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TMA4220 Numerical Solution of Partial Differential Equations Using Element Methods Fall 2012

Exercise set 6

1 The conjugate gradient (CG) algorithm for solving

$$A\mathbf{u} = \mathbf{b}$$

is given by

Compute $\mathbf{r}_0 = \mathbf{b} - A\mathbf{u}_0, \quad \mathbf{p}_0 = \mathbf{r}_0$.
1: **for** $k = 0, 1, 2, \cdots$ **do**
2: $\alpha_k = \dfrac{\mathbf{r}_k^T \mathbf{r}_k}{\mathbf{p}_k^T A \mathbf{p}_k}$
3: $\mathbf{u}_{k+1} = \mathbf{u}_k + \alpha_k \mathbf{p}_k$
4: $\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k A \mathbf{p}_k$
5: $\beta_k = \dfrac{\mathbf{r}_{k+1}^T \mathbf{r}_{k+1}}{\mathbf{r}_k^T \mathbf{r}_k}$
6: $\mathbf{p}_{k+1} = \mathbf{r}_{k+1} + \beta_k \mathbf{p}_k$
7: **end for**

In the following, we will assume that A is symmetric, positive definite.

In the lecture, it was proved that $\mathbf{r}_i^T \mathbf{r}_j = 0$ and $\mathbf{p}_i A \mathbf{p}_j = 0$ if $i \neq j$.

a) Prove that this algorithm coincide with the algorithm on p. 166 in Quarteroni, with no preconditioner ($P = I$).

Solution: There is an error in the CG algorithm in Q: β_k has the wrong sign. There were a few errors in the algorithm in the exercise as well, but they should have been corrected in this version.
The only differences between the two algorithms is how β_k and α_k is computed. For α_k, we have

$$\mathbf{p}_k^T \mathbf{r}_k = (\mathbf{r}_k + \beta_k \mathbf{p}_{k-1})^T \mathbf{r_k} = \mathbf{r}_k^T \mathbf{r}_k^T$$

since $\mathbf{p}_{k-1}^T \mathbf{r}_k = 0$. For β_k use

$$\mathbf{p}_k^T A \mathbf{r}_{k+1} = \frac{1}{\alpha_k}(\mathbf{r}_k - \mathbf{r}_{k+1})^T \mathbf{r}_{k+1} = -\frac{1}{\alpha_k} \mathbf{r}_{k+1}^T \mathbf{r}_{k+1}.$$

and

$$\mathbf{p}_k^T A \mathbf{p}_k = \frac{1}{\alpha_k} \mathbf{p}_k^T (\mathbf{r}_k - \mathbf{r}_{k+1}) = \frac{1}{\alpha_k} \mathbf{r}_k^T \mathbf{r}_k.$$

b) If A is symmetric positive definite, prove that so is A^{-1}. Thus A^{-1} can be used to define a norm: $\|\mathbf{y}\|_{A^{-1}} = \sqrt{\mathbf{y}^T A^{-1} \mathbf{y}}$ for all $\mathbf{y} \in \mathbb{R}^N$.

Solution: Choose some arbitrary $\mathbf{y} \neq 0$. *Let* $\mathbf{x} = A^{-1}\mathbf{y}$ *(which do exist, since* A *is SPD and then invertible). But then*

$$\mathbf{y}^T A^{-1}\mathbf{y} = (A\mathbf{x})^T A^{-1} A\mathbf{x} = \mathbf{x}^T A\mathbf{x} > 0.$$

So, A^{-1} *is SPD.*

c) From the derivation of the CG algorithm, we know that at each iteration, the method minimizes the *error* in th A-norm over all elements in $K^m(A; \mathbf{r}_0)$. Prove that, at each iteration, CG minimizes the *residual* in the A^{-1} norm.
Solution: Let $\mathbf{u}$ *be the exact solution to* $A\mathbf{u} = \mathbf{b}$. *Then*

$$\mathbf{u} - \mathbf{u}_m = A^{-1}(\mathbf{b} - A\mathbf{u}_m) = A^{-1}\mathbf{r}_m.$$

And

$$\|\mathbf{u} - \mathbf{u}_m\|_A^2 = (\mathbf{u} - \mathbf{u}_m)^T A(\mathbf{u} - \mathbf{u}_m) = \mathbf{r}_m A^{-1}\mathbf{r}_m = \|\mathbf{r}_0\|_{A^{-1}}^2.$$

d) Assume that the initial residual can be expressed as a sum of m eigenvectors of A, with $m \leq N$. Show that CG converges in m iterations in this case.
Solution: The Krylov space is given by

$$K^k(A; \mathbf{r}_0) = span\{\mathbf{r}_0, A\mathbf{r}_0, \ldots, A^{k-1}\mathbf{r}_0\}. \tag{1}$$

This is supposed to create a subspace of dimension k, *and the CG algorithm is essential a smart implementation of the Gram-Schmidt process to find an orthogonal basis,* $\{\mathbf{r}_0, \mathbf{r}_1, \ldots \mathbf{r}_{k-1}\}$ *of* $K^k(A; \mathbf{r}_0)$. *However, if* $\mathbf{r}_0 = \sum_{i=1}^m \gamma_i \mathbf{v}_i$, *where the* $\mathbf{v}_i$*'s are* m *of the eigenvectors of* A, *then*

$$A\mathbf{r}_0 = \sum_{i=1}^m \gamma_i \lambda_i \mathbf{v}_i, \qquad A^2\mathbf{r}_0 = \sum_{i=1}^m \gamma_i \lambda_i^2 \mathbf{v}_i, \qquad etc.$$

So $K^k(A, \mathbf{r}_0) \subseteq V_m = span\{\mathbf{v}_1, \mathbf{v}_2, \ldots \mathbf{v}_m\}$, *for all* $k \leq N$. *After* m *iterations there are no new directions to be found,* $K^m = V_m$, $\mathbf{r}_m = 0$ *and the exact solution has been found.*

2 Consider the diffusion-transport problem:

$$\begin{aligned} -\mu u_{xx} + b u_x &= f, \qquad in \quad \Omega = (0, L) \\ u(0) &= 0 \\ u(L) &= 1 \end{aligned}$$

where μ and b are given constants, and $\mu > 0$.

a) Find the weak formulation of the problem.

b) Set up the Galerkin approximation, using a space $V_h = \text{span}\{\varphi_1, \varphi_2, \ldots, \varphi_N\}$.

c) Let $V_h = X_h^1$. Set up the elemental matrix A^K for this problem.

d) Assume a uniform grid ($h = L/M$ is constant). Set up the global linear system to be solved in this case.

e) Let $L = 20$, $\mu = 0.04$ and $b = 2$. How small do you have to make the stepsize h to avoid oscillations in the numerical solution? How many elements would you need?

f) Confirm the results of **e)** numerically (MATLAB file enclosed).

g) How can you avoid the oscillations, while still using a solution based on finite element methods. Again, confirm your results numerically.

h) Explain the idea of the Gummel-Scharfetter scheme (bottom half of page 285). In particular, explain why the use of this scheme will solve the diffusion-transport equation exactly if the source term $f = 0$.
Confirm your results numerically.

i) Assume that you would rather use a variable stepsize scheme. Describe a typical row in the global linear system of equations.