
HPC for numerical methods and data analysis

Fall Semester 2024

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Arnoldi Process and application to GMRES

Exercise 1: Randomized GS

Consider the Randomized Gram-Schmidt algorithm (RGS) from Oleg and Grigori, <https://arxiv.org/pdf/2011.05090.pdf>.

Algorithm 1 Randomized Gram-Schmidt algorithm (RGS)

Input: $n \times m$ W and sketching matrix Ω of size $k \times n$ with $m \leq k \leq n$

Output: $n \times m$ factor Q and $m \times m$ upper triangular factor R .

for $j = 1 : m$ **do**

 Sketch $w_i : p_i = \Omega w_i$

 Solve the $k \times (i - 1)$ least squares problem:

$$R_{1:i-1,i} = \arg \min_y \|S_{i-1}y - p_i\|.$$

 Compute the projection of $w_i : q'_i = w_i - Q_{i-1}R_{1:i-1,i}$.

 Sketch $q'_i : s'_i = \Omega q'_i$.

 Compute the sketched norm $r_{i,i} = \|s'_i\|$.

 Scale vector $s_i = s'_i / r_{i,i}$.

 Scale vector $q_i = q'_i / r_{i,i}$

end for

Suppose you have an orthonormal set $Q_r = \{q_1, q_2, \dots, q_r\}$. Implement this algorithm in such way that it orthogonalizes a vector w_i against Q_r .

Exercise 2: GMRES

Recall that the Arnoldi process can be used to find eigenvalues. It can also be used to solve systems of equations $Ax^* = b$. The following diagram might be useful:

	$Ax = b$	$Ax = \lambda x$
$A = A^*$	CG	Lanczos
$A \neq A^*$	GMRES CGN BCG et al.	Arnoldi

This was taken from Trefethen and Bau's book <http://www.stat.uchicago.edu/~lekheng/courses/309/books/Trefethen-Bau.pdf>.

At each step GMRES approximates the solution x^* by a vector in the Krylov subspace $x_n \in \mathcal{K}_n$ that minimizes the residual $r_n = b - Ax_n$. This week we are going to implement GMRES from the lecture slides in a sequential fashion. Next week we are going to modify them so that they are implemented using MPI.

- a) Implement Algorithm 2.
- b) Test this method with the following matrices:
 - A from the file `VG_mat.csv` and b from the file `VG_b.csv`
 - A from the file `CTT_mat.csv` and b from the file `CTT_b.csv`
 - A and $b = f$ from session 9. Such matrix and vector had to do with kernel regression using the MNIST data set.
- c) Plot the number of GMRES iterations vs L_2 error
- d) Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be the eigenvalues of A . Plot $\max_j \lambda_j / \lambda_{j+1}$ vs the L_2 error.

To recall these algorithms:

Algorithm 2 Algorithm 2 GMRES with MGS

Input: $A, x_0, b, \max_{\text{iter}} = m$

Output: x^* approximation to the solution of $Ax^* = b$

$r_0 = b - Ax_0, \beta = \|r_0\|_2, q_1 = r_0/\beta$

for $j = 1 : m - 1$ **do**

$w_{j+1} = Aq_j$

MGS to orthogonalize w_{j+1} against $\{q_1, \dots, q_j\}$

Obtain $[r_0, AQ_j] = Q_{j+1}[\|r_0\|_2 e_1 \bar{H}_j]$

end for

Solve $y_m = \arg \min_y \|\beta e_1 - \bar{H}_m y\|_2$

You can find the data here: <https://www.dropbox.com/scl/fi/fissuao7legmz5cv588sv/Data.zip?rlkey=ccjry3318bmfaxqwp0odwsby3&dl=0>