CHAPTER	
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

$$Ax = b, (I.1)$$

with $A \in \mathbb{C}^{n \times n}(\mathbb{R}^{n \times n}), \ b \in \mathbb{C}^n(\mathbb{R}^n)$. 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
- . . .

3

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

Gaussian Elimination (LU-factorization):

We decompose A such that

$$A = LU, \quad L = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad U = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

We obtain, that

(1.1)
$$\Leftrightarrow LUx = b \Leftrightarrow x = U^{-1}(L^{-1}b).$$

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

$$A = \begin{bmatrix} * & \cdots & * \\ \vdots & \ddots & * \\ * & * \end{bmatrix} = \begin{bmatrix} 1 \\ \ddots & 1 \end{bmatrix} \begin{bmatrix} 1 \\ \ddots & 1 \end{bmatrix}.$$

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

Input: $A \in \mathbb{C}^{n \times n}, b \in \mathbb{C}^n$

Output: Orthonormal basis Q_k of (1.2)

1: Set
$$q_1=rac{b}{\|b\|}$$
 and $Q_q:=[q_1]$.
2: for $j=1,2,\ldots$ do

2: **for**
$$j = 1, 2, ...$$
 do

Set $z = Aq_j$.

Set $w = z - Q_j(Q_j^H z)$. 4:

 $\begin{aligned} &\text{Set } q_{j+1} = \frac{w}{\|w\|}. \\ &\text{Set } Q_{j+1} = [Q_j, q_{j+1}]. \end{aligned}$

7: 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 "\"-command: $x = A \setminus b$ or lu(A)-routine. (Never use inv(A)!)

Iterative methods

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

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

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

<u>Idea:</u> 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 $\operatorname{range}(Q_k) = \mathcal{Q}_k$ for a matrix $Q_k \in \mathbb{C}^{n \times k}$.

A good choice of the subspace is the Krylow-subspace

$$Q_k = \mathcal{K}_k(A, b) = \operatorname{span}\{b, Ab, \dots, A^{k-1}b\}.$$
(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 $x_k \in x_0 + Q_k$ by two common ways:

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

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

· Minimize the residual:

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

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 $A=A^{\rm H}$: Arnoldi \leadsto Lanczos)

In practice: Convergence acceleration by preconditioning:

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

for easily invertible $P \in \mathbb{C}^{n,n}$ and $P^{-1}A$ "nicer" than $A \ (\leadsto$ 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 $\Lambda(A) = \{\lambda_1, \dots, \lambda_n\}$ is called the *spectrum of* A.

Small, dense problems:

Computing the Jordan-Normal-Form (JNF)

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

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

$$Q^{\mathrm{H}}AQ = R = \begin{bmatrix} \lambda_1 & * \\ & \ddots & \\ 0 & \lambda_n \end{bmatrix}$$

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 $[Q,R]=\mathrm{schur}(A)$. Additionally, the routine $\mathrm{eigs}(A)$ 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 $\mathcal{K}_k(A,b) = \operatorname{range}(Q_k)$. 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:

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

which means (μ,y_k) are the eigenpairs of the $k \times k$ -dimensional eigenvalue problem for $Q_k^{\rm H}AQ_k$. This small eigenvalue problem is solvable by the Francis-QR-method. This is the basis of the ${\rm eigs}(A)$ 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 Equation	ons

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

$$F(X) = C, (II.1)$$

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:

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

b) discrete time:

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

- 4) algebraic Riccati equations:
 - a) continuous time:

$$A^{T}X + XA - XBR^{-1}B^{T}X + C^{T}QC = 0$$
, $X = X^{T}$.

b) discrete time:

$$A^{T}XA - X - (A^{T}XB)(R + B^{T}XB)^{-1}(B^{T}XA) + C^{T}QC = 0, \quad X = X^{T}.$$

II.1. Preliminaries 9

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 $C \in \mathbb{C}^{p \times s}$, $i = 1, \ldots, k$ 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 =

$$\begin{bmatrix} x_1 & \dots & x_m \end{bmatrix} = \begin{bmatrix} x_{11} & \dots & x_{1m} \\ \vdots & & \vdots \\ x_{n1} & \dots & x_{nm} \end{bmatrix} \in \mathbb{C}^{n \times m} \text{ and } Y \in \mathbb{C}^{p \times q}$$

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

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

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

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

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

and we find that (II.2) has a unique solution if and only if the linear system of equations $\mathcal{AX} = \mathcal{B}$ 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 $k \le 2$ 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

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

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:

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

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

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

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

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

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

d) discrete-time Lyapunov equations \rightarrow 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

$$X = -\int_{0}^{\infty} e^{At} W e^{Bt} dt$$

Proof. Exercise.

From now on

$$AX + XA^* = W, \quad W = W^*.$$
 (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 $\operatorname{rank}[B, AB, \dots A^{n-1}B] = n$.

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

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

Proof. We first prove that $\operatorname{rank}[A-\lambda I,B]=n \quad \forall \lambda \in \mathbb{C}$ is equivalent to Definition II.8. Assuming that $\operatorname{rank}[A-\lambda I,B] < n$ 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 $w^TB=0$ 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 $\operatorname{rank}[B,AB,\dots A^{n-1}B]< n$ 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

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

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

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 $w^TA = \lambda w^T$ and $w^TB = 0$ and therefore $\mathrm{rank}[A - \lambda i, B]$ not full. The proof of the equivalence is basically also done within this proof. \Box

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 $\Leftrightarrow \exists$ unique sol. $X=X^*>0$.
- b) Let (A,B) be controllable and assume there \exists 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

$$X = \int_{0}^{\infty} e^{At} B B^{T} e^{A^{*}t} dt$$

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

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

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

II.2.2 Direct Numerical Solution

We have seen that linear matrix equations are equivalent to linear systems. Why do we not just apply a linear solver? Consider a (real) Lyapunov equation where we obtain the system matrix $\mathcal{A}=I_n\otimes A+A\otimes I_n\in\mathbb{R}^{n^2\times n^2}$. For computing an LU-factorization of \mathcal{A} and a forward/backwards substitution we need approximately $\frac{2}{3}(n^2)^3=\frac{2}{3}n^6$ FLOPS and n^4 memory. This is only feasible for small n. If $n\gtrsim 50$, then this is already prohibitively expensive (even if we exploit the structure and symmetry).

Therefore, our first goal is to develop a basic algorithm with complexity $\mathcal{O}(n^3)$ for moderately sized linear matrix equations.

The Bartels-Stewart Algorithm

The idea of this method is the transformation of the matrix A into Schur form.

The Schur form can be computed in a numerically stable fashion by the QR algorithm and it is the backbone of many dense eigenvalue algorithms (MAT-LAB schur).

Consider (II.3) with $\Lambda(A) \cap \Lambda(-A^H) = \emptyset$ and let $Q^HAQ = T$ with be the (complex) Schur form of A.

Premultiplication of (II.3) by Q^H and postmultiplication by Q leads to

$$Q^{H}AXQ + Q^{H}XA^{T}Q = Q^{H}WQ$$

$$\Leftrightarrow Q^{H}AQ\underbrace{Q^{H}XQ}_{=:\tilde{X}} + Q^{H}XQQ^{H}A^{T}Q = \underbrace{Q^{H}WQ}_{=:\tilde{W}}$$

$$\Leftrightarrow T\tilde{X} + \tilde{X}T^{H} = \tilde{W}$$
(II.6)

We partition this in the form

$$\begin{bmatrix} T_1 & T_2 \\ 0 & T_3 \end{bmatrix} \begin{bmatrix} X_1 & X_2 \\ X_2^H & X_3 \end{bmatrix} + \begin{bmatrix} X_1 & X_2 \\ X_2^H & X_3 \end{bmatrix} \begin{bmatrix} T_1^H & 0 \\ T_2^H & T_3^H \end{bmatrix} = \begin{bmatrix} \tilde{W}_1 & \tilde{W}_2 \\ \tilde{W}_2^H & \tilde{W}_3 \end{bmatrix},$$

where $T_1 \in \mathbb{C}^{(n-1)\times(n-1)}$, $T_2 \in \mathbb{C}^{n-1}$, $T_3 \in \mathbb{C}$. Thus we get

$$\begin{cases} T_1X_1 + T_2X_2^H + X_1T_1^H + X_2T_2^H = \tilde{W}_1, \\ T_1X_2 + T_2X_3 + X_2T_3^H = \tilde{W}_2, \\ T_3X_3 + X_3T_3^H = \tilde{W}_3, \end{cases}$$

$$\Leftrightarrow \begin{cases} T_1X_1 + X_1T_1^H = \tilde{W}_1 - T_2X_2^H - X_2T_2^H, & (n-1) \times (n-1) \\ T_1X_2 + X_2\overline{T}_3 = \tilde{W}_2 - T_2X_3, & (n-1) \times 1 \\ (T_3 + \overline{T}_3)X_3 = \tilde{W}_3. & 1 \times 1 \end{cases}$$

Algorithm 2 Bartels-Stewart algorithm (complex version)

Input: $A, W \in \mathbb{C}^{n \times n}$ with $W = W^H$.

Output: $X = X^H$ solving (II.3).

- 1: Compute $T=Q^HAQ$ with the QR algorithm.
- 2: if $\operatorname{diag}(T) \cap \operatorname{diag}(-T^H) \neq \emptyset$ then
- 3: STOP (no unique solution)
- 4: end if
- 5: Set $\tilde{W} := Q^H W Q$.
- 6: Set k := n 1.
- 7: while k > 1 do
- 8: Solve (II.7a) with $\tilde{W}_3=\tilde{W}(k+1,k+1)$ and $T_3=T(k+1,k+1)$ to obtain X(k+1,k+1).
- 9: Solve (II.7b) with $T_1=T(1:k,1:k), T_2=T(1:k,k+1), \tilde{W}_2=\tilde{W}(1:k,k+1),$ and $X_3=X(k+1,k+1)$ to obtain X(1:k,k+1).
- 10: Set $\tilde{W} = \tilde{W}(1:k,1:k) T_2 X_2^H X_2 * T_2^H$
- 11: Set k := k 1.
- 12: end while
- 13: Solve (II.7c) with $T_1 = T(1,1)$ and $\hat{W}_1 = \tilde{W}(1,1)$.
- 14: Set $X := QXQ^H$.

Now we get

$$X_3 = \frac{\tilde{W}_3}{T_3 + \overline{T}_3},\tag{II.7a}$$

where $T_3 + \overline{T}_3 \neq 0$ since $T_3 \in \Lambda(A) \notin i\mathbb{R}$. Next we obtain

$$T_1X_2 + X_2\overline{T_3} = \tilde{W}_2 - T_2X_3 =: \hat{W}_2,$$
 (II.7b)

which is a special Sylvester equation that is equivalent to the linear system

$$(\overline{T_3}I_{n-1} + T_1)X_2 = \hat{W}_2,$$

and can easily be solved by backward substitution. Its solution always exists since $\Lambda(T_1) \cap \left\{ -\overline{T_3} \right\} = \varnothing$. It remains to solve the smaller $(n-1) \times (n-1)$ sized 'triangular' Lyapunov equation

$$T_1X_1 + X_1T_1^H = \tilde{W}_1 - T_2X_2^H - X_2T_2^H =: \hat{W}_1,$$
 (II.7c)

which is also solvable since $\Lambda(T_1) \cap \Lambda(-T_1^H) = \emptyset$ and $\hat{W}_1 = \hat{W}_1^H$. This leads to the complex Bartels-Stewart algorithm, see Algorithm 2. As a convention we use MATLAB notation, i.e., we denote the section of a matrix $A \in \mathbb{C}^{n \times n}$ consisting only of the rows r_1 to r_2 and the columns c_1 to c_2 by $A(r_1 : r_2, c_1 : c_2)$. If for example, $r_1 = r_2$, then we shortly write $A(r_1, c_1 : c_2)$.

Remark: a) In total this algorithm needs approximately

$$32n^3 \approx \underbrace{25n^3}_{\text{Schur}} + \underbrace{3n^3}_{\text{premult.}} + \underbrace{3n^3}_{\text{postmult.}} + \underbrace{n^3}_{\text{while loop}}$$

complex floating point operations.

- b) The algorithm uses only numerically backward stable parts and unitary transformations and thus it can be considered backward stable.
- c) The method is implemented in the MATLAB routine lyap and in SLICOT in SB03MD (real version only).
- d) The version for Sylvester equations works analogously (see exercise).

Major drawback: The algorithm uses complex arithmetic operations even if all data is real. Luckily, it can be reformulated to use real operations only.

Theorem II.11 (real Schur form): For every $A \in \mathbb{R}^{n \times n}$ there exists an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ such that A is transformed to *real Schur form*, i. e.

$$Q^{T}AQ = T = \begin{bmatrix} T_{11} & \dots & T_{1k} \\ & \ddots & \vdots \\ & & T_{kk} \end{bmatrix}, \tag{II.8}$$

where for $i=1,\ldots,k,$ $T_{ii}\in\mathbb{R}^{1\times 1}$ (corresponding to a real eigenvalue of A) or $T_{ii}=\begin{bmatrix}\alpha_i&\beta_i\\-\beta_i&\alpha_i\end{bmatrix}\in\mathbb{R}^{2\times 2}$ (corresponding to a pair of complex conjugate eigenvalues $\alpha_i\pm\mathrm{i}\beta_i$ of A).

Proof. See the course on "Numerical Linear Algebra".

To this end, we replace the Schur form by the real Schur form (II.8). Then T_3 may be a 2×2 block, i. e., $T_3=\left[\begin{smallmatrix}t_1&t_2\\t_3&t_4\end{smallmatrix}\right]$. We obtain

$$\begin{bmatrix} t_1 & t_2 \\ t_3 & t_4 \end{bmatrix} \begin{bmatrix} x_1 & x_2 \\ x_2 & x_3 \end{bmatrix} + \begin{bmatrix} x_1 & x_2 \\ x_2 & x_3 \end{bmatrix} \begin{bmatrix} t_1 & t_3 \\ t_2 & t_4 \end{bmatrix} = \begin{bmatrix} w_1 & w_2 \\ w_2 & w_3 \end{bmatrix}.$$

This is equivalent to

$$\begin{cases} w_1 = t_1x_1 + t_2x_2 + t_1x_1 + t_2x_2 = 2(t_1x_1 + t_2x_2), \\ w_2 = t_1x_2 + t_2x_3 + t_3x_1 + t_4x_2 = t_3x_1 + (t_1 + t_4)x_2 + t_2x_3, \\ w_3 = t_3x_2 + t_4x_3 + t_3x_2 + t_4x_3 = 2(t_3x_2 + t_4x_3). \end{cases}$$

We can write this as a linear system of equations

$$\begin{bmatrix} t_1 & t_2 & 0 \\ t_3 & t_1 + t_4 & t_2 \\ 0 & t_3 & t_4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \frac{w_1}{2} \\ w_2 \\ \frac{w_3}{2} \end{bmatrix}.$$

Additionally, one can exploit the fact that T_3 corresponds to a pair of complex conjugate eigenvalues $\lambda_{1,2}=a\pm \mathrm{i} b$ and $T_3=\begin{bmatrix} a & b \\ -b & a \end{bmatrix}$ which leads to

$$\begin{bmatrix} a & b & 0 \\ -b & 2a & b \\ 0 & -b & a \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \frac{w_1}{2} \\ w_2 \\ \frac{w_3}{2} \end{bmatrix}.$$

Now (II.7b) becomes

$$T_1X_2 + X_2T_3^T = \hat{W}_2 := \tilde{W}_2 - T_2X_3 \in \mathbb{R}^{n-2 \times 2}.$$
 (II.9)

Consider the partitions corresponding to the quasi-triangular structure of T_1 :

$$X_2 = \begin{bmatrix} x_1 \\ \vdots \\ x_{k-1} \end{bmatrix}, \quad \hat{W}_2 = \begin{bmatrix} \hat{w}_1 \\ \vdots \\ \hat{w}_{k-1} \end{bmatrix},$$

In general we have x_i , $\hat{w}_i \in \mathbb{R}^{n_i \times n_k}$, where n_i , $n_k \in \{1, 2\}$ and $i = 1, \dots, k-1$.

We now compute X_2 block-wise by progressing upwards from x_{k-1} to x_1 . It holds

$$T_{jj}x_j + x_jT_3^T = \hat{w}_j - \sum_{h=j+1}^k T_{jh}x_h =: \tilde{w}_j, \quad j = k-1, k-2, \dots, 1.$$

For the solution of this Sylvester equation four cases have to be considered:

- a) $n_j = n_k = 1$: We obtain a scalar equation such that $x_j = \tilde{w}_j/(T_{jj} + T_3)$.
- b) $n_j=2,\,n_k=1$: We obtain a linear system in \mathbb{R}^2 with unique solution given by

$$(T_{ij} + T_3 I_2) x_i = \tilde{w}_i.$$

c) $n_j=1,\,n_k=2$: We obtain a linear system in \mathbb{R}^2 with unique solution given by

$$(T_{jj}I_2 + T_3) x_j^T = \tilde{w}_j^T.$$

d) $n_j=2,\,n_k=2$: We obtain a linear system in \mathbb{R}^4 with unique solution given by

$$((I_2 \otimes T_{jj}) + (T_3 \otimes I_2)) \operatorname{vec}(x_j) = \operatorname{vec}(\tilde{w}_j).$$

Hence, we get X_2 and can set up a Lyap. eqn. for X_1 defined by T_1 . Repeat whole process until $T_1 \in \mathbb{R}$ or $T_1 \in \mathbb{R}^{2 \times 2}$. Then back-transform the solution.

Remark II.12: The Sylvester equation (II.9) can be solved alternatively by solving a linear system of the form

$$(T_1^2 + \alpha T_1 + \beta I_{n-2})X_2 = \tilde{W}_2,$$

where $X_2=[s,t],\ \tilde{W}_2=[y,z]\in\mathbb{R}^{n-2\times 2}$ and $\alpha,\beta\in\mathbb{R}$ (see exercise).

Hammarling's Method

Now we consider (II.3) with $W=-BB^T$. By Theorem II.10 we know that $X=X^T>0$, provided that $\Lambda(A)\subset\mathbb{C}^-$ and the pair (A,B) is controllable. Sometimes it is desirable to only compute a factor U of the solution, i.e., $X=UU^H$ with some matrix U. Later we will see that many further algorithms such as projection methods for large scale matrix equations proceed with factors rather than Gramians themselves.

Assume that we have already computed and applied the Schur decomposition of $A = Q^H T Q$, analogously to (II.6). So our starting point is

$$T\tilde{X} + \tilde{X}T^H = -\tilde{B}\tilde{B}^H$$
 with $\tilde{X} = Q^H X Q$, $\tilde{B} = Q^H B$. (II.10)

Since X>0, we also have $\tilde{X}>0$ by Sylvester's law of inertia. Our goal is to compute upper triangular Cholesky factors \tilde{U} of $\tilde{X}=\tilde{U}\tilde{U}^H$.

Partition

$$\tilde{U} = \begin{bmatrix} U_1 & u \\ 0 & \tau \end{bmatrix}, \quad U_1 \in \mathbb{C}^{n-1 \times n-1}, \ u \in \mathbb{C}^{n-1}, \ 0 < \tau \in \mathbb{R}.$$

Hammarlings method computes (similar to B.S.) first τ (scalar equation), then u (LS of size n-1), and finally U_1 as Cholesky factor or a $n-1\times n-1$ Lyap. equation defined by T_1 . As in B.S., repeat this until $T_1\in\mathbb{C}$, afterwards backtransform $U\leftarrow QU$. Complexity, stability, real version analog to BS. Details here omitted.

Remark: Iterative methods for small, dense Matrix Equations: There are several, iterative methods computing sequences X_k , $k \geqslant 0$ converging to the true solution, i.e., $\lim_{k \to \infty} X_k = X$. For instance:

- · Matrix sign function iteration
- Alternating directions implicit (ADI) iteration was later for large problems.

II.2.3 Iterative Solutions of Large and Sparse Matrix Equations

Now we consider

$$AX + XA^T = -BB^T, (II.11)$$

where $A \in \mathbb{R}^{n \times n}$ and n is 'large', but A is sparse, i. e., only a few entries in A are non-zero. Therefore, multiplication with A can be performed in $\mathcal{O}(n)$ rather than $\mathcal{O}(n^2)$ FLOPS. Also solves with A or A + pI can be performed efficiently.

However, $X \in \mathbb{R}^{n \times n}$ is usually dense and thus X cannot be stored for large n since we would need $\mathcal{O}(n^2)$ memory.

Thus the question arises whether it is possible to store the solution ${\cal X}$ more efficiently.

The Low-Rank Phenomenon

In practice we often have $B \in \mathbb{R}^{n \times m}$, where $m \ll n$, i. e., the right-hand side BB^T has a low rank. Recall that if (A,B) is controllable then $X=X^T\geqslant 0$ and $\mathrm{rank}(X)=n$.

It is a very common observation in practice that the eigenvalues of X solving (II.11) decay very rapidly towards zero, and fall early below the machine precision

This gives the concept of the numerical rank of X:

$$\operatorname{rank}(X,\tau) = \operatorname{argmin}_{j=1,\dots,\operatorname{rank}(X)} \{\sigma_j(X) \geqslant \tau\}, \quad \operatorname{e.g.}, \tau = \epsilon_{\operatorname{mach}} \sigma_1(X).$$

Can we also theoretically explain this eigenvalue decay?

Theorem II.13: Let A be diagonalizable, i. e., there exists an invertible matrix $V \in \mathbb{C}^{n \times n}$ such that $A = V \Lambda V^{-1}$. Then the eigenvalues of X solving (II.11) with $B \in \mathbb{C}^{n \times m}$ satisfy

$$\frac{\lambda_{km+1}(X)}{\lambda_1(X)} \le \|V\|_2^2 \|V^{-1}\|_2^2 \rho(M_k)^2$$

for any choice of shift parameters p_k used to construct

$$M_k = \prod_{i=1}^k (A - p_k I)(A + p_k I)^{-1}$$

(in particular, the optimal ones).

In the Theorem above the spectral radius ρ of a matrix is used:

$$\rho(A) = \max_{1 \le i \le n} |\lambda_i(A)|.$$

Remark II.14: • If the eigenvalues of A cluster in the complex plane, only a few p_k in the clusters suffice to get a small $\rho(M_k)$ and thus $\lambda_i(X)$ decay fast.

- If A is normal, then $\|V\|_2 \, \|V^{-1}\|_2 = 1$ and the bound gives a good explanation for the decay. The nonnormal case is much harder to understand.
- This bound (and most others) does not precisely incorporate the eigenvectors of A as well as the precise influence of B.

Consequence: If there is a fast decay of $\lambda_i(X)$, then X can be well approximated as $X = X^T \approx ZZ^H$, where $Z \in \mathbb{C}^{n \times r}$ with $r \ll n$ is a *low-rank solution factor*. Hence, only nr memory is required. Thus, in the next subsection we consider algorithms for computing the factor Z without explicitly forming X.

Projection Methods

Now we consider projection-based methods for the solution of large and sparse Lyapunov equations

The main idea consists of representing the solution X by an approximation extracted from a low-dimensional subspace $\mathcal{Q}_k = \operatorname{im} \mathcal{Q}_k$ with $\mathcal{Q}_k^T \mathcal{Q}_k = I_{km}$, i. e., $X \approx X_k = \mathcal{Q}_k Y_k \mathcal{Q}_k^T$ for some $Y_k \in \mathbb{R}^{mk \times mk}$. Impose a Galerkin condition

$$R(X_k) := AX_k + X_k A^T + BB^T \perp \mathcal{Z}_k,$$

where

$$\mathcal{Z}_k := \left\{ Q_k Z Q_k^T \in \mathbb{R}^{n \times n} \mid Q_k^T Q_k = I_{mk}, \text{ im } Q_k = \mathcal{Q}_k, \ Z \in \mathbb{R}^{km \times km} \right\}$$

and orthogonality is with respect to the trace inner product. Equivalently, Y_k solves the small-scale Lyapunov equation

$$H_k Y_k + Y_k H_k^T + Q_k^T B B^T Q_k = 0, \quad H_k := Q_k^T A Q_k,$$
 (II.12)

which can be solved by the Bartels-Stewart or Hammerling's method.

In case that the residual norm $\|R(X_k)\|$ is not small enough, we increase the dimension of \mathcal{Q}_k by a clever expansion (orthogonally expand Q_k), otherwise we prolongate to obtain $X_k = Q_k Y_k Q_k^T$ (never formed explicitly).

What are good choices for Q_k ?

a) Standard block Krylov subspaces

$$\mathcal{Q}_k = \mathcal{K}_k(A, B) := \operatorname{span}\{B, AB, \dots, A^{k-1}B\}$$
:

A matrix Q_k with orthonormal columns spanning \mathcal{Q}_k can be generated by a block Arnoldi process, i. e. in the kth iteration we have $Q_k = \begin{bmatrix} V_1 & \dots & V_k \end{bmatrix}$ fulfilling (assuming there is no breakdown in the process)

$$AQ_k = Q_k H_k + V_{k+1} H_{k+1,k} E_k^T,$$

where

$$H_k = \begin{bmatrix} H_{11} & H_{12} & \dots & \dots & H_{1k} \\ H_{21} & H_{22} & \dots & \dots & \vdots \\ 0 & H_{32} & H_{33} & \dots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & H_{k,k-1} & H_{kk} \end{bmatrix}$$

is a block upper Hessenberg matrix and ${\cal E}_k$ is a matrix of the last m columns of ${\cal I}_{km},$ and

$$H_k = Q_k^T A Q_k.$$

The residual norm computation for this method is cheap as shown by the following theorem.

Theorem II.15: Suppose that k steps of the block Arnoldi process have been taken. Assume that $\Lambda(H_k) \cap \Lambda(-H_k) = \emptyset$. Then the following statements are satisfied:

- a) It holds $Q_k^T R(Q_k Y Q_k^T) Q_k = 0$ if and only if $Y = Y_k$, where Y_k solves the Lyapunov equation (II.12).
- b) The residual norm is given by

$$||R(Q_k Y_k Q_k^T)||_F = \sqrt{2} ||H_{k+1,k} E_k^T Y_k||_F.$$

Unfortunately, this method often converges only slowly. Therefore, one often chooses modified Krylov subspaces as follows.

b) Extended block Krylov subspaces

$$\mathcal{EK}_a(A,B) := \mathcal{K}_a(A,B) \cup \mathcal{K}_a(A^{-1},A^{-1}B)$$
:

The resulting method is also known as EKSM (extended Krylov subspace method) or KPIK (Krylov plus inverted Krylov). We obtain a similar construction formula as for the block Arnoldi method above and also the residual norm formula is similar. However, the approximation quality is often significantly better than with $\mathcal{K}_q(A,B)$ only. On the other hand, the subspace dimension grows by 2m in each iteration step (until n is reached).

c) Rational Krylov subspaces

$$\mathcal{RK}_{q}(A, B, S)$$
 (II.13)
$$:= \mathrm{span}\{(s_{1}I_{n} - A)^{-1}B, (s_{2}I_{n} - A)^{-1}B, \dots, (s_{q}I_{n} - A)^{-1}B\},$$

$$S = \{s_{1}, \dots, s_{q}\} \subset \mathbb{C}^{+}, \ s_{i} \neq s_{j}, i \neq j : \ \text{(shifts)}$$

This choice often gives an even better approximation quality compared to $\mathcal{EK}_q(A,B)$, provided that good shifts S are known. Generating the basis requires solving LS $(s_iI-A)v=q_i$, but this is usually efficiently possible (cf. Intro).

The shifts s_i are crucial for a fast convergence, but finding good ones is difficult. For one possible shift selection approach, let m=1. One can show

$$\|R_k\| \sim \max |\psi_k(z)|$$
 with $\psi_k(z) = \prod_{j=1}^k \frac{z - \lambda_j}{z + s_j}, \ \lambda_j \in \Lambda(H_k).$

This leads to the following procedure for getting the next shift

$$s_{k+1} = \operatorname{argmax}_{z \in \partial D} |\psi_k(z)|,$$

where ∂D is a discrete set of point taken from the convex hull of $\Lambda(H_k)$ $(\partial D \subset \operatorname{conv}(\Lambda(H_k)))$.

For all choices of subspace **a)-c)**: Is the reduced Lyapunov equation (II.12) always uniquely solvable?

For general matrices A the answer is no. However, for *strictly dissipative matrices*, i. e., matrices A with $A + A^T < 0$ we have the following result.

Theorem II.16: Let $A \in \mathbb{R}^{n \times n}$ be strictly dissipative and $Q_k \in \mathbb{R}^{n \times mk}$ with $Q_k^T Q_k = I_{km}$. Then $\Lambda(H_k) \subset \mathbb{C}^-$ and the reduced Lyapunov equation (II.12) is always uniquely solvable.

Proof. Since $A+A^T$ is symmetric and negative definite, it holds $x^H(A+A^T)x < 0$ for all $x \in \mathbb{C}^n$. Then we have

$$z^{H}(H_k + H_k^T)z = z^{H}(Q_k^T A Q_k + Q_k^T A^T Q_k)z$$
$$= y^{H}(A + A^T)y < 0, \ y := Q_k z, \ \forall \ z \in \mathbb{C}^{km}$$
$$\Rightarrow H_k + H_k^T < 0$$

Now let $H_k \hat{x} = \hat{\lambda} \hat{x}$ for $\hat{x} \in \mathbb{C}^{km} \setminus \{0\}$. Then we have

$$\hat{x}^{H} (H_k + H_k^T) \hat{x} = \hat{\lambda} \hat{x}^{H} \hat{x} + \overline{\hat{\lambda}} \hat{x}^{H} \hat{x} = 2 \operatorname{Re}(\hat{\lambda}) \hat{x}^{H} \hat{x} < 0.$$

Thus $\Lambda(H_k)\subset\mathbb{C}^-$ and the reduced Lyapunov equation (II.12) is uniquely solvable. \qed