CHAPTER I

Introduction

In this lecture, we discuss theory, numerics and application of advanced problems in linear algebra:

(II) matrix equations (example: solve $AX + XB = C$),

(III) matrix functions: compute $f(A)$ or $f(A)b$, where $A \in \mathbb{C}^{n \times n}$, $b \in \mathbb{C}^n$,

(IV) randomized algorithms.

The main focus is on problems defined by real matrices/vectors. In most chapters, we have to make the distinction between problems defined by

- dense matrices of small /moderate dimensions and
- large, sparse matrices, e.g. $A \in \mathbb{C}^{n \times n}$, $n > 10^4$ or greater, but only $\mathcal{O}(n)$ nonzero entries, often from PDEs.

We first have to review two important standard problems in numerical linear algebra, namely solving linear systems of equations and eigenvalue problems.

I.1 Linear systems of equations

We consider the linear system

$$Ax = b, \tag{I.1}$$

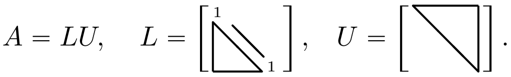
with $A \in \mathbb{C}^{n \times n}\, (\mathbb{R}^{n \times n}), \quad b \in \mathbb{C}^n\, (\mathbb{R}^n)$. The linear system (I.1) admits a unique solution, if and only if

- there exists an inverse A^{-1}
- $\det(A) \neq 0$
- no eigenvalues/ singular values are equal to zero
- $\ldots$

Numerical methods for small and dense $A \in \mathbb{C}^{n \times n}$

Gaussian Elimination (LU-factorization):

We decompose A such that



We obtain, that

$$(\text{I.1}) \quad \Leftrightarrow \quad LUx = b \quad \Leftrightarrow \quad x = U^{-1}(L^{-1}b).$$

Hence, we solve (I.1) in two steps:

1. Solve $Ly = b$ via backward substitution.
2. Solve $Ux = y$ via backward substitution.

This procedure is numerically more robust with pivoting $PAQ = LU$, where P, $Q \in \mathbb{C}^{n,n}$ are permutation matrices. This method has a complexity of $\mathcal{O}(n^3)$ and is, therefore, only feasible for small (moderate) dimensions.

QR-decomposition:

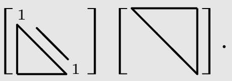
We decompose A into a product of Q and R where Q is an orthogonal matrix and R is an upper triangular matrix leading to the so-called Gram-Schmidt or the modified Gram-Schmidt algorithm. Numerically this can be done either with Givens rotations or with Householder transformations.

Methods for large and sparse $A \in \mathbb{C}^{n \times n}$

Storing and computing dense LU-factors is infeasible for large dimensions n ($\mathcal{O}(n^2)$ memory, $\mathcal{O}(n^3)$ flops). One possibility are *sparse direct solvers*, i.e. find permutation matrices P and Q, such that $PAQ = LU$ has sparse LU-factors (cheap forward/ backward substitution and $\mathcal{O}(n)$ memory).

Example: We consider the LU-factorization of the following matrix

$$A = \begin{bmatrix} * & \cdots & * \\ \vdots & \ddots & \\ * & & * \end{bmatrix} =$$



With the help of permutation matrices P and Q, we can factorize

$$PAQ = \begin{bmatrix} * & & * \\ & \ddots & \vdots \\ * & \cdots & * \end{bmatrix} = \begin{bmatrix} * & & \\ \vdots & \ddots & \\ * & & * \end{bmatrix} \begin{bmatrix} * & \cdots & * \\ & \ddots & \\ & & * \end{bmatrix}.$$

Algorithm 1 Arnoldi method

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Input: $A \in \mathbb{C}^{n\times n}$, $b \in \mathbb{C}^n$
Output: Orthonormal basis $Q_k$ of (I.2)
Set $q_1 = \frac{b}{\|b\|}$ and $Q_q := [q_1]$.
for $j = 1, 2, \dots$ do
    Set $z = Aq_j$.
    Set $w = z - Q_j(Q_j^{\mathrm{H}} z)$.
    Set $q_{j+1} = \frac{w}{\|w\|}$.
    Set $Q_{j+1} = [Q_j, q_{j+1}]$.
end for
```

Finding such P and Q and still ensuring numerical robustness is difficult and based e.g. on graph theory.

In MATLAB, sparse-direct solvers are found in the "$\backslash$"-command: $x = A\backslash b$ or $\mathrm{lu}(A)$-routine. (Never use $\mathrm{inv}(A)$!)

Iterative methods

Often an approximation $\hat{x} \approx x$ is sufficient. Hence, we generate a sequence $x_1, x_2, \dots, x_k$ by an iteration, such that

$$\lim_{k\to\infty} x_k = x = A^{-1}b$$

and each x_k, $k \geqslant 1$ is generated efficiently (only $\mathcal{O}(n)$ computations). Of course, we want $x_k \approx x$ for $k \ll n$.

Idea: Search approximated solution in a low-dimensional subspace $\mathcal{Q}_k \subset \mathbb{C}^n$, $\dim(\mathcal{Q}_k) = k$. Let $\mathcal{Q}_k$ be given as $\mathrm{range}(Q_k) = \mathcal{Q}_k$ for a matrix $Q_k \in \mathbb{C}^{n\times k}$.

A good choice of the subspace is the Krylow-subspace

$$\mathcal{Q}_k = \mathcal{K}_k(A, b) = \mathrm{span}\{b, Ab, \dots, A^{k-1}b\}. \tag{I.2}$$

It holds for $z \in \mathcal{K}_k(A, b)$, that $z = p(A)b$ for a polynomial of degree $k-1$ $p \in \Pi_{k-1}$. An orthonormal basis of $\mathcal{K}_k(A, b)$ can be constructed with the *Arnoldi process* presented in Algorithm 1.

The Arnoldi process requires matrix-vector products $z = Aq$. These are cheap for sparse A and therefore feasible for large dimensions.

We find an approximation $x_k \in x_0 + \mathcal{Q}_k$ by two common ways:

- Galerkin-approach:
  Impose $r = b - Ax_k \perp \mathrm{range}(Q_k) \quad \Leftrightarrow \quad (Q_k^{\mathrm{H}} A Q_k) y_k = Q_k^{\mathrm{H}} b$.

  We have to solve a k-dimensional system ⇒ low costs.

- Minimize the residual:

$$\min_{x_k \in \operatorname{range}(Q_k)} \|b - Ax_k\|$$

  in some norm. If x_k is not good enough, we expand Q_k.

There are many Krylov-subspace methods for linear systems. (Simplification for $A = A^{\mathrm{H}}$: Arnoldi $\rightsquigarrow$ Lanczos)

In practice: Convergence acceleration by *preconditioning*:

$$Ax = b \quad \Leftrightarrow \quad P^{-1}Ax = P^{-1}b$$

for easily invertible $P \in \mathbb{C}^{n,n}$ and $P^{-1}A$ "nicer" than A ($\rightsquigarrow$ Literature NLA I).

Another very important building block is the numerical solution of eigenvalue problems.

I.2 Eigenvalue problems (EVP)

For a matrix $A \in \mathbb{C}^{n,n}$ we want to find the eigenvectors $0 \neq x \in \mathbb{C}^n$ and the eigenvalues $\lambda \in \mathbb{C}$ such that

$$Ax = \lambda x.$$

The set of eigenvalues $\Lambda(A) = \{\lambda_1, \ldots, \lambda_n\}$ is called the *spectrum of* A.

Small, dense problems:

Computing the Jordan-Normal-Form (JNF)

$$X^{-1}AX = J = \operatorname{diag}(J_{s_1}(\lambda_1), \ldots, J_{s_k}(\lambda_k)), \quad J_{s_j}(\lambda_j) := \begin{bmatrix} \lambda_j & 1 & \\ & \ddots & 1 \\ & & \lambda_j \end{bmatrix}$$

to several eigenvalues and eigenvectors is numerically infeasible, unstable (NLA I).

Theorem I.1 (Schur)**:** For all $A \in \mathbb{C}^{n\times n}$ exists a unitary matrix $Q \in \mathbb{C}^{n,n}$ ($Q^{\mathrm{H}}Q = I$), such that

$$Q^{\mathrm{H}}AQ = R = \underbrace{\begin{bmatrix} \lambda_1 & & * \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix}}_{\text{Schur form of } A}$$

with $\lambda_i \in \Lambda(A)$ in arbitrary order.

The Schur form can be numerically stable computed in $\mathcal{O}(n^3)$ (NLA I) by the Francis-QR-algorithm. It is this basis for dense eigenvalue computations. In MATLAB we use $[\mathrm{Q}, \mathrm{R}] = \mathrm{schur}(\mathrm{A})$. Additionally, the routine $\mathrm{eigs}(\mathrm{A})$ uses the Schur form. In general, the columns of Q are no eigenvectors of A, but $Q_k = Q(:, 1 : k)$ spans an A-*invariant subspace* for all k:

$$AQ_k = Q_k R_k, \quad \text{for a matrix } R_k \in \mathbb{C}^{k \times k} \text{ with } \Lambda(R_k) \subseteq \Lambda(A).$$

But because of the $\mathcal{O}(n^3)$ complexity and $\mathcal{O}(n^2)$ memory, the Schur form is infeasible for large and sparse matrices A.

Eigenvalue problems defined by large and sparse matrices A can again be treaded with the Arnoldi-process and projections on the Krylov-subspace $\mathcal{K}_k(A, b) = \mathrm{range}(Q_k)$. We obtain the approximated eigenpair $x_k = Q_k y_k \approx x$, $\mu \approx \lambda$ by using the Galerkin-condition on the residual of the eigenvalue problem:

$$r_k = Ax_k - \mu\, x_k \perp \mathrm{range}(Q_k) \quad \Leftrightarrow \quad Q_k^{\mathrm{H}} A Q_k y_k = \mu\, y_k,$$

which means (μ, y_k) are the eigenpairs of the $k \times k$-dimensional eigenvalue problem for $Q_k^{\mathrm{H}} A Q_k$. This small eigenvalue problem is solvable by the Francis-QR-method. This is the basis of the $\mathrm{eigs}(\mathrm{A})$ routine in MATLAB for computing a few ($\ll n$) eigenpairs of A.

Summary: Solving linear systems and eigenvalue problems is for small or large and sparse matrices A no problem!

CHAPTER II

Matrix Equations

II.1 Preliminaries

Up to now we know linear systems of equations

$$Ax = b,$$

where $A \in \mathbb{R}^{n\times n}$ and $b \in \mathbb{R}^n$ are given and $x \in \mathbb{R}^n$ has to be found.

In this course we consider more general equations

$$F(X) = C, \tag{II.1}$$

where $F : \mathbb{R}^{q\times r} \to \mathbb{R}^{p\times s}$, $C \in \mathbb{R}^{p\times s}$ is given, and $X \in \mathbb{R}^{q\times r}$ has to be found. Equations of the form (II.1) are called *algebraic matrix equations*.

II.1.1 Examples of Algebraic Matrix Equations

1) $F(X) = AXB$, i. e., (II.1) is

$$AXB = C.$$

2) Sylvester equations:

$$AX + XB = C,$$

3) algebraic Lyapunov equations:

   a) continuous time:

   $$AX + XA^T = -BB^T, \quad X = X^T,$$

   b) discrete time:

   $$AXA^T - X = -BB^T, \quad X = X^T,$$

4) algebraic Riccati equations:

   a) continuous time:

   $$A^TX + XA - XBR^{-1}B^TX + C^TQC = 0, \quad X = X^T,$$

   b) discrete time:

   $$\begin{aligned} A^TXA - X - (A^TXB)(R + B^TXB)^{-1}(B^TXA) \\ + C^TQC = 0, \quad X = X^T. \end{aligned}$$

c) non-symmetric

$$AX + XM - XGX + Q = 0.$$

Examples 1) – 3) are *linear* matrix equations, since the map F is linear. Equations of the type 4) are called *quadratic* matrix equations. The goal of this lecture is to understand the solution theory as well as numerical algorithms for the above matrix equations. Our focus will be on the equations 2),3a) and 4a) since these are the equations mainly appearing in the applications.

The term *continuous-/discrete-time* in 3a,b), 4a,b) refers to applications in context of *continuous-time dynamical systems*

$$\dot{x}(t) = Ax(t), \quad t \in \mathbb{R}$$

or *discrete-time dynamical systems*

$$x_{k+1} = Ax_k, \quad k \in \mathbb{N},$$

respectively. More info in courses on *control theory* or *model order reduction*.

There are also variants of the above equations containing X^T or X^H – these will not play a prominent role here. Furthermore, there are matrix equations where $X = X(t)$ is a matrix-valued function and F contains derivative information of X. Such equations are called *differential matrix equations*, for example the *differential Lyapunov equation*

$$\dot{X}(t) + A(t)^T X(t) + X(t)A(t) + Q(t) = 0,$$

where $A,\ Q \in C([t_0, t_\mathrm{f}], \mathbb{R}^{n\times n})$, and $X \in C^1([t_0, t_\mathrm{f}], \mathbb{R}^{n\times n})$ with $Q(t) = Q(t)^T \geqslant 0$ and $X(t) = X(t)^T$ for all $t \in [t_0, t_\mathrm{f}]$ and the initial condition $X(t_0) = X_0$.

II.2 Linear Matrix Equations

In this chapter we discuss the solution theory and the numerical solution of linear matrix equations as defined precisely below.

Definition II.1 (linear matrix equation)**:** Let $A_i \in \mathbb{C}^{p\times q}$, $B_i \in \mathbb{C}^{r\times s}$, and $C \in \mathbb{C}^{p\times s}$, $i = 1, \dots, k$ be given. An equation of the form

$$\sum_{i=1}^{k} A_i X B_i = C \tag{II.2}$$

is called a *linear matrix equation*.

II.2.1 Solution Theory

To discuss solvability and uniqueness of solutions of (II.2) we need the following concepts.

Definition II.2 (vectorization operator and Kronecker product)**:** For $X = \begin{bmatrix} x_1 & \dots & x_m \end{bmatrix} = \begin{bmatrix} x_{11} & \dots & x_{1m} \\ \vdots & & \vdots \\ x_{n1} & \dots & x_{nm} \end{bmatrix} \in \mathbb{C}^{n\times m}$ and $Y \in \mathbb{C}^{p\times q}$

a) the vectorization operator $\operatorname{vec} : \mathbb{C}^{n\times m} \to \mathbb{C}^{nm}$ is given by

$$\operatorname{vec}(X) := \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix},$$

b) the Kronecker product is given by

$$X \otimes Y = \begin{bmatrix} x_{11}Y & \dots & x_{1m}Y \\ \vdots & & \vdots \\ x_{n1}Y & \dots & x_{nm}Y \end{bmatrix} \in \mathbb{C}^{np\times mq}.$$

Lemma II.3: For $\mathcal{T} \in \mathbb{C}^{n\times m}$, $\mathcal{O} \in \mathbb{C}^{m\times p}$, and $\mathcal{R} \in \mathbb{C}^{p\times r}$ it holds

$$\operatorname{vec}(\mathcal{T}\mathcal{O}\mathcal{R}) = \left(\mathcal{R}^T \otimes \mathcal{T}\right) \operatorname{vec}(\mathcal{O})$$

(Note that it has to be $\mathcal{R}^T$ in the above formula, even if all the matrices are complex.)

Proof. Exercise. □

By this lemma, and the obvious linearity of $\operatorname{vec}(\cdot)$, we see that

$$\sum_{i=1}^{k} A_i X B_i = C \quad \Leftrightarrow \quad \underbrace{\sum_{i=1}^{k} \left(B_i^T \otimes A_i\right)}_{\mathcal{A}} \underbrace{\operatorname{vec}(X)}_{\mathcal{X}} = \underbrace{\operatorname{vec}(C)}_{\mathcal{B}},$$

and we find that (II.2) has a unique solution if and only if the linear system of equations $\mathcal{A}\mathcal{X} = \mathcal{B}$ has one. Equivalently, $\mathcal{A}$ has to be nonsingular.

Theorem II.4: The linear matrix equation (II.2) with $ps = qr$ has a unique solution iff all eigenvalues of the matrix

$$\mathcal{A} = \sum_{i=1}^{k} \left(B_i^T \otimes A_i\right)$$

are non-zero.

In the following we will focus on the case $k \leqslant 2$ and $p = s = q = r$, since Lyapunov equations $(k = 2,\ A_1 = A,\ B_1 = A_2 = I_n,\ B_2 = A^T)$ and Sylvester equations $(k = 2,\ A_1 = A,\ B_2 = B,\ A_2 = I_n,\ B_1 = I_m)$ are important special cases of interest in applications.

To check the above condition for unique solvability, we do not want to evaluate the Kronecker products. Therefore, we now derive easily checkable conditions based on the original matrices.

Lemma II.5: a) Let W, X, Y, Z be matrices such that the products WX and YZ are defined. Then $(W \otimes Y)(X \otimes Z) = (WX) \otimes (YZ)$.

b) Let S, G be nonsingular matrices. Then $S \otimes G$ is nonsingular, too, and $(S \otimes G)^{-1} = S^{-1} \otimes G^{-1}$.

c) If A and B, as well as, C and D are similar matrices then $A \otimes C$ and $B \otimes D$ are similar (A similar to B if $\exists Q$ nonsingular s.t. $A = Q^{-1}BQ$).

d) Let $X \in \mathbb{C}^{n \times n}$ and $Y \in \mathbb{C}^{m \times m}$ be given. Then

$$\Lambda(X \otimes Y) = \{\lambda\mu \mid \lambda \in \Lambda(X),\ \mu \in \Lambda(Y)\}.$$

Proof. Exercise. □

Theorem II.6 (Theorem of Stephanos)**:** Let $A \in \mathbb{C}^{n\times n}$ and $B \in \mathbb{C}^{m\times m}$ with $\Lambda(A) = \{\lambda_1, \ldots, \lambda_n\}$, $\Lambda(B) = \{\mu_1, \ldots, \mu_m\}$ be given. For a bivariate polynomial $p(x, y) = \sum\limits_{i,j=0}^{k} c_{ij} x^i y^j$ we define by

$$p(A, B) := \sum_{i,j=0}^{k} c_{ij}(A^i \otimes B^j)$$

a polynomial of the two matrices. Then the spectrum of $p(A, B)$ is given by

$$\Lambda(p(A, B)) = \{p(\lambda_r, \mu_s) \mid r = 1, \ldots, n,\ s = 1, \ldots, m\}.$$

Proof. Use JNF or Schurforms of A, B + Lemma II.5. □

Now we are ready to consider our preferred special cases of (II.2).

a) $AXB = C$:

$$\begin{aligned}\mathcal{A} = B^T \otimes A \text{ invertible } &\Leftrightarrow \lambda \cdot \mu \neq 0 \quad \forall \lambda \in \Lambda(A) \text{ and } \mu \in \Lambda(B)\\ &\Leftrightarrow \lambda \neq 0 \text{ and } \mu \neq 0 \quad \forall \lambda \in \Lambda(A) \text{ and } \mu \in \Lambda(B)\\ &\Leftrightarrow \text{ both } A \text{ and } B \text{ are nonsingular.}\end{aligned}$$

b) continuous-time Sylvester equation $AX + XB = C$, where $A \in \mathbb{C}^{n\times n}$, $B \in \mathbb{C}^{m\times m}$, $C,\ X \in \mathbb{C}^{n\times m}$:

$$\begin{aligned}\mathcal{A} = I_m \otimes A + B^T \otimes I_n \text{ invertible } &\Leftrightarrow \lambda + \mu \neq 0 \quad \forall \lambda \in \Lambda(A) \text{ and } \mu \in \Lambda(B)\\ &\Leftrightarrow \Lambda(A) \cap \Lambda(-B) = \varnothing.\end{aligned}$$

c) continuous-time Lyapunov equation $AX + XA^H = W$, where $A,\ X \in \mathbb{C}^{n\times n}$, $W = W^H \in \mathbb{C}^{n\times n}$:

$$\mathcal{A} = I_n \otimes A + \overline{A} \otimes I_n \text{ invertible } \Leftrightarrow \Lambda(A) \cap \Lambda(-A^H) = \varnothing.$$

For example, this is the case when A is asymptotically stable.

d) discrete-time Lyapunov equations → exercise.

The following result gives some useful results about the solution structure of Sylvester equations.

Theorem II.7: Let $A \in \mathbb{C}^{n\times n}$, $B \in \mathbb{C}^{n\times n}$ with $\Lambda(A) \subset \mathbb{C}_-$,$\Lambda(B) \subset \mathbb{C}_-$. Then $AX + XB = W$ has a (unique) solution

$$X = -\int_0^\infty \mathrm{e}^{At} W \mathrm{e}^{Bt} \mathrm{d}t$$

Proof. Exercise. □

From now on

$$AX + XA^* = W, \quad W = W^*. \tag{II.3}$$

Definition II.8 (controllability)**:** Let $A \in \mathbb{C}^{n\times n}$ and $B \in \mathbb{C}^{n\times m}$. We say (A, B) is *controllable* if rank$[B, AB, \dots A^{n-1}B] = n$.

Lemma II.9: The above controllability condition is equivalent to

rank$[A - \lambda I, B] = n$ for all $\lambda \in \mathbb{C}$
$\iff y^*B \neq 0 \quad \forall y \neq 0 : \; y^*A = y^*\lambda$ (left. eigenvecs of) A

Proof. We first prove that rank$[A - \lambda I, B] = n \quad \forall \lambda \in \mathbb{C}$ is equivalent to Definition II.8. Assuming that rank$[A - \lambda I, B] < n$ for a $\lambda \in \mathbb{C}$ then there exists a $w \neq 0$ such that $w^T[A - \lambda I, B] = 0$ which means that $w^T(A - \lambda I) = 0$ and $w^T B = 0$ and that means that $w^T[B, AB, \dots A^{n-1}B] = 0$ which means (A, B) is not controllable. Assuming (A, B) is not controllable and therefore rank$[B, AB, \dots A^{n-1}B] < n$ we define a matrix M contains a basis of the image of $[B, AB, \dots A^{n-1}B]$. Then there is a matrix $\tilde{M}$ such that $T = [M, \tilde{M}]$ is invertible and

$$\tilde{A} = T^{-1}AT = \begin{bmatrix} \widetilde{A}_{11} & \widetilde{A}_{12} \\ 0 & \widetilde{A}_{22} \end{bmatrix} \tag{II.4}$$

$$\tilde{B} = T^{-1}B = \begin{bmatrix} \widetilde{B}_1 \\ 0 \end{bmatrix} \tag{II.5}$$

Let λ be an eigenvalue of $\tilde{A}_{22}$ and w_{22} a left eigenvector. Then

$$w := \begin{bmatrix} 0 \\ \tilde{w}_{22} \end{bmatrix} T^{-1} \neq 0.$$

It also holds that $w^T A = \lambda w^T$ and $w^T B = 0$ and therefore rank$[A - \lambda i, B]$ not full. The proof of the equivalence is basically also done within this proof. □

Theorem II.10: Consider Lyapunov equation (II.3) with $W = W^* = -BB^T \leqslant 0$, $B \in \mathbb{R}^{n\times m}$.

a) For $\Lambda(A) \subset \mathbb{C}_-$: (A, B) controllable ⇔ ∃ unique sol. $X = X^* > 0$.

b) Let (A, B) be controllable and assume there ∃ unique sol. $X = X^* > 0$. Then $\Lambda(A) \subset \mathbb{C}_-$.

Proof. a) If the spectrum of A is in the left half plane and $W = W^*$ then there exist a unique symmetric solution of the Lyapunov equation. What is left to prove is the equivalence of (A, B) being controllable and the solution being positive definite. The solution is given by

$$X = \int_0^\infty \mathrm{e}^{At} BB^T \mathrm{e}^{A^* t} \mathrm{d}t$$

which is positive if and only if (A, B) are controllable.

b) Take an eigenvalue $\lambda \in \Lambda(A)$ and a corresponding left eigenvector y. Then

$$0 > -y^* BB^T y = y^* AXy + y^* XA^* y = (\lambda + \bar{\lambda}) y^* Xy$$

Since $X = X^* > 0$ we must have that $\lambda + \bar{\lambda} = 2\mathrm{Re}\lambda < 0$ and since λ was arbitrary that $\Lambda(A) \subset \mathbb{C}_-$

□