Student ID mail Kevin Elezi s316685 kevin.elezi@studenti.polito.it Suyash Singh s307798 suyash.singh@studenti.polito.it 1. Homework Free Implementing the *Inverse Power* and *Deflation Methods* to determine the lowest M eigenvalues for a symmetric matrix. Importing the necessary libraries the only library that we used in this notebook is **numpy** import numpy as np In [3]: # To ignore the warnings import warnings warnings.filterwarnings('ignore') # Suppress warnings for cleaner output from google.colab import drive drive.mount('/content/drive') Mounted at /content/drive To test our program, we've made a symmetric and invertible matrix $A \in \mathbb{R}^{5x5}$ with $\lambda \neq 0$. This setup helps us check if our method for finding eigenvalues, specifically the smallest one, works as intended. Alongside, we've prepared an initial guess for both the **eigenvector** x_0 and **eigenvalue** λ_0 , which are crucial for starting the process of the Inverse Power Method, a technique used to find the **specific** eigenvalue we're interested in. This preparation ensures our method has a solid starting point for accurate and efficient computations. We added the diagonal dominance. More precisely, the matrix A is diagonally dominant if : $|a_{ii}| \geq \sum
olimits_{j
eq i} |a_{ij}| \quad orall i$ We know that the A strictly diagonally dominant matrix is **invertible**. In [4]: np.random.seed(min(316665,307798)) # Size of the matrix size = 5# Generate a random matrix matrix = np.random.rand(size, size) # Make the matrix symmetric matrix = (matrix + matrix.T) / 2 # Add diagonal dominance diagonal = np.diag(np.sum(np.abs(matrix), axis=1)) matrix = matrix + diagonal # Add positive definiteness eigenvalues, eigenvectors = np.linalg.eig(matrix) min_eigenvalue = np.min(eigenvalues) matrix = matrix + np.eye(size) * (abs(min_eigenvalue) + 1) 2. Shifted Inverse Power Method In the following cell, we have implemented the **Shifted** Inverse Power Method. This method ensures that given an α value of our choice, we are able to find the closest eigenvalue λ of A to α . Knowing that: $Ax = \lambda x$ $(A - \alpha I)x = (\lambda - \alpha)x$ $\frac{x}{\lambda - \alpha} = \frac{(A - \alpha I)^{-1}(\lambda - \alpha)x}{\lambda - \alpha}$ $(A - \alpha I)^{-1}x = \frac{1}{\lambda - \alpha}x$ If λ is an eigenvalue of A, x is the eigenvector corresponding the eigenvalue $(\lambda - \alpha)$ of the matrix $(A - \alpha I)$. We want to compute the closest eigenvalue to α making $(\lambda - \alpha)$ as small as possibile \Rightarrow Inverse Power Method. In this way we can find the eigenvalue λ (closest to α) since the truer the relationship $\lambda \sim \alpha$ is, the more the eigenvalue $\frac{1}{\lambda - \alpha}$ of the matrix $(A - \alpha I)^{-1}$ will become the largest in term of magnitude. # @title In [5]: from IPython.display import Image Image(filename='/content/drive/MyDrive/1_HMs_comptuational/HM3/porr.png', width=600) Out[5]: $1/\lambda - \alpha$ α The method takes as input: • matrix A• initial eigenvector x_0 • initial **eigenvalue** λ_0 , number of iterations MaxIter • tolerance auThe method returns the final and smallest eigenvalue $(\lambda - \alpha)$ and the corresponding eigenvector x. Knowing that : $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_i| \geq \alpha \geq |\lambda_{i+1}| \geq \ldots \geq |\lambda_{n-1}| \geq |\lambda_n|$ Where $\lambda = \; \left\{ egin{array}{ll} \lambda_i & ext{if} \quad (\lambda_i - lpha) < (\lambda_{i+1} - lpha) \ \lambda_{i+1} & ext{if} \quad (\lambda_i - lpha) > (\lambda_{i+1} - lpha) \end{array}
ight.$ Shifted Inverse Power Method: $v_0
eq 0, \quad v^{old} = rac{v_o}{||v_0||}, \quad \sigma = rac{1}{\lambda - lpha}$ 1. $v^{new}=(A-\alpha I)^{-1}v^{old} o ext{LU decompositzion}$ 2. $v^{new}=rac{v^{new}}{||v^{new}||}$ 3. $\lambda^{new}=rac{\lambda^TA\lambda}{\lambda^T\lambda} o ext{Rayleigh Quotient}$ 4. $\lambda^{old}=\lambda^{new}$ 5. $v^{old} = v^{new}$ 6. k + +7. $while~(k < MaxIter \wedge rac{|\lambda^{new} - \lambda^{old}|}{|\lambda^{new}|} > au)$ return λ The method works as follows: It begins by taking the size of the matrix. The eigenvalue and eigenvector variables are initialized to default values of 0.0 and None, respectively. The algorithm enters a loop that runs for a maximum of max iterations times. Inside the loop, it attempts to solve the linear system using matrix inversion. It calculates the inverse of the matrix by subtracting the target eigenvalue multiplied by the identity matrix. As suggested in lecture, we will use LU decomposition to find: $v^{new} = (A - \alpha I)^{-1} v^{old} \longrightarrow (A - \alpha I) v^{new} = v^{old}$ In this way we will decrease the computational effort required each time we want to calculate the new eigenvector v^{new} . If the matrix is singular and cannot be inverted, a LinAlgError is caught, and the method returns None value for both the eigenvalue and eigenvector. If the linear system is solvable, the algorithm computes the next eigenvector approximation. The next eigenvector is then normalized to ensure it has unit length using **np.linalg.norm**. To approximate the eigenvalue, the algorithm computes through the **Rayleigh Quotient** the eigenvalue λ^{new} . The algorithm checks for convergence by comparing the absolute difference between the new eigenvalue approximation and the previous eigenvalue with the specified tolerance au. If the difference is below the tolerance, the algorithm considers the iteration converged and breaks out of the loop. If convergence is not achieved, the eigenvalue and eigenvector are updated with the new values, and the algorithm proceeds to the next iteration. The initial eigenvector is updated with the next eigenvector for the next iteration. Finally, when the algorithm terminates (either due to convergence or reaching the maximum iterations), it returns the converged eigenvalue and eigenvector. def rayleigh_quotient(matrix, vector): numerator = np.dot(vector.T, np.dot(matrix, vector)) denominator = np.dot(vector.T, vector) return numerator / denominator In [7]: **import** numpy **as** np import matplotlib.pyplot as plt **from** scipy.linalg **import** lu_factor,lu_solve def inverse_power_method(matrix, initial_eigenvector , alpha, max_iterations=100, tolerance=1e-6): n = matrix.shape[0]eigenvalue = 0.0 # to initialize eigenvalue with a default value eigenvector = None lambda_values = [] # List to store the computed eigenvalues for iteration in range(max_iterations): # Solving the linear system using LU decomposition try: lu, piv = lu_factor(matrix - alpha * np.eye(n)) # Solve L * $y = v_old$ y = lu_solve((lu, piv), initial_eigenvector) # Solve U * x = ynext_vector = lu_solve((lu, piv), y) except np.linalg.LinAlgError: print("Matrix is singular. Inverse power method failed.") return None, None # Normalizing the next vector next_vector /= np.linalg.norm(next_vector) # Compute the eigenvalue approximation eigenvalue_next = rayleigh_quotient(matrix, next_vector) # Checking for convergence if np.abs(eigenvalue_next - eigenvalue) < tolerance:</pre> eigenvalue = eigenvalue_next eigenvector = next_vector break # Updating the eigenvalue and eigenvector eigenvalue = eigenvalue_next eigenvector = next_vector # Update the initial vector for the next iteration initial_eigenvector = next_vector # Store the computed eigenvalue lambda_values.append(eigenvalue) return eigenvalue, eigenvector In [8]: # Generate a random initial eigenvector initial_eigenvector = np.random.rand(size) # Normalize the initial eigenvector initial_eigenvector = initial_eigenvector / np.linalg.norm(initial_eigenvector) print('Initial eigenvector :', initial_eigenvector) Initial eigenvector : [0.60265916 0.65217018 0.01737863 0.43150893 0.1580317] In [9]: #using the inverse power method to find the smallest eigenvalue eigenvalue, eigenvector = inverse_power_method(matrix, initial_eigenvector, 4.2) print("Eigenvalue:", eigenvalue) Eigenvalue: 4.659995842026454 eigenvalues, eigenvectors = np.linalg.eigh(matrix) In [10]: print("Eigenvalues:", eigenvalues) Eigenvalues: [3.19361117 3.7137999 4.65999953 4.95290266 6.72487503] Therefore **np.linalg.eigh** function from NumPy to find all eigenvalues and their corresponding eigenvectors for a matrix, aiming to **verify the accuracy of our inverse power method**. After running this function, it prints out the eigenvalues, allowing us to compare these results with those obtained from our custom implementation to ensure they match up correctly. As you can see, the eigenvalue λ_{SIPM} coming from the Shifted Inverse Power Method is almost identical to the true (and nearest to α) eigenvalue λ of the A matrix : $|\lambda_{SIPM} - \lambda| pprox -3.687e^{-6}$ 3. Deflation Method Suppose we have found the largest eigenvalue of the matrix A with the power literation method, how do we find the second largest eigenvalue? One solution is, after finding the largest eigenvalue λ_1 , to make it into the smallest by deflation and then go on to find the new largest one, let say λ_2 . Deflation is a straightforward approach. Essentially, this is what we do: 1. First, we use the Power Method to find the largest eigenvalue and eigenvector of matrix A. 2. Multiply the largest eigenvector \mathbf{x}_1 by its transpose and then by the largest eigenvalue λ_1 . This produces the matrix $Z^* = \lambda_1 \mathbf{x}_1 \mathbf{x}_1^T$ 3. Compute a new matrix $A^* = A - Z^* = A - \lambda_1 \mathbf{x}_1 \mathbf{x}_1^T$. 4. Apply the Power Method to A^* to compute its largest eigenvalue λ_2 . This in turns should be the second largest eigenvalue of the initial matrix A. Consider: $\left(A - \lambda_1 \mathbf{x}_1 \mathbf{x}_1^T\right) \mathbf{x}_j = A \mathbf{x}_j - \lambda_1 \mathbf{x}_1 \mathbf{x}_1^T \mathbf{x}_j = \lambda_j \mathbf{x}_j - \lambda_1 \mathbf{x}_1 \left(\mathbf{x}_1^T \mathbf{x}_j\right)$ $\text{If } j = 1 \text{ then:} \qquad \left(A - \lambda_1 \mathbf{x}_1 \mathbf{x}_1^T\right) \mathbf{x}_j = \lambda_1 \mathbf{x}_1 - \lambda_1 \mathbf{x}_1 \left(\mathbf{x}_1^T \mathbf{x}_1\right) = 0 \mathbf{x}_1$ $\text{If } j \neq 1 \text{ then:} \qquad \left(A - \lambda_1 \mathbf{x}_1 \mathbf{x}_1^T\right) \mathbf{x}_j = \lambda_j \mathbf{x}_j - \lambda_1 \mathbf{x}_1 \left(0\right) = \lambda_j \mathbf{x}_j$ thus, $(A - \lambda_1 \mathbf{x}_1 \mathbf{x}_1^T) = A^*$ has the same eigenvectors as A and the same eigenvalues as A except that the largest one has been replaced by 0. Thus we can use the power method to find the next biggest one λ_2 and so on... Let's now see why this method works: The method of deflation proceeds by finding the largest eigenvalue by iteration, then reducing the $(n \times n)$ matrix to an $(n-1) \times (n-1)$ matrix, finding the largest eigenvalue of this matrix, reducing the matrix to an $(n-2) \times (n-2)$ matrix, and so on. Let A be an $n \times n$ matrix with largest eigenvalue λ_1 and associated eigenvector x_1 . If x_1 does not have 1 as the component of largest modulus, multiply x_1 by a **permutation matrix** P which interchanges the largest element and the first element. Suppose $Px_1=x_1^{'}$ We must find an elementary matrix R such that $Rx_{1}^{'}=e_{1}$, the elementary vector with first component 1 and all other components 0. Let: $B = RPAP^{-1}R^{-1} = RPAPR^{-1}$ Then: $Be_1=RPAPR^{-1}e_1=RPAPx_1^{'}=RPAx_1=\lambda_1RPx_1=\lambda_1e_1$ Thus e_1 is an eigenvector of B with eigenvalue λ_1 and B must be upper triangular with λ_1 as the first element on the leading diagonal. $B = \begin{bmatrix} \lambda_1 & & x_1 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & x_n \end{bmatrix}$ Delete the first column and row to give an $(n-1) \times (n-1)$ matrix B_1 . A, B are similar so have the same eigenvalues $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$. The eigenvalues $\lambda_2, \lambda_3, \dots, \lambda_n$ are eigenvalues of the $(n-1) \times (n-1)$ matrix B_1 . Let us now try to apply it: In [11]: def power_method(matrix, tolerance, max_iterations): # Step 1: Initialize a random vector n = matrix.shape[0] $x_k = np.random.rand(n)$ for _ in range(max_iterations): # Step 2: Compute $y = A * x_k$ $y = np.dot(matrix, x_k)$ # Step 3: Normalize the vector $x_k1 = y / np.linalg.norm(y)$ # Step 4: Check convergence if np.linalg.norm($x_k1 - x_k$) < tolerance: break $x_k = x_{1}$ # Compute the dominant eigenvalue eigenvalue = $np.dot(x_k, np.dot(matrix, x_k)) / np.dot(x_k, x_k)$ return eigenvalue, x_k In [12]: **import** numpy as np # Deflation method for updating the matrix to find subsequent eigenvalues def deflation(matrix, eigenvalue, eigenvector): # Create a copy of the input matrix to avoid modifying the original matrix_copy = np.copy(matrix) # Get the size of the matrix size = matrix_copy.shape[0] # Ensure the eigenvector is a numpy array for matrix operations eigenvector = np.array(eigenvector) # Compute the outer product of the eigenvector with itself Z = eigenvalue * np.outer(eigenvector, eigenvector.T) # Perform the deflation by subtracting the outer product scaled by the eigenvalue from the matrix matrix_copy -= Z # Remove the first row and column to reduce the matrix size for further eigenvalue computations matrix_copy = np.delete(matrix_copy, 0, axis=0) matrix_copy = np.delete(matrix_copy, 0, axis=1) return matrix_copy In [13]: def deflation_method(matrix, tolerance=1e-6, max_iterations=1000): eigenvalues = []matrices = [] $d_{count} = 0$ while True: eigvalue, eigvector = power_method(matrix, tolerance, max_iterations) eigenvalues.append(eigvalue) matrices.append(matrix) **if** matrix.shape[0] == 1: break matrix = deflation(matrix, eigvalue, eigvector) print('-----') **if** d_count **==** 0 : print(f'The largest eigenvalue for the original matrix is: {eigvalue}') print(f'The largest eigenvalue for the {d_count}-deflated matrix is: {eigvalue}') d_count += 1 print('-----') for i, mat in enumerate(matrices): plt.subplot(1, len(matrices), i+1) plt.imshow(mat) plt.title(f'matrix{i+1}') plt.axis('off') plt.show() return eigenvalues eigvalues = deflation_method(matrix, tolerance=1e-6, max_iterations=1000) The largest eigenvalue for the original matrix is: 6.724875034408807 ______ The largest eigenvalue for the 1-deflated matrix is: 4.941522582423315 ______ The largest eigenvalue for the 2-deflated matrix is: 4.533326869338119 The largest eigenvalue for the 3-deflated matrix is: 0.5666498122152445 matrix1 matrix2 matrix3 matrix4 matrix5 print("Eigenvalues of the original matrix:", eigenvalues) Eigenvalues of the original matrix: [3.19361117 3.7137999 4.65999953 4.95290266 6.72487503] We can use deflation to find subsequent eigenvector-eigenvalue pairs, but there is a point wherein rounding error reduces the accuracy below acceptable limits. As you can see from the fourth largest eigenvalue λ_4 there begins to be an error that cannot be underestimated at all : 0.566 vs 3.713. For this reason other methods, are preferred when one needs to compute many or all eigenvalues of a matrix. The peril is that deflation is numerically unstable, and repeated applications can lead to disaster. Using it to get λ_2 is usually fine except for ill-behaved eigen-problems, but it is **not** advisable to use it to find all the eigenvalues. Here is an another (and maybe more general) extreme example where there trouble can be find. Let $A = \lambda_1 extbf{v}_1 extbf{v}_1^T + \lambda_2 extbf{v}_2 extbf{v}_2^T$ where $\mathbf{v}_1^T\mathbf{v}_1=\mathbf{v}_2^T\mathbf{v}_2=1$. Then A has eigenvalues λ_1,λ_2 and eigenvectors $\mathbf{v}_1,\mathbf{v}_2$. Now suppose $\tilde{\lambda_1}\sim\lambda_1$ is computed. We then deflate $B = A - ilde{\lambda_1} extbf{v}_1 extbf{v}_1^T$ choosing $x = \mathbf{v}_1^T$ for simplicity (of the example). Then $B = (\lambda_1 - ilde{\lambda_1}) extbf{v}_1 extbf{v}_1^T + \lambda_2 extbf{v}_2 extbf{v}_2^T$ So B has an eigenvalue $\lambda_1 - \tilde{\lambda_1}.$ If say $\lambda_1 = 10^8, \quad \lambda_2 = 10^{-8}$ and $\tilde{\lambda_1}$ is computed to machine precision (relative error 10^{-16}) then $|\lambda_1 - ilde{\lambda_1}| \simeq 10^{-8}$ which is the same size as λ_2 . Thus the spurious 'leftover' from the deflation is actually the dominant part, and the power method cannot see λ_2 . References: 1. https://services.math.duke.edu/~jtwong/math361-2019/lectures/Lec10eigenvalues.pdf 2. https://astarmathsandphysics.com/university-maths-notes/matrices-and-linear-algebra/4554-the-deflation-method-for-finding-eigenvalues-and-eigenvectors.html