to be handed in until October 23, 2024, 11am.

Please hand in your solutions in groups of 2-4. Solutions submitted by only one person will not be graded. The solutions for non-programming problems may be either handed in online via Moodle or on paper (Mathematikon, 1st floor, letterbox to be determined). The solutions for programming problems have to be handed in online via Moodle. Specifics may be found in the respective problems. To receive the points for the exercises, write everyones first and last name on every hand-in. Details will be discussed in the exercise group on Thursday.

If you currently don't have access to Moodle, please contact your tutor Freya in the exercise group or via Mail (freya.jensen[at]iwr.uni-heidelberg.de).

Problem 1. Review the following items and write down at least one of the definitions and one of the theorems with proof in detail.

- Definition of a projection
- Definition of an orthogonal projection
- Theorem: Orthogonal projection is uniquely determined by subspace Consider a finite-dimensional space V with inner product $\langle \cdot, \cdot \rangle$ and a subspace $W \subset V$. Then, there exists a unique orthogonal projection

$$P_W: V \to W$$
.

• Theorem: Best Approximation Theorem

Let W be a subspace of \mathbb{R}^n , let \mathbf{x} be any vector in \mathbb{R}^n , and let $\tilde{\mathbf{x}}$ be the orthogonal projection of \mathbf{x} onto W. Then $\tilde{\mathbf{x}}$ is the closest point in W to \mathbf{x} , in the sense that

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| < \|\mathbf{x} - \mathbf{w}\|$$

for all \mathbf{w} in W distinct from \mathbf{x} .

• Theorem: Orthogonal projection in orthonormal basis

Let $B = \{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_p\}$ be an orthonormal basis of a subspace W of a finite-dimensional space V with inner product $\langle \cdot, \cdot \rangle$. Then, the orthogonal projection P_i of any vector $\mathbf{v} \in V$ onto \mathbf{u}_i , and the orthogonal projection P_W of any vector $\mathbf{v} \in V$ onto W have the following expressions, respectively:

$$P_i(\mathbf{v}) = \langle \mathbf{v}, \mathbf{u}_i \rangle \mathbf{u}_i, \qquad i = 1, 2, ..., p,$$
$$P_W(\mathbf{v}) = \sum_{i=1}^p \langle \mathbf{v}, \mathbf{u}_i \rangle \mathbf{u}_i,$$

and

$$\mathbf{v} = P_W(\mathbf{v}) + \mathbf{z}, \qquad \mathbf{z} \perp W.$$

• Theorem: Parseval identity

Suppose that W is a finite-dimensional linear space with inner product $\langle \cdot, \cdot \rangle$. Let $\{ \mathbf{e}_i \}$, i=1,...,n be an orthonormal basis of W. Then, for every $\mathbf{w} \in W$ it holds

$$\sum_{i=1}^{n} |\langle \mathbf{w}, \mathbf{e}_i \rangle|^2 = \|\mathbf{w}\|^2.$$

Problem 2 (Programming). To familiarize yourself with the C++ library Armadillo write a function $gauss_eliminiation$ that performs the Gaussian elimination for a system of linear equations Ax = b. You should use the armadillo matrix class and vector class to store the system of linear equations, handle the result and perform the vector matrix multiplication in the end. Write a main function in which you test your implementation with the following system of linear equations:

In order to test the correctness of your result you should perform a matrix vector multiplication to see whether the original matrix A multiplied with the resulting vector x yields the vector b. We will also discuss this problem in the programming tutorial on Thursday.

Numerical Linear Algebra - Sheet 1 Solutions

Solution 1.

Solution 2.

Solution 3.

Solution 4 (Programming).

to be handed in until October 30, 2024, 11am.

Problem 1. Problem 1.2.7 in the Lecture Notes.

Problem 2. Problem 1.2.9 in the Lecture Notes.

Problem 3. Compute the eigenvalues and eigenvectors of the matrix

$$\begin{bmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{bmatrix},$$

for $\alpha \in \mathbb{R}$.

Problem 4. Given a normal matrix A and a right eigenvector v of A with eigenvalue λ . Show that then the complex conjugate of v, \bar{v} , is a left eigenvector of A with the same eigenvalue λ , i.e.

$$v^*A = \lambda v^*$$
.

Numerical Linear Algebra - Sheet 2 Solutions

Solution 1.
Solution 2.
Solution 3.
Solution 4. 1.
2.
3. (Programming)

4.

to be handed in until November 6, 2024, 11am.

- **Problem 1.** Problem 2.1.23 in the Lecture Notes.
- **Problem 2.** Problem 2.1.24 in the Lecture Notes.
- **Problem 3.** Problem 2.2.14 in the Lecture Notes.

Problem 4.

- 1. Write a function Compute_Givens which takes two values a and b and returns the Givens parameters c and s.
- 2. Write a function Apply_Givens_left which applies a Givens rotation (matrix) from the left to a matrix M.
- 3. Test the functions by computing and applying the Givens rotation to pairs of values from the vector $x = (10, ..., 1)^T$ beginning with the last two entries and ending with the first two entries, thereby transforming the vector into a multiple of the first unit vector.
- 4. Apply the same computation to randomly generated vectors (which you find in the template file).

Numerical Linear Algebra - Sheet 3 Solutions

Solution 1.

Solution 2.

Solution 3.

Solution 4 (Programming).

to be handed in until November 15, 2023,11am.

$\mathbf{Problem}$ 1. Write a program $\mathtt{COMPUTE_EIGENVALUES}$ that

- 1. computes the dominant eigenvalue of a matrix using the power method.
- 2. computes all further eigenvalues using suitable matrix polynomials.

Test your program with the following matrix

$$\mathbf{A} = \begin{pmatrix} 1+i & 1 & 0 & 0 & 0 \\ 0 & 1+i & 1 & 0 & 0 \\ 0 & 0 & 1+i & 1 & 0 \\ 0 & 0 & 0 & 1+i & 1 \\ 1 & 0 & 0 & 0 & 1+i \end{pmatrix}.$$

Problem 2. Let **A** be a symmetric tridiagonal matrix. Show that the QR-iteration (see Algorithm 2.4.2 in the lecture notes) preserves the tridiagonal structure of the matrix, i.e., all iterates $\mathbf{A}^{(n)}$ generated by the QR-iteration are tridiagonal.

Problem 3. Rewrite the QR factorization of a tridiagonal (complex) symmetric matrix such that its complexity is of order O(n) (this proves the second part of Corollary 2.4.17 in the lecture notes).

Numerical Linear Algebra - Sheet 4 Solutions

Solution 1.

Solution 2.

Solution 3.

Solution 4.

Solution 5 (Programming). The eigenvalues of \mathbf{A}_n are

$$\lambda_{n,j} = 4\sin^2\left(\frac{j\pi}{2n+2}\right)$$

https://math.stackexchange.com/questions/3875168/eigenvalues-of-a-tridiagonal-matrix-with-1-2-1-as-entries

https://math.stackexchange.com/questions/177957/eigenvalues-of-tridiagonal-symmetric-matrix-with-diagonal-entries-2-and-subdiago?rq=1

to be handed in until November 22, 2023, 11am

Problem 1. Problem 2.4.16 in the Lecture Notes:

- 1. How many operations do the two versions of the Hessenberg QR step require?
- 2. Show that if **H** is Hermitian, the result of the Hessenberg QR step is Hermitian as well.

Problem 2. Problem 2.4.20 in the Lecture Notes:

Show that every (complex) Hermitian matrix is orthogonally similar to a symmetric tridiagonal matrix with real entries.

Problem 3.

- (a) Implement the implicit Hessenberg QR step (Algorithm 2.4.9 in the lecture notes) in real arithmetic.
- (b) Test your code with the tridiagonal matrix $\mathbf{A}_n = \text{tridiag}(-1, 2, -1)$ in dimension n = 4.
- (c) Use your implementation to run several steps of the QR iteration (Algorithm 2.4.19 in the lecture notes) for the matrix \mathbf{A}_{10} . You should obtain the following eigenvalues:

$$\lambda_j = 2 - 2\cos(j\vartheta) = 4\sin^2\left(\frac{j\vartheta}{2}\right)$$

where $\vartheta = \frac{\pi}{n+1}$, $1 \le j \le n$.

(d) Discuss the observed convergence of the off-diagonal and diagonal entries, respectively.

Problem 4.

- (a) Implement the QR iteration with shift (Algorithm 2.4.25 in the Lecture Notes) using the Wilkinson shift (Definition 2.4.30).
- (b) Test your implementation with the matrix \mathbf{A}_{10} . Run several steps of the iteration and observe the behaviour of the subdiagonal elements, especially the last one.
- (c) For the curious: Implement the QR iteration with deflation (cf. Algorithm 2.4.35).

Numerical Linear Algebra - Sheet 5 Solutions

Solution 1.

Solution 2.

Solution 3.

Solution 4 (Programming).

to be handed in until November 29, 2023, 11am.

Problem 1. Prove Lemma 2.5.2:

Let $\mathbf{T} \in \mathbb{R}^{n \times n}$ be a real, symmetric, tridiagonal matrix and $\mathbf{Q}\mathbf{R} = \mathbf{T}$ its QR factorization. Then, $\tilde{\mathbf{T}} = \mathbf{R}\mathbf{Q}$ is also symmetric and tridiagonal. Furthermore, \mathbf{R} is zero except for its main and the first two upper diagonals.

The same holds for the shifted version with $\sigma \in \mathbb{R}$,

$$\mathbf{Q}\mathbf{R} = \mathbf{T} - \sigma \mathbb{I}, \qquad \tilde{\mathbf{T}} = \mathbf{R}\mathbf{Q} + \sigma \mathbb{I}.$$

Problem 2. Prove that in case of a normal real matrix, for each complex eigenvalue pair there is a 2×2 matrix with according invariant subspace.

- (a) Show that complex eigenvalues and their associated eigenvectors of a real matrix come in complex conjugate pairs.
- (b) Choose real linear combinations of these vectors to obtain the 2×2 block.

Problem 3. Let **H** be a real Hessenberg matrix. Let $\mathbf{Q}_1, \mathbf{R}_1, \mathbf{Q}_2, \mathbf{R}_2$ be the matrices obtained in the explicit double-shift QR step (Algorithm 2.5.14). Let σ_1 and σ_2 are the shifts in Lemma 2.5.16. Show that the following equation in the proof of Lemma 2.5.16 holds:

$$\mathbf{Q}_1\mathbf{Q}_2\mathbf{R}_2\mathbf{R}_1 = \mathbf{M} = (\mathbf{H} - \sigma_1\mathbb{I})(\mathbf{H} - \sigma_2\mathbb{I})$$

Problem 4. Consider the $n \times n$ tridiagonal matrix

$$\mathbf{T}_{\alpha} = \begin{pmatrix} \alpha & -1 \\ -1 & \alpha & -1 \\ & \ddots & \ddots & \ddots \\ & & -1 & \alpha & -1 \\ & & & -1 & \alpha \end{pmatrix}$$

where α is a real parameter. Verify that the eigenvalues of \mathbf{T}_{α} are given by

$$\lambda_j = \alpha - 2\cos(j\vartheta),$$

where

$$\vartheta = \frac{\pi}{n+1},$$

and the eigenvectors associated with each λ_i are given by

$$\mathbf{v}_j = (\sin(j\vartheta), \sin(2j\vartheta), \dots, \sin(nj\vartheta))^T.$$

What are the conditions on α , such that the matrix \mathbf{T}_{α} becomes positive-definite?

Problem 5. Implement the inverse power method (Algorithm 2.6.1 in the lecture notes). To solve the system of linear equations use the functions numpy.linalg.solve and numpy.linalg.lstsq. Test your implementations with the matrix \mathbf{A}_{20} and $\alpha=2$ from Problem 4 and shift parameters $\sigma=\lambda_1,\lambda_2,\lambda_{10}$. Compare your results for the two different solvers.

Numerical Linear Algebra - Sheet 6 Solutions

- Solution 1.
- Solution 2.
- Solution 3.
- Solution 4.

to be handed in until December 4, 2024, 11am.

Problem 1. Prove Theorem 3.2.15 in the Lecture Notes (Convergence of Richardson Iteration).

Problem 2. Problem B.3.13 in the lecture notes.

Problem 3 (Programming). Let \mathbf{L}_d be the discretization of the d-dimensional Laplace operator on the unit square by the five-point stencel with a uniform Dirichlet boundary condition to the mesh size $h = \frac{1}{n+1}$. In 1D it is given in terms of the matrix \mathbf{T}_2 defined in Problem 4 of Sheet 6 by

$$\mathbf{L}_1 = \frac{1}{h^2} \mathbf{T}_2 \in \mathbb{R}^{n \times n}.$$

In 2D it is given by

where $\mathbb{I} \in \mathbb{R}^{n \times n}$ and $\mathbf{D} \in \mathbb{R}^{n \times n}$ are defined as

$$\mathbb{I} = \begin{pmatrix} 1 & & & \\ & \ddots & \\ & & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{D} = \begin{pmatrix} 4 & -1 & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{pmatrix}.$$

Details may be found in appendix B.3 on finite difference methods in the lecture notes

Let $\mathbf{A} = \mathbf{L}_2 \in \mathbb{R}^{n^2 \times n^2}$ as defined above and $\mathbf{b} \in \mathbb{R}^{n^2}$. Write a program that solves the 2D Laplace problem

$$Ax = b$$
,

with the Richardson iteration by observing the following steps:

- (a) Have a look at the function vmult that performs the matrix-vector product Av of A with a given vector v, and returns a vector w. You can find it in Moodle.
- (b) Write a function richardson_step that implements a single step of the Richardson iteration. Similar to (a) this function should take vectors \mathbf{v} and \mathbf{b} , optionally n, and return the resulting vector \mathbf{w} . Hint: The eigenvalues of \mathbf{L}_2 are given by the pairwise sums of the eigenvalues of \mathbf{T}_2 , see B.3.13.

(c) Use the null-vector $\mathbf{x}^{(0)} = (0, ..., 0)^T$ as initial guess and test your program for the constant vector $\mathbf{b} = (1, ..., 1)^T$ with n = 20 and n = 100. Observe the evolution of the residual in the 2-norm

$$r^{(k)} = \|\mathbf{A} \cdot \mathbf{x}^{(k)} - \mathbf{b}\|_2$$

for 50 steps of the Richardson iteration.

- (d) Plot the obtained result vector after 1, 5, 15, 30, and 50 iterations as a two-dimensional function. Hint: For plotting you have to invert the numbering of the vector (use, for example, np.reshape) and then plot the two dimensional grid using a numpy color map (greyscale).
- (e) Compute and discuss the observed convergence rate (see Definition 3.2.22 in the Lecture Notes).

Numerical Linear Algebra - Sheet 7 Solutions

Solution 1. The Richardson iteration can be written as

$$F(x) = (1 - \omega \mathbf{A})x + \omega b.$$

Using the Banach fixed-point theorem, the method converges if $||1 - \omega \mathbf{A}|| < 1$.

Since **A** is symmetric, $1-\omega \mathbf{A}$ is symmetrix and thus the spetral norm of $1-\omega \mathbf{A}$ is given by the maximum of the absolute values of its eigenvalues. We can compute the new eigenvalues from the eigenvalues of **A**. Let **x** denote an eigenvector of **A** with eigenvalue λ :

$$(1 - \omega \mathbf{A})\mathbf{x} = \mathbf{x} - \omega \lambda \mathbf{x} = (1 - \omega \lambda)\mathbf{x}.$$

For any eigenvalue λ of **A** we have: $\omega \lambda < \frac{2\lambda}{\lambda_{\text{max}}}$. Since **A** is positive definite, we have

$$0<\frac{2\lambda_{\min}}{\lambda_{\max}}<\frac{2\lambda_{\min}}{\lambda_{\max}}=2.$$

. Thus, $-1 < 1 - \omega \lambda < 1$ for any eigenvalue λ of ${\bf A}$. This proves that $\|1 - \omega {\bf A}\| < 1$

Solution 2. 1. First equality is for the first entry in the vector:

$$(2 - 2\cos(j\vartheta))\sin(j\vartheta) = 2\sin(j\vartheta) - 2\cos(j\vartheta)\sin(j\vartheta) = 2\sin(j\vartheta) - \sin(2j\vartheta)$$

Here we have used the addition theorem for trigonometric functions.

2. For all other entries in $\mathbf{T}\mathbf{v}_j$ we have to show:

$$2\cos(i\theta)\sin(ki\theta) = \sin((k-1)i\theta) + \sin((k+1)i\theta).$$

But

$$\sin((k-1)j\vartheta) + \sin((k+1)j\vartheta) = \sin(kj\vartheta - j\vartheta) + \sin(kj\vartheta + j\vartheta)$$

$$= \sin(kj\vartheta)\cos(j\vartheta) - \cos(kj\vartheta)\sin(j\vartheta)$$

$$\sin(kj\vartheta)\cos(j\vartheta) + \cos(kj\vartheta)\sin(j\vartheta)$$

$$= 2\cos(j\vartheta)\sin(kj\vartheta).$$

3. For the last row keep in mind that $\sin((n+1)j\vartheta) = \sin(j\pi) = 0$.

Solution 3.

Solution 4 (Programming). C++ sample code ./programs/gauss—seidel.cc without assembling the system matrix. Convergence

to be handed in until December 11, 2024, 11am.

Problem 1. Let $\mathbf{A}\mathbf{x} = \mathbf{b}$ be a linear system with a symmetric, positive definite matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ that has extremal eigenvalues λ_{\min} and λ_{\max} and spectral condition number $\operatorname{cond}(\mathbf{A})$. Consider the sequence $\{\mathbf{x}^{(k)}\}$ of one-dimensional projection processes with $K = L = \operatorname{span}\{\mathbf{e}_i\}$, where \mathbf{e}_i denotes the *i*-th unit vector in \mathbb{R}^n . The index *i* is selected at each step *k* to be the index of a component of largest absolute value in the current residual vector $\mathbf{r}^{(k)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(k)}$.

(a) For $\mathbf{d}^{(k)} = \mathbf{A}^{-1}\mathbf{b} - \mathbf{x}^{(k)}$ show that

$$\|\mathbf{d}^{(k+1)}\|_{\mathbf{A}} \le \left(1 - \frac{1}{n \operatorname{cond}(\mathbf{A})}\right)^{\frac{1}{2}} \|\mathbf{d}^{(k)}\|_{\mathbf{A}}.$$

Hint: You can use the expression

$$\left\langle \mathbf{A}\mathbf{d}^{(k+1)}, \mathbf{d}^{(k+1)} \right\rangle = \left\langle \mathbf{A}\mathbf{d}^{(k)}, \mathbf{d}^{(k)} \right\rangle - \frac{\left\langle \mathbf{r}^{(k)}, \mathbf{e}_i \right\rangle^2}{a_{ii}},$$

as well as the inequality $\|\mathbf{r}^{(k)}\|_{\infty} = |\mathbf{e}_i^T \mathbf{r}^{(k)}| \ge n^{-1/2} \|\mathbf{r}^{(k)}\|_2$. a_{ii} denotes the *i-th diagonal element of* A.

(b) Does (a) prove that the algorithm converges? Why do we care about its convergence?

Problem 2. Consider the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$, where \mathbf{A} is a symmetric positive definite matrix. We define a projection method which uses a two-dimensional space at each step. At a given step, take $L = K = \text{span}\{\mathbf{r}, \mathbf{A}\mathbf{r}\}$, where $\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}$ is the current residual.

- (a) For a basis of K use the vector \mathbf{r} and the vector \mathbf{p} obtained by orthogonalizing \mathbf{Ar} against \mathbf{r} with respect to the \mathbf{A} -inner product. Give the formula for computing \mathbf{p} (no need to normalize the resulting vector).
- (b) Write the algorithm for performing the projection method described above.
- (c) Can you explain, not compute, why the algorithm converges for any initial guess \mathbf{x}_0 ? Hint: Exploit the convergence results for one-dimensional projection techniques.

Problem 3 (Programming).

- (a) Implement the steepest decent method (Algorithm 3.3.14 in the lecture notes).
- (b) Use your implementation of the steepest decent method to solve the 2D Laplace problem

$$\mathbf{L}_2\mathbf{x} = \mathbf{b}$$

as in Problem 3 on Sheet 7 with right hand side vector $\mathbf{b} = (1, ..., 1)^T$ and initial guess $\mathbf{x}^{(0)} = (0, ..., 0)^T$ with n = 50 and n = 100.

(c) Compute and discuss the observed convergence rate (see 3.2.21/Definition 3.2.22 in the Lecture Notes).

Problem 4 (Programming).

- (a) Implement the minimal residual method (Algorithm 3.3.21 in the lecture notes).
- (b) Use your implementation of the steepest decent method to solve the 2D Laplace problem

$$\mathbf{L}_2\mathbf{x}=\mathbf{b}$$

as in Problem 3 on Sheet 7 with right hand side vector $\mathbf{b} = (1,...,1)^T$ and initial guess $\mathbf{x}^{(0)} = (0,...,0)^T$ with n = 50 and n = 100.

(c) Compute and discuss the observed convergence rate (see 3.2.21/Definition 3.2.22 in the Lecture Notes). Compare it with the convergence rate observed in Problem 3.

Numerical Linear Algebra - Sheet 8 Solutions

Solution 1 ([?, P-5.1 b]).

Part (a):

Hint 1:

$$\left\langle \mathbf{A}\mathbf{d}^{(k+1)}, \mathbf{d}^{(k+1)} \right\rangle = \left\langle \mathbf{A}\mathbf{d}^{(k)}, \mathbf{d}^{(k)} \right\rangle - \frac{\left\langle \mathbf{r}^{(k)}, \mathbf{e}_i \right\rangle^2}{a_{ii}}$$

Hint 2:

$$|\mathbf{e}_i^T \mathbf{r}^{(k)}| \ge n^{-1/2} ||\mathbf{r}^{(k)}||_2$$

With the help of hint 1 and 2 we get

$$\begin{aligned} \|\mathbf{d}^{(k+1)}\|_{\mathbf{A}}^2 &= \left\langle \mathbf{A} \mathbf{d}^{(k+1)}, \mathbf{d}^{(k+1)} \right\rangle \overset{\text{Hint } 1}{=} \left\langle \mathbf{A} \mathbf{d}^{(k)}, \mathbf{d}^{(k)} \right\rangle - \frac{\left\langle \mathbf{r}^{(k)}, \mathbf{e}_i \right\rangle^2}{a_{ii}} \\ &= \left(1 - \frac{\left\langle \mathbf{r}^{(k)}, \mathbf{e}_i \right\rangle^2}{a_{ii}} \frac{1}{\left\langle \mathbf{A} \mathbf{d}^{(k)}, \mathbf{d}^{(k)} \right\rangle} \right) \|\mathbf{d}^{(k)}\|_{\mathbf{A}}^2 \\ &\overset{\text{Hint } 2}{\leq} \left(1 - \frac{1}{na_{ii}} \frac{\|\mathbf{r}^{(k)}\|_2^2}{\left\langle \mathbf{A} \mathbf{d}^{(k)}, \mathbf{d}^{(k)} \right\rangle} \right) \|\mathbf{d}^{(k)}\|_{\mathbf{A}}^2 \end{aligned}$$

The result follows by the following two estimates of Rayleigh quotients:

$$a_{ii} = \langle \mathbf{A} \mathbf{e}_i, \mathbf{e}_i \rangle = \frac{\langle \mathbf{A} \mathbf{e}_i, \mathbf{e}_i \rangle}{\langle \mathbf{e}_i, \mathbf{e}_i \rangle} \le \lambda_{\max},$$

and

$$\frac{\left\langle \mathbf{A}\mathbf{d}^{(k)},\mathbf{d}^{(k)}\right\rangle}{\|\mathbf{r}^{(k)}\|^2} = \frac{\left\langle \mathbf{r}^{(k)},\mathbf{A}^{-1}\mathbf{r}^{(k)}\right\rangle}{\|\mathbf{r}^{(k)}\|^2} \leq \lambda_{\max}(\mathbf{A}^{-1}) = \frac{1}{\lambda_{\min}}.$$

Part (b): For n > 1, $1 - \frac{1}{n \operatorname{cond}(\mathbf{A})} < 1$, and thus

$$\|\mathbf{d}^{(k+1)}\|_{\mathbf{A}} \leq \left(1 - \frac{1}{n \operatorname{cond}(\mathbf{A})}\right)^{\frac{k+1}{2}} \|\mathbf{d}^{(0)}\|_{\mathbf{A}} \to 0 \text{ for } n \to \infty.$$

That shows that $x^{(k)}$ converges to the solution $x = \mathbf{A}^{-1}\mathbf{b}$.

Final remarks:

1. Since $\mathbf{e}_i \in K = L$, it holds the Galerkin-orthogonality

$$\left\langle \mathbf{r}^{(k)} - \alpha \mathbf{A} \mathbf{e}_i, \mathbf{e}_i \right\rangle = 0,$$

where according to Example 2.3.10

$$\alpha = \frac{\left\langle \mathbf{r}^{(k)}, \mathbf{e}_i \right\rangle}{\left\langle \mathbf{A} \mathbf{e}_i, \mathbf{e}_i \right\rangle} = \frac{\left\langle \mathbf{r}^{(k)}, \mathbf{e}_i \right\rangle}{a_{ii}}.$$

This would have been used to show hint 1.

2. To show hint 2, notice that by the choice of i as maximal value of the residual vector

$$\|\mathbf{r}^{(k)}\|_2 \le \sqrt{n} \|\mathbf{r}^{(k)}\|_{\infty} = \sqrt{n} |\mathbf{e}_i^T \mathbf{r}^{(k)}|$$

Solution 2. Part (a):

$$\mathbf{p} = \mathbf{A}\mathbf{r} - \frac{\left\langle \mathbf{A}\mathbf{r}, \mathbf{r} \right\rangle_{\mathbf{A}}}{\left\langle \mathbf{r}, \mathbf{r} \right\rangle_{\mathbf{A}}} \mathbf{r}.$$

Then $\langle \mathbf{Ar}, \mathbf{p} \rangle = \langle \mathbf{r}, \mathbf{p} \rangle_{\mathbf{A}} = 0.$

Part(b): As defined in Definition 3.3.3, we choose $\mathbf{v} \in K = L$, i.e. \mathbf{v} is a linear combination of \mathbf{p} and \mathbf{r} . From the second condition $\mathbf{r}^{(k)} - \mathbf{A}\mathbf{v} \perp L$, we can deduce the coefficients for \mathbf{v} :

$$\mathbf{r}^{(k)} - \mathbf{A}\mathbf{v} \perp L \Rightarrow \langle \mathbf{r} - \mathbf{A}\mathbf{v}, \mathbf{r} \rangle = 0, \langle \mathbf{r} - \mathbf{A}\mathbf{v}, \mathbf{p} \rangle = 0.$$

Let $\mathbf{v} = \alpha \mathbf{r} + \beta \mathbf{p}$.

$$\langle \mathbf{r} - \mathbf{A}\mathbf{v}, \mathbf{r} \rangle = 0$$

$$\Leftrightarrow \langle \mathbf{r}, \mathbf{r} \rangle - \langle \alpha \mathbf{A}\mathbf{r} + \beta \mathbf{A}\mathbf{p}, \mathbf{r} \rangle = 0$$

$$\Leftrightarrow \langle \mathbf{r}, \mathbf{r} \rangle - \alpha \langle \mathbf{A}\mathbf{r}, \mathbf{r} \rangle - \beta \langle \mathbf{A}\mathbf{p}, \mathbf{r} \rangle = 0$$

$$\Leftrightarrow \langle \mathbf{r}, \mathbf{r} \rangle - \alpha \langle \mathbf{A}\mathbf{r}, \mathbf{r} \rangle - \beta \langle \mathbf{p}, \mathbf{A}\mathbf{r} \rangle = 0$$

$$\Leftrightarrow \langle \mathbf{r}, \mathbf{r} \rangle - \alpha \langle \mathbf{A}\mathbf{r}, \mathbf{r} \rangle = 0$$

$$\Leftrightarrow \alpha = \frac{\langle \mathbf{r}, \mathbf{r} \rangle}{\langle \mathbf{A}\mathbf{r}, \mathbf{r} \rangle}$$

$$\langle \mathbf{r} - \mathbf{A}\mathbf{v}, \mathbf{p} \rangle = 0$$

$$\Leftrightarrow \langle \mathbf{r}, \mathbf{p} \rangle - \langle \alpha \mathbf{A}\mathbf{r} + \beta \mathbf{A}\mathbf{p}, \mathbf{p} \rangle = 0$$

$$\Leftrightarrow \langle \mathbf{r}, \mathbf{p} \rangle - \alpha \langle \mathbf{A}\mathbf{r}, \mathbf{p} \rangle - \beta \langle \mathbf{A}\mathbf{p}, \mathbf{p} \rangle = 0$$

$$\Leftrightarrow \langle \mathbf{r}, \mathbf{p} \rangle - \beta \langle \mathbf{A}\mathbf{p}, \mathbf{p} \rangle = 0$$

$$\Leftrightarrow \beta = \frac{\langle \mathbf{r}, \mathbf{p} \rangle}{\langle \mathbf{A}\mathbf{p}, \mathbf{p} \rangle}$$

$$\Leftrightarrow \beta = \frac{\langle \mathbf{r}, \mathbf{p} \rangle}{\langle \mathbf{A}^2\mathbf{r}, \mathbf{p} \rangle}$$

In each step, first update **p**, then compute α and β and then update **x**.

Part (c): The method is similar to the steepest decent method. In the steepest decent method we choose $K_{\rm sd} = L_{\rm sd} = {\rm span}\{{\bf r}\}$ and in the method described here we choose $K = L = {\rm span}\{{\bf r},{\bf Ar}\}$. In each step $K_{\rm sd} \subset K$ and $L_{\rm sd} \subset L$. Thus, the method is not converging worse than the steepest decent method. Therefore, it converges.

 ${\bf Solution~3~(Programming).~C++~sample~code~./programs/steepest-decent.cc}$ without assembling the system matrix.

Convergence rate (Definition 2.2.18 in lecture notes). As can be seen in the plot, the convergence of the steepest decent method is sublinear.

to be handed in until December 18, 2024, 11am.

Problem 1. Consider a matrix of the form

$$\mathbf{A} = \mathbb{I} + \alpha \mathbf{B},$$

where **B** is skew symmetric (real), i.e., such that $\mathbf{B}^T = -\mathbf{B}$.

- (a) Show that $\langle \mathbf{A}\mathbf{x}, \mathbf{x} \rangle / \langle \mathbf{x}, \mathbf{x} \rangle = 1$ for all $\mathbf{x} \neq 0$.
- (b) Consider the Arnoldi process for **A**. Show that the resulting Hessenberg matrix will have the following tridiagonal form:

$$\mathbf{H}_{m} = \begin{pmatrix} 1 & -\eta_{2} \\ \eta_{2} & 1 & -\eta_{3} \\ & & \cdots \\ & & \eta_{m-1} & 1 & -\eta_{m} \\ & & & \eta_{m} & 1 \end{pmatrix}.$$

(c) Using the result of part (b), explain why the CG algorithm applied as is to a linear system with the matrix **A**, which is nonsymmetric, will still yield residual vectors that are orthogonal to each other.

Problem 2. Consider the CG Method described in Algorithm 3.4.31. Assume, in line 4, $\langle \mathbf{A}\mathbf{p}_m, \mathbf{p}_m \rangle = 0$ and thus the algorithm terminates there. Why is the Krylov space K_m invariant? Why have we found the exact solution then?

Problem 3. Consider again matrix T_{α} as introduced in Problem 3 on sheet Sheet 7.

- (a) Implement a method that computes the smallest eigenvalue of the matrix \mathbf{L}_2 using the inverse iteration (Algorithm 2.6.2 in the lecture notes). Do not calculate the inverse explicitly for solving the appearing linear system, but use the conjugate gradient iteration (Algorithm 3.4.31 in the lecture notes) for this matter.
- (b) Use your implementation to calculate the smallest eigenvalue of L_2 with n=20.

Numerical Linear Algebra - Sheet 9 Solutions

Solution 1. (a) We want to show that $\langle \mathbf{A}x, x \rangle / \langle x, x \rangle = 0$.

$$\langle \mathbf{B}\mathbf{x}, \mathbf{x} \rangle = \langle \mathbf{x}, \mathbf{B}\mathbf{x} \rangle = \langle \mathbf{B}^T \mathbf{x}, \mathbf{x} \rangle = -\langle \mathbf{B}\mathbf{x}, \mathbf{x} \rangle$$
 (1)

Thus, $\langle \mathbf{B} \mathbf{x}, \mathbf{x} \rangle = 0$ and therefore,

$$\langle \mathbf{A}\mathbf{x}, \mathbf{x} \rangle = \langle \mathbf{x} + \alpha \mathbf{B}\mathbf{x}, \mathbf{x} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle + \alpha \langle \mathbf{B}\mathbf{x}, \mathbf{x} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle.$$
 (2)

(b) Using Lemma 3.4.12 we have

$$\mathbf{A}\mathbf{Q}_m = \mathbf{Q}_m \mathbf{H}_m + \mathbf{w}_m \mathbf{e}_m^T. \tag{3}$$

Using this and $\mathbf{A} = \mathbb{I} + \alpha \mathbf{B}$ we can rearrange into

$$\mathbf{H}_m = \mathbb{I} + \alpha \mathbf{Q}_m^T \mathbf{B} \mathbf{Q}_m - \mathbf{Q}_m^T \mathbf{w}_m \mathbf{e}_m^T. \tag{4}$$

From the Arnoldi algorithm (Algorithm 3.4.11) we get that \mathbf{w}_m is chosen such that it is orthogonal to $\mathbf{q}_1, \dots, \mathbf{q}_m$ and therefore $\mathbf{Q}_m^T \mathbf{w}_m \mathbf{e}_m^T = 0$. Furthermore,

$$(\mathbf{Q}_m^T \mathbf{B} \mathbf{Q}_m)^T = \mathbf{Q}_m^T \mathbf{B}^T \mathbf{Q}_m = -\mathbf{Q}_m^T \mathbf{B} \mathbf{Q}_m, \tag{5}$$

i.e. $\mathbf{Q}_m^T \mathbf{B} \mathbf{Q}_m$ is skew-symmetric with zeros on the diagonal. This shows that \mathbf{H}_m admits the desired structure.

(c) ...

Solution 2.

Solution 3.

discussion in the first tutorials of January, 2025

This exercise sheet reviews some topics of this lecture. Try first to answer withour looking at the notes. Your answers do not have to be handed in, but the exercises will be discussed in the tutorials of the first week of January.

Problem 1. Recapitulate the concept of an orthogonal projection and an oblique projection. What are use cases of both and why are they important for numerical linear algebra?

Problem 2. How can the QR factorization of a given matrix be computed? Discuss downsides and benefits of the different methods.

Problem 3. Householder reflections vs. Givens rotations: Which one is more cost-efficient in the general case? When is using the other one advantageous?

Problem 4. Which of the discussed methods for solving eigenvalue problems can be implemented without explicitly forming a matrix?

Problem 5. Consider an $n \times n$ matrix that has n distinct eigenvalues such that $|\lambda_i| \neq |\lambda_j|$ for $i \neq j$. How can the eigenvalue with the second largest absolute value be computed?

Problem 6. When does one step of the Gauss-Seidel iteration provide the direct solution of a linear system? Consider an upper triangular matrix to visualize this matter.

Problem 7. What are drawbacks of the orthogonal subspace iteration? When does it converge?

Problem 8. Why is the implicit double shift better than the explicit?

Problem 9. What is deflation? Why do we use it?

Problem 10. What is polynomial filtering?

Problem 11. Why do we use iterative solvers?

Problem 12. How does the Gauss-Seidel method converge for an upper triangular matrix?

Problem 13. What is the difference between the steepest descent and the minimal residual method?

Problem 14. What is the difference between the steepest descent and the conjugate gradient method?

Problem 15. Why do we use conjugate gradient and not a straight forward implementation of a Lanczos solver?

Problem 16. What is a Krylov space?

Problem 17. What is the difference between the Arnoldi and the Lanczos processes?

Problem 18. Is there a short recurrence for the GMRES method?

Problem 19. What is preconditioning?

Problem 20. What complicates preconditioning for the conjugate gradient method?

Numerical Linear Algebra -Sheet 10 Solutions

Solution 1.

Solution 2.

Solution 3.

Solution 4 (Programming).

to be handed in until January 15, 2025, 11am.

Problem 1. Use your implementation of the Conjugate Gradient Method (Problem 3 on Sheet 9) and augment it such that you can compute the eigenvalues of the projected matrix \mathbf{H}_m in each step. For the computation of the eigenvalues you could, for example, use your implementation of the QR iteration (Problem 3 on Sheet 5). Test your implementation with \mathbf{L}_2 as in Problem 3 on Sheet 9 and observe the convergence of extremal eigenvalues λ_{\min} and λ_{\max} .

Problem 2. Show that GMRES and Arnoldi with modified Gram-Schmidt will convwerge on the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ when

$$\mathbf{A} = \begin{pmatrix} 1 & & & 1 \\ 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

and $\mathbf{x}_0 = \mathbf{0}$.

Numerical Linear Algebra -Sheet 11 Solutions

Solution 1.

Solution 2 (Programming).

to be handed in until February 22, 2025, 2pm.

Problem 1. Let **A** and **B** be symmetric positive-definite matrices in $\mathbb{R}^{n \times n}$. Let there be constants c_1, c_2 auch that

$$c_1 \mathbf{x}^T \mathbf{A} \mathbf{x} \le \mathbf{x}^T \mathbf{B} \mathbf{x} \le c_2 \mathbf{x}^T \mathbf{A} \mathbf{x}.$$

Derive an estimate for the convergence of the conjugate gradient iteration for $\mathbf{A}\mathbf{x} = \mathbf{b}$ with preconditioner \mathbf{B}^{-1} depending on c_1 and c_2 .

Hints: Lemma 3.4.72 in the lecture notes and Theorem 2.2.17 (note that the definition of the Rayleigh quotient is independent of the choice of inner product).

Problem 2. Develop a modified version of the non-Hermitian Lanczos algorithm that produces a sequence of vectors \mathbf{v}_i , \mathbf{w}_i that are such that each \mathbf{v}_i is orthogonal to every \mathbf{w}_i with $j \neq i$ and $\|\mathbf{v}_i\| = \|\mathbf{w}_i\| = 1$ for all i.

Problem 3. Find an example of a matrix with a real spectrum for which the QR method will not converge to an upper triangular matrix.

Numerical Linear Algebra -Sheet 12 Solutions

Solution 1. A and B are symmetric, positive-definite, thus

$$\left\langle \mathbf{B}^{-1}\mathbf{A}\mathbf{x},\mathbf{x}\right\rangle _{\mathbf{B}}=\left\langle \mathbf{A}\mathbf{x},\mathbf{x}\right\rangle =\left\langle \mathbf{x},\mathbf{A}\mathbf{x}\right\rangle =\left\langle \mathbf{x},\mathbf{B}\mathbf{B}^{-1}\mathbf{A}\mathbf{x}\right\rangle =\left\langle \mathbf{x},\mathbf{B}^{-1}\mathbf{A}\mathbf{x}\right\rangle _{\mathbf{B}}.$$

For the CG-method we have the estimate:

$$\|e^{(m)}\|_{\mathbf{A}} \le 2 * \left(\frac{\sqrt{\operatorname{cond}(\mathbf{A})} - 1}{\sqrt{\operatorname{cond}(\mathbf{A})} + 1}\right)^m \|e^{(0)}\|_{\mathbf{A}}.$$

The condition number for $\mathbf{B}^{-1}\mathbf{A}$ is given by

$$\operatorname{cond}(\mathbf{B}^{-1}\mathbf{A}) = \frac{\sigma_{\max}(\mathbf{B}^{-1}\mathbf{A})}{\sigma_{\max}(\mathbf{B}^{-1}\mathbf{A})}.$$

We want to find an estimate for the condition number, using the Rayleigh quotient.

$$R_{\mathbf{B}^{-1}\mathbf{A}}(\mathbf{x}) = \frac{\left\langle \mathbf{B}^{-1}\mathbf{A}\mathbf{x}, \mathbf{x} \right\rangle_{\mathbf{B}}}{\left\langle \mathbf{x}, \mathbf{x} \right\rangle_{\mathbf{B}}} = \frac{\left\langle \mathbf{A}\mathbf{x}, \mathbf{x} \right\rangle}{\left\langle \mathbf{x}, \mathbf{x} \right\rangle_{\mathbf{B}}} = \frac{\mathbf{x}^T \mathbf{A}\mathbf{x}}{\mathbf{x}^T \mathbf{B}\mathbf{x}}.$$

Thus, for all \mathbf{x} in \mathbb{R}^n , we have the estimate

$$1/c_2 \le R_{\mathbf{B}^{-1}\mathbf{A}}(\mathbf{x}) \le 1/c_1.$$

Using Courant-Fischer, we get

$$1/c_2 \le \sigma_{\min}(\mathbf{B}^{-1}\mathbf{A}) \le 1/c_1$$

and

$$1/c_2 \le \sigma_{\max}(\mathbf{B}^{-1}\mathbf{A}) \le 1/c_1.$$

For the condition number we then have

$$0 < c_1/c_2 \le \text{cond}(\mathbf{B}^{-1}\mathbf{A}) \le c_2/c_1$$
.

For the convergence of the CG-method with preconditioner \mathbf{B}^{-1} this means

$$\begin{aligned} \|e^{(m)}\|_{\mathbf{B}^{-1}\mathbf{A}} &\leq 2 * \left(\frac{\sqrt{\operatorname{cond}(\mathbf{B}^{-1}\mathbf{A})} - 1}{\sqrt{\operatorname{cond}(\mathbf{B}^{-1}\mathbf{A})} + 1}\right)^{m} \|e^{(0)}\|_{\mathbf{B}^{-1}\mathbf{A}} \\ &\leq 2 * \left(\frac{\sqrt{c_{2}/c_{1}} - 1}{\sqrt{c_{1}/c_{2}} + 1}\right)^{m} \|e^{(0)}\|_{\mathbf{B}^{-1}\mathbf{A}} \\ &\leq 2 * \left(\frac{c_{2} - \sqrt{c_{1}c_{2}}}{c_{1} + \sqrt{c_{1}c_{2}}}\right)^{m} \|e^{(0)}\|_{\mathbf{B}^{-1}\mathbf{A}}. \end{aligned}$$

Solution 2. Consider for example the matrix

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Then **A** is orthonormal and the QR-decomposition of **A** is given by **A** and \mathbb{I} . In each iteration step we have $\mathbf{A}_k = \mathbf{A}$, which is not an upper tridiagonal matrix.

Choosing

$$\mathbf{Q} = 1/\sqrt{2} * \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

gives us the correct Schur form

$$\mathbf{R} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Problems for presentation on Thursday, 30 January

Problem 1. Problem 1.2.9 in the lecture notes.

Problem 2. Problem 2.1.24 in the lecture notes.

Problem 3. Let **A** be a symmetric tridiagonal matrix. Show that the QR-iteration (see Algorithm 2.4.2 in the lecture notes) preserves the tridiagonal structure of the matrix, i.e., all iterates $\mathbf{A}^{(n)}$ generated by the QR-iteration are tridiagonal.

Problem 4. Problem 2.4.18 in the lecture notes.

Problem 5. Let **H** be a real Hessenberg matrix. Let $\mathbf{Q}_1, \mathbf{R}_1, \mathbf{Q}_2, \mathbf{R}_2$ be the matrices obtained in the explicit double-shift QR step (Algorithm 2.5.14). Let σ_1 and σ_2 are the shifts in Lemma 2.5.16. Show that the following equation in the proof of Lemma 2.5.16 holds:

$$\mathbf{Q}_1\mathbf{Q}_2\mathbf{R}_2\mathbf{R}_1 = \mathbf{M} = (\mathbf{H} - \sigma_1\mathbb{I})(\mathbf{H} - \sigma_2\mathbb{I})$$

Problem 6. Prove Theorem 3.2.15 in the lecture notes.

Problem 7. Consider the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$, where \mathbf{A} is a symmetric positive definite matrix. We define a projection method which uses a two-dimensional space at each step. At a given step, take $L = K = \mathrm{span}\{\mathbf{r}, \mathbf{A}\mathbf{r}\}$, where $\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}$ is the current residual.

- (a) For a basis of K use the vector \mathbf{r} and the vector \mathbf{p} obtained by orthogonalizing \mathbf{Ar} against \mathbf{r} with respect to the \mathbf{A} -inner product. Give the formula for computing \mathbf{p} (no need to normalize the resulting vector).
- (b) Write the algorithm for performing the projection method described above.
- (c) Can you explain, not compute, why the algorithm converges for any initial guess \mathbf{x}_0 ? Hint: Exploit the convergence results for one-dimensional projection techniques.

Problem 8. Consider a matrix of the form

$$\mathbf{A} = \mathbb{I} + \alpha \mathbf{B},$$

where **B** is skew symmetric (real), i.e., such that $\mathbf{B}^T = -\mathbf{B}$.

(a) Show that $\langle \mathbf{A}\mathbf{x}, \mathbf{x} \rangle / \langle \mathbf{x}, \mathbf{x} \rangle = 1$ for all $\mathbf{x} \neq 0$.

(b) Consider the Arnoldi process for ${\bf A}.$ Show that the resulting Hessenberg matrix will have the following tridiagonal form:

$$\mathbf{H}_{m} = \begin{pmatrix} 1 & -\eta_{2} & & & \\ \eta_{2} & 1 & -\eta_{3} & & \\ & & \cdots & & \\ & & \eta_{m-1} & 1 & -\eta_{m} \\ & & & \eta_{m} & 1 \end{pmatrix}.$$

(c) Using the result of part (b), explain why the CG algorithm applied as is to a linear system with the matrix \mathbf{A} , which is nonsymmetric, will still yield residual vectors that are orthogonal to each other.