Kungl. Tekniska Högskolan **2012**
CSC / NA
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Deadline 2012-04-05

Homework set 1.
Advanced numerical methods for science and engineering - DN3250

http://www.csc.kth.se/~eliasj/DN3250/

Gaussian elimination, LU decomposition and Krylov subspace

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1. (a) Implement Algorithm 20.1 in [TB]. In this homework [TB] refers to the book in [Trefethen & Bau, Numerical linear algebra] and the programming should in this homework set be done in MATLAB.

   (b) Combine your implementation of Algorithm 20.1 and the function `back_fw_subs.m` (downloadable from the course web page) as a solver for linear systems. Verify and show that your algorithm works for the linear system $Ax = b$ with
   `A=[-4,12,-3,8;5,6,-4,15;10,-1,0,4;-12,-2,0,-3];`
   `b=[4;20;14;-15];`

2. (a) Implement the partial pivoting described in Algorithm 21.1 in [TB]. Check that the expression `P*A-L*U` for the problem in exercise 1 and solve the linear system.
   Hint: `back_fw_subs(L,U,P*b)`

   (b) Test the accuracy of both the algorithm in exercise 1 and the partial pivoting algorithm (in exercise (a)) with the following linear system of equations
   `A=[0.01,-0.2,-0.6,1;-0.5,10+1e-8,-0.3,10;-0.8,1.3,-1.9,0.3;1,-5,-1.2,-1.3]`
   `b=(1:4)'`
   Is the result consistent with theory? Explain what happens in the algorithm and what is special with the given matrix.

3. In your introductory numerical analysis course (e.g., from the literature in DN1260 [Peter Pohl, Numeriska Metoder, Section 6:3]) you learned how to discretize the boundary value problem

$$\begin{aligned} \frac{d^2u}{dx^2} &= f(x), \quad x \in [-1, 1] \\ u(-1) &= a, \\ u(1) &= b, \end{aligned}$$

   using finite differences. We will here use $f(x) = 10\sin(2\pi x) + \exp(x)$ and $a = b = 2$. The matrix and vector stemming from the finite difference discretization with central differences and N equidistant gridpoints, is given by

```
h=2/(N+1);
x=h:h:(2-h);
e = ones(N,1);
A = 1/h^2*spdiags([e -2*e e], -1:1, N,N)
b=10*sin(2*pi*x)+exp(x);
```

   (a) Use your algorithm in exercise 2 to solve the linear system. Make sure your implementation does not store any matrix in a dense format. Plot the your approximation of $u(x)$.

(b) Inspect the structure of L, U, P and describe the relevant properties, e.g., with the command `spy`. How would the algorithm in exercise 1 compare with this? Explain your reasoning.

(c) Improve your implementation of algorithm 20.1 by exploiting the sparsity structure and modifying the inner loop.

(d) Plot the processing time against N and increase N until the computer takes approximately 1 minute.

4. In your introductory numerical analysis course you also learned how to compute integrals with the *trapezoidal rule.*

   (a) Derive the matrix and vector corresponding to the discretization of

$$\begin{aligned} \frac{d^2u}{dx^2} + \frac{1}{2}\int_{-1}^{1} u(\xi)\, d\xi &= f(x), \quad x \in [-1,1] \\ u(-1) &= a, \\ u(1) &= b. \end{aligned}$$

   where a, b and f are as before.

   (b) Generate the matrices in matlab and solve it with the algorithm developed in exercise 2.

   (c) Carefully consider the structure and reformulate the problem such that it only involves a sparse matrix. Solve the problem using the reformulation and the modified algorithm in exercise 3. Compare the largest system you can solve in 1 minutes with and without exploiting the reformulation and structure.
   Hint: Sherman-Morrison formula

5. The concept of *Krylov matrices* is relevant for algorithms for linear systems of equations and eigenvalue problems, and is defined as the matrix

$$K_k = (c, Ac, \cdots, A^{k-1}c) \in \mathbb{R}^{n\times k},$$

   where $A \in \mathbb{R}^{n\times n}$ and $c \in \mathbb{R}^n$. In your introduction to numerical analysis course, you also solved least squares problem. Assume that an approximate solution to $Ax = b$ can be written as $x \approx K_k z$. Solve the approximation problem $b = Ax \approx AK_k z$ in a least squares sense when $c = b$. Use A and b generated by

```
n=100
A=expm((ones(n,n)+diag(1:n))/n)
b=(1:n)'
```

   Plot the residual norm, i.e., $\|AK_k z - b\|$ as a function of k, for $k = 2, \ldots 20$. How good solution can you get? In this exercise you are allowed to use the \ operator in matlab.

   You will observe some numerical difficulties with the approach above, which we will later overcome when studying the algorithms GMRES and CG. These are the topic of the next set of homework.

The deadline for this homework is April 5, 2012. Please hand in the source code, plots and answers to the questions.