Numerical Linear Algebra for Computational Science and Information Engineering

Problems

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Each problem refers to one, or more, specific lectures, which we covered in class. The lectures are labeled as follows:

- Lecture 01 – Essentials of linear algebra (Pbs. 1-6)
- Lecture 02 – Essentials of the Julia language
- Lecture 03 – Floating-point arithmetic and error analysis (Pbs. 7-10)
- Lecture 04 – Direct methods for dense linear systems (Pbs. 11-14)
- Lecture 05 – Sparse data structures and basic linear algebra subprograms (Pb. 15)
- Lecture 06 – Introduction to direct methods for sparse linear systems (Pb. 16)
- Lecture 07 – Orthogonalization and least-squares problems (Pb. 17)
- Lecture 08 – Basic iterative methods for linear systems (Pb. 18)
- Lecture 09 – Basic iterative methods for eigenvalue problems (Pbs. 19-20)
- Lecture 10 – Locally optimal block preconditioned conjugate gradient (Pbs. 21-22)
- Lecture 11 – Arnoldi and Lanczos procedures (Pbs. 23-24)
- Lecture 12 – Jacobi-Davidson method (Pbs. 25-26)
- Lecture 13 – Krylov subspace methods for linear systems
- Lecture 14 – Preconditioned iterative methods for linear systems
- Lecture 15 – Restarted Krylov subspace methods
- Lecture 16 – Elements of randomized numerical linear algebra
- Lecture 17 – Introduction to communication-avoiding algorithms (Pbs. 35-36)
- Lecture 18 – Matrix function evaluation

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. (L01)

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 $A = uv^T$. (L01)

Problem 3

Show that $\|xy^T\|_2 = \|x\|_2 \cdot \|y\|_2 \ \forall \ x, y \in \mathbb{R}^n$. (L01)

Problem 4

Determine the orthogonal projector P onto the subspace spanned by a non-zero vector $w \in \mathbb{R}^n$. (L01)

Problem 5

Let $A \in \mathbb{R}^{m \times n}$ have $p \leq \min(m, n)$ non-zero singular values $\sigma_1 \geq \cdots \geq \sigma_p > 0$ with corresponding $U := [u_1, \ldots, u_p]$ and $V := [v_1, \ldots, v_p]$ 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 $\Sigma := \mathrm{diag}(\sigma_1 \ldots, \sigma_p)$. (L01)

b. $P := AA^\dagger$ is an orthogonal projector onto range(A). (L01)

c. $P := I_n - A^\dagger A$ is an orthogonal projector onto null(A). (L01)

Problem 6

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 $(\cdot, \cdot)_A : (x, y) \in \mathbb{R}^n \times \mathbb{R}^n \mapsto (x, y)_A := x^T A y$. (L01)

Problem 7

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 $u = 2^{-p}$. (L03)

Problem 8

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 $\tilde{f} : (x, y, z) \mapsto \mathrm{fl}(\mathrm{fl}(x + y) + z)$. Show that

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

in which u is the unit roundoff of the system. (L03)

Problem 9

Show that the perturbations

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

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. (L03)

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

Problem 10

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? (L01, L04)

b. Is A singular? (L01)

c. Is A defective? (L01)

d. Is A diagonalizable? (L01)

e. Is A normal? (L01)

f. What is the conditioning number of the smallest eigenvalue of A? (L03)

g. What is the conditioning number of each eigenvalue of $B := A + A^T$? (L01, L03)

Problem 11

Show that, if a leading principal sub-matrix of A, i.e., $A[1:k, 1:k]$ with k such that $1 \le k < n$, 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. (L04)

Problem 12

Answer the following questions, and provide proper explanations:

a. Are the principal sub-matrices of a Hermitian positive-definite (HPD) matrix also HPD? (L01, L04)

b. Let $A = XBX^H$ be HPD and X be non-singular. Is B also HPD? (L01, L04)

c. Are the principal sub-matrices of a non-singular matrix also non-singular? (L01, L04)

Problem 13

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

a. Construct, with a pen and paper, the Cholesky factor L with positive diagonal components such that $A = LL^T$. (L04)

b. Form the square root $A^{1/2}$ of A. (L01)

Problem 14

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:

a. Is A singular? (L01)

b. Assuming exact arithmetic, can (Doolittle's) forward elimination procedure be successfully applied to A, without pivoting? (L04)

Problem 15

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). (L05)

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

Problem 16

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. (L06)

Problem 17

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. (L07)

(b) Find the least-squares problem solution $x = \arg\min_x \|Ax - b\|_2$ making use of the QR factorization. (L07)

Problem 18

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. (L08)

(b) A Gauss-Seidel iteration would converge. (L08)

(c) A SOR iteration would converge with $\omega = 1/2$. (L08)

Problem 19

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

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

is given by $\nabla r(x) = \frac{2}{x^T x}(Ax - r(x)x)$. (L09)

Problem 20

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. (L09)

Problem 21

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

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

is $\nabla\rho(x) = \frac{2}{x^T B x}(Ax - \rho(x)Bx)$. (L10)

Problem 22

Let A be symmetric and B be SPD. Then show that the matrix $X = [x_1, \ldots, x_k]$ of the smallest general eigenvectors $x_1, \ldots, x_k$ 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 $X^T B X = I_k$. (L10)

Problem 23

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 range(V). (L11)

(b) Assemble the reduced eigenvalue problem to solve in order to find the harmonic Ritz values of A with respect to range(V) for $\sigma = 0$. (L11)

Problem 24

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 $H_2 = Q_2^T A Q_2$. (L11)

Problem 25

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. (L12)

Problem 35

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. (L17)

Problem 36

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. (L17)