Course of Numerical Methods for Engineering
Lab 7

Luca Bonaventura, Tommaso Benacchio

MOX - Politecnico di Milano

PHYS-ENG, A.Y. 2020-21

26-27/10/2020

Topics of this session:

- **Sparsity-enhancing permutations**
- **Error estimates for linear systems and ill conditioned problems**

Sparsity-enhancing permutations

- **In general, the inverse of a sparse matrix is not sparse and the LU factors of a sparse matrix can be much less sparse than the matrix itself: the horrible fill-in phenomenon!**

- **Given a sparse matrix A and the system $Ax = b$, for some permutation matrices P, the matrices PA (permutation by rows), AP^T (permutation by columns), or PAP^T (permutation by both rows and columns) have sparser LU factors, and so it might be more convenient to solve the equivalent systems $PAx = Pb$, $AP^T y = b;\ y = Px$ or $PAP^T y = Pb; y = Px$.**

Sparsity-enhancing permutations in MATLAB

- **Column permutations: commands `colamd` and (for symmetric matrices) `symamd`. For banded matrices: `symrcm`.**
- **Given the sparse $\mathtt{n} \times \mathtt{n}$ matrix `As`, the permutation matrix `P_` is found by:**

```
p = {colamd or symamd or symrcm}( As );
I = speye(n);
P_ = I(p,:);
```

Exercise 1

Consider the matrix A and vector b as defined in Exercise 7 of the previous exercise session.

(a) **Using the command `spy`, visualize the sparsity structure of the LU factors of A;**

(b) **Use the command `colamd` to build a sparsity enhancing permutation of the columns of A;**

(c) **Determine the solution of $\mathsf{Ax} = \mathsf{b}$ solving with LU factorization the appropriate modification of the system induced by the column permutation at point b);**

(d) **Compare the execution times of the solutions with and without permutations.**

Exercise 2

Build the $n \times n$ matrix A that has elements equal to 100 on the main diagonal, 1 on the first and last rows and columns (outside the main diagonal), and -1 on the sub and superdiagonal $n/2$ (leaving the first and last element of those diagonals equal to 1). Represent the matrix in sparse storage format.

(a) **Check that the matrix is symmetric and positive definite, using the command `eigs` to compute the smallest eigenvalue of the matrix;**

(b) **Consider $n = 100$. Define $\mathrm{b} = [1, -1, \dots, 1, -1]^T \in \mathbb{R}^{100}$ and solve the system $\mathrm{Ax} = \mathrm{b}$ using the Cholesky factorization method, both in the sparse storage form and in the full storage form. Check that the results are the same and compare the execution times for the solution by the two storage formats;**

(c) **Repeat the exercise for the case of $n = 500$ and $n = 2000$;**

(d) **Using the command `spy`, visualize the sparsity structure of the $\mathbf{L}$ and $\mathbf{L}^T$ factors of A;**

(e) **Use the commands `symamd` and `symrcm` to build sparsity enhancing permutations of the columns of A;**

(f) **Determine the solution of $\mathrm{Ax} = \mathrm{b}$ solving with Cholesky factorization the appropriate modification of this system induced by the permutations. Compare the execution times.**

Error estimates and condition number

- **When we solve** $\mathsf{A}\mathsf{x} = \mathsf{b}$ **in finite precision, we are actually solving the system** $\tilde{\mathsf{A}}\tilde{\mathsf{x}} = \tilde{\mathsf{b}}$**, with** $\tilde{\mathsf{A}} = \mathsf{A} + \mathsf{E}, \tilde{\mathsf{b}} = \mathsf{b} + \mathsf{e}$**.**
- **We look for an error bound:**

$$\frac{\|\tilde{\mathsf{x}} - \mathsf{x}\|}{\|\mathsf{x}\|} \leq f\left(\frac{\|\mathsf{E}\|}{\|\mathsf{A}\|}, \frac{\|\mathsf{e}\|}{\|\mathsf{b}\|}\right)$$

Definition

Given an invertible $n \times n$ **matrix** A**, the number**

$$\kappa(\mathsf{A}) = \|\mathsf{A}\|\|\mathsf{A}^{-1}\|$$

is called the condition number of A **in the matrix norm** $\|\cdot\|$**.**

Error estimates

Theorem

Given an $n \times n$ invertible matrix A and considering the solution of the linear system $\mathrm{A}\tilde{\mathrm{x}} = \tilde{\mathrm{b}}$, one has the a priori error estimate:

$$\frac{\|\tilde{\mathrm{x}} - \mathrm{x}\|}{\|\mathrm{x}\|} \leq \kappa(\mathrm{A}) \frac{\|\mathrm{e}\|}{\|\mathrm{b}\|},$$

where x is such that $\mathrm{A}\mathrm{x} = \mathrm{b}$. Note: When roundoff is the only source of error, $\frac{\|\mathrm{e}\|}{\|\mathrm{b}\|}$ is bounded by the machine precision.

Definition

If $\tilde{\mathrm{x}}$ is a numerical solution computed for the linear system $\mathrm{A}\mathrm{x} = \mathrm{b}$, the vector $\mathrm{r} = \mathrm{b} - \mathrm{A}\tilde{\mathrm{x}}$ is in general different from zero; this vector is called the residual associated to the numerical solution $\tilde{\mathrm{x}}$.

Theorem

The following a posteriori error estimate holds:

$$\frac{\|\tilde{\mathrm{x}} - \mathrm{x}\|_2}{\|\mathrm{x}\|_2} \leq \kappa_2(\mathrm{A}) \frac{\|\mathrm{r}\|_2}{\|\mathrm{b}\|_2}.$$

Preconditioning

- **If a linear system** $\mathsf{Ax} = \mathsf{b}$ **is such that** $\kappa(\mathsf{A}) \gg 1$, **the system is called ill conditioned.**

- **A preconditioner is a matrix** P **such that** $\kappa(\mathsf{PA}) \ll \kappa(\mathsf{A})$**, so instead of** $Ax = b$ **one can more conveniently solve** $\mathsf{PAx} = \mathsf{Pb}$

Exercise 3

Build the Hilbert matrix H_n using the function `hilb` for $n = 1, \ldots, 20$. Build the right hand sides of systems $\mathrm{H}_n \mathrm{x} = \mathrm{b}$ so that $\mathrm{x}_{ex} = [1, 1, \ldots, 1, 1]^T$.

(a) **Determine for which value of n the matrices cannot be guaranteed to be positive definite;**

(b) **Solve these linear systems by the LU factorization algorithm, checking whether pivoting has been performed, and with the backslash $\backslash$ command;**

(c) **Compute the absolute and relative error of the computed solutions with respect to x_{ex} in the l^2 and l^∞ norm;**

(d) **Compute the** *a posteriori* **and** *a priori* **error estimates;**

(e) **Display these errors on a semi-logarithmic plot.**

Exercise 4

Let $A = 10^{-8}I + H_{20}$ **and consider the linear system** $Ax = b$ **so that** $x_{ex} = [1, 1, \ldots, 1, 1]^T$. **Consider then the perturbed system** $A\tilde{x} = b + e$, **where** e **is a vector of independent, identically distributed Gaussian variables of zero mean and variance** σ **built using the command** `randn`**. Say which is the maximum value of** σ **for which an** *a priori* **error bound of** 10^{-2} **on the computation of** x **can be guaranteed.**

Exercise 5

Consider the Vandermonde matrix A **associated to the vector** $[1.0, 1.1, 1.2, 1.3, 1.4, 1.5, 100]^T$ **(use the command** `vander`**). Build the right hand side of the system** $\mathrm{Ax} = \mathrm{b}$ **so that** $\mathrm{x}_{ex} = [1, -1, 1, -1, 1, -1, 1]^T$.

(a) **Solve the linear system by the LU factorization algorithm, checking if pivoting has been performed, and with the backslash** $\backslash$ **command;**

(b) **Compute the absolute and relative error of the computed solutions with respect to** x_{ex} **in the** l^2 **and** l^∞ **norm;**

(c) **Compute the** *a posteriori* **and** *a priori* **error estimates;**

(d) **Build the diagonal matrix** P **whose main diagonal elements are the reciprocals of the elements on the first column of** A**;**

(e) **Solve the linear system** $\mathrm{PAx} = \mathrm{Pb}$ **and compare the quality of the results with those obtained for the previous system, explaining the differences on the basis of the theory.**

Exercise 6

Consider the $n \times n$ tridiagonal matrix A with elements equal to $1, 4, \dots n^2$ on the main diagonal, -1 on the $80-$th superdiagonal and 1 on the $80-$th subdiagonal. In the case $n = 1000$,

(a) **Represent A in sparse format. Build the right hand side of the system $\mathrm{Ax} = \mathrm{b}$ so that $\mathrm{x}_{ex} = [1, \dots, 1]^T$.**

(b) **Solve the linear system by the LU factorization algorithm, checking if pivoting has been performed, and with the backslash $\backslash$ command;**

(c) **Compute the absolute and relative error of the computed solutions with respect to x_{ex} in the l^2 and l^∞ norm;**

(d) **Compute the *a posteriori* and *a priori* error estimates in the l^1 norm, using the command `condest` to estimate the condition number of a sparse matrix.**