12. Assignment „Numerische Mathematik für Ingenieure II“

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Conjugate directions and gradients

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1. Exercise: Conjugate direction method **6 points**

Consider the conjugated directions method, generating a sequence $x_{k+1} = x_k + \gamma_k d_k$ from given set of directions d_k. The sequence is supposed to converge to the solution of $Ax = b$ with $A \in \mathbb{R}^{n\times n}$ a SPD matrix. We have the error $e_k = x_k - x$ and the residual $r_k = b - Ax_k$. Consider a set of given linearly independent vectors $(d_0, ..., d_{n-1})$ where $d_i \in \mathbb{R}^n$ and $d_i^\top A d_j = 0$ for all $0 \le i, j \le n-1$, $i \ne j$. The for some δ_k the error e_0 is represented by

$$e_0 = \sum_{k=0}^{n-1} \delta_k d_k.$$

(a) With $x_{k+1} = x_k + \gamma_k d_k$ derive γ_k from the requirement $d_k^\top A e_{k+1} = 0$ and derive an explicit expression for e_k.

(b) Show that x_k is the exact solution after at most n iterations.

2. Exercise: Conjugate gradient method **6 points**

Consider the CG method as defined in the lecture, where for a given $A \in \mathbb{R}^{n\times n}$ symmetric, positive definite and given $b \in \mathbb{R}^n$ we define the following algorithm to solve $Ax = b$. Let $x_0 \in \mathbb{R}^n$ the initial guess of x and $r_0 = b - Ax_0$, $d_0 = r_0$.

$$\begin{aligned}
\gamma_k &= \frac{r_k^\top r_k}{d_k^\top A d_k} \\
x_{k+1} &= x_k + \gamma_k d_k \\
r_{k+1} &= r_k - \gamma_k A d_k \\
\beta_k &= \frac{r_{k+1}^\top r_{k+1}}{r_k^\top r_k} \\
d_{k+1} &= r_{k+1} + \beta_k d_k
\end{aligned}$$

(a) Show $r_i^\top r_j = 0$ for $i \ne j$.

(b) Show $d_i^\top A d_j = 0$ for $i \ne j$.

(c) Let $v_i \in \mathbb{R}^n$ the set of eigenvectors of A for $i = 1, \dots, n$ with eigenvalues λ_i (in no particular order). Assume we can write

$$b = \sum_{i=1}^{\rho} \alpha_i v_i$$

for some $1 < \rho < n$ and $x_0 = b$ (or $x_0 = 0$). How many iterations (at most) are required to get the exact solution (without rounding errors)? **Hint:** What is the dimension of the Krylov space $K_k = \operatorname{span}(r_0, Ar_0, A^2 r_0, \dots, A^{k-1} r_0)$, from which the CG method can recruit its directions d_k?

3. Programming exercise: Conjugate gradient method **12 points**

(a) Write a `function [x,iter,err]=cgm(A,b,tol,x0)` which solves $Ax = b$ using the CG method. Perform the iteration as long as $(r_k^\top r_k)^{1/2} \geq$ `tol`. If `x0` is not provided use $x_0 = b$. Return `x` $= x_k$, the number of iterations `iter` $= k$. As additional output provide the vector `err(i)` $= \|e_{i-1}\|_A$ of errors in the A-norm.

(b) Let `A` $= K_{100}$ with K_n from assignment 1, and $b = (1, ..., 1)^\top$. Compare i) CG method with `x0=b`, ii) CG method with `x0(i)=i`, iii) steepest descent with `x0=b`. Plot error $\|e_k\|_A$ versus iteration number k using `semilogy` and compare with your expectations. **Remark:** Modify steepest descent to return $\|e_k\|_A$.

(c) Modify (a) and write a `function [x,iter,err]=pcgm(A,b,tol,x0,L)` which solves $B^{-1}Ax = B^{-1}b$ using preconditioned CG with given $B = (LL^\top)^{-1}$. Other input/output as before. Using $r_0 = b - Ax_0$, $z_0 = (LL^\top)^{-1}r_0$, $d_0 = z_0$ we have

$$\begin{aligned}
\gamma_k &= \frac{r_k^\top z_k}{d_k^\top A d_k}, \\
x_{k+1} &= x_k + \gamma_k d_k, \\
r_{k+1} &= r_k - \gamma_k A d_k, \\
z_{k+1} &= (LL^\top)^{-1} r_{k+1}, \\
\beta_k &= \frac{r_{k+1}^\top z_{k+1}}{r_k^\top z_k}, \\
d_{k+1} &= z_{k+1} + \beta_k d_k.
\end{aligned}$$

For the purpose of this assignment it suffices to solve $z_k = (LL^\top)^{-1}r_k$ directly using `zk=(L*L')\rk` or more efficiently solving $Ly = r_k$, $L^\top z_k = y$. **Remark:** If L is a upper/lower triangular matrix, then these could be efficiently solved by back substitution.

(d) Use $A = -\Delta_h$ the finite differences Laplace operator on the unit square $[0,1]^2$ in the reduced form for the problem

$$-\Delta u = f, \quad \text{in } (0,1)^2, \qquad u = 0, \quad \text{on } \Gamma = \partial(0,1)^2.$$

For the corresponding discrete problem $Ax = b$ compare the error $\|e_k\|_A$ of the CG method with the PCG method. As preconditioner for PCG use the incomplete Cholesky decomposition with `L1=cholinc(A,0.1)` and `L2=cholinc(A,0.01)` and $x_0 = b$. Study the cases i) $f(x,y) = 1$ and ii) $f(x,y) = \sin(\pi x)\sin(\pi y) + \sin(2\pi x)\sin(2\pi y) + \sin(5\pi x)\sin(3\pi y)$. Create separate plots for both f and plot the error versus iteration number using `semilogy`. Interprete what you observe. **Remark:** In the notation of previous assignments use $p = 5$ and remove boundary points from A. If neccessary the matrix A will be provided via the ISIS 2 page.

total sum: 24 points

As usual, use sparse matrices (where this is useful).