it identifies e.g. the range (column space), null space, rank, and many more. In applications, the primary reason SVD is so important is that it gives the optimal low-rank approximation.

Let  $A = U \Sigma V^T$  be the SVD and write  $U = [u_1, \dots, u_n]$ ,  $V = [v_1, \dots, v_n]$ . Let  $r$  be any integer  $r \leq n$ , and define the "tall-skinny matrices"  $U_r = [u_1, \dots, u_r]$ ,  $V_r = [v_1, \dots, v_r]$ , and  $\Sigma_r = \text{diag}(\sigma_1, \dots, \sigma_r)$ . Then set

$$A_r = U_r \Sigma_r V_r^T = \sum_{i=1}^r \sigma_i u_i v_i^T.$$

Note that  $\text{rank}(A_r) = r$ . Also note that  $A = \sum_{i=1}^n \sigma_i u_i v_i^T$ , which is another way of expressing the SVD.  $A_r$  is called the (rank- $r$ ) *truncated SVD* of  $A$ , as  $A_r$  is obtained by truncating the trailing components of the SVD of  $A$ .

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<sup>1</sup>Also known as the 2-norm or the operator norm. We return to the topic of norms later in the course.

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We are now ready to state the result.

**Theorem.** Let  $r \leq n$  be an integer. For any  $B \in \mathbb{C}^{m \times n}$  with  $\text{rank}(B) \leq r$ ,

$$\|A - A_r\|_2 = \sigma_{r+1} \leq \|A - B\|_2. \quad (2)$$

In other words, the truncated SVD  $A_r$  is the best rank- $r$  approximant to  $A$  in the spectral norm.

**Proof.** The first equality  $\|A - A_r\|_2 = \sigma_{r+1}$  can be seen by noting that  $A - A_r = \sum_{i=r+1}^n \sigma_i u_i v_i^T$  with singular values  $\sigma_{r+1}, \dots, \sigma_n$ , along with  $r$  0's. For the inequality:

1. Since  $\text{rank}(B) \leq r$ , we can write  $B = B_1 B_2^T$  where  $B_1, B_2$  have  $r$  columns. Therefore, there exists an orthonormal null space  $W \in \mathbb{C}^{n \times (n-r)}$  s.t.  $BW = 0$ .
2. Then  $\|A - B\|_2 \geq \|(A - B)W\|_2 = \|AW\|_2 = \|U\Sigma(V^T W)\|_2$ . Now since  $W$  is  $(n - r)$ -dimensional, there is an intersection between  $W$  and  $[v_1, \dots, v_{r+1}]$ , the  $(r + 1)$ -dimensional subspace spanned by the leading  $r + 1$  left singular vectors ( $[W, v_1, \dots, v_{r+1}] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 0$  has a nonzero solution; then  $Wx_1$  is such a vector).
3. Scale  $x_1$  to have unit norm, and by orthogonal invariance  $\|U\Sigma V^T Wx_1\|_2 = \|\Sigma V^T Wx_1\|_2 = \|\Sigma_{r+1} y_1\|_2$ , where  $\|y_1\|_2 = 1$  (b.c.  $Wx_1$  lies in  $\text{span}[v_1, \dots, v_{r+1}]$ ) and  $\Sigma_{r+1}$  is the leading  $r + 1$  part of  $\Sigma$ .
4. Then  $\|U\Sigma_{r+1} y_1\|_2 \geq \sigma_{r+1}$  can be verified by direct calculations.

□

In fact, more generally it is known that

$$\|A - A_r\| \leq \|A - B\| \quad (3)$$

for any so-called unitarily invariant norm  $\|\cdot\|$  (non-examinable).

In many applications  $\sigma_{r+1} \ll \sigma_1$  for some  $r \ll n$ , in which case  $A \approx U_r \Sigma_r V_r^T$ . Now, storing  $U_r, \Sigma_r, V_r$  requires  $\approx (m + n + 1)r$  memory, as opposed to  $mn$  for the full  $A$ , so when  $r \ll \min(m, n)$ , this can be used for data compression; this fact is used everywhere e.g. in data science!

**Illustration of low-rank approximation:** A traditional example to illustrate low-rank approximation via the truncated SVD is image compression. A grayscale image can be represented by a matrix  $A$ , with each entry representing the intensity of a pixel. One can then approximate  $A$  by a truncated SVD, and use that to get a compressed image that hopefully looks similar to the original image to human eyes. Images tend to have structure that lends  $A$  to be approximately low-rank.

Below we take an image of the Oxford logo, represent it as a matrix  $A \in \mathbb{R}^{589 \times 589}$  and compute its SVD (just `[U,S,V] = svd(A)` in MATLAB). Using the truncated SVD we then compute a rank- $r$  approximation for different values of  $r$ . With a rank-1 matrix the rows (and columns) are all parallel so the image is uninformative; but as  $r$  increases the image becomes clear, and with rank 50 the image is almost indistinguishable from the

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original, while still giving some data compression. For larger images, such savings can be significant. (This is however not how images are usually compressed in practice; e.g. the algorithm behind the jpg format is completely different).

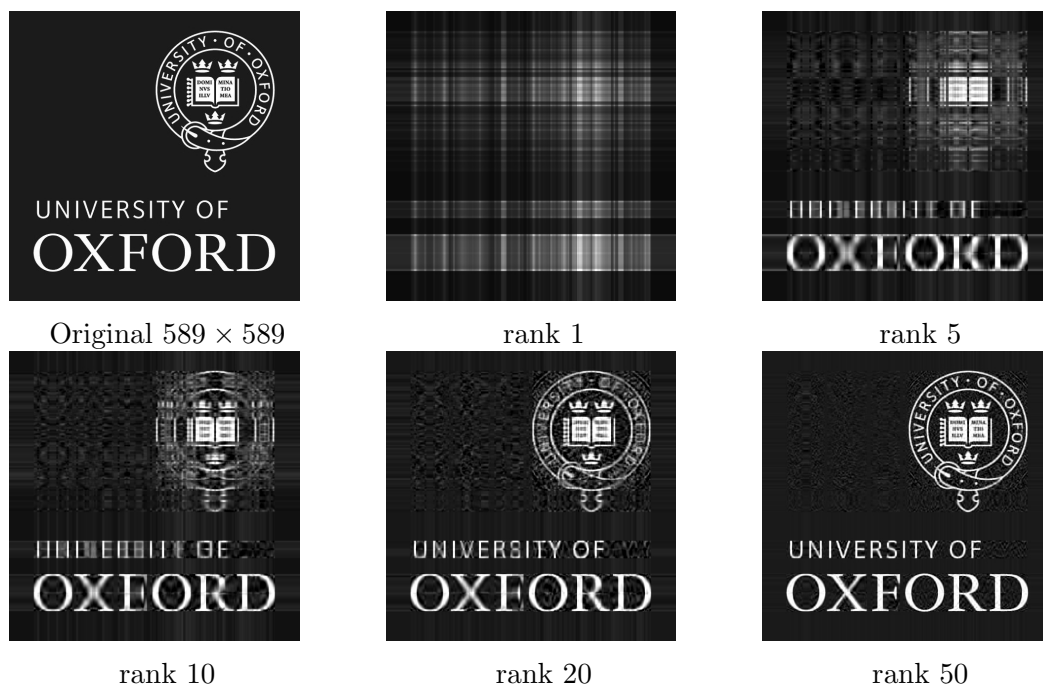


Figure 1: The Oxford logo and its low-rank approximations via the truncated SVD.

The SVD  $A = U\Sigma V^T$  and symmetric eigenvalue decomposition  $A = V\Lambda V^T$  have many properties and results in common (e.g. Courant-Fisher min-max theorem; nonexam-inable), stemming from the fact that they are both decompositions of the form “orthogonal-diagonal-orthogonal”. In fact the SVD proof given above suggests an algorithm for computing the SVD via a symmetric eigenvalue decomposition of  $A^T A$  (this is not exactly how the SVD is computed in practice, but that is outside the scope); we now turn to eigenvalue problems  $Ax = \lambda x$  and describe an algorithm for solving them.