Notation

We denote by $\sigma(A)$ the spectrum of A, that is the set of the eigenvalues of A. The set $\mathcal{M}_n(\Omega)$ will be the set of complex $n \times n$ matrices whose spectrum is contained in Ω.

For a diagonal matrix, we use the notation

$$\mathrm{diag}(a_1, \dots, a_n) = \bigoplus_{i=1}^{n} [a_i] = \begin{bmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & a_n \end{bmatrix}.$$

For a upper triangular Toeplitz matrix we use the notation

$$\mathrm{utoep}(a_1, \dots, a_n) = \begin{bmatrix} a_1 & a_2 & a_3 & \cdots & a_n \\ 0 & a_1 & a_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a_1 & a_2 \\ 0 & \cdots & \cdots & 0 & a_1 \end{bmatrix}.$$

Let $A = [c_1|c_2|\dots|c_n] \in \mathbb{C}^{m \times n}$, whose columns are $c_1, \dots, c_n$, then we define

$$\mathrm{vec}(A) = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}.$$

Let $F : \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n}$ be a linear function, then there exists a matrix $M \in \mathbb{C}^{n^2 \times n^2}$ such that $\mathrm{vec}(F(A)) = M\,\mathrm{vec}(A)$. We say that M represents F in the vec basis.

The symbol $f[a, b]$ means $\frac{f(b)-f(a)}{b-a}$ for $a \neq b$ and $f'(a)$ for $a = b$ (it is said to be a divided differences of f).

Let A be a square matrix and $p(z) = \sum_{i=0}^{m} a_i z^i$ be a polynomial, then $p(A) = \sum_{i=0}^{m} a_i A^i$.

The Euclidean or Frobenius norm of a matrix M is $\|M\|_F = \sqrt{\sum_{i,j} |m_{ij}|^2}$.

Useful concepts

Let $f : \Omega \to \mathbb{C}$ be analytic and let A be a diagonalizable matrix such that $\sigma(A) \subseteq \mathbb{C}$ one can define $f(A)$ as

1. $f(A) := M \bigoplus_i [f(\lambda_i)] M^{-1}$, where $M^{-1}AM = \bigoplus_i [\lambda_i]$;
2. $f(A) := p(A)$, where $p(z)$ is any polynomial verifying the interpolation conditions $p(\lambda_i) = f(\lambda_i)$ for $\lambda \in \sigma(A)$.
3. Let γ be a contour enclosing $\sigma(A)$ then
$$f(A) := \frac{1}{2\pi i} \int_\gamma f(z)(zI - A)^{-1} dz.$$

Notice that the first two definitions require only that f is defined in Ω.

In most exercises we will assume that matrices are diagonalizable but the three definitions are equivalent and can be extended to nondiagonalizable matrices. Definition 1 requires the function of a Jordan block of size ν, that is

$$f(J) = f\big(\mathrm{utoep}(\lambda, 1, 0, \cdots, 0)\big) = \mathrm{utoep}\left(f(\lambda), f'(\lambda), \frac{f''(\lambda)}{2}, \cdots, \frac{f^{(\nu-1)}(\lambda)}{(\nu-1)!}\right).$$

Definition 2 requires $p(z)$ to interpolate the function $f(z)$ not only at the eigenvalues of A but, for each eigenvalue λ_i, $p^{(j)}(\lambda_i) = f^{(j)}(\lambda_i)$ for $j = 0, \dots, \nu_i - 1$, where ν_i is the largest size of the Jordan blocks relative to λ_i. Definition 3 generalizes in the same form to nondiagonalizable matrices. For further details see [1].

Let $\Omega \subseteq \mathbb{C}$ and f be a function differentiable in Ω. The Fréchet derivative of the function $f : \mathcal{M}_n(\Omega) \to \mathbb{C}^{n\times n}$ at a point A in the direction $H \in \mathbb{C}^{n\times n}$ is

$$Df(A)[H] := \lim_{t\to 0} \frac{1}{t}(f(A + tH) - f(A)).$$

Let $f : \Omega \to \mathbb{R}$ be a function differentiable in $\Omega \subseteq \mathbb{C}$ and let X be a matrix such that $\sigma(X) \subseteq \Omega$. The gradient with respect to the scalar product $\langle\cdot,\cdot\rangle$ of f at A is the matrix $\nabla(A)$ such that

$$\langle \nabla(A), H\rangle = Df(A)[H],$$

for each $H \in \mathbb{C}^{n\times n}$. Observe that the gradient depends on the scalar product.

The geometric mean of two positive definite matrices is $A\#B = A(A^{-1}B)^{1/2}$, the Riemannian distance of two positive definite matrices is $\delta(A, B) = \| \log(A^{-1/2}BA^{-1/2})\|_F$, while the Riemannian scalar product in the space tangent to the set of positive definite matrices at the point X is $\langle A, B\rangle_X = \mathrm{trace}(X^{-1}AX^{-1}B)$, for Hermitian A, B.

Operation counts

Let A be a positive definite matrix, then there exists unique a upper triangular matrix R with positive diagonal entries, such that $A = R^*R$. This is called *Cholesky factorization* of A and can be computed with $n^3/3 + o(n^3)$ arithmetic operations (ops).

For any matrix $A \in \mathbb{C}^{n\times n}$, there exist U unitary and T upper triangular such that $U^*AU = T$. This is called Schur decomposition and its computation requires about $25n^3$ ops; if A is Hermitian T is diagonal real and the (spectral) decomposition can be computed with about $9n^3$ ops [3].

Using the customary algorithms, the product of two square matrices requires $2n^3 + o(n^3)$ ops, while multiplying a triangular matrix by a full matrix requires $n^3 + o(n^3)$ ops. Inverting a full matrix requires $2n^3 + o(n^3)$ ops, while inverting a triangular matrix requires $n^3/3 + o(n^3)$ ops.

Exercises

Exercise 1. Prove that the three definitions are equivalent for a diagonalizable matrix.

Exercise 2. Prove in an elementary way that, for any invertible matrix A, A^{-1} can be written as a polynomial of the matrix A, say $p(A)$. Find a strict lower bound for the degree of $p(z)$.

Exercise 3. Show that the definition of the exponential of a matrix A as a function of A agrees with the usual definition $\exp(A) = \sum_{k=0}^{\infty} \frac{A^k}{k!}$. Using the latter definition, prove that the exponential of a matrix A is a polynomial of A.

Exercise 4. Let $f : \Omega \to \mathbb{C}$ be a function and A be a matrix such that $\sigma(A) \subseteq \Omega$. Prove that $f(A)^T = f(A^T)$. Discuss the existence of an analogous formula for $f(A^*)$.

Exercise 5. Prove that if A is Hermitian and $f : \mathbb{R} \to \mathbb{R}$ then $f(A)$ is Hermitian and if, moreover $f : \mathbb{R} \to \mathbb{R}_+$, then $f(A)$ is positive definite. Deduce that if P is positive definite and H is Hermitian, then $\exp(H)$ is positive definite, $P^{1/2}$ is positive definite, $\log(P)$ is Hermitian, where $z^{1/2}$ and $\log(z)$ denote the principal branches of the square root and the logarithm, respectively.

Exercise 6. Prove that if $f : \Omega \to \mathbb{C}$ is defined on the diagonalizable matrix A, and K is an invertible matrix, then $f(KAK^{-1}) = Kf(A)K^{-1}$.

Exercise 7. Prove that A is a normal matrix if and only if A^* is a function of A. Prove that a matrix which is normal and triangular, is necessarily diagonal.

Exercise 8. Let A, B be positive definite matrices and let $f : \mathbb{R}^+ \to \mathbb{R}$, show that $Af(A^{-1}B)$ is well defined and Hermitian, moreover if $f : \mathbb{R}^+ \to \mathbb{R}^+$ then $Af(A^{-1}B)$ is positive.

Exercise 9. If A and B are positive, show that $(AB)^{1/2}$ is well defined, but in general it can be different from $A^{1/2}B^{1/2}$. Show that if A, B commute and are positive definite then $(AB)^{1/2} = A^{1/2}B^{1/2}$.

Exercise 10 ([2])**.** Let $A = C^*C$ and $B = D^*D$, with C, D nonsingular. Prove that

$$A\#B = C^* \,\mathrm{polar}(CD^{-1})D,$$

where $\mathrm{polar}(M) = M(M^*M)^{-1/2}$ is the unitary polar factor of the matrix M.

Exercise 11 ([2])**.** Let $A = K^*K = C^*C$ be full rank factorization of A, then KC^{-1} is unitary and, in particular, $KC^{-1} = \mathrm{polar}(KC^*)$. Use this to prove that if $A = C^*C$ is a full rank factorization of A and B is positive definite then, for the Riemannian distance, we have

$$\delta(A,B) := \|\log(A^{-1/2}BA^{-1/2})\|_F = \|\log(C^{-*}BC^{-*})\|_F.$$

Exercise 12. Let A, B positive definite and let $K(A,B) = A\#B$ be their geometric mean, show that the derivative of $K(A,B)$ is such that

$$\mathrm{vec}(DK(A,B)[H_A,H_B]) = (I\otimes Z^{-1} + Z^{-1}\otimes I)^{-1}\,\mathrm{vec}(H_A) + (I\otimes Z + Z\otimes I)^{-1}\,\mathrm{vec}(H_B),$$

where $Z = (BA^{-1})^{1/2}$.

Exercise 13. Design an algorithm to evaluate $f(A)$ for A being Hermitian, using the spectral decomposition of A. Estimate its computational cost. Discuss the diagonalizable, non Hermitian case.

Exercise 14. Compare the three algorithms for computing $Af(A^{-1}B)$, for A and B being positive definite:

(i) use the formula $Af(A^{-1}B)$;

(ii) use the formula $A^{1/2}f(A^{-1/2}BA^{-1/2})A^{1/2}$;

(iii) use the formula $R^*f(R^{-*}BR^{-1})R$, where $A = R^*R$ is the Cholesky factorization.

Exercise 15. Compare the two algorithms for computing $\delta(A,B)$, for A and B being positive definite:

(i) use the formula $\delta(A,B) = \|\log(A^{-1/2}BA^{-1/2})\|_F$;

(ii) use the formula $\delta(A,B) = \|\log(R^{-*}BR^{-1})\|_F$, where $A = R^*R$ is the Cholesky factorization.

Exercise 16. Let $b > a > 0$ and let

$$a_{k+1} = \frac{1}{2}(a_k + b_k), \qquad b_{k+1} = \frac{2}{\frac{1}{a_k} + \frac{1}{b_k}},$$

with $a_0 = a$ and $b_0 = b$. Show that for each k

$$a_k \le a_{k+1} < \sqrt{ab} < b_{k+1} \le b_k,$$

$a_kb_k = ab$ and that $\lim_k a_k = \lim_k b_k = \sqrt{ab}$.

The same properties hold by substituting scalar with positive definite matrices, the real order with the order on positive matrices and the geometric mean of scalars with the geometric mean of matrices (difficult to prove, compare [2]).

Exercise 17 ([2])**.** Consider the iteration $A_0 = A$, $B_0 = B$ and

$$A_{k+1} = \frac{1}{2}(A_k + B_k), \qquad B_{k+1} = 2(A_k^{-1} + B_k^{-1})^{-1}.$$

Show that the iteration

$$C_{k+1} = \varphi(C_k) := \frac{1}{2}(C_k + AC_k^{-1}B), \qquad C_0 = A,$$

generates a sequence such that $A_k = C_k$. Prove that the limit, if exists, is $A\#B$. Moreover, prove that the sequence may be not locally convergent in a neighborhood of the fixed point $A\#B$ (it is sufficient to prove that $\rho(D\varphi(A\#B)) > 1$).

Exercise 18. Let f be analytic in Ω.
(i)Using the Cauchy formulae prove that, for $a, b \in \Omega$, we have

$$\frac{1}{2\pi i}\int_\gamma \frac{f(z)}{(z-a)(z-b)}dz = f[a,b],$$

where γ is a contour in Ω enclosing a and b.
(ii) Let $\Lambda = \bigoplus_i [\lambda_i]$ be such that $\sigma(\Lambda) \subseteq \Omega$, use the Sherman-Morrison formula

$$(A + uv^*)^{-1} = A^{-1} - \frac{A^{-1}uv^*A^{-1}}{1 + v^*A^{-1}u},$$

to show that

$$Df(\Lambda)[e_i e_j^T] = f[\lambda_i, \lambda_j] e_i e_j^T$$

(iii) Prove that $Df(\Lambda)[H] = [f[\lambda_i, \lambda_j]] \circ H$, for each $H \in \mathbb{C}^{n \times n}$.
(iv) Prove that if A is normal and U is such that $U^* AU = \Lambda = \bigoplus_i [\lambda_i]$ and with $\lambda_i \in \Omega$, then

$$Df(A)[H] = UDf(\Lambda)[U^* HU]U^*.$$

Exercise 19. Let $f, g : \Omega \to \mathbb{C}$ differentiable, and let X be a normal matrix such that $\sigma(X) \subseteq \Omega$. Show that

$$\operatorname{trace}(f(X)Dg(X)[H]) = \operatorname{trace}(f(X)g'(X)H).$$

Exercise 20. Let X, H be Hermitian matrices of the same size, with X positive definite.
(i) Let $\varphi(X) = \|X\|^2$, show that $D\varphi(X) = 2\operatorname{trace}(XH)$.
(ii) Let $\psi(X) = \|\log(X)\|^2$, show that $D\psi(X)[H] = 2\operatorname{trace}(X^{-1}\log(X)H)$.
(iii) Let A be positive definite and set $\delta_A^2(X) = \delta(X, A)^2$. Use the fact that $\delta_A^2(X) = \delta_I^2(A^{-1/2}XA^{-1/2}) = \psi(A^{-1/2}XA^{-1/2})$, to prove that

$$D\delta_A^2(X)[H] = 2\operatorname{trace}(X^{-1}\log(XA^{-1})H)$$

(iv) Let $A_1, \dots, A_m$ be positive definite and set $f(X) = \sum_{i=1}^m \delta^2(A, X)$. Show that the Euclidean gradient of f is

$$\sum_{i=1}^m 2X^{-1}\log(XA_i^{-1}),$$

while the gradient with respect to the Riemannian scalar product is

$$\sum_{i=1}^m 2X\log(A_i^{-1}X).$$

References

[1] N. Higham, *Functions of Matrices: Theory and Computation*, SIAM, 2008.

[2] B. Iannazzo, *The geometric mean of matrices from a computational viewpoint*, arXiv:1201.0101 [math.NA], 2011.

[3] G. Golub, C. Van Loan, *Matrix Computation*, Third edition, John Hopkins University Press, 1996.