to be handed in until October 28, 2022, 2pm.

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

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

Problem 2. Proof that every finite-dimensional vector space with scalar product has an orthonormal basis.

Hint: Gram-Schmidt orthogonalization

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 (Programming). Write a program that:

- ullet Generates an orthonormal basis from a given set of n n-dimensional complex vectors.
- Computes the Gram matrix of the obtained orthonormal basis

Test your program on the set of vectors: $\{\mathbf{v}_k\}$, k=1,...,n, $(\mathbf{v}_k)_j=e^{\frac{i\alpha_k j}{n}}$, $\alpha_k=1+\frac{1}{k}$. Investigate the obtained Gram matrix.

to be handed in until November 04, 2022, 2pm.

Problem 1. Show that a matrix is normal, if and only if it is unitarily similar to a normal matrix. Namely, matrix \mathbf{A} is normal, if and only if there exists a matrix \mathbf{Q} and a normal matrix \mathbf{B} such that

$$\mathbf{A} = \mathbf{Q}^{-1} \mathbf{B} \mathbf{Q}.$$

Problem 2. Show that for normal matrices the left and right eigenvectors for a given eigenvalue coincide.

Problem 3. Construct a counterexample that the problem of finding eigenvectors is *not* well-posed, if the eigenspaces are almost parallel.

Problem 4. Consider the following matrix

$$\mathbf{A} = \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix}^T \begin{pmatrix} 1 \\ c \end{pmatrix} \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix}$$

with parameters $\varphi \in [0, 2\pi]$ and $c \in (0, 1)$.

- 1. Compute the eigenvalues and eigenvectors of **A**.
- 2. (Programming) Write a program which computes the sequence $\mathbf{x}^{(n)} \in \mathbb{R}^2$ defined as

$$\mathbf{x}^{(n)} = \mathbf{A}\mathbf{x}^{(n-1)},$$
$$\mathbf{x}^{(0)} = \mathbf{x}^*,$$

for $\mathbf{x}^* = (1,\ 0)^T,\ c = 0.1,$ and $\varphi = \frac{\pi}{4}.$ Try playing with different values of those parameters.

- 3. Is there a limit of $\mathbf{x}^{(n)}$? What is about the case c=1?
- 4. Compute the limit: $\lim_{n\to\infty} \mathbf{A}^n$.

to be handed in until November 11, 2022, 2pm.

Problem 1. Consider a Hermitian matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ and a unitary linear operator $\mathbf{Q} \in \mathbb{C}^m \to \mathbb{C}^n$, m < n. Prove, that an eigenvalue $\lambda_k(\mathbf{B})$ of the matrix $\mathbf{B} = \mathbf{Q}^* \mathbf{A} \mathbf{Q} \in \mathbb{C}^{m \times m}$ is either equal to 0, or the following estimate holds

$$|\lambda_{\min}(\mathbf{A})| \le |\lambda_k(\mathbf{B})| \le |\lambda_{\max}(\mathbf{A})|,$$

where $\lambda_{\min}(\mathbf{A})$ and $\lambda_{\max}(\mathbf{A})$ denote the smallest and largest eigenvalues of \mathbf{A} measured by their magnitude.

Problem 2. A diagonalizable real matrix **A** has the following spectrum:

$$\sigma(\mathbf{A}) = \{-2, 1-2i, 1+2i, 1, -i, i, 2\}.$$

Consider using the inverse power method (vector iteration) to compute its eigenvalues.

- (a) Find a set of all shift parameters for which the inverse power method may not converge. Draw a sketch.
- (b) For every *real* eigenvalue find a *real* range of shifts that, if used in the inverse power method, will reduce the error of approximation of the eigenvalue by a factor of 10 in each iteration.

Problem 3. Propose shift parameters that will allow you to compute *all* eigenvalues and eigenvectors of the matrix

$$\begin{pmatrix} 100 & 15 & 3 \\ 15 & 20 & 5 \\ 3 & 5 & 65 \end{pmatrix}.$$

Prove that your choice is correct. Hint: Gershgorin circle theorem

Problem 4 (Programming). Write a program that computes all eigenvectors and eigenvalues of the matrix

$$\mathbf{A}_{\varepsilon} = \begin{pmatrix} 100 & 15 & 3 & 0 & 0 & \varepsilon \\ 15 & 20 & 5 & 0 & \varepsilon & 0 \\ 3 & 5 & 65 & \varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon & 110 & 20 & 5 \\ 0 & \varepsilon & 0 & 20 & 80 & 4 \\ \varepsilon & 0 & 0 & 5 & 4 & 30 \end{pmatrix}$$

using the shifted (inverse) power method by observing the following steps:

(a) Consider the matrix \mathbf{A}_0 with $\varepsilon=0$ and examine the structure of the eigenvalue problem.

- (b) Compute all eigenvalues and eigenvectors of \mathbf{A}_0 .
- (c) Would the strategy you proposed in Problem 3 allow you to compute all 6 eigenvalues?

Rewrite: Does the algorithm work, if you use Gerschgorin for ...

(d) Make an educated guess of the eigenvalues of \mathbf{A}_1 and try computing those.

Can you use part (a) to get something better

to be handed in until November 18, 2022, 2pm.

Problem 1. Let **A** be a symmetric tridiagonal matrix. Show that the QR-iteration (see Algorithm 1.4.3 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 2. Show that a (complex) symmetric matrix can be transformed to a tridiagonal matrix by using similarity transformations (this proves Theorem 1.4.14 in the lecture notes).

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 1.4.13 in the lecture notes).

Problem 4. Find an example of a matrix with a real spectrum for which the QR method will *not* converge to an upper triangular matrix.

Problem 5 (Programming).

- (a) Implement the Hessenberg QR step (Algorithm 1.4.12 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 and check, if your results are correct.

Give eigenvalues of A_n . Compare Sheet 6. See solution notes.

- (c) Use your implementation to run several steps of the QR iteration (Algorithm 1.4.3 in the lecture notes) for the matrix \mathbf{A}_{10} .
- (d) Discuss the observed convergence of the off-diagonal and diagonal entries, respectively.

to be handed in until November 25, 2022, 2pm.

Problem 1. Show that a normal triangular matrix is diagonal. *Hint:* look at the norms of Ae_i and A^*e_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 of a real matrix come in complex conjugate pairs.

Show that complex eigenvalues and their associated eigenvectors of a real matrix come in complex conjugate pairs.

Delete (b)

- (b) Show that the eigenvectors are of the form $\mathbf{u} \pm i\mathbf{v}$.
- (c) Choose real linear combinations of these vectors to obtain the 2×2 block.

Problem 3. Provide the following steps of Lemma 1.5.11 in the lecture notes (explicit double shift).

- (a) Show that $\mathbf{Q}_1\mathbf{Q}_2\mathbf{R}_2\mathbf{R}_1$ represents the QR factorization of a real matrix $\mathbf{M} = (\mathbf{H} \sigma_1\mathbb{I})(\mathbf{H} \sigma_2\mathbb{I}).$
- (b) Show that $\mathbf{Q}_1\mathbf{Q}_2$ is the orthogonal matrix that implements the similarity transformation of \mathbf{H} to obtain \mathbf{H}_2 .

Adjust this exercise according to tutorial notes of Laura

Problem 4 (Programming). Implement the symmetric QR step with implicit shift (Algorithm 1.5.6 in lecture notes) for a symmetric, unreduced, tridiagonal matrix **T** by observing the following steps:

- (a) Store **T** in two vectors, one for the diagonal, and one for the subdiagonal entries.
- (b) Implement the Givens rotation G_{12} and think about where to store the additional non-zero entry t_{31} .
- (c) Implement the additional Givens rotations for this data structure.
- (d) Use this to compute the eigenvalues of the matrix $\mathbf{A}_n = \operatorname{tridiag}(-1., 2., -1.)$ in dimension n = 10.

to be handed in until December 2, 2022, 2pm.

Problem 1. Prove that a matrix iteration converges *if and only if* the spectral radius of the iteration matrix is less than 1. *Hint:* You can use Lemma 2.2.10 in the lecture notes.

Problem 2. 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_j 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 3. Let **A** be a real symmetric positive-definite $n \times n$ matrix and **b** a vector in \mathbb{R}^n . Consider the Richardson iteration defined as

$$\mathbf{x}_{k+1} = (\mathbb{I} - \omega \mathbf{A}) \mathbf{x}_k + \omega \mathbf{b} = \mathbf{x}_k - \omega (\mathbf{A} \mathbf{x}_k - \mathbf{b})$$

where ω is a constant real parameter.

(a) Show that the sequence of iterates \mathbf{x}_k generated by the Richardson iteration converges to $\mathbf{A}^{-1}\mathbf{b}$ for any initial vector \mathbf{x}_0 if and only if

$$0<\omega<\frac{2}{\lambda_{\max}}.$$

(b) Show that the optimal value of ω is

$$\omega_{opt} = \frac{2}{\lambda_{\max} + \lambda_{\min}}.$$

Moreover

$$\|\mathbb{I} - \omega_{opt}\mathbf{A}\|_2 = \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} = \frac{\operatorname{cond}_2(\mathbf{A}) - 1}{\operatorname{cond}_2(\mathbf{A}) + 1},$$

where $\operatorname{cond}_2(\mathbf{A}) = \frac{\lambda_{\max}}{\lambda_{\min}}$.

Problem 4. Apply the obtained results of Problem 3 to a one-dimensional Laplace problem. To this end, take matrix \mathbf{T}_{α} from Problem 2 with $\alpha=2$ and work on the following tasks.

(a) Will the Richardson iteration coverge for this matrix? If so, what will be its covergence rate?

How do you have to choose ω , such that the Richardson iteration converges? What is the best choice?

- (b) How many iterations are needed to reduce the error by a factor of 10^{-6} depending on the number n of dicretization points?
- (c) Estimate the cost of a single iteration (depending on n, use $\mathcal{O}(\cdot)$ notation).
- (d) Estimate the cost of reducing the error by a given factor (depending on n, use $\mathcal{O}(\cdot)$ notation).

to be handed in until December 9, 2022, 2pm.

Problem 1. Let **A** be a real symmetric matrix with eigenvalues λ_j , $1 \leq j \leq n$. Show that for any polynomial $p(t) = \sum_{j=0}^k a_j t^j$ the matrix

$$p(\mathbf{A}) = \sum_{j=0}^{k} a_j \mathbf{A}^j$$

is also symmetric. Moreover, the eigenvectors of **A** and $p(\mathbf{A})$ are identical, while the eigenvalues of $p(\mathbf{A})$ are equal to $p(\lambda_j)$ for $1 \leq j \leq n$.

Definition missing: scalar $a_i \in \mathbb{R}$

Problem 2 (Eigenvalues and eigenvectors of a tensor product operator). For vectors $\mathbf{u} \in \mathbb{R}^n$ and $\mathbf{v} \in \mathbb{R}^m$ we define the tensor product as a (block) vector

$$\mathbf{u} \otimes \mathbf{v} = \begin{pmatrix} u_1 v & u_2 v & \cdots & u_n v \end{pmatrix}^T \in \mathbb{R}^{nm}.$$

Let **A** and **B** be matrices in $\mathbb{R}^{n\times n}$ and $\mathbb{R}^{m\times m}$ respectively. We define their tensor product $\mathbf{A}\otimes\mathbf{B}\in\mathbb{R}^{nm\times nm}$ as

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{n1}\mathbf{B} & \cdots & a_{nn}\mathbf{B} \end{pmatrix}.$$

- (a) Show that $(\mathbf{A} \otimes \mathbf{B})(\mathbf{u} \otimes \mathbf{v}) = (\mathbf{A}\mathbf{u}) \otimes (\mathbf{B}\mathbf{v})$.
- (b) Prove that the eigenvectors of the tensor product are the pairwise tensor products of the eigenvectos of the individual matrices. What are the corresponding eigenvalues?

Problem 3. 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 2 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

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

(a) Use the results of Problem 2 to show that L_2 could be expressed as

$$\mathbf{L}_2 = (\mathbf{L}_1 \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbf{L}_1).$$

(b) List the four smallest eigenvalues of L_2 . What is their multiplicity?

Problem 4 (Programming). Write a program that solves the 2D Laplace problem

$$Ax = b$$
,

with the Gauss-Seidel iteration, where the system matrix $\mathbf{A} = \mathbf{L}_2 \in \mathbb{R}^{n^2 \times n^2}$ is defined in Problem 3, and the right hand side is given by the constant vector $\mathbf{b} = (1, ..., 1)^T$, by observing the following steps. Try to avoid explicitly forming the system matrix.

- (a) Implement a function vmult that performs the matrix-vector product $\mathbf{A} \cdot \mathbf{v}$ of \mathbf{A} with a given vector \mathbf{v} , and returns a vector \mathbf{w} .
- (b) Write a function gauss_seidel_step that implements a single step of the Gauss-Seidel iteration. As in (a) this function should take a vector \mathbf{v} and return the resulting vector \mathbf{w} .
- (c) Use the null-vector $\mathbf{x}^{(0)} = (0,...,0)^T$ as initial guess and test your program 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 Gauss-Seidel iteration. Plot the obtained result vector after 1, 5, 15, 30, and 50 iterations.

Note: Be careful not to crash your computer when starting your program with n = 100 or more, if you explicitly build the system matrix, because of the possibly high memory usage.

b has not been defined: $\mathbf{b} = (1, ..., 1)^T$

to be handed in until December 16, 2022, 2pm.

Problem 1.

(a) Estimate the sparsity pattern, that is, the possible positions of nonzero entries, of the LU decomposition for the 5-diagonal sparse matrix

$$\begin{pmatrix} 2 & 0 & -1 & & & & \\ 0 & 2 & 0 & -1 & & & \\ -1 & 0 & 2 & 0 & -1 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 2 & 0 & -1 \\ & & & -1 & 0 & 2 & 0 \\ & & & & -1 & 0 & 2 \end{pmatrix}.$$

- (b) Make an educated guess how this sparsity pattern will change if the nonzero off-diagonal entries are further away from the diagonal.
- (c) Will the inverse have similar sparsity? To this end, consider how information flows between far away vector entries using $A^{-1} = LU$.

Rewrite as $\mathbf{A}^{-1} = \mathbf{U}^{-1} \mathbf{L}^{-1}$

Problem 2 ([?, P-5.1 b]). 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 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 . Assume that *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

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

1

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

Definition of a_{ii} is missing

(b) Does (a) prove that the algorithm converges?

Problem 3 ([?, P-5.6]). 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) Will the algorithm converge for any initial guess \mathbf{x}_0 ? Justify the answer. Hint: Exploit the convergence results for one-dimensional projection techniques.

Problem 4 (Programming).

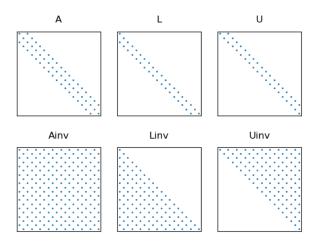
- (a) Implement the steepest decent method (Algorithm 2.3.15 in the lecture notes).
- (b) Use your implementation of the steepest decent method to solve the 2D Laplace problem

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

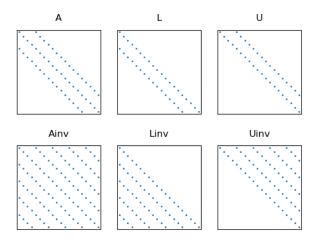
as in Problem 4 on Sheet 7 with right hand side vector $\mathbf{b} = (1, ..., 1)^T$ and initial guess $\mathbf{x}^{(0)} = (0, ..., 0)^T$ with n = 50 and n = 100. Observe the convergence for the first 50 steps. What convergence rate do you expect?

Numerical Linear Algebra - Sheet 8 Solutions

Solution 1. (a) Sample calculation of LU factorization in ./programs/lu.py. Sparsity patterns in figure below.



(b) The width of the zero diagonals gets transported to the matrices of the LU factorization



(c) The inverse is dense up to the zero diagonals that get scattered over the whole inverse

Solution 2 ([?, P-5.1 b]).

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

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

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

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

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

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

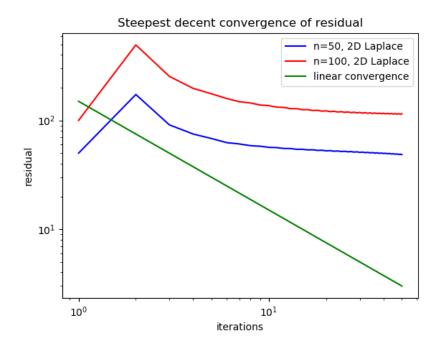
This would have been used to show hint 1.

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

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

Solution 3.

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.



discussion in the first tutorials of January, 2023

This exercise sheet reviews some topics of this lecture. 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. What methods presented in the lecture can be used for computing or estimating the eigenvalues of a matrix A? Sort by properties of the methods, as well as by conditions on A.

Problem 3. How can the QR factorization of a given matrix be computed? Discuss downsides and benefits of the different methods.

Problem 4. Householder reflections vs. Givens rotations: which one is more cost-efficient in the general case? When using the other one is advantageous?

Problem 5. Which of the discussed methods for solving eigenvalue problems can be implemented without explicitly forming a matrix?

Problem 6. 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 7. 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.

to be handed in until January 20, 2023, 2pm.

Problem 1 ([?, Exercise 6.21]). Consider a matrix of the form:

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

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

(a) Show that

$$\frac{\langle \mathbf{A}\mathbf{x}, \mathbf{x} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle} = 1$$

for all nonzero \mathbf{x} .

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

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

- (c) Using the result of part (b), explain why the conjugate gradient method applied to a linear system with the matrix **A** will still yield residual vectors that are orthogonal to each other.
- (d) Can this algorithm break down before the solution is reached?

Problem 2 ([?, Exercise 6.8]). Show how GMRES (Algorithm 2.3.41 in the lecture notes) and Arnoldi with modified Gram-Schmidt (Algorithm 2.3.29 in the lecture notes) will converge 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 $\mathbf{x}_0 = \mathbf{0}$.

Problem 3 (Programming).

(a) Implement the conjugate gradient method (Algorithm 2.3.57 in the lecture notes).

(b) Use your implementation to solve the 2D Laplace problem

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

as in Problem 4 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. Observe the convergence for the first 50 steps. What convergence rate do you expect? Compare your results of the conjugate gradient method with the steepest decent method from Problem 4 of Sheet 8.

to be handed in until January 27, 2023, 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 such 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 2.3.80 in the lecture notes, and Thereom 1.2.5 (note, that the definition of the Rayleigh quotient is independent of the choice of the inner product).

Problem 2. Consider again the 2D Laplace operator L_2 , discretized by the five-point-stencel, as in Problem 4 on Sheet 7.

- (a) Implement a method that computes the smallest eigenvalue of \mathbf{L}_2 using the inverse iteration (Algorithm 1.3.6 in the lecture notes). Do not calculate the invers explicitly for solving the appearing linear system, but use the conjugate gradient iteration (Algorithm 2.3.57 in the lecture notes) for this matter.
- (b) Use your implementation to calculate the smallest eigenvalue of \mathbf{L}_2 for n=50 and n=100.

to be handed in until February 3, 2023, 2pm.

Problem 1 ([?, P-6.8]). Show that the vector \mathbf{v}_{m+1} obtained at the last step of Arnoldi's method is of the form

$$\mathbf{v}_{m+1} = \gamma p_m(\mathbf{A})\mathbf{v}_1,$$

in which γ is a certain normalizing scalar and p_m is the characteristic polynomial of the Hessenberg matrix \mathbf{H}_m .

Problem 2 ([?, P-6.9]). 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}_j with $j \neq i$ and $\|\mathbf{v}_i\| = \|\mathbf{w}_i\| = 1$ for all i. What does the projected problem become?

Problem 3. The coefficients of the Hessenberg matrix \mathbf{H}_m in the conjugate gradient iteration can be used to compute the eigenvalues of a matrix \mathbf{A} . Use this to develop a method that approximates the eigenvalues of a symmetric positive definit matrix \mathbf{A} .