Project 2 : Krylov Space Methods

1. Programming:

We compare the different Krylov space methods.

a) Implement the steepest descent method (Algorithm 7.1), CG (Algorithm 8.1) and GMRES (Algorithm 10.1).

b) Compare the convergence rates for the 2D Poisson model problem by plotting the residual in the 2-norm over number of iterations. Which method performs best?

For moderate N, we can compute the exact solution x_* via $x_* = A \setminus b$. Compare the true error in the energy norm for CG and GMRES for a fixed number of iterations. Which method is better in this metric? Why?

c) Matlab provides efficient implementations of the CG and GMRES method (see *help pcg* and *help gmres*). Compare the run times of your implementations with the run-times of the Matlab functions.

d) We look at the condition number / speed of convergence for the 1D Poisson model problem.

- What do you expect for the condition number of A? Derive a bound of the form $\kappa(A) \leq Cn^\alpha$ for some parameter $\alpha \in \mathbb{R}$ and constant $C > 0$ independent of n. (Hint: For small x, one can approximate $\cos(x) \approx 1 + \frac{x^2}{2}$)
- Apply the CG method to this matrix with the right-hand side $b := (1, \dots, 1)^T$. How fast does the method converge? Does it match the prediction of Theorem 8.2?
- Plot the convergence of the relative residuals $\|b - Ax_m\|/\|b\|$ for different choices of n, e.g. $n = 2^{10}, 2^{11}, 2^{12}, 2^{13}$. How does the number of iterations needed to reach a certain accuracy change (for example to get a relative error of 10%) as you increase n?

e) For $n = 1000$, we look at the $n \times n$ matrix given by

$$A := \begin{pmatrix} 1 & 1 & & & \\ & 1 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 1 \\ & & & & 1 \end{pmatrix}, \qquad b := \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}. \tag{1}$$

- Apply the GMRES method to solve $Ax = b$ and plot the convergence of the residual. What do you observe?
- How does the computational cost for reaching good accuracy (say $\|Ax - b\|_2 < 10^{-5}$) compare to a direct solver?

2. Theory:

a) Let $A \in \mathbb{R}^{n\times n}$ be SPD, set $\phi(x) := \frac{1}{2}(Ax, x) - (b, x)$, and let x_* be the exact solution of $Ax_* = b$.

- Show that
$$\phi(x) - \phi(x_*) = \frac{1}{2}\|x - x_*\|_A^2.$$
- Fix $x_0 \in \mathbb{R}^n$ and let $(x_0, x_1, \dots, x_k)$ be the sequence of CG approximations. Let $\widehat{x}_k \in \mathbb{R}^n$ be the result of a steepest-descent iteration step with search direction $0 \neq d = r_{k-1} = b - Ax_{k-1}$, starting from the CG-vector x_{k-1}. Show
$$\|x_k - x_*\|_A \leq \|\widehat{x}_k - x_*\|_A,$$
i.e. the CG-step is at least as good as the SD-step.
Conclude the local contraction property
$$\|x_k - x_*\|_A \leq q\|x_{k-1} - x_*\|_A \qquad \text{with} \qquad q := \frac{\kappa_2(A) - 1}{\kappa_2(A) + 1} < 1.$$

b)
- Let $A \in \mathbb{R}^{n\times n}$ be an invertible matrix, and $x_0 \in \mathbb{R}^n$ an arbitrary starting value. Show that the approximation x_n obtained by the GMRES minimization criterion
$$\|b - A\,x_n\|_2 = \min_{x \in x_0 + \mathcal{K}_n} \|b - A\,x\|_2$$
is the exact solution x_* of $A\,x = b$.
- Assume additionally that for some $m \leq n$ there holds $\mathcal{K}_m = \mathcal{K}_n$. Show that then already
$$x_m = x_{m+1} = \cdots = x_*$$
Hint: Show that $\mathcal{K}_k = \mathcal{K}_m = \mathcal{K}_n$ also for all $k > m$.

c) Let A be of the form
$$A = \begin{pmatrix} I_{d\times d} & Y_1 & & & & \\ & I_{d\times d} & Y_2 & & & \\ & & \ddots & \ddots & & \\ & & & I_{d\times d} & Y_{k-1} & \\ & & & & I_{d\times d} & Y_k \\ & & & & & I_{d\times d} \end{pmatrix}$$
with sub-matrices $Y_1, \dots Y_k \in \mathbb{R}^{d\times d}$, $d \in \mathbb{N}$ and $I_{d\times d}$ is the $d \times d$ identity matrix.
Show that $(I - A)^k = 0$. How many iterations does the GMRES method take (at most) to converge?