University of Vienna
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Introductory Seminar
Advanced Numerical Analysis

Exercise sheet 4, due date: 28.03.2022

Exercise 1 (CG iteration).
In this exercise we wish to solve linear systems $Ax = b$ using the conjugate gradient method.

(1) Write a program in Python which takes as input parameters a SPD matrix $A \in \mathbb{R}^{n\times n}$, a vector $b \in \mathbb{R}^n$ and a number of steps and performs the conjugate gradient iteration for $Ax = b$.
(2) For testing, take the matrix Q of Exercise 3, Sheet 2 with dimension $n = 20$ and right-hand side $b = (1, 1, \dots, 1)^T$. Compare the output of the algorithm with the setting where we use the command `numpy.linalg.inv`.
(3) What can happen if the matrix is not positive definite? E.g. consider

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

Exercise 2 (CG and Krylov spaces).
Consider the linear system $Ax = b$ where

$$A = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}, \quad b = \begin{pmatrix} 4 \\ 0 \\ 0 \end{pmatrix}.$$

(1) Carry out by hand iterations $x_0, x_1, x_2, \dots, x_n$ of the CG method with initial guess $x_0 = 0$ on $Ax = b$ until you reach the exact solution x_n.
(2) Determine the vectors defining the Krylov spaces $\mathcal{K}_k(A, b)$ for $k = 1, \dots, n$.
(3) Verify that $\dim(\mathcal{K}_k(A, b)) = k$ for $k = 1, \dots, n$. Further show that the residuals $r_0, \dots, r_{k-1}$ form an orthogonal basis for $\mathcal{K}_k(A, b)$ for $k = 1, \dots, n$.

Exercise 3 (A^TA inner product, part 1).
Let $\{v_i : i = 1, \dots, k\} \subset \mathbb{R}^n$ be linearly independent vectors and let $\langle\cdot,\cdot\rangle$ be an inner product on $\mathbb{R}^n$.

(1) Show that the $k \times k$ matrix with entries $a_{ij} = \langle v_i, v_j\rangle$ is SPD.

Now let $\mathcal{K} \subset \mathbb{R}^n$ be any linear subspace.

(2) Show that there is a unique $\hat{x} \in \mathcal{K}$ so that

$$w^T A^T A\hat{x} = w^T A^T b \quad \forall w \in \mathcal{K}$$

and that $\hat{x}$ satisfies

$$\|b - A\hat{x}\|_2 \le \|b - Aw\|_2 \quad \forall w \in \mathcal{K}.$$

In the rest of this exercise we consider the situation above, but where the vector space $\mathcal{K}$ is taken to be the Krylov space

$$\mathcal{K}_k(A, b) = \operatorname{span}\{b, Ab, \dots, A^{k-1}b\}.$$

We use the inner product in $\mathbb{R}^n$ given by

$$\langle v, w \rangle_A = v^T A^T A w.$$

The associated approximations of x, corresponding to $\hat{x}$ in $\mathcal{K}_k(A, b)$ are then denoted by x_k. Assume that $x_k \in \mathcal{K}_k(A, b)$ is already determined. In addition, assume that we already computed a search direction $p_k \in \mathcal{K}_{k+1}(A, b)$ such that $\|Ap_k\|_2 = \|p_k\|_A = 1$ and such that

$$\langle p_k, w \rangle_A = 0 \quad \forall w \in \mathcal{K}_k(A, b).$$

(3) Show that $x_{k+1} = x_k + \alpha_k p_k$ for suitable $\alpha_k \in \mathbb{R}$.

Exercise 4 ($A^T A$ inner product, part 2).
This is a continuation of Exercise 3.

(1) Express α_k in terms of the residual r^k and p_k.
(2) Assume that A is symmetric but not necessarily positive definite. Assume further that the vectors p_{k-2}, p_{k-1}, p_k are already known with properties as above. Show that

$$Ap_{k-1} \in \operatorname{span}\{p_{k-2}, p_{k-1}, p_k\}.$$

(3) Use this to suggest how the search vectors p_k can be computed recursively.