Entropy Distance: New Quantum Phenomena

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Entropy Distance as an Information Functional

Definition

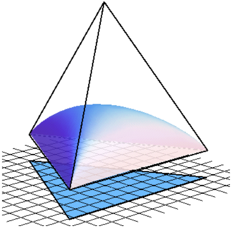
Entropy distance $d_{\mathcal{E}}$ is the relative entropy distance from an exponential family $\mathcal{E}$ in a finite-dimensional matrix algebra $\mathcal{A}$. Classical algebra $\mathcal{A} \cong \mathbb{C}^N$, quantum otherwise.

Overview of exponential families in statistics: Amari and Nagaoka, *Methods of information geometry* (2000).
Applications of entropy distance include

- MLE through the log-likelihood function (classical),
- the stochastic interaction measure of multi-information, this is the entropy distance from the independence model (classical & quantum).

Previous Work on $d_{\mathcal{E}}$ in Classical Probability Theory

Barndorff-Nielsen ('78),
Čencov ('82),
Ay ('02),
Csiszár and Matúš ('03, '05, '08)



Rough Idea:

- Pythagorean theorem of relative entropy implies projection theorem along the normal space,
- mean value chart maps $\mathcal{E}$ to the mean value set (convex support),
- extension of $\mathcal{E}$ implies optimal projection theorem and optimal Pythagorean theorem.

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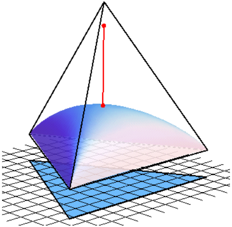

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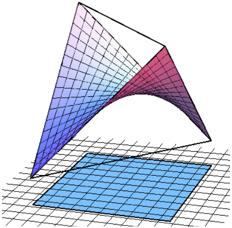

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Previous Work on $d_{\mathcal{E}}$ in the Quantum Case

Classical extension of $\mathcal{E}$ is compact, the mean value set is a polytope and $d_{\mathcal{E}}$ is continuous. All wrong for quantum case!

Well-known in the quantum case:

- Pythagorean theorem implies (only in a restriction!) a projection theorem along the normal space, see Petz ('08),
- mean value chart and mean value set are known, see Wichmann ('63).

New in our work: Convex structure of mean value set includes non-exposed faces; extensions of $\mathcal{E}$; optimal projection theorem and Pythagorean theorem.

Exponential Families

Definition

State space $\overline{\mathcal{S}} := \{\rho \in \mathcal{A} \mid \rho \geq 0, \mathrm{tr}(\rho) = 1\}$. Real vector space $\mathcal{A}_{\mathrm{sa}} \subset \mathcal{A}$ of self-adjoint matrices, Hilbert-Schmidt inner product. Analytic diffeo. $\exp_1 : \mathcal{A}_{\mathrm{sa}}/\mathbb{R}\mathbb{1} \to \mathcal{S} := \{\rho \in \overline{\mathcal{S}} | \rho^{-1}$ exists $\}$, $a \mapsto \frac{e^a}{\mathrm{tr}(e^a)}$, canonical chart $\ln_0 = \exp_1^{-1}$ to traceless matrices.
Exponential family $\mathcal{E} := \exp_1($ linear subspace of $\mathcal{A}_{\mathrm{sa}}$ $)$,
$V := \ln_0(\mathcal{E})$ tangent space, $V^\perp$ normal space,
orth. projection $\pi_V : \mathcal{A}_{\mathrm{sa}} \to V$, mean value set $\mathrm{mv}(V) := \pi_V(\overline{\mathcal{S}})$.

Theorem (Wichmann '63)

$\pi_V \circ \exp_1|_V : V \to \mathrm{Int}(\mathrm{mv}(V))$ *real analytic bijection.*

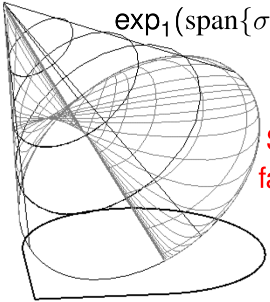
Two Examples

Definition (Mean value chart)

The analytic chart $\pi_V|_{\mathcal{E}}$ onto $\mathrm{Int}(\mathrm{mv}(V))$ is called **mean value chart**.

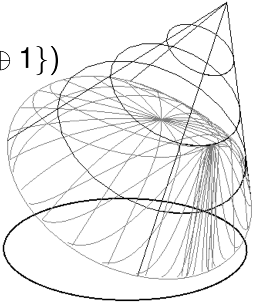
$\exp_1(\mathrm{span}\{\sigma_1 \oplus 1, \sigma_2 \oplus 1\})$

$\exp_1(\mathrm{span}\{\sigma_1 \oplus 0, \sigma_2 \oplus 1\})$



Swallow family

Staffelberg family



$\mathcal{A} := \mathrm{Mat}(2, \mathbb{C}) \oplus \mathbb{C}$

2D Mean Value Sets in $\mathcal{A} := \mathrm{Mat}(2, \mathbb{C}) \oplus \mathbb{C}$

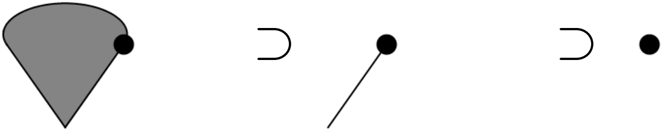
- $\overline{\mathcal{S}}$ is the 4D cone $\mathrm{conv}($ Bloch ball $\oplus\, 0, 0_2 \oplus 1)$,
- every 2D exponential family $\mathcal{E}$ of $\mathcal{A}$ is included in a 3D cone,
- modulo automorphism take $z := -\frac{1}{2}\mathbb{1}_2 \oplus 1$, $W := \mathrm{span}\{\sigma_1 \oplus 0, \sigma_2 \oplus 0, z\}$, $V \subset W$ and the cone $C := (\frac{1}{3}\mathbb{1} + W) \cap \overline{\mathcal{S}} = \overline{\exp_1(W)} \supset \mathcal{E}$,
- a complete orbit invariant of 2D planes V is the angle $\measuredangle(V, z) \in [0, \frac{\pi}{2}]$.

Exposed Faces, Poonems and Access Sequences

Definition (Rockafellar, Grünbaum, Csiszár and Matúš)

Let M be a convex set. The intersection F of M with a supporting hyperplane of M is called exposed face of M. $\emptyset$ and M are expsed faces by definition. In these cases we write $F \overset{\text{Ex}}{<} M$. A sequence $F = F_1 \overset{\text{Ex}}{<} \cdots \overset{\text{Ex}}{<} F_k \overset{\text{Ex}}{<} M$ is called access sequence and F is called poonem of M. A poonem, which is not an exposed face is called non-exposed face.

Concept of poonem is equivalent to the more popular concept of face.



The Pythagorean Theorem (Restricted Form)

Definition

The relative entropy of two states $\rho, \sigma \in \overline{\mathcal{S}}$ is $S(\rho, \sigma) := \infty$ unless $\mathrm{Im}(\sigma) \supset \mathrm{Im}(\rho)$ and then $S(\rho, \sigma) := \mathrm{tr}\rho(\ln \rho - \ln \sigma)$.

Theorem (Monograph Petz '08 for an overview)

If $\rho, \sigma, \tau \in \overline{\mathcal{S}}$ are states, σ and τ are invertible and $\rho - \sigma \perp \ln(\tau) - \ln(\sigma)$ holds, then we have $S(\rho, \sigma) + S(\sigma, \tau) = S(\rho, \tau)$.

- The Pythagorean theorem induces the projection $\pi_{\mathcal{E}} : \mathcal{E} + V^{\perp} \to \mathcal{E}$, $a \mapsto (a + V^{\perp}) \cap \mathcal{E}$ to an exponential family $\mathcal{E}$.
- For a state $\rho \in \mathcal{E} + V^{\perp}$ we have $d_{\mathcal{E}}(\rho) := \inf_{\sigma \in \mathcal{E}} S(\rho, \sigma) = S(\rho, \pi_{\mathcal{E}}(\rho))$.

Lattice Isomorphisms and Compressions

Assignment of an orth. projector $F \mapsto p^F$ to each face F of $\mathrm{mv}(V)$ through

- inverse projection $F \mapsto (F + V^\perp) \cap \overline{\mathcal{S}}$ lifts faces of $\mathrm{mv}(V)$ to faces of $\overline{\mathcal{S}}$,
- (face lattice of $\overline{\mathcal{S}}$) $\cong$ (projector lattice of $\mathcal{A}$).

Definition

Orth. projector p defines projection $\mathcal{A} \to p\mathcal{A}p := \{pap \mid a \in \mathcal{A}\}$ by $a \mapsto pap$. We denote by $\exp_1^p$ and $\ln^p$ the trace normalized exponential and the logarithm in $p\mathcal{A}p$.
A face F of $\mathrm{mv}(V)$ defines the compressed exponential family $\mathcal{E}^{p^F} := \exp_1^{p^F}(p^F V p^F)$.

The Geodesic Closure

Definition

The e-geodesic through $\theta \in \mathcal{A}_{\mathrm{sa}}$ in the direction of $v \in \mathcal{A}_{\mathrm{sa}}$ is the curve $\gamma \mapsto g_{\theta,v}(\lambda) = \exp_1(\theta + \lambda v) \subset \mathcal{S}$.

If p is the maximal projector of v (spectral projector of the largest eigenvalue), then $\mathcal{E}^p = \{\lim_{\lambda\to\infty} g_{\theta,v}(\lambda) \mid \theta \in V\}$.

Definition

The geodesic closure of $\mathcal{E}$ is $\mathrm{cl}_{\mathrm{geo}}(\mathcal{E}) := \bigcup_F \mathcal{E}^{p^F}$. Here F extends over the exposed faces ($\neq \emptyset$) of $\mathrm{mv}(V)$.

The geodesic closure $\mathrm{cl}_{\mathrm{geo}}(\mathcal{E})$ exceeds $\mathcal{E}$ by the limit points of e-geodesics in $\mathcal{E}$.

The rI-Closure

Definition (Csiszár and Matúš)

The rI-closure of $\mathcal{E}$ is $\mathrm{cl}_{\mathrm{rI}}(\mathcal{E}) := \{\rho \in \overline{\mathcal{S}} \mid d_{\mathcal{E}}(\rho) = 0\}$.

- E-geodesic asymptotics show $\mathrm{cl}_{\mathrm{geo}}(\mathcal{E}) \subset \mathrm{cl}_{\mathrm{rI}}(\mathcal{E})$.
- The proof idea to the following theorem is to concatenate e-geodesic asymptotics. For every poonem F in an access sequence of $\mathrm{mv}(V)$ we form the geodesic closure of the compressed exponential family $\mathcal{E}^{p^F}$ and take the union:

$$\mathrm{cl}_{\mathrm{rI}}(\mathcal{E}) = \bigcup_F \mathcal{E}^{p^F}.$$

- Equality $\mathrm{cl}_{\mathrm{geo}}(\mathcal{E}) = \mathrm{cl}_{\mathrm{rI}}(\mathcal{E})$ holds if and only if all faces of $\mathrm{mv}(V)$ are exposed. Examples: independence model, convex family or classical algebra.

The Optimal Projection Theorem

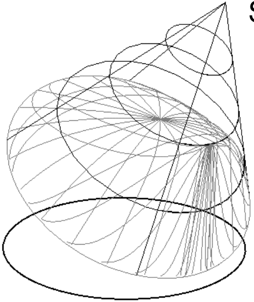
Theorem (Weis '09)

Let $\mathcal{E}$ be an exponential family with tangent space V.

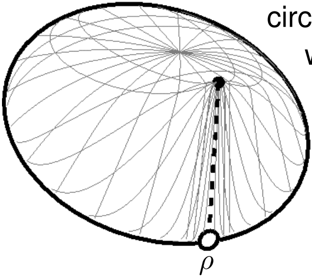
(1) *If $\rho \in \overline{\mathcal{S}}$, then $\rho + V^{\perp}$ intersects the reverse information closure $\mathrm{cl}_{\mathrm{rI}}(\mathcal{E})$ in a unique point denoted by $\pi_{\mathcal{E}}(\rho)$.*

(2) *If $\rho \in \overline{\mathcal{S}}$, then the relative entropy $S(\rho, \cdot)$ has a unique local minimum on $\mathrm{cl}_{\mathrm{rI}}(\mathcal{E})$ and*
$\min_{\sigma \in \mathrm{cl}_{\mathrm{rI}}(\mathcal{E})} S(\rho, \sigma) = S(\rho, \pi_{\mathcal{E}}(\rho)) = S_{\mathcal{E}}(\rho)$.

A Discontinuous Entropy Distance is Possible



Staffelberg family: Discontinuity on the base circle of the cone C where $d_{\mathcal{E}} \equiv 0$ except $d_{\mathcal{E}}(\rho) = \ln(2)$ for $\rho := \frac{1}{2}(\mathbb{1}_2 \oplus \sigma_2) \oplus 0$.

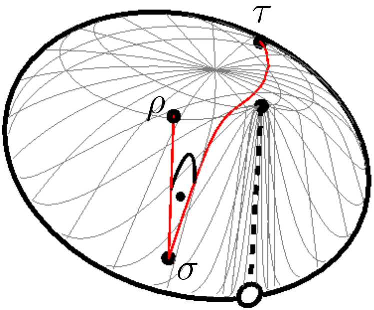


- The discontinuous $d_{\mathcal{E}}$ at $\varphi = \measuredangle(V, z) = \frac{\pi}{3}$ separates mean value sets with non-exposed faces from those without.
- According to the Pinsker-Csiszár inequality $\mathrm{cl}_{\mathrm{rI}}(\mathcal{E}) \subset \overline{\mathcal{E}}$ holds. Equality $\mathrm{cl}_{\mathrm{rI}}(\mathcal{E}) = \overline{\mathcal{E}} \iff d_{\mathcal{E}}$ is continuous. E.g. indep. model, convex family or (Ay '02) classical algebra.

The Optimal Pythagorean Theorem

Theorem (Weis '10)

Let $\mathcal{E}$ be an exponential family with tangent space V. If $\rho \in \overline{\mathcal{S}}$ and $\sigma, \tau \in \mathrm{cl}_{\mathrm{rI}}(\mathcal{E})$ are states such that $\sigma - \rho \perp V$, then $S(\rho, \sigma) + S(\sigma, \tau) = S(\rho, \tau)$ holds.



Maximization of Entropy Distance

Previous work e.g. by Ay, Knauf, Matúš

Definition

If $\rho \in \overline{\mathcal{S}}$ then the support projector of ρ is the ortho. projector $s(\rho) \in \mathcal{A}$ with the image $\mathrm{Im}(s(\rho)) = \mathrm{Im}(\rho)$. For $a \in \mathcal{A}_{\mathrm{sa}}$ denote the free energy $F(a) := \ln \mathrm{tr} e^a$ and use F^p for free energy in $p\mathcal{A}p$.

Theorem (Knauf and Weis '10)

Let $\rho \in \overline{\mathcal{S}}$, $p := s(\rho)$ and $q := s(\pi_{\mathcal{E}}(\rho))$. For every traceless self-adjoint matrix $u \in p\mathcal{A}p$ we have the directional derivative $\mathrm{D}|_\rho d_{\mathcal{E}}(u) = \langle u, \ln^p(\rho) - \ln^q \circ \pi_{\mathcal{E}}(\rho)\rangle$.
If ρ is a local maximizer of $d_{\mathcal{E}}$ then for $\theta := \ln^q \circ \pi_{\mathcal{E}}(\rho)$ we have $\rho = \exp_1^p(p\theta p)$ and $d_{\mathcal{E}}(\rho) = F^q(\theta) - F^p(p\theta p)$.

Maximum Entropy (Wichmann '63, Ingarden et al. '97)

Let $U \subset \mathcal{A}_{\mathrm{sa}}$ be a vector space and let $u \in U$.

Definition

The von Neumann entropy of a state $\rho \in \overline{\mathcal{S}}$ is $S(\rho) := -\mathrm{tr}\rho \ln \rho$. The constraint set of (U, u) is $C_{U,u} := \{\rho \in \overline{\mathcal{S}} \mid \pi_U(\rho) = u\}$. Let $\mathcal{E} := \exp_1(U)$.

Theorem (Weis '09)

We have $\mathrm{argmax}_{\rho \in C_{U,u}} S(\rho) = C_{U,u} \cap \mathrm{cl}_{\mathrm{rI}}(\mathcal{E})$.

Idea: replace $\max_\rho S(\rho) - \ln \mathrm{tr}\mathbb{1} = \max_\rho -S(\rho, \frac{\mathbb{1}}{\mathrm{tr}\mathbb{1}})$ by $\min_\rho S(\rho, \frac{\mathbb{1}}{\mathrm{tr}\mathbb{1}})$ and use Pythagorean theorem $\min_\rho [S(\rho, \pi_\mathcal{E}(\rho)) + S(\pi_\mathcal{E}(\rho), \frac{\mathbb{1}}{\mathrm{tr}\mathbb{1}})] = S(\pi_\mathcal{E}(\rho), \frac{\mathbb{1}}{\mathrm{tr}\mathbb{1}})$.

Coordinates for Maximum Entropy Ensembles

We fix $a_1, \dots, a_k \in \mathcal{A}_{\mathrm{sa}}$ (observables) and put $V := \mathrm{span}\{a_1, \dots, a_k, \mathbb{1}\} \cap \{\mathrm{tr}(\cdot) = 0\}$. Then we choose a tuple of mean values $(\xi_i)_{i=1}^k \in \{\{\mathrm{tr}(a_i\rho)\}_{i=1}^k \mid \rho \in \overline{\mathcal{S}}\} \cong \mathrm{mv}(V)$.

Theorem (Weis '10)

There exists a unique face G of $\mathrm{mv}(V)$ and unique coefficients $\beta_1, \dots, \beta_k \in \mathbb{R}$ such that for $a(\beta) := -\sum_{i=1}^k \beta_i p^G a_i p^G$ and for $j = 1, \dots, k$ we have

$$-\frac{\partial}{\partial \beta_j} F(a(\beta)) = \xi_j \langle p^G, \exp_1(a(\beta)) \rangle.$$

The maximizer of von Neumann entropy S with mean $(\xi_i)_{i=1}^k$ is $\rho := \exp_1^{p^G}(a(\beta))$ and $S(\rho) = \sum_{i=1}^k \beta_i \xi_i + F^{p^G}(a(\beta))$.

General Properties of the Entropy Distance $d_{\mathcal{E}}$

- Entropy distance $d_{\mathcal{E}}(\rho) = S(\rho, \pi_{\mathcal{E}}(\rho))$ of a state ρ given by projection $\pi_{\mathcal{E}} : \overline{\mathcal{S}} \to \mathrm{cl}_{\mathrm{rI}}(\mathcal{E})$ along the normal space $V^{\perp}$.
- Optimal Pythagorean theorem, for states $\rho \in \overline{\mathcal{S}}$ and $\tau \in \mathrm{cl}_{\mathrm{rI}}(\mathcal{E})$ we have $S(\rho, \tau) = d_{\mathcal{E}}(\rho) + S(\pi_{\mathcal{E}}(\rho), \tau)$.
- Geo. closure $\mathrm{cl}_{\mathrm{geo}}(\mathcal{E}) \subset$ rI-closure $\mathrm{cl}_{\mathrm{rI}}(\mathcal{E}) \subset$ topo. closure $\overline{\mathcal{E}}$,
  - $\mathrm{cl}_{\mathrm{geo}}(\mathcal{E}) = \mathrm{cl}_{\mathrm{rI}}(\mathcal{E}) \iff$ no non-exposed faces,
  - $\mathrm{cl}_{\mathrm{rI}}(\mathcal{E}) = \overline{\mathcal{E}} \iff$ entropy distance is continuous.

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Open Questions

- What can be said about special families, e.g. independence model, Boltzmann machines?
- Where are the discontinuities of entropy distance?
- What are the one-sided directional derivatives?
- Are there connections to the geometry of entanglement?

Evidence

- A. Knauf and S. Weis.
  Entropy Distance: New Quantum Phenomena.
  arXiv:1007.5464
- S. Weis.
  The Pythagorean Theorem of Relative Entropy.
  arXiv:1003.5671
- S. Weis.
  Exponential Families with Incompatible Statistics and Their Entropy Distance, PhD thesis, Erlangen (2009).
  www.opus.ub.uni-erlangen.de/opus/volltexte/2010/1580

Thanks!

The Staffelberg Mountain