Case Studies in High-Performance Computing

Assignment 2 - Krylov Subspace Methods and GMRES

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1 The Arnoldi Iteration

1.1 Pseudocode

We base our solution on the explanation given in BYU (2025a).

Algorithm 1 The Arnoldi Iteration

$\quad$ **procedure** ARNOLDI(A, u, m)
$\quad\quad n \leftarrow \text{length}(u)$
$\quad\quad Q \leftarrow \text{zeros}(n, m + 1)$
$\quad\quad H \leftarrow \text{zeros}(m + 1, m)$
$\quad\quad Q[:, 0] \leftarrow u/\|u\|_2$
$\quad\quad$ **for** $j = 0$ to $m - 1$ **do**
$\quad\quad\quad Q[:, j + 1] \leftarrow A \cdot Q[:, j]$
$\quad\quad\quad$ **for** $i = 0$ to j **do**
$\quad\quad\quad\quad H[i, j] \leftarrow \langle Q[:, i], Q[:, j + 1] \rangle$
$\quad\quad\quad\quad Q[:, j + 1] \leftarrow Q[:, j + 1] - H[i, j] \cdot Q[:, i]$
$\quad\quad\quad$ **end for**
$\quad\quad\quad H[j + 1, j] \leftarrow \|Q[:, j + 1]\|_2$
$\quad\quad\quad Q[:, j + 1] \leftarrow Q[:, j + 1]/H[j + 1, j]$
$\quad\quad$ **end for**
$\quad\quad$ **return** Q, H
$\quad$ **end procedure**

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2 The GMRES Algorithm

2.1 Pseudocode

We base our solution on the explanation given in BYU (2025b).

Algorithm 2 The GMRES Algorithm

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procedure GMRES(A, b, m)
    $n \leftarrow \text{length}(b)$
    $Q \leftarrow \text{zeros}(n, m+1)$
    $H \leftarrow \text{zeros}(m+1, m)$
    $x_0 \leftarrow \text{zeros}(n)$
    $r_0 \leftarrow b - A(x_0)$
    $\beta \leftarrow \|r_0\|_2$
    $Q[:, 0] \leftarrow r_0/\beta$
    $residuals \leftarrow [\beta]$
    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
        $H[j+1, j] \leftarrow \|q\|_2$
        $Q[:, j+1] \leftarrow q/H[j+1, j]$
        $e_1 \leftarrow \text{zeros}(j+2)$
        $e_1[0] \leftarrow \beta$
        Solve the least squares problem $\min \|H[: j+2, : j+1]y - e_1\|_2$ for y
        $res \leftarrow \|\beta e_1 - H[: j+2, : j+1] \cdot y\|_2$
        $residuals.\text{append}(res)$
    end for
    $x \leftarrow x_0 + Q[:, : m] \cdot y$
    return $x, \text{array}(residuals)$
end procedure

References

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

for a course discussing Krylov subspaces.

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