An integral formula for quantum relative entropy

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“All identities are trivial.”

(Littlewood)

The formula

Definition (Umegaki, 1959)

The quantum relative entropy of matrices $\rho \geq 0$ *and* $\sigma \geq 0$ *is*

$$D(\rho\|\sigma) = \begin{cases} \operatorname{tr} \rho(\log \rho - \log \sigma) \text{ if } \operatorname{im} \rho \subseteq \operatorname{im} \sigma \\ +\infty \text{ otherwise.} \end{cases}$$

Theorem (Integral formula)

$$D(\rho\|\sigma) = \operatorname{tr}(\rho - \sigma) + \int_{-\infty}^{\infty} \frac{dt}{|t|(t-1)^2} \operatorname{tr}^-((1-t)\rho + t\sigma)$$

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Lemma (Elementary data processing inequality)

For any trace-preserving positive linear map

$$\mathcal{E} : M_n(\mathbb{C}) \to M_{n'}(\mathbb{C}),$$

$$\operatorname{tr}^{\pm} \mathcal{E}A \leq \operatorname{tr}^{\pm} A \qquad (A = A^* \in M_n(\mathbb{C})).$$

Proof.

It suffices to treat the $+$ case because passing from A to $-A$ interchanges tr^+ and tr^-.

$$\operatorname{tr}^+ \mathcal{E}A = \operatorname{tr}^+ \mathcal{E}(A^+ - A^-) = \operatorname{tr}^+(\mathcal{E}A^+ - \mathcal{E}A^-) \leq$$
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Data processing inequality

Let $\rho, \sigma \geq 0$. For any trace-preserving positive linear map

$$\mathcal{E} : M_n(\mathbb{C}) \to M_{n'}(\mathbb{C}),$$

we have

$$D(\mathcal{E}\rho \| \mathcal{E}\sigma) \leq D(\rho \| \sigma).$$

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- for completely positive $\mathcal{E}$: Lindblad (1975); equivalent to strong subadditivity of von Neumann entropy (Lieb, Ruskai 1973); implies Holevo bound (1973)

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Derived formula

Definition (John von Neumann, 1932)

$S(\rho) = -\operatorname{tr}\rho\log\rho$ *for* $\rho \geq 0$

Theorem (derivatives of von Neumann entropy)

Let $\rho \geq 0$, $\sigma = \sigma^*$, *and* $\operatorname{im}\sigma \subseteq \operatorname{im}\rho$.

(a) *For all* $m \geq 2$, *we have*

$$-\frac{1}{m!}S(\rho + t\sigma)^{(m)}(0) = \int_{-\infty}^{\infty} \frac{dt}{|t|t^m} \operatorname{tr}^-(\rho + t\sigma). \qquad (1)$$

(b) *When* $m \geq 2$ *is even, the quantity* (1) *is nonnegative and convex as a function of the pair* (ρ, σ).

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Derivative of matrix logarithm

Let $X(t)$ be a differentiable curve whose values are positive definite matrices.

$$(\log X)' = \int_0^\infty (X + r\mathbf{1})^{-1} X' (X + r\mathbf{1})^{-1} \, dr.$$

From this, we infer

Lemma (Intertwining)

If, for a given t, $X(t)$ commutes with a matrix Y, then

$$\operatorname{tr} Y (\log X)'(t) = \operatorname{tr} Y X'(t) X(t)^{-1}.$$

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Negative eigenvalues of matrix pencils

Let $A(t) = (1-t)\rho + t\sigma$ with $A(0) = \rho \geq 0$ and $A(1) = \sigma = \sigma^*$.

Lemma (negative real eigenvalues only occur for real t)

If $A(t)e = -re$ for a unit vector e and a positive real number r, then $t((\rho - \sigma)e, e) > 0$, and therefore t is real.

Proof.

We have $-r = (A(t)e, e) = (1-t)(\rho e, e) + t(\sigma e, e)$,
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Characteristic polynomial

Define $f(t,r) = \det(A(t) + r\mathbf{1})$.
We have $f(t,r) = 0$ if and only if $-r$ is an eigenvalue of $A(t)$.

Lemma (ratio of partial derivatives)

If $A(t)e = -re$ for a unit vector e, then

$$f_t(t,r) = ((\sigma - \rho)e, e) f_r(t,r).$$

Corollary (signs of partial derivatives)

Assume $f(t,r) = 0$ and $r > 0$. Then t is real, and

$$t f_r(t,r) f_t(t,r) = t((\sigma - \rho)e, e) f_r(t,r)^2 \leq 0.$$

Equality $\Leftrightarrow f_r(t,r) = 0 \Leftrightarrow -r$ is a multiple eigenvalue of $A(t)$

We may and do assume, for convenience:
all negative eigenvalues of all $A(t)$ are simple.

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Joining the pair (ρ, σ) to infinity

Lemma (limit at infinity)

$\lim_{r\to\infty} D(\rho + r\mathbf{1}\|\sigma + r\mathbf{1}) = \mathrm{tr}(\rho - \sigma)$.

Proof.

$D(\rho + r\mathbf{1}\|\sigma + r\mathbf{1}) = rD(\mathbf{1} + \rho/r\|\mathbf{1} + \sigma/r) \sim r\,\mathrm{tr}(\rho - \sigma)/r.$ □

Lemma (derivative)

(a) *For all* $r > 0$, *we have*

$$\frac{d}{dr}D(\rho + r\mathbf{1}\|\sigma + r\mathbf{1}) = \log f(0, r) - \log f(1, r) + (\log f)'(1, r)$$

(b) *If* $\mathrm{im}\,\rho \subseteq \mathrm{im}\,\sigma$, *then this is* $o(1/r)$ *as* $r \to 0$ *or* $r \to \infty$.

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Residues appear

From these two lemmas, we have

$$D(\rho\|\sigma) - \operatorname{tr}(\rho - \sigma) =$$
$$= -\int_0^\infty \left(\log f(0,r) - \log f(1,r) + (\log f)'(1,r)\right)\, dr =$$
$$= \int_0^\infty r\left((\log f)_r(0,r) - (\log f)_r(1,r) + (\log f)'_r(1,r)\right)\, dr$$

if $\operatorname{im}\rho \subseteq \operatorname{im}\sigma$.

Let

$$g(t) = \frac{1}{t} - \frac{1}{t-1} + \frac{1}{(t-1)^2} = \frac{1}{t(t-1)^2},$$

then

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Residue Theorem

Fix $r > 0$.
$g \cdot (\log f)_r = gf_r/f$ holomorphic for $t \in \mathbb{C} \setminus \{0, 1\}$, $f(t, r) \neq 0$.
$f(t, r) = 0 \Rightarrow \mathrm{Res}_t(gf_r/f) = gf_r/f_t$.
$gf_r/f = O\left(|t|^{-3}\right)$ as $t \to \infty$.
Contour integrals on circles $|t| = T$ tend to zero as $T \to \infty$.
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$$D(\rho\|\sigma) - \mathrm{tr}(\rho - \sigma) = -\int_0^\infty r \sum_{f(t,r)=0} \frac{gf_r}{f_t}\, dr = \int_{-\infty}^{\infty} \frac{dt}{|t|(t-1)^2} \sum_{f(t,r)=0} r^+$$

Indeed, for a simple negative eigenvalue $-r$ of $A(t)$, we have
$t \in \mathbb{R}$, $f_r(t, r) \neq 0$, $f_t(t, r) \neq 0$, $|dr/dt| = |f_t/f_r| = -(\mathrm{sgn}\, t) f_t/f_r$
as we move along the algebraic plane curve $f = 0$.
The last sum that has appeared is $\mathrm{tr}^- A(t)$.

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Fix $r > 0$.
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Theorem (F. Hiai, M. Ohya, M. Tsukada, 1981)

$$D(\rho_1 \| \rho_0) \geq \|\rho_1 - \rho_0\|_1^2 / 2$$

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Let $\rho_0, \rho_1 \in M_n(\mathbb{C})$ be density matrices.

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Let $E_\pm$ be the orthogonal projection onto $V_\pm$.

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Let Δ be any function depending on two density matrices and satisfying $\Delta(\mathcal{E}\rho_0\|\mathcal{E}\rho_1) \leq \Delta(\rho_0\|\rho_1)$
for any quantum measurement $\mathcal{E}$ with two possible outcomes.
Examples:

- concavity of von Neumann entropy (A. Holevo):

$$\chi(\rho_0, \rho_1; q_0, q_1) = S(q_0\rho_0 + q_1\rho_1) - q_0 S(\rho_0) - q_1 S(\rho_1)$$

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Theorem (Lower bound for generalized divergence)

For any quantum states $\rho_0, \rho_1 \in M_n(\mathbb{C})$, there exist binary classical states ρ_0' and ρ_1' such that $\|\rho_1' - \rho_0'\|_1 = \|\rho_1 - \rho_0\|_1$ and $\Delta(\rho_0'\|\rho_1') \leq \Delta(\rho_0\|\rho_1)$.

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Lower bound for Holevo quantity

- The entropy of the binary classical state with distribution $(x, 1-x)$ is given by the binary entropy function $h(x) = -x \log x - (1-x)\log(1-x)$.
- The mutual information between two binary classical states is given by $I(t_0, t_1; q_0, q_1) := h(q_0 t_0 + q_1 t_1) - q_0 h(t_0) - q_1 h(t_1)$.

Theorem (Sharp lower bound for Holevo quantity)

$$\chi(\rho_0, \rho_1; q_0, q_1) \geq$$
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Lemma (Lower bound for mutual information)

$$I(t_0, t_1; q_0, q_1) \geq 4q_0q_1 \left(h\left(\frac{1}{2}\right) - h\left(\frac{1 + t_1 - t_0}{2}\right)\right)$$

Note that $h(1/2) = \log 2$.

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$$\chi(\rho_0, \rho_1; q_0, q_1) \geq 4q_0q_1 \left(h\left(\frac{1}{2}\right) - h\left(\frac{2 + \|\rho_1 - \rho_0\|_1}{4}\right)\right)$$

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