

10. Positive definite matrices

Def: A self-adjoint map  $H: X \rightarrow X$  is positive (or positive definite) if  $(x, Hx) > 0$  for all  $x \neq 0$ . It is nonnegative (or positive semidefinite) if  $(x, Hx) \geq 0$ .

We denote these as e.g.,  $H > 0$ , and  $H \geq 0$ , resp.

Theorem (O.1): Let  $X$  be a Euclidean space.

- (i) The identity map  $I$  is positive.
- (ii) If  $M, N > 0$  then  $M+N > 0$  and  $aM > 0$  for  $a > 0$ .
- (iii) If  $H > 0$  and  $Q$  invertible, then  $Q^*HQ > 0$ .
- (iv)  $H > 0$  iff all eigenvalues are positive.
- (v) If  $H > 0$  then  $H$  is invertible.
- (vi) Every positive map has a unique positive square root.
- (vii) The set of positive maps is an open subset of the space of self-adjoint maps.
- (viii) The boundary points of the set of positive maps are the nonnegative maps that are not positive.

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Proof: (i)  $(x, \mathbb{I}x) = (x, x) > 0$  if  $x \neq 0$ . ✓

(ii)  $(x, (M+N)x) = (x, Mx) + (x, Nx) > 0$  if  $x \neq 0$ . ✓

and  $(x, aMx) = a(x, Mx) > 0$  ✓

(iii)  $(x, Q^*HQx) = (\alpha x, HQx)$ . Put  $y = Qx \neq 0$  if  $x \neq 0$ .

$$= (y, Hy) > 0. \quad \checkmark$$

(iv) ( $\Rightarrow$ ) Say  $H > 0$  and  $Hv = \lambda v$ ,  $v \neq 0$ .

Then  $(v, Hv) = (v, \lambda v) = \lambda(v, v) > 0 \Rightarrow \lambda > 0$ . ✓

( $\Leftarrow$ ) Let  $v_1, \dots, v_n$  be an orthonormal basis of eigenvectors with eigenvalues  $\lambda_1, \dots, \lambda_n > 0$ . Pick  $x \neq 0$ , write  $x = a_1 v_1 + \dots + a_n v_n$ , and  $Hx = a_1 \lambda_1 v_1 + \dots + a_n \lambda_n v_n$ .

$$(x, Hx) = \sum_{i=1}^n \lambda_i |a_i|^2 > 0 \text{ for all } x \neq 0. \quad \checkmark$$

Note:  $(x, Hx) = \sum_{i=1}^n \lambda_i |a_i|^2 \geq \lambda_{\min} \|x\|^2$  (\*).

(V) If  $H$  is not invertible, then  $Hv = 0$  for some  $v \neq 0 \Rightarrow \lambda = 0$  ↗.

(Vi) Write  $\sqrt{H}x = \sum_{i=1}^n a_i \sqrt{\lambda_i} v_i$  (clearly positive). ✓

(Vii) Fix  $H > 0$ , and let  $N$  be any self-adjoint map such that  $\|N - H\| < \lambda_{\min}$ .

Claim:  $N$  is positive.

Put  $M = N - H$ .

Since  $\|M\| < d_{\min}$ , we know  $\|Mx\| < \lambda_{\min} \|x\|$  for all  $x \neq 0$ .

By Cauchy-Schwarz,  $|(\langle x, Mx \rangle)| \leq \|x\| \|Mx\| < d_{\min} \|x\|^2$

Together, we get for  $x \neq 0$ :

$$\begin{aligned} (\langle x, Nx \rangle) &= (\langle x, (H+M)x \rangle) = (\underbrace{\langle x, Hx \rangle}_{< d_{\min} \|x\|, \text{ see above}} + \underbrace{\langle x, Mx \rangle}) \\ &> \lambda_{\min} \|x\|^2 - \lambda_{\min} \|x\|^2 = 0. \\ &\geq \lambda_{\min} \|x\| \text{ by (A)} \end{aligned}$$

Therefore,  $N = H + M$  is positive.  $\square$

(viii) By definition, if  $K$  is on the boundary of positive maps, then  $\exists$  sequence  $H_n \rightarrow K$  of positive maps, i.e.,  $\|H_n - K\| \rightarrow 0$ .

By Cauchy-Schwarz,  $\lim_{n \rightarrow \infty} (\langle x, H_n x \rangle) = (\langle x, Kx \rangle)$ .  $\square$

Put a partial order onto the set of self-adjoint maps:

Say  $M < N$  iff  $N - M > 0$

$M < N$  iff  $N - M \geq 0$ .

We get the following properties (almost) for free:

Additive:  $M_1 < N_1$  and  $M_2 < N_2 \Rightarrow M_1 + M_2 < N_1 + N_2$

Transitive:  $L < M < N \Rightarrow L < N$

Multiplicative:  $M < N$ ,  $Q$  invert  $\Rightarrow Q^* M Q < Q^* N Q$ .

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Theorem 10.2: Suppose  $0 < M < N$ . Then  $M^{-1} > N^{-1} > 0$ .

Proof: First, suppose  $N = I$ .

Then  $M < I \Rightarrow I - M > 0$ .

$\Rightarrow$  Eigenvalues of  $I - M$  are positive.

Say:  $(I - M)v = \lambda v$  for  $v \neq 0$ .

Then  $Mv = v - \lambda v = (1 - \lambda)v$ . Since  $1 - \lambda > 0$ ,  $0 < \lambda < 1$ .

In summary:  $\lambda$  eigenvalue of  $I - M \Rightarrow 0 < \lambda < 1$

$\Rightarrow 1 - \lambda$  eigenvalue of  $M$ , and  $0 < 1 - \lambda < 1$ .

$\Rightarrow \frac{1}{1-\lambda}$  eigenvalue of  $M^{-1}$ , and  $\frac{1}{1-\lambda} > 1$

$\Rightarrow$  Eigenvalues of  $M^{-1} - I > 0$

$\Rightarrow M^{-1} - I > 0 \Rightarrow M^{-1} > I$ . ✓

Now, consider arbitrary  $N > M > 0$ .

Factor  $N = R^2$ ,  $R > 0$  and invertible.

We'll use  $0 < M < N \Rightarrow 0 < Q^* M Q < Q^* N Q$  twice.

First:  $Q = R^{-1}$  (so  $Q^* = R^{-1}$ )

$$0 < R^{-1} M R^{-1} < R^{-1} N R^{-1} = I$$

From what we showed above,  $(R^{-1} M R^{-1})^{-1} = R M^{-1} R > I$ .

Second:  $Q = R^{-1}$

$$0 < I < R M^{-1} R \Rightarrow 0 < R^{-1} I R^{-1} < R^{-1} (R M^{-1} R) R^{-1}$$

$$\Rightarrow 0 < R^{-2} = N^{-1} < M^{-1}$$

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Caveat: The product of self-adjoint maps is in general, not self-adjoint.

Example: Let  $A = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$ ,  $B = \begin{pmatrix} 1 & -2 \\ -2 & 5 \end{pmatrix}$ ,  $x = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$Ax = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \quad Bx = \begin{pmatrix} 1 \\ -2 \end{pmatrix}, \quad (x, ABx) = (Ax, Bx) = -3$$

Def: If  $A, B$  are self-adjoint, define their symmetrized product as  $S = AB + BA$ .

$$\text{Note that } (x, Sx) = (x, ABx) + (x, BAx) = (Ax, Bx) + (Bx, Ax).$$

$$\text{In the real case: } (x, Sx) = 2(Ax, Bx).$$

$$\text{In the example above, } AB + BA = \begin{pmatrix} -6 & 0 \\ 0 & 42 \end{pmatrix}.$$

Thus, it is false that  $A > 0, B > 0 \Rightarrow AB + BA > 0$ .

But a similar statement is true:

Theorem 10.3: Let  $A, B$  be self-adjoint. If  $A > 0$  and  $AB + BA > 0$ , then  $B > 0$ .

Proof: Define  $B(t) = B + tA$ . (Note: We must show  $B(0) > 0$ .)

Claim 1: The symmetrized product of  $A$  and  $B(t)$  is positive for  $t \geq 0$ .

$$S(t) = AB(t) + B(t)A = A(B + tA) + (B + tA)A = AB + BA + 2tA^2 = S + 2tA^2 > 0$$

(since  $S > 0$  and  $2tA^2 \geq 0$ ) ✓

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Claim 2: For  $t$  large enough,  $B(t) > 0$ :

$$(x, B(t)x) = (x, (B + tA)x) = (x, Bx) + t(x, Ax).$$

Recall:  $(x, Ax) \geq \lambda_{\min} \|x\|^2$  (min e-value of  $A$ )

$$\text{and } |(x, Bx)| \leq \|x\| \|Bx\| \leq \|B\| \|x\|^2$$

$$\begin{aligned} \text{Together, } (x, B(t)) &= t(x, Ax) + (x, Bx) \\ &\geq t \lambda_{\min} \|x\|^2 - \|B\| \|x\|^2 = (t \lambda_{\min} - \|B\|) \|x\|^2 \end{aligned}$$

Thus, if  $t > \|B\| / \lambda_{\min}$ ,  $B(t) > 0$ .

Claim 3:  $B = B(0) > 0$ .

If not, then for some  $t_0$ ,  $0 \leq t_0 \leq \|B\| / \lambda_{\min}$  such that

$B(t_0)$  is on the boundary of the set of positive maps, i.e.,  $B(t_0) \geq 0$  but  $B(t_0) \not\succeq 0$ .

Such a  $B(t_0)$  has a  $\lambda = 0$ , so  $B(t_0)y = 0$  for some  $y \neq 0$ .

However,  $(y, S(t_0)y) = (Ay, B(t_0)y) + (B(t_0)y, Ay) = 0$ .  $\$$

Thus  $B > 0$ .

Corollary 10.4: If  $0 < M < N$ , then  $0 < \sqrt{M} < \sqrt{N}$ .

Proof: Put  $A(t) = M + t(N - M)$ .

For  $0 \leq t \leq 1$ ,  $A(t) = (1-t)M + tN > 0$ ,  $\dot{A}(t) = N - M > 0$ .

Thus we can define  $R(t) = \sqrt{A(t)}$  for  $0 \leq t \leq 1$ .

Since  $A = R^2$ ,  $\dot{A} = \dot{R}R + R\dot{R}$ . (Symmetrized product of  $R$  and  $\dot{R}$ ).

We know  $\dot{A} = N - M > 0$  and thus so is  $R > 0$ . (on  $[0, 1]$ )

Claim:  $R(t)$  is an increasing function on  $[0, 1]$ .

Pf: For any  $x \neq 0$ ,  $\frac{d}{dt}(x, R_x) = (x, \dot{R}x) > 0$ .

By calculus,  $(x, R(t)x)$  is increasing

$$\Rightarrow (x, R(s)x) < (x, R(t)x) \text{ for } s < t$$

$$\Rightarrow R(t) - R(s) > 0 \Rightarrow R(t) > R(s) \quad \checkmark$$

In particular,  $R(0) < R(1)$

$$R(0) = \sqrt{A(0)} = \sqrt{M}, \quad R(1) = \sqrt{A(1)} = \sqrt{N} \Rightarrow \sqrt{M} < \sqrt{N}.$$

Def: A real-valued function  $f(s)$ ,  $s > 0$  is a monotone matrix function (mmf) if for all self-adjoint mappings,

$$0 < M < N \Rightarrow f(M) < f(N).$$

Recall that for  $H$  self-adjoint with eigenvalues  $\lambda_1, \dots, \lambda_n$  and orthonormal eigenvectors  $v_1, \dots, v_n$ , we define

$$F(H) = \sum_{i=1}^n f(\lambda_i) P_i \quad \text{for a spectral resolution } H = \sum_{i=1}^n \lambda_i P_i.$$

Example:

(i)  $f(s) = -\frac{1}{s}$  is a mmf (immediate from Theorem 10.2;

$$0 < M < N \Rightarrow M^{-1} > N^{-1} > 0 \Rightarrow -M^{-1} < -N^{-1} < 0.$$

(Note that  $f(M) = -M^{-1}$ ).

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(ii)  $f(s) = s^{1/2}$  is a mmf (immediate from Corollary 10.4;  
 $0 < M < N \Rightarrow 0 < \sqrt{M} < \sqrt{N}$ . Note that  $f(M) = \sqrt{M}$ )

(iii)  $f(s) = s^2$  is not a mmf

Take any  $A, B > 0$  with  $s = AB + BA \neq 0$ .

Claim: For small  $t$ , if  $M = A$ ,  $N = A + tB$ , then

$0 < M < N$  but  $M^2 \neq N^2$ .

Note that  $N^2 = A^2 + t(\underbrace{AB + BA}_{\text{not negligible}}) + \underbrace{t^2 B^2}_{\text{negligible for } t \approx 0}$

so  $N^2 = M^2 + [\text{something nonpositive}] \neq M^2$ .

(iv)  $f(s) = s^{(-2^k)}$  and  $f(s) = \log s$  are mmf. (Exercise)

Additionally, positive multiples, sums, and limits of mmf's are mmf's.

For example,  $-\sum \frac{m_j}{s+t_j}$   $m_j > 0$ ,  $t_j > 0$  is an mmf,

and so is  $f(s) = as + b - \int_0^\infty \frac{dm(t)}{s+t}$   $a > 0$ ,  $b \in \mathbb{R}$ , (\*\*)

and  $m(t)$  non-negative measure for which the integral converges.

In fact, every mmf has the form of (\*\*).

(Theorem of C. Loewner - very nontrivial!)

Surprisingly, functions of the form (\*\*\*) are easy to characterize:

Theorem (Herglotz, Riesz): Every function  $f$  which is analytic on the upper half-plane with  $\operatorname{Im}(f) > 0$  there, and  $\operatorname{Im}(f) = 0$  on the positive real axis, has the form (\*\*\*).

Conversely, every function of the form (\*\*\*\*) can be extended to be analytic on the upper half-plane, with  $\operatorname{Im}(f) > 0$  there.

Proof: See "Functional Analysis" by Peter Lax.

How to construct (all) positive matrices:

Def: Let  $f_1, \dots, f_m$  be a sequence of vectors in a Euclidean space  $X$ . Define the  $m \times m$  matrix  $G$ , where  $G_{ij} = (f_i, f_j)$ .

This is called the Gram matrix of  $f_1, \dots, f_m$ .

Theorem 10.5:

- (i) Every Gram matrix is nonnegative.
- (ii) The Gram matrix of a set of linearly independent vectors is positive.
- (iii) Every positive matrix can be represented as a Gram matrix.

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Proof:

$$(i), (ii): (x, Gx) = \sum_{i,j} x_i \bar{G}_{ij} \bar{x}_j = \sum_{ij} (f_i, f_j) x_i \bar{x}_j \\ = \left( \sum_{i=1}^m x_i f_i, \sum_{j=1}^m x_j f_j \right) = \left\| \sum x_i f_i \right\|^2.$$

(iii) Let  $H = (h_{ij})$  be positive, and define the nonstandard inner product by  $(x, y)_H = (x, Hy)$ .

Note that under this inner product, the Gram matrix of the unit vectors  $e_1, \dots, e_m$  has  $ij$ -entry

$$(e_i, e_j)_H = (e_i, He_j) = h_{ij}.$$

□

Examples:

$$(i) \text{ Let } X = \{f: [0, 1] \rightarrow \mathbb{R}\}, (f, g) := \int_0^1 f(t) g(t) dt.$$

If  $f_1 = 0, f_2 = t, \dots, f_i = t^{i-1}$ , then

$$G = (G_{ij}) \quad \text{where} \quad G_{ij} = \frac{1}{i+j-1}.$$

$$(ii) \text{ Define } (F, g) = \int_0^{2\pi} F(\theta) \bar{g}(\theta) w(\theta) d\theta, \quad w: \mathbb{R} \rightarrow \mathbb{R}^+.$$

If  $f_j = e^{ij\theta}, j = -n, \dots, n$ , then the corresponding Gram matrix is  $G_{kj} = C_{kj}$ , where

$$C_p = \int w(\theta) e^{-ip\theta} d\theta.$$

Theorem 10.6 (Schur): Let  $A = (A_{ij})$  and  $B = (B_{ij})$  be positive matrices. Then  $M = (M_{ij}) := (A_{ij} B_{ij})$  is positive.

We need to employ tensor products for the proof.

Given two vector spaces  $U, V$ , their tensor product, denoted  $U \otimes V$ , is a related vector space of dimension  $(\dim U)(\dim V)$ .

Definition 1: If  $\{e_i\}_{i=1}^n$  is a basis of  $U$  and  $\{f_j\}_{j=1}^m$  a basis of  $V$ , then  $\{e_i \otimes f_j\}$  is a basis of  $U \otimes V$ .

Analogy:  $\langle 1, x, \dots, x^n \rangle, \langle 1, y, \dots, y^m \rangle$  vs.  $\langle x^i y^j : i \leq n, j \leq m \rangle$ .

There's a better, basis-free way to construct  $U \otimes V$ .

Definition 2:  $U \otimes V = \left\{ \sum u_i \otimes v_i : u_i \in U, v_i \in V \right\} / N$

$$\text{where } N = \left\langle (u_1 + u_2) \otimes v - u_1 \otimes v - u_2 \otimes v, \right. \\ \left. u \otimes (v_1 + v_2) - u \otimes v_1 - u \otimes v_2 \right\rangle$$

Basically, we are forcing the distributive law, i.e.

$$(u_1 + u_2) \otimes v = u_1 \otimes v + u_2 \otimes v, \text{ etc.}$$

Theorem 10.7: There is a natural isomorphism

$$U \otimes V \longrightarrow L(U, V).$$

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Proof: (sketch). Define the map as follows:

$$U \otimes V \longrightarrow \mathcal{L}(U', V)$$

$$u \otimes v \longmapsto \{l \mapsto (l, u)v\} \quad \text{and extend linearly.}$$

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} \otimes \begin{bmatrix} v_1 \\ \vdots \\ v_m \end{bmatrix} \longmapsto \begin{bmatrix} v_1 \\ \vdots \\ v_m \end{bmatrix} [u_1 \dots u_n] = \begin{bmatrix} v_1 u_1 & v_1 u_2 & \dots & v_1 u_n \\ \vdots & \vdots & \ddots & \vdots \\ v_m u_1 & v_m u_2 & \dots & v_m u_n \end{bmatrix}_{m \times n}$$

Note that  $(l, u)v$  is:

$$\begin{bmatrix} v_1 \\ \vdots \\ v_m \end{bmatrix} [u_1 \dots u_n] \begin{bmatrix} l_1 \\ \vdots \\ l_n \end{bmatrix} \quad \mathbb{R} \xrightarrow{l} \mathbb{R}^n \xrightarrow{u} \mathbb{R} \xrightarrow{v} \mathbb{R}^m$$

Analogy: Let  $U = \langle 1, x, \dots, x^n \rangle$ ,  $V = \langle 1, y, \dots, y^m \rangle$ .

Think of  $U \times V$  as  $\langle (x^i, y^j) : 0 \leq i \leq n, 0 \leq j \leq m \rangle$

and  $U \otimes V$  as  $\langle x^i y^j : 0 \leq i \leq n, 0 \leq j \leq m \rangle$

Remark: We could similarly define an isomorphism  $U \otimes V \rightarrow \mathcal{L}(V', U)$ , where the dual of  $L: U' \rightarrow V$  is a map  $L': V' \rightarrow U$ .

If  $U, V$  are Euclidean spaces (so  $U' = U$ ), there is a natural way to endow  $U \otimes V$  with a Euclidean structure.

For  $M, L \in \mathcal{L}(U, V)$ , define  $(M, L) = \text{tr}(L^* M) = \sum_{i,j} l_{ji} m_{ij}$

Note that  $\|M\|^2 = (M, M) = \sum_{ij} m_{ji}^2$

So  $e_i \otimes e_j$  under the isomorphism is the matrix  $E_{ij}$  (i.e., the  $ij$ -entry is 1, all others 0).

Clearly these form an orthonormal basis of  $U \otimes V$ .

Proof of Thm 10.6 (Schur):  $(A_{ij}), (B_{ij}) > 0 \Rightarrow M := (A_{ij} B_{ij}) > 0$ .

Since every positive matrix can be written as a Gram matrix, write  $A_{ij} = (u_i, u_j)$ ,  $B_{ij} = (v_i, v_j)$

where  $u_1, \dots, u_n$  and  $v_1, \dots, v_n$  are linearly independent sets.

Define  $g_i \in U \otimes V$  as  $g_i = u_i \otimes v_i$ .

Note that  $(g_i, g_j) = (u_i, u_j)(v_i, v_j) = A_{ij} B_{ij}$ .

Hence,  $M$  is a Gram matrix, and positive by Theorem 10.5.  $\square$

Another way to view tensor products:

Let  $X$  be an  $n$ -dimensional real vector space

Note that  $\mathbb{C}$  is a 2-dimensional real vector space ( $\{1, i\}$  is a basis).

Suppose  $A: X \rightarrow X$  is a linear map with minimum polynomial  $A(s) = s^2 + 1$ .

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Then  $i$  and  $-i$  are eigenvalues of  $A$ , but  $i \notin \mathbb{R}$ .

So if  $v$  is an eigenvector with eigenvalue  $\lambda = i$ ,  $v \notin X$ .

However,  $v$  should live in some "extension" of  $X$ .

In this bigger vector space, we want to have vectors like  $zv$ ,  $z \in \mathbb{C}$ ,  $v \in X$ .

What we really want is  $\mathbb{C} \otimes X$ .

This has basis  $\{x_1, \dots, x_n, ix_1, \dots, ix_n\}$ , where  $x_1, \dots, x_n$  is a basis of  $X$ .

Note that we need certain associativity, such as

$$(3i)v = (i3)v = i(3v)$$

$$\text{i.e., } 3i \otimes v = i \otimes 3v.$$

But this comes for free with the construction!