Case Studies in High-Performance Computing

Assignment 2 - Krylov Subspace Methods and GMRES

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1 The Arnoldi Iteration

We present the pseudocode of the Arnoldi iteration algorithm exactly as is given in BYU (2025):

procedure ARNOLDI($A, u, m, \mathrm{tol} = 1\mathrm{E}-8$)
  $n \leftarrow \mathrm{length}(u)$
  $Q \leftarrow \mathrm{zeros}(n, m+1)$, with `dtype=complex` ▷ Initialise matrix to hold orthonormal basis vectors
  $H \leftarrow \mathrm{zeros}(m+1, m)$, with `dtype=complex` ▷ Initialise Hessenberg matrix
  $Q[:, 0] \leftarrow u/\|u\|_2$
  for $j = 0$ to $m-1$ **do**
    $Q[:, j+1] \leftarrow A \cdot Q[:, j]$
    for $i = 0$ to j **do**
      $H[i, j] \leftarrow \langle Q[:, i], Q[:, j+1]\rangle$ ▷ Use complex inner product
      $Q[:, j+1] \leftarrow Q[:, j+1] - H[i, j] \cdot Q[:, i]$ ▷ Orthogonalise against $Q[:, i]$
    end for
    $H[j+1, j] \leftarrow \|Q[:, j+1]\|_2$
    if $|H[j+1, j]| < \mathrm{tol}$ **then**
      return $Q[:, 0{:}j+1], H[0{:}j+1, 0{:}j+1]$
    end if
    $Q[:, j+1] \leftarrow Q[:, j+1]/H[j+1, j]$
  end for
  return Q, H
end procedure

References

BYU. Lab 1 - krylov subspaces. https://acme.byu.edu/0000017a-1bb8-db63-a97e-7bfa0bdf0000/krylov1-pdf, 2025. A lab handout for a course discussing Krylov subspaces.