MA5233 Computational Mathematics

Homework Sheet 4

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Recommended deadline: 19 September 2019
Final deadline: 19 September 2019, 7pm

Consider the following definitions.

- A matrix $A \in \mathbb{R}^{n\times n}$ is called *column-wise diagonally dominant* if for all $j \in \{1,\dots,n\}$ we have
$$A_{jj} \geq \sum_{i\neq j} |A_{ij}|.$$
The notation $i \neq j$ below the sum indicates that the sum is taken over $i \in \{1,\dots,n\} \setminus \{j\}$.
- A matrix $A \in \mathbb{R}^{n\times n}$ is called *symmetric positive semi-definite* (SPSD) if A is symmetric ($A^T = A$) and for all $v \in \mathbb{R}^n$ we have $v^T A v \geq 0$.

This homework sheet will

- examine the relationships between these two classes of matrices, and
- study the consequences of the above properties regarding pivoting in the LU factorisation.

You may have noticed that this homework sheet is somewhat longer than usual. To compensate for this, there will be no homework sheet released on the 12 September (next week), and this sheet will carry twice the weight compared to the sheets so far.

1 Alternative definition of symmetric positive semi-definite

Show that a symmetric matrix A is positive semi-definite if and only if all of its eigenvalues λ_k are nonnegative.

Solution. Since A is symmetric, it can be written as $A = X\Lambda X^T$ where $X \in \mathbb{R}^{n\times n}$ is the orthogonal matrix of eigenvectors $X[:,k] = x_k$ and $\Lambda \in \mathbb{R}^{n\times n}$ is the diagonal matrix with the eigenvalues $\Lambda[k,k] = \lambda_k$ on the diagonal.

Let us first assume that all eigenvalues λ_k are nonnegative. Then,
$$v^T A v = v^T X \Lambda X^T v = \sum_{k=1}^{n} \lambda_k \, (x_k^T v)^2 \geq 0$$
and hence A is positive semi-definite. Conversely, if one of the λ_k is negative, then
$$x_k^T A x_k = \lambda_k < 0$$
and hence A is not positive semi-definite.

2 Diagonally dominant vs. symmetric positive semi-definite

1. Show Gershgorin's circle theorem, which states that the eigenvalues of a matrix $A \in \mathbb{C}^{n\times n}$ are contained in the union of all disks with centres $c = A_{jj}$ and radii $r = \sum_{i\neq j} |A_{ij}|$.

   Hints.

   - An alternative formulation of Gershgorin's circle theorem is

     $$Ax = \lambda x \qquad \Longrightarrow \qquad \lambda \in \bigcup_{j=1}^{n} D\Big(A_{jj},\, \textstyle\sum_{i\neq j} |A_{ij}|\Big)$$

     where $D(c, r) := \{z \in \mathbb{C} \mid |z - c| \le r\}$ denotes the disk in the complex plane with centre $c \in \mathbb{C}$ and radius $r > 0$.
   - Consider a left eigenvector y, i.e. a vector y such that $y^T A = \lambda y^T$ for some $y \in \mathbb{R}^n$, and assume y is scaled such that $\|y\|_\infty = 1$. The claim then follows from the equation $y^T A = \lambda\, y^T$.

   Solution. Let y be as in the hint, and assume j is one of the indices such that $|y_j| = 1$. Then,

   $$(y^T A)_j = \sum_{i\neq j} A_{ij} y_i + A_{jj}\, y_j = \lambda\, y_j$$

   and hence

   $$|\lambda - A_{jj}| = |\lambda - A_{jj}|\, |y_j| \le \sum_{i\neq j} |A_{ij}|\, |y_i| \le \sum_{i\neq j} |A_{ij}|$$

   where in the last step we used $|y_i| \le 1$ for all i. Thus,

   $$|\lambda - A_{jj}| \le \sum_{i\neq j} |A_{ij}| \qquad \Longleftrightarrow \qquad \lambda \in D\Big(|A_{jj}|, \textstyle\sum_{i\neq j} |A_{ij}|\Big).$$

2. Show that a symmetric column-wise diagonally dominant matrix A is symmetric positive semi-definite.

   Solution. Gershgorin's circle theorem implies

   $$A_{jj} - \lambda \le \sum_{i\neq j} |A_{ij}| \qquad \Longleftrightarrow \qquad \lambda \ge A_{jj} - \sum_{i\neq j} |A_{ij}| \ge 0.$$

   Hence, A is positive semi-definite according to Exercise 1.

3. Provide a symmetric positive semi-definite 2×2 matrix which is not column-wise diagonally dominant.

Solution. Consider the matrix

$$A = \begin{pmatrix} 4 & 2 \\ 2 & 1 \end{pmatrix} = \begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 1 & \\ & 0 \end{pmatrix} \begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}^T.$$

This matrix is positive semi-definite (its eigenvalues are 1 and 0), but it is not diagonally dominant.

3 Pivoting for diagonally dominant matrices

Assume the matrix

$$A = \begin{pmatrix} \alpha & b^T \\ c & D \end{pmatrix}$$

with $\alpha \in \mathbb{R}$, $c, b \in \mathbb{R}^{n-1}$ and $D \in \mathbb{R}^{n-1 \times n-1}$ is column-wise diagonally dominant, and consider a single step of LU factorisation applied to this matrix,

$$\begin{pmatrix} \alpha & b^T \\ c & D \end{pmatrix} = \begin{pmatrix} 1 & \\ \frac{c}{\alpha} & I \end{pmatrix} \begin{pmatrix} \alpha & b^T \\ & D - \frac{cb^T}{\alpha} \end{pmatrix}.$$

1. Show that the lower-right block $\tilde{A} := D - \frac{cb^T}{\alpha}$ of the resulting matrix is column-wise diagonally dominant.

   Hint. You will need the inequalities

   $$D_{jj} - |b_j| \geq \sum_{i \neq j} |D_{ij}| \qquad \text{and} \qquad \alpha - |c_j| \geq \sum_{i \neq j} |c_j|$$

   which hold for all $j \in \{1, \ldots, n-1\}$ and follow from the diagonal dominance of A. The notation $i \neq j$ below the sums indicates that the sum is taken over $i \in \{1, \ldots, n-1\} \setminus \{j\}$.

   Solution. We compute using the provided hint that

   $$\begin{aligned} \tilde{A}_{jj} &= D_{jj} - \frac{c_j b_j}{\alpha} \\ &\geq D_{jj} - \frac{|c_j||b_j|}{\alpha} \\ &= D_{jj} - |b_j| + \left(\alpha - |c_j|\right) \frac{|b_j|}{\alpha} \\ &\geq \sum_{i \neq j} \left(|D_{ij}| + \frac{|c_i||b_j|}{\alpha} \right) \\ &\geq \sum_{i \neq j} \left| D_{ij} - \frac{c_i b_j}{\alpha} \right| \\ &= \sum_{i \neq j} |\tilde{A}_{ij}|. \end{aligned}$$

2. Show that column-pivoting does not swap any rows when selecting the pivot for the first column of A.

   Solution. It follows from $A_{11} \geq \sum_{i \neq 1} |A_{i1}|$ that $A_{11} \geq |A_{i1}|$ for all i, hence A_{11} is the largest element in the first column of A.

3. Conclude that LU factorisation with column pivoting applied to A does not swap any rows.

   Solution. According to Task 2, column pivoting does not swap any rows in the first step of LU factorisation. The full factorisation can then be obtained by applying LU factorisation recursively to $\tilde{A} = D - \frac{cb^T}{\alpha}$, and since this matrix is again column-wise diagonally dominant according to Task 1, no pivoting will occur in this recursion.

4 Further remarks (unmarked)

One can show that if A is column-wise diagonally dominant, then its LU factors satisfy

$$\max_{ij} |L_{ij}| \leq 1, \qquad \max_{ij} |U_{ij}| \leq 2 \max_{ij} |A_{ij}| \tag{1}$$

(the statement regarding L is easy to show, the statement regarding U requires quite a bit of work). If we assume e.g. the norm $\|M\|_\infty = \max_i \sum_j |M_{ij}|$, then this implies

$$\|L\|_\infty \leq n, \qquad \|U\|_\infty \leq 2n \, \|A\|_\infty$$

and hence the exponential growth of the entries of the U-factor that we observed for the Wilkinson matrix on sheet 2 is not possible for column-wise diagonally dominant matrices.

If A is symmetric positive semi-definite, then column pivoting may swap rows. However, it can be shown that even without column pivoting, similar entry-wise bounds as in (1) hold; hence exponential blow-up of rounding errors as we have observed in the LU factorisation of the Wilkinson matrix is again not possible if A is symmetric positive semi-definite.

The following books contain more details regarding the above statements.

- B. Wendroff. *Theoretical Numerical Analysis.* DOI:10.1016/C2013-0-12559-7
- N. Highan. *Accuracy and Stability of Numerical Algorithms* DOI:10.1137/1.9780898718027