HPC for numerical methods and data analysis

Fall Semester 2023

Prof. Laura Grigori

Assistant: Mariana Martinez

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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 $Q_r = \{q_1, q_2, ..., q_r\}$. 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 $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$ 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 $\{q_1, ..., q_j\}$
    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=ccjry33l8bmfaxqwp0odwsby3&dl=0`