Chapter 1
Introduction

Remark 1.1. Contents of the lecture notes. These lecture notes consider solvers for a linear system of equation

$$A\underline{x} = \underline{b}, \quad A \in \mathbb{R}^{n\times n}, \underline{x}, \underline{b} \in \mathbb{R}^n, \tag{1.1}$$

with a non-singular matrix A. The solution of such systems is the core of many algorithms.

In particular, systems with the following features will be considered in these notes:

- the dimension n of the systems is very large,
- the system matrix A is sparse, i.e., the number of non-zero entries in A is only a small percentage, usually $\mathcal{O}(n)$, of the total number of entries that is n^2.

Systems with these features arise, e.g., in the discretization of partial differential equations.

Throughout the lecture notes, vectors are denoted by small underlined letters, components of vectors by small letters, matrices by capital letters, scalars by Greek letters, and indices by the letters i, j, l, m. The iteration index in iterative scheme is denoted by k.

Main parts of these lecture notes follow Starke (2001). □

Chapter 2
Some Basics on Vectors and Matrices

Remark 2.1. Contents. This chapter gives an overview on vector and matrix properties that will be used in these lecture notes. □

Remark 2.2. Norms of vectors. Let $\underline{x} = (x_1, \ldots, x_n)^T \in \mathbb{R}^n$ be a vector. The l^p-norm is defined by

$$\begin{aligned} \|\underline{x}\|_p &:= \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}, \quad p \in [1, \infty), \\ \|\underline{x}\|_\infty &:= \max_{i=1,\ldots,n} |x_i| . \end{aligned}$$

If $p = 1$, the norm is called sum norm, in the case $p = 2$ one speaks of the Euclidean norm, and for $p = \infty$ of the maximum norm. □

Remark 2.3. Norms of matrices. Let

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

The induced matrix p-norm is defined by

$$\|A\|_p := \max_{\underline{x} \in \mathbb{R}^n, \underline{x} \neq \underline{0}} \frac{\|A\underline{x}\|_p}{\|\underline{x}\|_p} = \max_{\underline{x} \in \mathbb{R}^n, \|\underline{x}\|_p \leq 1} \|A\underline{x}\|_p = \max_{\underline{x} \in \mathbb{R}^n, \|\underline{x}\|_p = 1} \|A\underline{x}\|_p. \quad (2.1)$$

Special cases are

$$\begin{aligned} \|A\|_1 &= \max_{j=1,\ldots,n} \sum_{i=1}^n \left| a_{ij} \right|, \quad \text{(maximum absolute) column sum norm}, \\ \|A\|_2 &= \left(\lambda_{\max} \left(A^T A \right) \right)^{1/2}, \quad \text{spectral norm}, \end{aligned}$$

$$\|A\|_\infty = \max_{i=1,\ldots,n} \sum_{j=1}^{n} \left|a_{ij}\right|, \quad \text{(maximum absolute) row sum norm.}$$

Another norm is the Frobenius[1] norm given by

$$\|A\|_F = \left(\sum_{i,j=1}^{n} \left|a_{ij}\right|^2 \right)^{1/2}.$$

□

Remark 2.4. Properties of matrix norms. From (2.1), it follows immediately for all $\underline{x} \in \mathbb{R}^n \setminus \{\underline{0}\}$ that

$$\|A\|_p \geq \frac{\|A\underline{x}\|_p}{\|\underline{x}\|_p} \quad \Longleftrightarrow \quad \|A\underline{x}\|_p \leq \|A\|_p \|\underline{x}\|_p .$$

The right-hand side estimate holds also for $\underline{x} = \underline{0}$. It holds also $\|A\underline{x}\|_2 \leq \|A\|_F \|\underline{x}\|_2$. Matrix and vector norms that allow an estimate of this type are called compatible.

By induction, it follows for $B \in \mathbb{R}^{n\times n}$ that

$$\|AB\underline{x}\|_p \leq \|A\|_p \|B\underline{x}\|_p \leq \|A\|_p \|B\|_p \|\underline{x}\|_p \quad \Longleftrightarrow$$
$$\|AB\|_p = \max_{\underline{x}\in\mathbb{R}^n, \underline{x}\neq\underline{0}} \frac{\|AB\underline{x}\|_p}{\|\underline{x}\|_p} \leq \|A\|_p \|B\|_p .$$

□

Definition 2.5. Eigenvalues, eigenvectors, spectral radius. A complex number $\lambda \in \mathbb{C}$ is called eigenvalue of $A \in \mathbb{R}^{n\times n}$, if there is a vector $\underline{x} \in \mathbb{C}^n, \underline{x} \neq \underline{0}$, such that

$$A\underline{x} = \lambda\underline{x}.$$

The vector $\underline{x}$ is called eigenvector. Note that all real (complex) eigenvalues will be associated to real (complex) eigenvectors.

The spectral radius of a matrix A is defined by

$$\rho(A) = \max\{|\lambda| \ : \ \lambda \text{ is eigenvalue of A}\}.$$

□

Lemma 2.6. Properties of non-singular quadratic matrices. *Let $A \in \mathbb{R}^{n\times n}$. The following properties are equivalent:*

- *A is non-singular.*
- *The inverse A^{-1} of A exists.*

[1] Ferdinand Georg Frobenius (1849 – 1917)

- *The linear system* (1.1) *possesses for each right-hand side* $\underline{b}$ *a unique solution.*
- *The determinant of* A *does not vanish:* $\det(A) \neq 0$.
- *All eigenvalues of* A *are different from zero.*

Proof. This lemma was proved in the course on basic linear algebra. ■

Remark 2.7. On eigenvalues. For every eigenvalue $\lambda_j \in \mathbb{C}$ of A, it holds $\left|\lambda_j\right| \le \|A\|$ for any matrix norm which is given in Remark 2.3, see Numerical Mathematics I for a proof of this statement. It follows that $\rho(A) \le \|A\|$. □

Lemma 2.8. Existence of a matrix norm that is arbitrarily close to the spectral radius. *Let* $A \in \mathbb{R}^{n\times n}$ *and* $\varepsilon > 0$ *be given. Then, there is a vector norm* $\|\cdot\|_*$ *such that for the induced matrix norm, it holds*

$$\rho(A) \le \|A\|_* \le \rho(A) + \varepsilon.$$

Proof. The proof uses Schur's[2] triangulation theorem: Every matrix $A \in \mathbb{R}^{n\times n}$ can be factored in the form $A = U^*TU$, where $U \in \mathbb{C}^{n\times n}$ is a unitary matrix, $U^* = U^{-1}$ (the adjoint matrix is the inverse matrix), and T is an upper triangular matrix of the form

$$T = \begin{pmatrix} \lambda_1 & t_{12} & \cdots & t_{1n} \\ 0 & \lambda_2 & \cdots & t_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \in \mathbb{R}^{n\times n},$$

with the eigenvalues $\lambda_1, \ldots, \lambda_n$ of A, e.g., see (Marcus & Minc, 1992, p. 67). The vector norm $\|\cdot\|_*$ is defined with the diagonal matrix $D_\delta = \operatorname{diag}\left(1, \delta, \ldots, \delta^{n-1}\right)$, $\delta > 0$, to be determined:

$$\|\underline{x}\|_* := \left\|D_\delta^{-1} U \underline{x}\right\|_\infty.$$

For the induced matrix norm, it follows, using the Schur triangulation of A, that

$$\|A\|_* := \max_{\underline{x}\in\mathbb{R}^n, \underline{x}\neq\underline{0}} \frac{\left\|D_\delta^{-1} U A \underline{x}\right\|_\infty}{\left\|D_\delta^{-1} U \underline{x}\right\|_\infty} = \max_{\underline{x}\in\mathbb{R}^n, \underline{x}\neq\underline{0}} \frac{\left\|D_\delta^{-1} U U^* T U \underline{x}\right\|_\infty}{\left\|D_\delta^{-1} U \underline{x}\right\|_\infty}. \tag{2.2}$$

Setting $\underline{y} = D_\delta^{-1} U \underline{x}$, it follows that $\underline{x} = U^* D_\delta \underline{y}$ since the matrices U and D_δ are non-singular and $D_\delta^{-1} U$ is a bijection from $\mathbb{R}^n$ to $\mathbb{R}^n$. Inserting this expression in (2.2) and using the definition of the row sum norm gives

$$\|A\|_* = \max_{\underline{y}\in\mathbb{R}^n, \underline{y}\neq\underline{0}} \frac{\left\|D_\delta^{-1} U U^* T U U^* D_\delta \underline{y}\right\|_\infty}{\left\|\underline{y}\right\|_\infty} = \left\|D_\delta^{-1} T D_\delta\right\|_\infty.$$

The diagonal matrix D_δ^{-1} scales just the rows of T and the matrix D_δ just the columns of T. Thus, the product is again an upper triangular matrix and a straightforward calculation shows that

[2] Issai Schur (1875 – 1941)

$$D_\delta^{-1} T D_\delta = \begin{pmatrix} \lambda_1 & \delta t_{12} & \cdots & \delta^{n-1} t_{1n} \\ 0 & \lambda_2 & \cdots & \delta^{n-2} t_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \delta t_{n-1,n} \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$$

and hence $\left\| D_\delta^{-1} T D_\delta \right\|_\infty \leq \rho(A) + \varepsilon$ if δ is chosen sufficiently small. ■

Definition 2.9. Spectral condition number. The spectral condition number $\kappa_2(A)$ of a non-singular matrix $A \in \mathbb{R}^{n\times n}$ is defined by

$$\kappa_2(A) = \|A\|_2 \left\| A^{-1} \right\|_2 .$$

□

Definition 2.10. Definiteness. The matrix $A \in \mathbb{R}^{n\times n}$ is called positive definite if

$$\underline{x}^T A \underline{x} > 0 \quad \forall\, \underline{x} \in \mathbb{R}^n \setminus \{\underline{0}\}. \tag{2.3}$$

If the equal sign can occur, A is called positive semi-definite. □

Remark 2.11. On definiteness. Applying the standard basis vectors (Cartesian[3] basis vectors)

$$\underline{e}^{(i)} = (0, \ldots, 0, \underbrace{1}_{i}, 0, \ldots, 0)^T, \quad i = 1, \ldots, n,$$

in (2.3) shows that if A is positive (semi-)definite then also the diagonal matrix $\operatorname{diag}(a_{ii})$ is positive (semi-)definite. □

Remark 2.12. On symmetric matrices. A matrix $A \in \mathbb{R}^{n\times n}$ is called symmetric if $A = A^T$. It is called skew-symmetric if $A^T = -A$.

One of the most important properties of symmetric matrices is that all eigenvalues are real numbers. It holds, e.g., see Saad (2003),

$$\lambda_{\max}(A) = \max_{\underline{x}\in\mathbb{R}^n, \underline{x}\neq\underline{0}} \frac{\underline{x}^T A \underline{x}}{\underline{x}^T \underline{x}}, \quad \lambda_{\min}(A) = \min_{\underline{x}\in\mathbb{R}^n, \underline{x}\neq\underline{0}} \frac{\underline{x}^T A \underline{x}}{\underline{x}^T \underline{x}}. \tag{2.4}$$

The quotient on the right-hand side is called Rayleigh[4] quotient. A symmetric matrix is positive definite (s.p.d.) if and only if all of its eigenvalues are positive. It is positive semi-definite if and only if all of its eigenvalues are non-negative.

In the case of $A \in \mathbb{R}^{n\times n}$ being symmetric and positive definite, one obtains for the spectral norm of A

[3] René Descartes (1596 – 1650)

[4] John William Strutt (Lord Rayleigh) (1842 – 1919)

$$\|A\|_2 = \left(\lambda_{\max}\left(A^T A\right)\right)^{1/2} = \left(\lambda_{\max}\left(A^2\right)\right)^{1/2} = \left(\left(\lambda_{\max}\left(A\right)\right)^2\right)^{1/2}$$
$$= \lambda_{\max}\left(A\right).$$

It was used that the eigenvalues of A^2 are the squares of the eigenvalues of A, which is obtained by

$$A^2 \underline{x} = A\left(A\underline{x}\right) = A\left(\lambda\underline{x}\right) = \lambda A\underline{x} = \lambda^2\underline{x}.$$

Since

$$A\underline{x} = \lambda\underline{x} \quad \Longleftrightarrow \quad A^{-1}\underline{x} = \frac{1}{\lambda}\underline{x},$$

the eigenvalues of A^{-1} are the inverses of the eigenvalues of A. In particular, one finds that $\lambda_{\max}\left(A^{-1}\right) = \left(\lambda_{\min}\left(A\right)\right)^{-1}$. With the same arguments as for $\|A\|_2$, it follows that $\left\|A^{-1}\right\|_2 = \left(\lambda_{\min}\left(A\right)\right)^{-1}$ and finally

$$\kappa_2\left(A\right) = \frac{\lambda_{\max}\left(A\right)}{\lambda_{\min}\left(A\right)} \geq 1.$$

For each symmetric matrix $A \in \mathbb{R}^{n\times n}$ there is an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ such that

$$A = Q\ \mathrm{diag}(\lambda_i)\ Q^T,$$

where λ_i, $i = 1, \ldots, n$, are the eigenvalues of A. If A is in addition positive definite, then all eigenvalues are positive and the square root of A is defined by

$$A^{1/2} := Q\ \mathrm{diag}\left(\lambda_i^{1/2}\right)\ Q^T.$$

□

Definition 2.13. Diagonal dominance. A matrix A is called diagonally dominant if

$$|a_{ii}| \geq \sum_{j=1, j\neq i}^{n} \left|a_{ij}\right| \quad \text{for all } i = 1, \ldots, n.$$

If for all i the larger sign holds, then A is called strongly diagonally dominant. □

Definition 2.14. Normal matrix. The matrix $A \in \mathbb{R}^{n\times n}$ is called normal, if $A^T A = AA^T$. □

Remark 2.15. On normal matrices.

- It is known that A is normal if and only if it is unitary similar to a diagonal matrix, i.e., there is a unitary matrix $Q \in \mathbb{R}^{n\times n}$ (orthogonal matrix) such that

$$A = Q^* \Lambda Q, \quad \Lambda = \mathrm{diag}\left(\lambda_1, \ldots, \lambda_n\right),$$

  where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of A.

- From Definition 2.14, it follows directly that symmetric matrices are normal.

□