Numerical Linear Algebra Homework Project 2: Least Squares, Orthogonalization, and the SVD

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Problem 3

(1) Let $A \in \mathbb{R}^{m \times n}$, with $\text{rank}(A) = n$. The singular value decomposition of A can be written as $A = U\Sigma V^T$ or, equivalently, as $A = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$, where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ represent the singular values of A, while $\{\mathbf{u}_i\}_{i=1,\ldots,n}$ and $\{\mathbf{v}_i\}_{i=1,\ldots,n}$ are, respectively, left and right singular vectors of A.

Express the singular values and singular vectors of the following matrices in terms of those of A.

(a) $(A^TA)^{-1}$

$$(A^TA)^{-1} = (V^T)^{-1}\Sigma^{-2}V^{-1} = V\Sigma^{-2}V^T$$

In order to obtain this expression we used that $U^TU = \mathbb{1}$ and that $V^{-1} = V^T$, since U and V are orthogonal. We can conclude that both left and right singular vectors of $(A^TA)^{-1}$ are equal to the right singular vectors of A, while singular values of the former matrix are equal to those of A raised to the -2 power. Note that, since singular values of A are in increasing order and in this expression they are raised to a negative power, they must appear in reverse order.

(b) $(A^TA)^{-1}A^T$

$$(A^TA)^{-1}A^T = V\Sigma^{-2}V^TV\Sigma U^T = V\Sigma^{-1}U^T$$

Analogously to the previous case, we know that $V^TV = \mathbb{1}$. Here we see that left singular vectors of $(A^TA)^{-1}A^T$ are equal to the right singular vectors of A, right singular vectors of $(A^TA)^{-1}A^T$ are equal to the left singular vectors of A, while singular values of this matrix are equal to the inverse of singular values of A.

(c) $A(A^TA)^{-1}$

$$A(A^TA)^{-1} = U\Sigma V^TV\Sigma^{-2}V^{-T} = U\Sigma^{-1}V^T$$

Note that this result can also be obtained from the previous case, by noting that $A(A^TA)^{-1} = ((A^TA)^{-1}A^T)^T$. We can see that left and right singular vectors of $(A^TA)^{-1}$ coincide with that of A, while singular values of this matrix are equal to the inverse of singular values of A.

(d) $A(A^TA)^{-1}A^T$

$$A(A^TA)^{-1}A^T = U\Sigma^{-1}V^TV\Sigma U^T = UU^T$$

In this case, both left and right singular vectors of $A(A^TA)^{-1}A^T$ are equal to left singular vectors of A, while singular values of this matrix are all equal to 1.

(2) Given the following matrix:

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 2 \end{bmatrix}, \tag{1}$$

its singular values can be computed by considering the square root of the eigenvalues of the matrix $A^T A$, which has the form:

$$A^T A = \begin{bmatrix} 1 & 2 \\ 2 & 8 \end{bmatrix}. \tag{2}$$

Hence, by imposing that $p(\lambda) = \det(A^T A - \lambda \mathbb{1}) = 0$, we find the two eigenvalues of $A^T A$ and, therefore, the two singular values of A, which are:

$$\sigma_{1,2} = \sqrt{\frac{9 \pm \sqrt{65}}{2}}. \tag{3}$$

Finally, knowing that the spectral condition number is defined as $k_2(A) = \frac{\sigma_{\max}}{\sigma_{\min}}$, we can find the condition number of A:

$$k_2(A) = \sqrt{\frac{9 + \sqrt{65}}{9 - \sqrt{65}}} \simeq 4.26. \tag{4}$$

We want now to see how the unit ball is modified by the transformation described by the matrix A. In other words, we want to see what is the image of a vector $\mathbf{x} = (\cos(\theta), \sin(\theta))$, parametrizing the unit ball on a plane, when considering the linear transformation $\mathbf{y} = A\mathbf{x}$. The vector $\mathbf{y}$ under the transformation A assumes the form:

$$\mathbf{y} = (\cos(\theta) + 2\sin(\theta), 2\sin(\theta)) \quad \theta \in [0, 2\pi).$$

Graphically, we have:

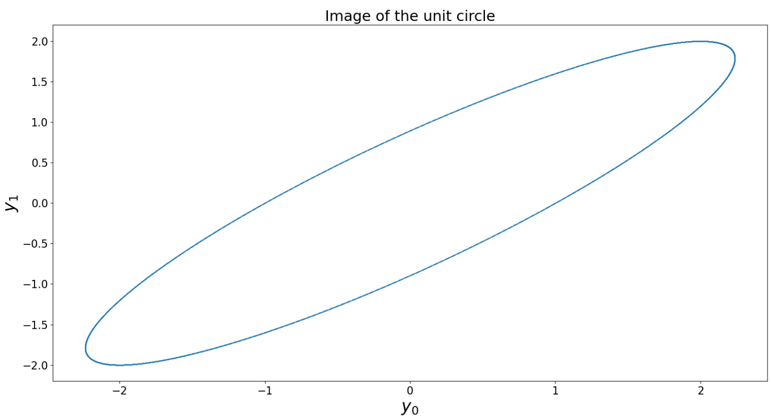


Figure 1: Image of the unit circle

(3) jvejkvbkdjf

(4) Given a matrix

$$A = \begin{bmatrix} -4 & -2 & -4 & -2 \\ 2 & -2 & 2 & 1 \\ -800 & 200 & -800 & -401 \end{bmatrix}. \tag{5}$$

we want to compute the the singular values of A, the Moore-Penrose pseudoinverse of A and its spectral condition number. We report in the following the Python script that we used to do it.

```python
import numpy as np

A = np.array([[-4.,-2.,-4.,-2.],[2.,-2.,2.,1.],[-800,200,-800,-401]])
U, singular_values, V_transpose = np.linalg.svd(A, compute_uv=True)
pseudoinverse = np.linalg.pinv(A)
spectral_cond_num = np.linalg.cond(A)
print(f'singular values of A = {singular_values}')
print(f'pseudoinverse of A = {pseudoinverse}')
print(f'spectral condition number of A = {spectral_cond_num}')
```

The results we obtained are reported below:

```
singular values of A = [1.21689895e+03 3.30829410e+00 4.21538860e-03]
pseudoinverse of A = [[-2.50833333e+01  5.00833333e+01  2.50000000e-01]
                      [-1.66666667e-01 -3.33333333e-01  7.57226996e-16]
                      [-2.50833333e+01  5.00833333e+01  2.50000000e-01]
                      [ 1.00000000e+02 -2.00000000e+02 -1.00000000e+00]]
spectral condition number of A = 288680.1350686104
```

Given the obtained results, we can say that $\text{rank}(A) = 3$.

(5) The best rank-k approximation of a matrix A, in the Frobenius norm, is obtained by computing the singular value decomposition of A and then by considering only the first k terms in that expression. In other words, given a matrix A written in terms of its singular value decomposition as $A = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$, its best rank-k approximation is given by $\tilde{A}_k = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$. Below is reported the Python code that we used to obtain the best rank-1 and rank-2 approximations of the matrix A mentioned in the previous point of this exercise.

```python
A_rank_1 = singular_values[0]*np.outer(U[:,0],V_transpose[0])
A_rank_2 = A_rank_1 + singular_values[1]*np.outer(U[:,1],V_transpose[1])
spectral_cond_num_A_rank_2 = singular_values[0]/singular_values[1]
print(f'A_rank_1 = {A_rank_1}')
print(f'A_rank_2 = {A_rank_2}')
print(f'Spectral condition number of A_rank_2 =
↪ {spectral_cond_num_A_rank_2}')
```

We obtained the following two matrices:

```
A_rank_1 = [[-3.67478811e+00  9.18652344e-01 -3.67478811e+00 -1.84198740e+00]
            [ 2.16152803e+00 -5.40355726e-01  2.16152803e+00  1.08346585e+00]
            [-8.00001057e+02  1.99990537e+02 -8.00001057e+02 -4.01000500e+02]]

A_rank_2 = [[  -3.99955481   -2.00000178   -3.99955481   -2.00177721]
            [   1.99910978   -1.99999645    1.99910978    1.00355377]
            [-800.00000445  200.00000002 -800.00000445 -400.99998223]]

Spectral condition number of A_rank_2 = 367.8327598758788
```

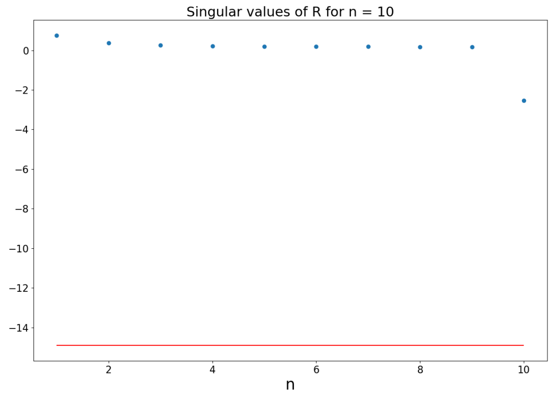
As we can see, the best rank-1 approximation of A returns a matrix that is already quite similar to the initial one, and the approximation improves when considering the best rank-2 approximation of A. This can be seen, in a more quantitative way, by considering the Frobenius norm of the difference between the approximated matrix and the initial matrix, both for the rank-1 and rank-2 approximation. By doing this, one obtains:

```
Frobenious norm between A and A_rank_1 = 3.308296788282531
Frobenious norm between A and A_rank_2 = 0.004215388599497665
```

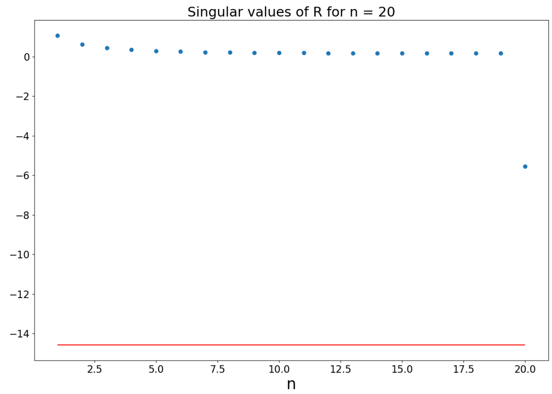
(6) Consider an upper triangular matrix matrix $R = (r_{ij})$, whose entries are given by $r_{ii} = 1$ and $r_{ij} = -1$ for $j > i$. We defined a function `R_matrix(n)` that allows us to compute this matrix for a given dimension n:

```
def R_matrix(n):
 R = np.triu(-np.ones((n,n)),k=1) + np.eye(n)
 return R
```

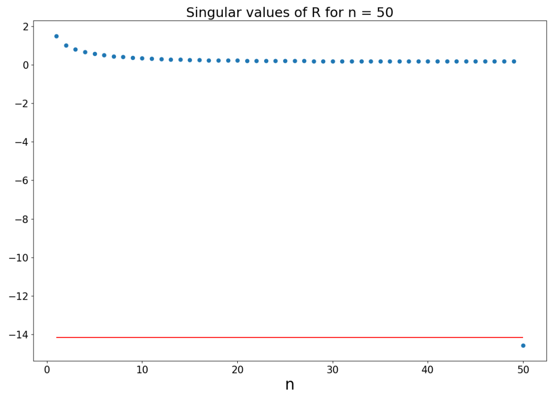
Note that we used an upper triangular mask to obtain the entries r_{ij}. Once derived R, we computed its singular values for $n = 10, 20, 50, 100$, as required. The plot of the singular values are reported below.



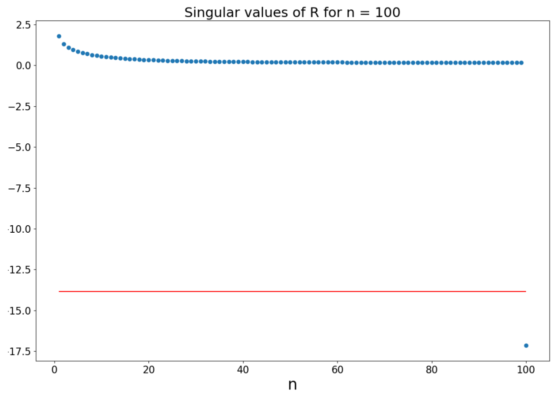
(a) n=10



(b) n=20



(c) n=50



(d) n=100

Figure 2: Singular values of the matrix R defined at the beginning of this exercise for $n = 10, 20, 50, 100$.

It can be observed that for $n = 50$ and for $n = 100$ the last singular value becomes smaller than the threshold value fixed by $u\sigma_1$, where u is the machine precision. This means that, when this happens, the matrix R becomes numerically singular.

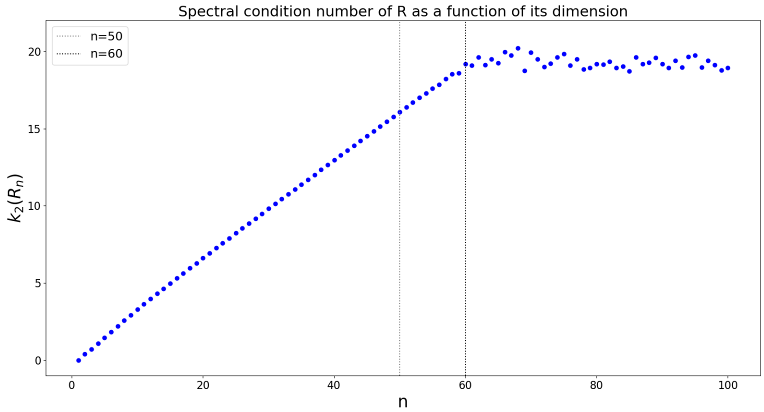


Figure 3: Spectral condition number of R as a function of its dimension.