Lecture 7: Lieb's concavity theorem CSE 599I, Spring 2021
Instructor: James R. Lee

1 Block magic

Recall that our goal is to prove that $(A, B) \mapsto \mathsf{S}(A \parallel B)$ is jointly convex on positive matrices, where

$$\mathsf{S}(A \parallel B) = \operatorname{Tr}\left(A(\log A - \log B) - (A - B)\right),$$

and that we established the following result as a first step.

Lemma 1.1. *The map $(A, B) \mapsto A : B$ is jointly concave on positive matrices, where $A : B = (A^{-1} + B^{-1})^{-1}$.*

Our approach is via another concavity theorem of Lieb.

Theorem 1.2. *For any matrix $X \in \mathbb{M}_n(\mathbb{C})$ and $0 \leqslant t \leqslant 1$, it holds that*

$$(A, B) \mapsto \operatorname{Tr}\left(X^* A^t X B^{1-t}\right)$$

is jointly concave on $A, B \succ 0$.

Indeed, with Theorem 1.2 in hand, let us define the function, for $0 \leqslant t \leqslant 1$,

$$I_t(A, X) := \operatorname{Tr}\left(X^* A^t X A^{1-t} - X^* X A\right).$$

Note that $A \mapsto I_t(A, X)$ is concave by Theorem 1.2 because $A \mapsto \operatorname{Tr}(X^* X A)$ is linear in A.

Because $I_0(A, X) = 0$, the function

$$I(A, X) := \left.\frac{d}{dt}\right|_{t=0^+} I_t(A, X) = \lim_{\varepsilon \to 0^+} \frac{I_\varepsilon(A, X) - I_0(A, X)}{\varepsilon} = \lim_{\varepsilon \to 0} \frac{I_\varepsilon(A, X)}{\varepsilon}$$

is also concave in A, since it is a limit of concave functions. Observe that

$$\frac{d}{dt} A^t = \frac{d}{dt} e^{t \log A} = (\log A) A^t, \quad \frac{d}{dt} A^{1-t} = -(\log A) A^{1-t},$$

hence

$$I(A, X) = \operatorname{Tr}\left(X^* (\log A) X A - X^* X (\log A) A\right)$$

Now comes the amazing twist: Define the block matrices

$$T = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix}, \quad X = \begin{bmatrix} 0 & 0 \\ I & 0 \end{bmatrix}.$$

Then $I(T, X) = -\mathsf{S}(A \parallel B)$. Since $T \mapsto I(T, X)$ is concave, it follows that $(A, B) \mapsto \mathsf{S}(A \parallel B)$ is jointly convex, establishing our goal. We are left to prove Theorem 1.2.

2 Tensor magic

We are left to prove Theorem 1.2. The magic is that it is **equivalent** to the assertion that the function $F(A, B) = A^t \otimes B^{1-t}$ is jointly *operator* concave on $A, B \succeq 0$.

2.1 Tensor products of operators

The tensor product $\mathcal{H} = \mathbb{C}^m \otimes \mathbb{C}^n$ is an mn-dimensional complex inner product space spanned by the orthonormal basis $\{u_i \otimes v_j\}$, where $\{u_1, \ldots, u_m\}$ and $\{v_1, \ldots, v_n\}$ are any orthonormal bases for $\mathbb{C}^m$ and $\mathbb{C}^n$. For vectors $u, u' \in \mathbb{C}^m, v, v' \in \mathbb{C}^n$, the inner product is given by

$$\langle u \otimes v, u' \otimes v' \rangle_{\mathcal{H}} = \langle u, u' \rangle \langle v, v' \rangle.$$

Of course, the space $\mathcal{H}$ contains more vectors than just those of the form $u \otimes v$. For instance, $u_1 \otimes u_2 + u_2 \otimes u_1$. The inner product is extended to such vectors by linearity. As an inner product space, $\mathcal{H}$ is isomorphic to $\mathbb{C}^{mn}$.

We can represent this isomorphism as follows: Given $u \in \mathbb{C}^m, v \in \mathbb{C}^n$, there is a canonical representation of $u \otimes v$ as an $m \times n$ matrix:

$$(u \otimes v)_{ij} = u_i v_j.$$

Moreover, it holds that $\langle u \otimes v, u' \otimes v' \rangle_{\mathcal{H}} = \mathrm{Tr}\left((u \otimes v)^*(u' \otimes v')\right)$, where in the second expression we consider the 2-tensors as matrices.

Note that the space $\mathbb{C}^m$ is isomorphic to the collection of univariate polynomials of degree at most $m-1$: $p(x) = a_{m-1}x^{m-1} + a_{m-2}x^{m-2} + \cdots + a_1 x + a_0$, where x is a complex variable. It holds that $\mathbb{C}^m \otimes \mathbb{C}^n$ is isomorphic to the collection of bivariate polynomials of degree at most $m-1$ in x and $n-1$ in y: $q(x, y) = \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} a_{ij} x^i y^j$.

If we have linear operators $A : \mathbb{C}^m \to C^{m'}$ and $B : \mathbb{C}^n \to \mathbb{C}^{n'}$, one defines the linear operator $A \otimes B : \mathbb{C}^m \otimes \mathbb{C}^n \to \mathbb{C}^{m'} \otimes \mathbb{C}^{n'}$ by

$$(A \otimes B)(x \otimes y) = (Ax) \otimes (By),$$

with the extension of to all of $\mathbb{C}^m \otimes \mathbb{C}^n$ given by linearity.

If A and B are represented by $m \times m'$ and $n \times n'$ matrices, respectively, then we can represent $A \otimes B$ as the $mn \times m'n'$ matrix given by

$$(A \otimes B)_{ij, i'j'} = A_{ii'} B_{j'j'}.$$

If additionally we have $m = n$ and $m' = n'$ (so that both A and B are square matrices), then

$$\mathrm{Tr}(A \otimes B) = \sum_{i=1}^{m} \sum_{j=1}^{n} (A \otimes B)_{ij,ij} = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ii} B_{jj} = \mathrm{Tr}(A)\mathrm{Tr}(B).$$

If we recall the Schur product $A \circ B$ given by $(A \circ B)_{ij} = A_{ij} B_{ij}$, then we can confirm our earlier claim that $A \circ B$ is a principal submatrix of $A \otimes B$:

$$A \circ B = (A \otimes B)_{ii,jj}.$$

2.2 Ando's idenity

Lemma 2.1. *Consider $A \in \mathbf{H}_m$ and $B \in \mathbf{H}_n$, and $X \in \mathbb{M}_{m \times n}(\mathbb{C})$ arbitrary. Then,*

$$\langle X, (A \otimes B)X \rangle = \mathrm{Tr}(X^* A X \bar{B}),$$

where on the LHS, X is considered as a vector in $\mathbb{C}^m \otimes \mathbb{C}^n$, and $\bar{B}$ denotes the matrix whose entries are the complex conjugates of those in B.

Proof. Considered as a matrix, we have

$$[(A \otimes B)X]_{ij} = \sum_{k,\ell} A_{ik} X_{k\ell} B_{j\ell}.$$

Since B is Hermitian, we can write the latter sum as

$$\sum_{k,\ell} A_{ik} X_{k\ell} \bar{B}_{\ell j} = [AX\bar{B}]_{ij}.$$

Hence:

$$\langle X, (A \otimes B)X \rangle = \mathrm{Tr}(X^*[(A \otimes B)X]) = \mathrm{Tr}(X^* A X \bar{B}).$$

□

We conclude that

$$\mathrm{Tr}(X^* A X \bar{B}) \geqslant 0 \quad \forall X \in \mathbb{M}_{m\times n}(\mathbb{C}) \iff A \otimes B \geq 0.$$

In particular, we have the following corollary.

Corollary 2.2. *The mapping* $(A, B) \mapsto \mathrm{Tr}(X^* A^p X B^q)$ *is jointly concave on positive matrices for every* $X \in \mathbb{M}_{m\times n}(\mathbb{C})$ *if and only if the mapping* $(A, B) \mapsto A^p \otimes B^q$ *is* jointly operator concave *on PSD matrices.*

Thus we reduce Theorem 1.2 to the following theorem.

Theorem 2.3. *For every* $0 \leqslant t \leqslant 1$*, the mapping* $(A, B) \mapsto A^t \otimes B^{1-t}$ *is jointly operator concave on PSD matrices.*

Proof. Recall the representation proved in Lecture 4: For $0 < p < 1$, we have

$$A^p = C_p \int_0^\infty t^p A(t + A)^{-1}\, dt = C_p \int_0^\infty t^p ((A/t)^{-1} + I)^{-1}\, dt = C_p \int_0^\infty t^p \left(A/t : I\right) dt.$$

Note that $A^t \otimes B^{1-t} = (I \otimes B)(A \otimes B^{-1})^t$, so using this representation, we can write

$$A^t \otimes B^{1-t} = C_p \int_0^\infty t^p (I \otimes B) \left((A \otimes B^{-1})/t : I\right) dt = C_p \int_0^\infty t^p \left((A \otimes I)/t : I \otimes B\right) dt.$$

Thus we are done by Lemma 1.1 since the mapping $(A, B) \mapsto A : B$ is jointly operator concave on positive matrices. □

3 Discussion

3.1 Extension of the Golden-Thompson inequality to three matrices

Given a function F, let us define the Fréchet derivative (when it exists) by

$$\mathsf{D}_K F(A) = \left.\frac{d}{dt}\right|_{t=0} F(A + tK).$$

For $A \succ 0$ and K Hermitian, define the operator

$$T_A(K) := \mathsf{D}_K \log(A).$$

Note that

$$\log(x) = \int_1^x \frac{1}{t}\, dt = \int_0^{x-1} \frac{1}{1+t}\, dt = \int_0^{\infty} \frac{1}{1+t} - \frac{1}{x+t}\, dt,$$

hence for a Hermitian matrix A,

$$\log(A) = \int_0^{\infty} (1+t)^{-1} I - (tI + A)^{-1}\, dt.$$

Recalling that $\mathsf{D}_K A^{-1} = -A^{-1} K A^{-1}$, we calculate

$$T_A(K) = \mathsf{D}_K \log(A) = \int_0^{\infty} (tI + A)^{-1} K (tI + A)^{-1}\, dt.$$

In particular, this implies that T_A is a positive operator: $T_A(K) \geq 0$ when $K \geq 0$. (This is equivalent to the fact we established earlier that $A \mapsto \log(A)$ is operator monotone.)

Theorem 3.1 (Lieb)**.** *For all $A, B, C \in \mathbf{H}^n$, it holds that*

$$\mathrm{Tr}(e^{A+B+C}) \leqslant \mathrm{Tr}\left(e^C T_{e^{-A}}(e^B)\right).$$

This simplifies to $\mathrm{Tr}(e^{A+B+C}) \leqslant \mathrm{Tr}(e^A e^B e^C)$ *if A and B commute.*

Note that if A, B commute, then $T_{e^{-A}}(e^B) = e^{A+B}$ since $\frac{d}{dt}\big|_{t=0} \log(e^{-a} + te^b) = e^{a+b}$ holds for numbers. In particular, taking $B = 0$ recovers the Golden-Thompson inequality $\mathrm{Tr}(e^{A+C}) \leqslant \mathrm{Tr}(e^A e^C)$. We will need two basic results.

Lemma 3.2. *If $f : I \to \mathbb{R}$ is continuously differentiable on an open interval I and* $\mathrm{spec}(A) \subseteq I$, *then*

$$\left.\frac{d}{dt}\right|_{t=0} \mathrm{Tr}\big(f(A+tB)\big) = \mathrm{Tr}\big(f'(A)B\big). \tag{3.1}$$

This follows from "first order perturbation theory" which is the following simple idea: Consider the case where $f(A) = A^n$, $n \geqslant 1$ an integer. Then as $\varepsilon \to 0$,

$$\mathrm{Tr}\left((A + \varepsilon B)^n - A^n\right) = \varepsilon \mathrm{Tr}\left(BA^{n-1} + ABA^{n-2} + \cdots + A^{n-1}B\right) + O(\varepsilon^2) = \varepsilon n \mathrm{Tr}(BA^{n-1}) + O(\varepsilon^2),$$

hence (3.1) holds. More generally, this shows that (3.1) holds when f is any polynomial. Now approximating f by polynomials yields the general claim.

Lemma 3.3. *Let $\mathscr{C}$ be a convex cone, and consider a differentiable convex function $F : \mathscr{C} \to \mathbb{R}$ that is 1-homogeneous in the sense that $F(\lambda A) = \lambda A$ for $\lambda > 0$. Then,*

$$\mathsf{D}_B(A) \leqslant F(B), \quad \forall A, B \in \mathscr{C}.$$

Proof. Since F is 1-homogeneous and convex, it holds that

$$F(A+B) = 2 \cdot F((A+B)/2) \leqslant 2 \cdot (F(A)/2 + F(B)/2) = F(A) + F(B),$$

hence $F(A + tB) - F(A) \leqslant F(tB) = tF(B)$, and the result follows by taking $t \to 0$. □

Recall that Lieb's concavity theorem asserts that for any Hermitian H, the map $X \mapsto \mathrm{Tr}(e^{H+\log X})$ is concave on positive matrices, hence the map $X \mapsto -\mathrm{Tr}(e^{H+\log X})$ is convex and 1-homogeneous. Therefore Lemma 3.3 gives

$$\mathrm{Tr}\left(e^{H+\log(Y)}\right) \leqslant \left.\frac{d}{dt}\right|_{t=0} \mathrm{Tr}\left(e^{H+\log(X+tY)}\right) \overset{(3.1)}{=} \mathrm{Tr}\left(e^{H+\log X}\mathsf{D}_Y \log(X)\right) = \mathrm{Tr}\left(e^{H+\log X}T_X(Y)\right),$$

for $H \in \mathbf{H}_n$ and $X, Y \succ 0$.

Thus taking $H = A + C$, $X = e^{-A}$ and $Y = e^B$ gives

$$\mathrm{Tr}(e^{A+B+C}) \leqslant \mathrm{Tr}\left(e^C T_{e^{-A}}(e^B)\right),$$

proving Theorem 3.1.

3.2 Integral representations

In the proof of Theorem 2.3, we once again used the integral representation: For $0 < p < 1$ and $a > 0$,

$$a^p = C_p \int_0^\infty t^p \frac{a}{t+a}\, dt,$$

where C_p is a constant depending on p.

In fact, a generalization of this approach is the only way to establish operator concavity. Let us state a characterization of Loewner. Define $\mathcal{M}_\infty(0,\infty)$ as the set of functions $f : (0,\infty) \to \mathbb{R}$ that are matrix monotone, i.e., satisfy $A \geq B \implies f(A) \geq f(B)$ for $\mathrm{spec}(A), \mathrm{spec}(B) \subseteq (0,\infty)$.

Denote the upper complex halfplane by $\mathbb{C}_+ := \{z \in \mathbb{C} : \mathrm{Im}\, z > 0\}$. Let $\mathscr{P}$ denote the class of *Pick functions:* Analytic functions $f : \mathbb{C}_+ \to \mathbb{C}_+$. Examples include $f(z) = z^p$ for $p \leqslant 1$, noting that if $z = re^{\mathrm{i}\theta}$, then $z^p = r^p e^{\mathrm{i}p\theta}$. This class also includes the principal branch of the logarithm $f(z) = \log r + \mathrm{i}\theta$.

Theorem 3.4 (Loewner)**.** *The following are equivalent:*

(a) $f \in \mathcal{M}_\infty(0,\infty)$

(b) There exists a positive measure μ *on* $(0,\infty)$ *and* $\beta \geqslant 0$ *such that*

$$f(x) = f(0) + \beta x + \int_0^\infty \frac{tx}{x+t}\, d\mu(t).$$

(c) f *admits an analytic extension to a Pick function on* $\mathbb{C}_+ \cup (0,\infty)$.

(d) f *is matrix concave on* $(0,\infty)$.

Observe that $(b) \Rightarrow (a) \wedge (d)$: Note that $\frac{x}{x+t} = 1 - \frac{t}{x+t}$, hence for Hermitian A, (b) gives

$$f(A) = f(0) + \beta A + \int_{-1}^1 t\left(1 - t(A+tI)^{-1}\right)\, d\mu(t).$$

Since the map $A \mapsto -(A+tI)^{-1}$ is matrix monotone, it follows that $f \in \mathcal{M}_\infty(0,\infty)$. Since the map $A \mapsto (A+tI)^{-1}$ is matrix convex, it follows that f is matrix concave. The hard direction of the theorem is $(a) \Rightarrow (c)$, and we will not go into it here (see B. Simons' extensive book *Loewner's Theorem on Monotone Matrix Functions*).

Dirichlet problem on the unit disk. But we can still understand why complex analysis arises naturally. Let $\mathbb{D} := \{z \in \mathbb{C} : |z| < 1\}$ denote the open unit disk, and suppose that $g : \partial\mathbb{D} \to \mathbb{R}$ is a continuous function on the boundary. Then there is a unique harmonic function $u : \overline{\mathbb{D}} \to \mathbb{R}$ such that $u|_{\partial\mathbb{D}} = g$. Harmonic means that $u(z)$ is given by its averages on small circles around z: As $\varepsilon \to 0$,

$$u(z) = \frac{1}{2\pi} \int u(z + \varepsilon e^{\mathrm{i}\theta})\, d\theta + O(\varepsilon).$$

If we let $\{B_t\}$ denote a 2-dimensional Brownian motion, and let T denote the first time at which B_t exits $\mathbb{D}$, then for $z \in \mathbb{D}$,

$$u(z) = \mathbb{E}[g(B_T) \mid B_0 = z].$$

In other words, u is specified by the boundary values, and its value at z is prescribed by the distribution of where Brownian motion started at z exits the disk. Fortunately, this has a nice expression given by the Poisson integral formula.

Since u is harmonic, it holds that

$$u(0) = \frac{1}{2\pi} \int g(e^{\mathrm{i}\theta})\, d\theta.$$

In other words, the exit measure for B_t started at the origin is uniform on the unit circle, as we would expect. Define the linear fractional transformation

$$T_z(w) := \frac{w + z}{1 + \bar{z}w}.$$

This is a conformal mapping that sends $\overline{\mathbb{D}}$ to $\overline{\mathbb{D}}$ and $0 \mapsto z$. If we define $v_z(w) := u(T_z(w))$, then v_z is also harmonic. (Intuitively, this is because a conformal map sends infinitesimal circles around 0 to infinitesimal circles around z.) Therefore for $z \in \mathbb{D}$, we can write

$$u(z) = v_z(0) = \frac{1}{2\pi} \int g(T_z(e^{\mathrm{i}\theta}))\, d\theta.$$

If we denote $T_z(e^{\mathrm{i}\theta}) = e^{\mathrm{i}\phi}$, then $e^{\mathrm{i}\phi} = T_{-z}(e^{\mathrm{i}\theta})$, and substituting in the integral gives

$$u(z) = \frac{1}{2\pi} \int g(e^{\mathrm{i}\phi}) \frac{d\theta}{d\phi}\, d\phi = \int \underbrace{\frac{1 - |z|^2}{|1 - ze^{-\mathrm{i}\phi}|^2}}_{\text{Poisson kernel}} \underbrace{g(e^{\mathrm{i}\phi}) \frac{d\phi}{2\pi}}_{d\nu(\phi)}. \tag{3.2}$$

The kernel describes the exit measure of 2-dimensional Brownian motion (started at z) from the unit disk. (The pedagogical value of introducing the Brownian motion is that the "physical" formulation seems more intuitive.) Note that if we additionally assume that g is nonnegative, then we obtain $u(z)$ as an integral of the Poisson kernel against a positive measure.

The analytic perspective. In the plane, every harmonic function is the real part of an analytic function. Suppose that a function f is analytic on an open neighborhood $\mathcal{D}$ of $\overline{\mathbb{D}}$. This means that f can be written as a convergent power series about every point in $\mathcal{D}$. Or, equivalently, that the complex derivative $\frac{d}{dz} f(z)$ exists for all $z \in \mathcal{D}$.

In this case, f satisfies the Cauchy-Riemann equations which, in particular, imply that $\operatorname{Re} f$ and $\operatorname{Im} f$ are harmonic functions. We can use the preceding discussion with $u = \operatorname{Re} f$ to write

$$\operatorname{Re} f(z) = \int \frac{1 - |z|^2}{|1 - ze^{-\mathrm{i}\phi}|^2} \operatorname{Re} f(e^{\mathrm{i}\phi}) \frac{d\phi}{2\pi} = \int \operatorname{Re} K(e^{\mathrm{i}\phi}, z) \operatorname{Re} f(e^{\mathrm{i}\phi}) \frac{d\phi}{2\pi}.$$

where we define

$$K(e^{i\theta}, z) := \frac{1 + ze^{-i\theta}}{1 - ze^{-i\theta}}.$$

Note that

$$\operatorname{Re}\left(f(z) - \int K(e^{i\phi}, z) \operatorname{Re} f(e^{i\phi}) \frac{d\phi}{2\pi}\right) = 0.$$

Since the quantity in parentheses is an analytic function whose real part vanishes, the Cauchy-Riemann equations dictate that this quantity is constant on $\overline{\mathbb{D}}$, hence we obtain a representation for f on $\overline{\mathbb{D}}$:

$$f(z) = i \operatorname{Im} f(0) + \int K(e^{i\phi}, z) \operatorname{Re} f(e^{i\phi}) \frac{d\phi}{2\pi}.$$

If $\operatorname{Re} f > 0$, we have

$$f(z) = i \operatorname{Im} f(0) + \int K(e^{i\phi}, z)\, d\nu(\phi),$$

for some positive measure $d\nu$ on $\partial\mathbb{D}$. (This is called the *Herglotz representation on* $\mathbb{D}$.)

Recall that we're concerned with functions $g : (0, \infty) \to \mathbb{R}$. Let's suppose that g is the restriction of a function $f : \mathbb{C} \to \mathbb{C}$ that is analytic on $\mathbb{C}_+ \cup (0, \infty)$. If $T : \mathbb{C}_+ \cup \{\infty\} \to \mathbb{D}$ is a conformal map, then we can obtain integral representations of f by applying the preceding argument to $f \circ T^{-1}$, with the caveat that we need $\operatorname{Re}(f \circ T^{-1}) > 0$. This is where the class of Pick functions $\mathscr{P}$ come into play: If $f : \mathbb{C}_+ \to \mathbb{C}_+$, then we have $-if \circ T^{-1} : \mathbb{D} \to \{z \in \mathbb{C} : \operatorname{Re} z > 0\}$.

Applying this to $-if \circ T^{-1}$ and working through the computation gives

$$f(z) = \operatorname{Re} f(i) + i \int K(T(t), T(z))\, d\mu(t)\,,$$

where μ is the pullback of the measure ν under T, i.e., $\mu(A) = \nu(T[A])$.

If $t \neq \infty$, then

$$i\, K(T(t), T(z)) = \frac{1 + tz}{t - z}.$$

And since $T(\infty) = 1$, it holds that $i\, K(T(\infty), T(z)) = z$. It follows that

$$f(z) = \operatorname{Re} f(i) + \mu(\mathbb{R})z + \int \frac{1 + tz}{t - z}\, d\mu(t).$$

While this is not quite the form of Theorem 3.4(c), one can get there with some further manipulation. (Briefly: It turns out that $\mu((0, \infty)) = 0$, hence the integral can be restricted to $(-\infty, 0)$.)