Course of Numerical Methods for Engineering
Lab 11

Luca Bonaventura, Tommaso Benacchio

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Topic of this session:

- **Overdetermined systems**

Linear systems of the form

$$
\begin{aligned}
&a_{1,1}x_1 + a_{1,2}x_2 + \cdots + a_{1,n}x_n = b_1 \\
&a_{2,1}x_1 + a_{2,2}x_2 + \cdots + a_{2,n}x_n = b_2 \\
&\ldots \\
&a_{m,1}x_1 + a_{m,2}x_2 + \cdots + a_{m,n}x_n = b_m
\end{aligned}
$$

with a number of equations m different from the number of unknowns n are called underdetermined if $m < n$, and overdetermined if $m > n$.

Least square solution

Definition

Let A be an $m \times n$ matrix, $\mathrm{x} \in \mathrm{R}^n$ and $\mathrm{b} \in \mathrm{R}^m$. The vector $\mathrm{x}^* \in \mathrm{R}^n$ is called a least square solution of $\mathrm{Ax} = \mathrm{b}$ if it is such that

$$\|\mathrm{Ax}^* - \mathrm{b}\|_2 = \min_{\mathrm{x} \in \mathrm{R}^n} \|\mathrm{Ax} - \mathrm{b}\|_2.$$

For overdetermined systems with full rank, the normal equation matrix $\mathrm{A}^T\mathrm{A}$ is symmetric and positive definite, so the solution of the normal equations exists and is unique.

QR factorization

Definition

A generic $m \times n$ matrix A has a QR factorization if there are a unitary $m \times m$ matrix Q and an $m \times n$ matrix R with all the elements below the main diagonal are zero which satisfy

$$\mathrm{A} = \mathrm{QR}.$$

Theorem

*(***QR factorization for full rank rectangular matrices***)* **For any $m \times n$ full rank matrix A with $m > n$, there are a $m \times m$ unitary matrix Q and a unique $n \times n$ upper triangular matrix $\tilde{\mathrm{R}}$ such that $\tilde{\mathrm{R}}$ is invertible and**

$$\mathrm{A} = \mathrm{QR} \qquad \mathrm{Q}^T\mathrm{Q} = \mathrm{Q}\mathrm{Q}^T = \mathrm{I} \qquad \mathrm{R} = \begin{bmatrix} \tilde{\mathrm{R}} \\ 0 \end{bmatrix}.$$

Singular value decomposition

Definition

A generic $m \times n$ matrix A has a singular value decomposition (SVD) if there are a unitary $m \times m$ matrix U, a unitary $n \times n$ matrix V and an $m \times n$ matrix Σ such that all the elements out of the main diagonal are zero and all the elements σ_i on the main diagonal are non negative which satisfy

$$A = U\Sigma V^T.$$

The numbers σ_i are are called singular values of A.

Theorem

*(***Existence of SVD for square invertible matrices***)* **The singular value decomposition exists and is unique for any invertible square matrix** A. **The singular values σ_i are the square roots of the eigenvalues of** $A^T A$.

Pseudo-inverse

Definition

For any $m \times n$ **matrix** A, **its pseudoinverse or Moore-Penrose inverse is defined by**

$$\mathrm{A}^{\dagger} = \mathrm{V} \begin{bmatrix} \mathrm{S}^{-1} & 0 \\ 0 & 0 \end{bmatrix} \mathrm{U}^{T}.$$

In Octave/MATLAB, the `pinv` **command can be used to compute the pseudo-inverse.**

Definition

Let A **be an** $m \times n$ **matrix,** $\mathrm{x} \in \mathrm{R}^{n}$ **and** $\mathrm{b} \in \mathrm{R}^{m}$. **The vector** $\mathrm{x}^{*} \in \mathrm{R}^{n}$ **is called a minimum norm least square solution of** $\mathrm{Ax} = \mathrm{b}$ **if it is such that**

$$\|\mathrm{Ax}^{*} - \mathrm{b}\|_{2} = \min_{\mathrm{x} \in \mathrm{R}^{n}} \|\mathrm{Ax} - \mathrm{b}\|_{2}$$

and $\|\mathrm{x}^{*}\|_{2} \leq \|\mathrm{y}\|_{2}$ **for any other** y **that may minimize the least square error.**

Theorem

For any $m \times n$ A **the minimum norm least square solution of the associated linear system** $\mathrm{Ax} = \mathrm{b}$ **is given by**

$$\mathrm{x}^{*} = \mathrm{A}^{\dagger}\mathrm{b}.$$

Exercise 1

Build the overdetermined linear system arising from the least square fitting of the paraboloid $z = f(x, y) = \frac{x^2}{10} + \frac{y^2}{5} - 1$ with a plane $\alpha x + \beta y + \gamma$ where the data consist of the values of f at the points

$$(0, 0),\ (0, 0.1),\ (0.1, 0),\ (0.1, 0.1),\ (0, 0.2),\ (0.1, 0.2),\ (0.2, 0.2),\ (0.2, 0.1),\ (0.2, 0).$$

Check that the resulting matrix is of full rank. Solve the system:

(a) **with the Octave/MATLAB command** $\backslash$

(b) **solving the normal equations by the Cholesky method**

(c) **using the QR decomposition approach**

(d) **using the SVD decomposition approach**

(e) **using the Octave/MATLAB command** `pinv`**.**

Compare all the numerical solutions obtained with the reference solution obtained with the Octave/MATLAB command $\backslash$ **by computing relative** l_2 **and** l_∞ **errors.**

Exercise 2

Repeat the previous exercise in the case in which the data consist of the values of f at the points

$$(0, 0.2),\ (0.1, 0.2),\ (0.2, 0.2),\ (0.3, 0.2), (0.4, 0.2),$$
$$(0.5, 0.2),\ (0.6, 0.2),\ (0.7, 0.2),\ (0.8, 0.2).$$

Explain what are the differences with respect to the previous case.

Exercise 3

Build the 20×20 **matrix** $\tilde{\mathrm{A}}$ **that has elements equal to 2 on the main diagonal and -1 on the first super and subdiagonal and the vector** $\tilde{\mathrm{b}} = [1, 1, \ldots, 1, 1]^T \in \mathrm{R}^{20}$. **Build then the** 200×20 **matrix** A **which contains 10 blocks equal to** $\tilde{\mathrm{A}}$ **and the vector** $\mathrm{b} \in \mathrm{R}^{200}$ **which contains 10 blocks equal to** $\tilde{\mathrm{b}}$ **multiplied by the integers** $1, \ldots, 10$. **Check that the resulting matrix** A **is of full rank. Solve the system** $\mathrm{Ax} = \mathrm{b}$**:**

(a) **with the Octave/MATLAB command** $\backslash$

(b) **solving the normal equations by the Cholesky method, after representing the corresponding matrix in sparse format**

(c) **using the QR decomposition approach**

(d) **using the SVD decomposition approach**

(e) **using the Octave/MATLAB command** `pinv`**.**

Compare all the numerical solutions obtained with the reference solution obtained with the Octave/MATLAB command $\backslash$ **by computing relative** l_2 **and** l_∞ **errors. Compare the time required to compute the solution by each method.**

Exercise 4

Build the $N \times N$ matrix $\tilde{\mathrm{A}}$ that has elements equal to 4 on the main diagonal, -1 on the first super and subdiagonal and $-1/2$ in the positions $(1, N)$ and $(N, 1)$. Build the vector $\tilde{\mathrm{b}} = [1, 1, \ldots, 1, 1]^T \in \mathrm{R}^N$. Build then the $10N \times N$ matrix A which contains 10 blocks equal to $\tilde{\mathrm{A}}$ and the vector $\mathrm{b} \in \mathrm{R}^{10N}$ which contains 10 blocks equal to $\tilde{\mathrm{b}}$ multiplied by the integers $1, \ldots, 10$. Check that the resulting matrix A is of full rank. Solve the system $\mathrm{Ax} = \mathrm{b}$ for $N = 300$ and $N = 1000$:

(a) **with the Octave/MATLAB command $\backslash$ to obtain the reference solution $x_\backslash$;**

(b) **using the QR decomposition approach;**

(c) **solving the normal equations by the Cholesky method, after representing the corresponding matrix in sparse format;**

(d) **solving the normal equations with `pcg`, after representing the corresponding matrix in sparse format (use as tolerance the 2-norm of the residual for the Cholesky solution, and $x_\backslash + 10$ as an initial guess);**

Compare all the numerical solutions with $x_\backslash$ by computing relative l_2 and l_∞ errors. Compare the time required to compute the solution by each method. Check what happens trying to employ the SVD method in this case.