

Problem 1: Where do you belong, Krylov?

Solution

a

$$Aq^i = \frac{q^{i+1}}{\|q^{i+1}\|} + \sum_k^i \langle Aq^i, q^k \rangle q^k \in \mathcal{K}_{i+1}$$

b

We firstly note that $q^1 = \frac{b}{\|b\|}$, and so we can note that it is a scaled version of b . Take this to be the first element of a Krylov subspace $\mathcal{K}^1 = q^1$. Furthermore, note that the definition of q^2 (or more generally, q^{i+1}) is equivalent to multiplying Aq^i and subtracting the projection of the prior q 's. Critically, because the subspace is defined as the *span* of a set of vectors, the resulting set of orthonormal vectors define an equivalent Krylov subspace – they are, in fact, an orthonormal basis of this subspace.

So, we can say:

$$\mathcal{K}^i = \text{span}\left(\left\{\frac{b}{\|b\|}, Aq_1, \dots, Aq_{i-1}\right\}\right)$$

$$[Aq_1 \mid \dots \mid Aq_n] = [Qh_1 \mid \dots \mid Qh_n]$$

$$\implies Aq_1 = Qh_1$$

$$Aq_1 \in \mathcal{K}_2 \implies Qh_1 \in \mathcal{K}_2$$

$$Aq_1 = \begin{bmatrix} * \\ * \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, Aq_2 = \begin{bmatrix} * \\ * \\ * \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \dots Aq_n = \begin{bmatrix} * \\ * \\ * \\ * \\ \vdots \\ * \end{bmatrix}$$

c

See the code section at the end for the implementation. The result is:

Did arnoldi work:

True

Q:

```
[[0.58  0.31 -0.75]
 [-0.58 0.81 -0.11]
 [0.58  0.50 0.65]]
```

H:

```
[[0.33  3.09 0.00]
 [3.09  7.56 0.95]
 [0.00  0.95 -0.90]]
```

Wow its upper Hessenberg, whoda thunk it

Wow its lower Hessenberg, whoda thunk it

Wow it's tridiagonal, its cuz the matrix A is Hermitian (or Symmetric cuz its real)

Problem 2: Ask Gram, Schmidt, or Givens for QR

Solution

a

Taken from “Linear Algebra Done Right” by Sheldon Axler.

Suppose v_1, \dots, v_m is a lin. ind. list of vectors in V . Let $e_1 = \frac{v_1}{\|v_1\|}$. For $j = 2, \dots, m$, define e_j inductively by:

$$e_j = \frac{v_j - \langle v_j, e_1 \rangle e_1 - \dots - \langle v_j, e_{j-1} \rangle e_{j-1}}{\|v_j - \langle v_j, e_1 \rangle e_1 - \dots - \langle v_j, e_{j-1} \rangle e_{j-1}\|}$$

(i.e. the Gram-Schmidt process definition). Then, e_1, \dots, e_m is an orthonormal list of vectors in V s.t.:

$$\text{span}(v_1, \dots, v_j) = \text{span}(e_1, \dots, e_j) \forall j = 1, \dots, m$$

Note that for $j = 1$, $\text{span}(v_1) = \text{span}(e_1)$ because v_1 is a positive multiple of e_1 .

Suppose $1 < j < m$ and it has been verified that:

$$\text{span}(v_1, \dots, v_{j-1}) = \text{span}(e_1, \dots, e_{j-1})$$

Note that $v_j \notin \text{span}(v_1, \dots, v_{j-1})$ because v_1, \dots, v_m are linearly independent. Thus, $v_j \notin \text{span}(e_1, \dots, e_{j-1})$. As such, we are not dividing by zero in the definition of e_j . We can also see that $\|e_j\| = 1$ by its definition.

Let $k \in [1, j)$. Then:

$$\begin{aligned} \langle e_j, e_k \rangle &= \left\langle \frac{v_j - \langle v_j, e_1 \rangle e_1 - \dots - \langle v_j, e_{j-1} \rangle e_{j-1}}{v_j - \langle v_j, e_1 \rangle e_1 - \dots - \langle v_j, e_{j-1} \rangle e_{j-1}}, e_k \right\rangle \\ &= \frac{\langle v_j, e_k \rangle - \langle v_j, e_k \rangle}{v_j - \langle v_j, e_1 \rangle e_1 - \dots - \langle v_j, e_{j-1} \rangle e_{j-1}} \\ &= 0 \end{aligned}$$

Thus e_1, \dots, e_j is an orthonormal list.

From the definition of e_j , we see that $v_j \in \text{span}(e_1, \dots, e_j)$. Combined with the equivalency of the spans provided above, we know:

$$\text{span}(v_1, \dots, v_j) \subset \text{span}(e_1, \dots, e_j)$$

Both these lists are lin. ind., thus both subspaces have dimension j and are equal. \square

b

The inner loop requires:

$$(4m-1)(1-1) + (4m-1) + (2-1) + \dots + (4m-1)(n-1) = (4m-1)(0+1+\dots+n-1) = (4m-1)\left(\frac{1}{2}n(n+1)-1\right)$$

The outer portion requires $(4m-1) * n$ operations. Summing:

$$= (4m+1)\left(\frac{1}{2}n(n+1)-1\right) + (4m+1)(n) = (4m+1)\left(\frac{1}{2}n(n)-1+n\right)$$

Simplifying and discarding lower order terms we find:

$$= 2mn^2$$

Algorithm 1 Classical Gram-Schmidt, annotated with FLOP counts

```

for  $j = 1, \dots, n$  do
   $v \leftarrow a^j$ 
  for  $i = 1, \dots, j - 1$  do
     $R_{ij} \leftarrow \langle v, q^i \rangle$  { $m$  multiplications,  $(m - 1)$  additions  $\implies 2m - 1$ }
     $v \leftarrow v - R_{ij}q^i$  { $m$  multiplications,  $m$  subtractions  $\implies 2m$ }
  end for {Total cost is }
   $q^j \leftarrow \frac{v}{\|v\|}$  { $m$  multiplications,  $m - 1$  additions, 1 for sqrt  $\implies 2m$ }
   $R_{jj} \leftarrow \langle a^j, q^j \rangle$  { $m$  multiplications,  $(m - 1)$  additions  $\implies 2m - 1$ }
end for
 $Q = (q^1 | \dots | q^n)$ 

```

c

An upper Hessenberg matrix of size $n \times n$ will require $n - 1$ operations to zero out the non-zero elements below the diagonal, which will result in a QR decomposition. Givens matrices take the form:

$$G_n = \begin{bmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & c & \cdots & -s & \cdots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & s & \cdots & c & \cdots & \vdots \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix}$$

The location of the c and s terms correspond to zeroing element i and j ; that is, to zero element $A_{i,j}$, we set $s = G_{ji} = -G_{ij}$ and $G_{k,k} = c$ for $k = i, j$ (and 1 for $k \neq i, j$). The resulting algorithm is as follows:

Algorithm 2 QR Factorization of an Upper Hessenberg Matrix using Givens rotations

```

Input:  $A^1 \in \mathbb{R}^{n \times n}$ ,  $A_{ij} = 0 \forall i > j + 1$  {This could be a parfor}
for  $j = 1, \dots, n - 1$  do
   $i \leftarrow j + 1$ 
   $r^j \leftarrow \sqrt{[A_{jj}^j]^2 + [A_{ij}^j]^2}$ 
   $c \leftarrow A_{jj}^j / r$ 
   $s \leftarrow -A_{ij}^j / r$ 
   $G_{ji}^j \leftarrow s$ 
   $G_{ij}^j \leftarrow -s$ 
   $G_{ii}^j \leftarrow c$ 
   $G_{jj}^j \leftarrow c$ 
   $A^{j+1} \leftarrow G^j A^j$ 
end for
 $Q = \Pi_{j=1}^{n-1} G^j$ 
 $R = A^{n-1}$ 

```

Code

Problem 1

```

1  #!/usr/bin/env python3
2  import numpy as np
3
4  float_formatter = "{:.2f}".format
5
6  np.set_printoptions(formatter={"float_kind": float_formatter})
7
8
9  def is_upper_hessenberg(A: np.ndarray) -> bool:
10     return np.isclose(np.tril(A, k=-2), 0.0, atol=1e-3).all()
11
12
13  def is_lower_hessenberg(A: np.ndarray) -> bool:
14     return np.isclose(np.triu(A, k=2), 0.0, atol=1e-3).all()
15
16
17  # Adapted from: https://relate.cs.illinois.edu/course/cs450-s18/file-version/587
18     fb0505883e0622b9b144b532b5e9a4e7a3684/demos/upload/04-eigenvalues/Arnoldi%20iteration.html
19  def arnoldi_iteration(A, b):
20     n = A.shape[0]
21     H = np.zeros((n, n))
22     Q = np.zeros((n, n))
23     # Normalize the input vector
24     Q[:, 0] = b / np.linalg.norm(b) # Use it as the first Krylov vector
25     for k in range(n):
26         u = A @ Q[:, k]
27         for j in range(k + 1):
28             qj = Q[:, j]
29             H[j, k] = qj @ u
30             u -= H[j, k] * qj
31         if k + 1 < n:
32             H[k + 1, k] = np.linalg.norm(u)
33             Q[:, k + 1] = u / H[k + 1, k]
34
35     return Q, H
36
37  if __name__ == "__main__":
38     A = np.array([[1, 2, 3], [2, 2, 4], [3, 4, 4]])
39     b = np.array([1, -1, 1])
40
41     q, h = arnoldi_iteration(A, b)
42     print("Did arnoldi work:")
43     print(np.isclose((q.T @ A @ q - h) / np.linalg.norm(A), 0.0, atol=1e-3).all())
44
45     print("Q:")
46     print(q)
47     print("H:")
48     print(h)
49     uh = is_upper_hessenberg(h)
50     lh = is_lower_hessenberg(h)
51     if uh:
52         print("Wow its upper Hessenberg, whoda thunk it")
53     if lh:
54         print("Wow its lower Hessenberg, whoda thunk it")
55     if lh and uh:
56         print(
57             "Wow it's tridiagonal, its cuz the matrix A is Hermitian (or Symmetric cuz its real)"
58         )

```