

Numerical Linear Algebra for Computational Science and
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Problems

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The listed problems are distributed as follows:

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L01. Essentials of Linear Algebra

Problem 1 Let $A \in \mathbb{R}^{n \times n}$ be symmetric positive-definite. Show that

$$(\cdot, \cdot)_A : (x, y) \in \mathbb{R}^n \times \mathbb{R}^n \mapsto (x, y)_A := x^T A y$$

is an inner-product on \mathbb{R}^n , and $\|\cdot\|_A := (\cdot, \cdot)_A^{1/2}$ is a norm.

Problem 2 Show that $A \in \mathbb{R}^{m \times n}$ has rank 1 if and only if there exist non-zero vectors $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$ such that $A = uv^T$.

Problem 3 Show that $\|xy^T\|_2 = \|x\|_2 \cdot \|y\|_2 \forall x, y \in \mathbb{R}^n$.

Problem 4 Determine the orthogonal projector P onto the subspace spanned by a non-zero vector $w \in \mathbb{R}^n$.

Problem 5 Let $A \in \mathbb{R}^{m \times n}$ have $p \leq \min(m, n)$ non-zero singular values $\sigma_1 \geq \dots \geq \sigma_p > 0$ with corresponding $U := [u_1, \dots, u_p]$ and $V := [v_1, \dots, v_p]$ as left and right singular vectors. Then, show that

- a. $A^\dagger := V\Sigma^{-1}U^T$ is the Moore-Penrose inverse of A where $\Sigma := \text{diag}(\sigma_1 \dots, \sigma_p)$.
- b. $P := AA^\dagger$ is an orthogonal projector onto $\text{range}(A)$.
- c. $P := I_n - A^\dagger A$ is an orthogonal projector onto $\text{null}(A)$.

Problem 6 Answer the following questions, and provide proper explanations:

- a. Are the principal sub-matrices of a Hermitian positive-definite (HPD) matrix also HPD?
- b. Let $A = XBX^H$ be HPD and X be non-singular. Is B also HPD?
- c. Are the principal sub-matrices of a non-singular matrix also non-singular?

Problem 7 Let $A \in \mathbb{R}^{n \times n}$ be symmetric positive-definite. Determine the A -orthogonal projector P onto the subspace spanned by a non-zero vector $w \in \mathbb{R}^n$, i.e., for which orthogonality is stated with respect to the inner product $(\cdot, \cdot)_A : (x, y) \in \mathbb{R}^n \times \mathbb{R}^n \mapsto (x, y)_A := x^T A y$.

L03. Floating-point arithmetic and error analysis

Problem 8 Show that the unit roundoff of a (binary) floating-point number system which uses $p - 1$ fraction bits, i.e., where p denotes the precision of the numerical system, is given by $u = 2^{-p}$.

Problem 9 Let x, y, z be floating-point numbers such that $x + y + z \neq 0$, and consider the functions given by $f : (x, y, z) \mapsto x + y + z$ and $\tilde{f} : (x, y, z) \mapsto \text{fl}(\text{fl}(x + y) + z)$. Show that

$$\tilde{f}(x, y, z) = (1 + \delta)f(x, y, z) \quad \text{where} \quad |\delta| \lesssim \left(1 + \left|\frac{x + y}{x + y + z}\right|\right) u$$

in which u is the unit roundoff of the system.

Problem 10 Show that the perturbations

$$\delta A = \frac{\|A\|_2 r \tilde{x}^T}{\|\tilde{x}\|_2 \cdot (\|A\|_2 \cdot \|\tilde{x}\|_2 + \|b\|_2)} \quad \text{and} \quad \delta b = -\frac{\|b\|_2 r}{\|A\|_2 \cdot \|\tilde{x}\|_2 + \|b\|_2}$$

are such that $(A + \delta A)\tilde{x} = b + \delta b$ is exactly solved by the approximation \tilde{x} of $A^{-1}b$, with residual $r = b - A\tilde{x}$. Show also that they attain the minimal 2-norms achievable by such perturbations.

Hint: Remember that $\|xy^T\|_2 = \|x\|_2\|y\|_2 \forall x, y \in \mathbb{R}^n$.

Problem 11 Let $A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 0 & 5 & 6 \\ 0 & 0 & 7 & 8 \\ 0 & 0 & 0 & 9 \end{bmatrix}$, answer the following questions, and provide proper explanations:

- a. What is the spectrum of A ?
- b. Is A singular?
- c. Is A defective?
- d. Is A diagonalizable?
- e. Is A normal?
- f. What is the conditioning number of the smallest eigenvalue of A ?
- g. What is the conditioning number of each eigenvalue of $B := A + A^T$?

L04. Direct methods for dense linear systems

Problem 12 Show that, if a leading principal sub-matrix of A , i.e., $A[1:k, 1:k]$ with k such that $1 \leq k < n$, is singular, then Doolittle's forward elimination procedure, if applied to A without pivoting, will break down. Explain when precisely and how the breakdown will happen.

Problem 13 Consider the symmetric positive-definite matrix given by $A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$, with eigenpairs $(4, \begin{bmatrix} 1 \\ 1 \end{bmatrix})$ and $(2, \begin{bmatrix} -1 \\ 1 \end{bmatrix})$.

- Construct, with a pen and paper, the Cholesky factor L with positive diagonal components such that $A = LL^T$.
- Form the square root $A^{1/2}$ of A .

Problem 14 Show that, if $A \in \mathbb{R}^{n \times n}$ is SPD, then it admits an LU decomposition without pivoting.

Problem 15 Let $A = \begin{bmatrix} 1 & 6 & 1 & 0 \\ 0 & 1 & 9 & 0 \\ 1 & 6 & 1 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$, answer the following questions, and provide proper explanations:

- Is A singular?
- Assuming exact arithmetic, can (Doolittle's) forward elimination procedure be successfully applied to A , without pivoting?

L05. Sparse data structures and basic linear algebra subprograms

Problem 16 Consider the matrices

$$A = \begin{bmatrix} \bullet & \bullet & 0 & \bullet & 0 & 0 \\ 0 & \bullet & 0 & 0 & 0 & \bullet \\ 0 & \bullet & \bullet & 0 & 0 & 0 \\ 0 & \bullet & 0 & 0 & \bullet & 0 \\ 0 & 0 & 0 & 0 & \bullet & 0 \\ 0 & 0 & 0 & 0 & 0 & \bullet \end{bmatrix} \text{ and } B = \begin{bmatrix} \bullet & 0 & 0 & 0 & 0 & 0 \\ \bullet & 0 & \bullet & 0 & \bullet & 0 \\ 0 & \bullet & 0 & 0 & 0 & 0 \\ \bullet & \bullet & 0 & 0 & 0 & 0 \\ 0 & \bullet & 0 & \bullet & \bullet & 0 \\ 0 & 0 & \bullet & 0 & 0 & \bullet \end{bmatrix}$$

where each \bullet denotes a non-zero component.

Show the adjacency graphs of A , B , AB and BA . You may assume that there are no numerical cancellations in computing the products AB and BA .

Problem excerpted from Pb. 4 in Chap. 3 of Saad (2003).

Saad, Y. (2003). Iterative methods for sparse linear systems. Society for Industrial and Applied Mathematics.

L06. Introduction to direct methods for sparse linear systems

Problem 17 Find the non-zero pattern of the Cholesky factor L for the following matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & a_{14} \\ a_{12} & a_{22} & 0 & a_{24} \\ 0 & 0 & a_{33} & 0 \\ a_{14} & a_{24} & 0 & a_{44} \end{bmatrix}$$

Show your work using the up-looking Cholesky factorization algorithm.

L07. Orthogonalization and least-squares problems

Problem 18 Let $A = \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix}$ and $b = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$.

- (a) Find a QR decomposition of A applying a Gram-Schmidt procedure with a pen and paper.
- (b) Find the least-squares problem solution $x = \arg \min_x \|Ax - b\|_2$ making use of the QR factorization.

L08. Basic iterative methods for linear systems

Problem 19 Let $A = \begin{bmatrix} 1 & 2 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$. Analyze the spectrum of the iteration matrix and show whether

- (a) A Jacobi iteration would converge.
- (b) A Gauss-Seidel iteration would converge.
- (c) A SOR iteration would converge with $\omega = 1/2$.

L09. Basic iterative methods for eigenvalue problems

Problem 20 Show that the gradient of the Rayleigh quotient of a symmetric matrix A given by

$$r(x) = \frac{x^T Ax}{x^T x} \text{ for } x \neq 0$$

is given by $\nabla r(x) = \frac{2}{x^T x}(Ax - r(x)x)$.

Problem 21 Let (λ, x) be a right eigen-pair of A , (μ, y) be a left eigen-pair of A and μ be distinct from λ . Show that x and y are orthogonal.

L10. Locally optimal block preconditioned conjugate gradient

Problem 22 Show that the gradient of the generalized Rayleigh quotient of a symmetric pencil (A, B) with symmetric A and SPD B given by

$$\rho(x) = \frac{x^T Ax}{x^T Bx} \text{ for } x \neq 0$$

is $\nabla \rho(x) = \frac{2}{x^T Bx}(Ax - \rho(x)Bx)$.

Problem 23 Let A be symmetric and B be SPD. Then show that the matrix $X = [x_1, \dots, x_k]$ of the smallest general eigenvectors x_1, \dots, x_k of (A, B) with $x_i^T B x_j = \delta_{ij}$ is such that $\text{trace}(X^T A X)$ is minimized, subjected to $X^T B X = I_k$.

L11. Arnoldi and Lanczos procedures

Problem 24 For the matrices

$$A = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} \quad \text{and} \quad V = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix},$$

- (a) Find the Rayleigh Ritz pairs of A with respect to $\text{range}(V)$.
- (b) Assemble the reduced eigenvalue problem to solve in order to find the harmonic Ritz values of A with respect to $\text{range}(V)$ for $\sigma = 0$.

Problem 25 For the matrix $A = \begin{bmatrix} 2 & 3 & 0 \\ 1 & 2 & 3 \\ 0 & 1 & 2 \end{bmatrix}$ and $q_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, use the Arnoldi process to build an orthonormal basis $Q_2 = [q_1, q_2]$ of the Krylov subspace $\mathcal{K}_2(A, q_1)$, and compute the projected matrix $H_2 = Q_2^T A Q_2$.

L12. Jacobi-Davidson methods

Problem 26 Show that if a matrix $A \in \mathbb{F}^{n \times n}$ has constant diagonal components, i.e., $D_A \propto I_n$, then, assuming exact arithmetic, the Davidson method is equivalent to applying a Rayleigh-Ritz projection to a Krylov subspace generated by a Arnoldi procedure with the same starting vector q .

L13. Krylov subspace methods for linear systems

Problem 27 Recall that the approximation $\tilde{x} \in x_0 + \mathcal{K}$ to the solution of $Ax = b$ s.t. $b - A\tilde{x} \perp \mathcal{L}$ is formed by $\tilde{x} = x_0 + V_m(W_m^H A V_m)^{-1} W_m^H r_0$, which requires that $W_m^H A V_m$ is not singular, where $\mathcal{K} = \text{range}(V_m)$ and $\mathcal{L} = \text{range}(W_m)$. Show that $W_m^H A V_m$ is not singular if and only if no vector of the subspace $A\mathcal{K}$ is orthogonal to the constraints subspace \mathcal{L} , i.e., $A\mathcal{K} \cap \mathcal{L}^\perp = \{0\}$. Do so considering the dot product as the inner product.

Problem 28 For any $y \in \mathbb{F}^n$ and approximation space $\mathcal{K} \subset \mathbb{F}^n$, show that among all $x \in \mathcal{K}$, $\|y - x\|_2$ is minimized if and only if $y - x \perp \mathcal{K}$.

Problem 29 Using the result of Pb. 27, prove that the GMRES iterate defined as

$$x_m \in x_0 + \mathcal{K}_m(A, r_0) \text{ such that } r_m := b - Ax_m \perp A\mathcal{K}_m(A, r_0)$$

is equivalently given as the constrained minimizer of residual norm:

$$\|b - Ax_m\|_2 = \min_{x \in x_0 + \mathcal{K}_m(A, r_0)} \|b - Ax\|_2.$$

Problem 30 Let $A \in \mathbb{R}^{n \times n}$ be SPD and $x_j \in x_0 + \mathcal{K}_j(A, r_0)$ denote the CG iterate approximating the solution of $Ax = b$. Show that x_j minimizes the A -norm of the error over the search space, i.e.,

$$\|x - x_j\|_A = \min_{y \in x_0 + \mathcal{K}_j(A, r_0)} \|x - y\|_A \quad \text{where} \quad \|x\|_A := (Ax, x)^{1/2}.$$

L14. Preconditioned iterative methods for linear systems

Problem 31 Let $A \in \mathbb{R}^{n \times n}$ be a non-singular coefficient matrix for the linear system $Ax = b$, and $M \in \mathbb{R}^{n \times n}$ be a non-singular preconditioner which admits a decomposition $M = M_L M_R$.

- a. Show that $M^{-1}A$, AM^{-1} and $M_L^{-1}AM_R^{-1}$ are similar.
- b. Given a right-eigenvector y of $M^{-1}A$, find an associated right-eigenvector for AM^{-1} , and another one for $M_L^{-1}AM_R^{-1}$.

Problem 32 Let $A \in \mathbb{R}^{n \times n}$ be any matrix. Then, show that

- a. $\|I_n - AM^{-1}\|_F$ is minimized by $M^{-1} \in \mathbb{R}^{n \times n}$ if $A^T AM^{-1} = A^T$.
- b. $\|I_n - M^{-1}A\|_F$ is minimized by $M^{-1} \in \mathbb{R}^{n \times n}$ if $M^{-1}AA^T = A^T$.

L15. Restarted Krylov subspace methods

Problem 33 Consider the Arnoldi relation achieved after an implicit restart:

$$AV_m^{(p)} = V_m^{(p)} H_m^{(p)} + r_k^{(p)} e_m^{(m)T}$$

where $V_m^{(p)} := V_m Q^{(p)}$ and

$$H_m^{(p)} = Q_{p+1} R_{p+1} + \mu_{p+1} I_m = Q_p^T H_m^{(p-1)} Q_p = Q^{(p)T} H_m Q^{(p)}$$

with $Q^{(p)} := Q_1 \cdots Q_p$. Show that

$$v_1^{(r)} := V_m^{(p)} e_1^{(p)} \propto (A - \mu_p I_n) \cdots (A - \mu_1 I_n) v_1.$$

Extra. Introduction to communication-avoiding algorithms

Problem 34 Consider a sparse matrix A of size $10^6 \times 10^6$ with $5 \cdot 10^6$ non-zero values. Analyze the worst case memory access pattern in terms of number of read and write accesses and find the corresponding arithmetic intensity of standard CSR-based SpMV for this matrix.

Problem 35 Consider a sparse matrix A of size $10^6 \times 10^6$ with $5 \cdot 10^6$ non-zero values spread in dense 4×4 blocks. Let the matrix be stored in BSR format with a block size of $r \times c = 4 \times 4$. You may further assume that all stored blocks of the BSR data structure are perfectly aligned with the non-zero pattern of the matrix. Assuming that, within blocks, there is a perfect reuse of data from the source and destination vectors in registers, analyze the worst case memory access pattern in terms of number of read and write accesses, and find the corresponding arithmetic intensity of the BSR-based SpMV kernel for this matrix. Ignore indexing arithmetic in your account of floating-point operations.