Case Studies in High-Performance Computing

Assignment 2 - Krylov Subspace Methods and GMRES

Ion Lipsiuc

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1 The GMRES Algorithm

We present the pseudocode of the GMRES algorithm as is given in BYU (2025) with some minor adjustments:

procedure GMRES(A, b, m)
    Ensure A is a function that applies the matrix to a vector
    $n \leftarrow \text{length}(b)$
    $Q \leftarrow \text{zeros}(n, m+1)$
    $H \leftarrow \text{zeros}(m+1, m)$
    $x_0 \leftarrow \text{zeros}(n)$
    $r_0 \leftarrow b - A(x_0)$
    $\beta \leftarrow \|r_0\|_2$
    $Q[:, 0] \leftarrow r_0/\beta$
    $residuals \leftarrow [\beta]$
    for $j = 0$ to $m-1$ **do**
        $q \leftarrow A(Q[:, j])$
        for $i = 0$ to j **do**
            $H[i, j] \leftarrow Q[:, i]^T \cdot q$
            $q \leftarrow q - H[i, j] \cdot Q[:, i]$
        end for
        $H[j+1, j] \leftarrow \|q\|_2$
        if $H[j+1, j] > 10^{-12}$ **then**
            $Q[:, j+1] \leftarrow q/H[j+1, j]$
        end if
        $e_1 \leftarrow \text{zeros}(j+2)$
        $e_1[0] \leftarrow \beta$
        Solve the least squares problem $\min \|H[0 : j+2, 0 : j+1]y - e_1\|_2$ for y
        $res \leftarrow \|\beta e_1 - H[0 : j+2, 0 : j+1] \cdot y\|_2$
        $residuals$.append(res)
    end for
    $x \leftarrow x_0 + Q[:, 0 : m] \cdot y$
    return $x, \text{array}(residuals)$
end procedure

References

BYU. Lab 1 - gmres. `https://acme.byu.edu/0000017a-1bb8-db63-a97e-7bfa0be30000/vol1lab23gmres-pdf`, 2025. A lab handout for a course discussing the GMRES algorithm.