The *rI*-Closure of an Exponential Family and Ground Spaces

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Introduction

The maximum-entropy inference and the entropy distance from an exponential family of quantum states are geometrically described by the rI-closure of the exponential family and by the rI-projection onto the rI-closure.

- An exponential family $\mathcal{E}$ consists of thermal states of maximal rank. The rI-closure $\operatorname{cl}\mathcal{E}$ contains states of non-maximal rank, for example ground states.
- The set of maximum-entropy inference states under linear constraints (Boltzmann 1877, Jaynes 1957) equals $\operatorname{cl}\mathcal{E}$. If $\operatorname{cl}\mathcal{E}$ is not norm closed, then the inference map has discontinuities (W and Knauf 2012) which correspond to ground energy level crossings (Leake et al. 2014, Chen et al. 2015, W 2016, W and Spitkovsky preprint).
- The entropy distances from $\mathcal{E}$ equals that from $\operatorname{cl}\mathcal{E}$ and quantifies interaction (Ay 2002), irreducible correlation (Linden et al. 2002, Zhou 2008), stochastic interdependence (Ay and Knauf 2006); see also Amari 2001, Rauh 2011, W et al. 2015, Gühne et al. 2017.

Preliminaries

Algebra M_n of n-by-n matrices, Hilbert-Schmidt inner product $\langle a,b\rangle := \operatorname{tr}(a^*b)$, $a,b\in M_n$, hermitian matrices $M_n^{\mathrm{h}} := \{a\in M_n \mid a^*=a\}$,

$$\textbf{linear subspace } U\subset M_n^{\mathrm{h}},$$

orthogonal projection $\pi_U : M_n^{\mathrm{h}}\to M_n^{\mathrm{h}}$ onto U.

State space $\mathcal{D}_n := \{\rho\in M_n \mid \rho\succeq 0, \operatorname{tr}(\rho)=1\}$ of M_n, asymmetric distance of **relative entropy** $D:\mathcal{D}_n\times\mathcal{D}_n\to[0,\infty]$,

$$D(\rho,\sigma) = \begin{cases} \langle \rho, \log(\rho)-\log(\sigma)\rangle, & \text{if image}(\rho)\subset\text{image}(\sigma),\\ +\infty, & \text{else,}\end{cases}$$

entropy distance $D(\rho,X) := \inf_{\sigma\in X} D(\rho,\sigma)$ of $\rho\in\mathcal{D}_n$ from $X\subset\mathcal{D}_n$.

Exponential map $R(a)=e^a/\operatorname{tr}(e^a)$, **exponential family** $\mathcal{E}=\mathcal{E}(U)=\{R(u)\mid u\in U\}$; in thermodynamics, $R(-\beta H)$ is the thermal state of $H\in M_n^{\mathrm{h}}$ at inverse temperature $\beta>0$.

Information Geometry of an Exponential Family

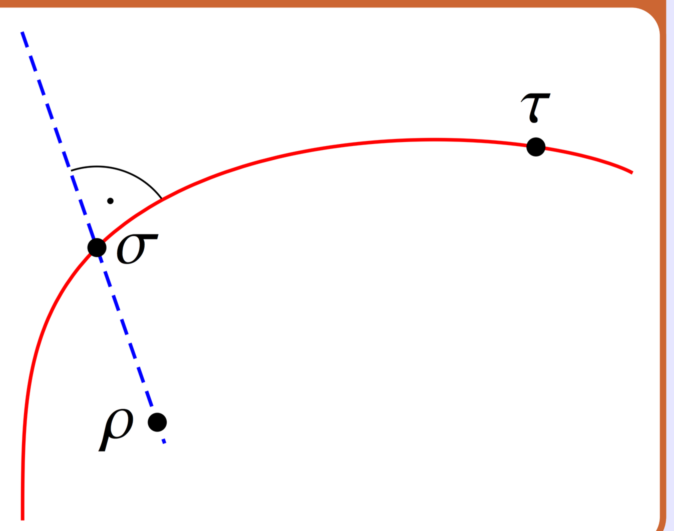
Information geometry studies the differential geometry of manifolds of probability vectors (Amari 1987) and quantum states (Petz 1994, Nagaoka 1995).

Pythagorean Theorem for Curves

Let $\rho,\sigma,\tau\in\mathcal{D}_n$, let σ,τ be of full rank n, and $\langle\rho-\sigma,\log(\tau)-\log(\sigma)\rangle=0$. Then

$$D(\rho,\sigma)+D(\sigma,\tau)=D(\rho,\tau).$$

Figure: (+1)-geodesic (solid, red)
$\mu\mapsto R[\log(\sigma)+\mu(\log(\tau)-\log(\sigma))]$
(−1)-geodesic (dashed, blue)
$\lambda\mapsto\sigma+\lambda(\rho-\sigma)$



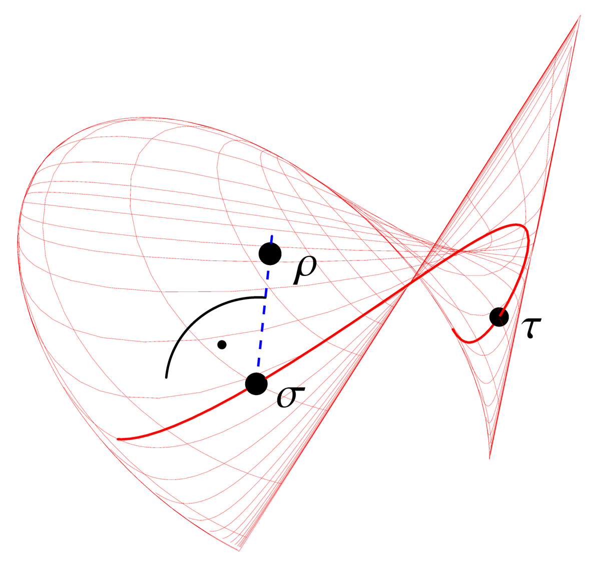
Proof: $D(\rho,\tau)-D(\rho,\sigma)-D(\sigma,\tau)=\langle\rho,\log(\sigma)-\log(\tau)\rangle-\langle\sigma,\log(\sigma)-\log(\tau)\rangle=0$. □

Pythagorean Theorem

Let $\rho\in\mathcal{D}_n$, let $\sigma,\tau\in\mathcal{E}(U)$, and $\langle\rho-\sigma,U\rangle=0$. Then

$$D(\rho,\sigma)+D(\sigma,\tau)=D(\rho,\tau).$$

Figure: Two-dimensional exponential family $\mathcal{E}(U)$ where U is spanned by $X\oplus 1$ and $Y\oplus 1\in M_3$ and where $X=\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$ and $Y=\left(\begin{smallmatrix}0&-i\\i&0\end{smallmatrix}\right)$; (+1)-geodesic included in $\mathcal{E}$ (solid, red) intersects (−1)-geodesic orthogonal to U (dashed, blue) in σ



Proof: Use $\langle\rho-\sigma,\log(\tau)-\log(\sigma)\rangle=0$ and the Pythagorean Theorem for Curves. □

Transversality and Projection Theorem

Let $\rho\in(\mathcal{E}(U)+U^\perp)\cap\mathcal{D}_n$.

- There exists a unique state $\pi_{\mathcal{E}}(\rho)\in\mathcal{E}$ such that $\rho-\pi_{\mathcal{E}}(\rho)\perp U$.
- We have $D(\rho,\mathcal{E})=\min_{\sigma\in\mathcal{E}}D(\rho,\sigma)=D(\rho,\pi_{\mathcal{E}}(\rho))$.

Proof: Use the Pythagorean Theorem and distance properties of the relative entropy. □

Notice. If $\rho\in\mathcal{D}_n$ is the state of the system, then the **expected value** of $u\in U$ is $\langle\rho,u\rangle$, so $\pi_U(\mathcal{E})$ represents **expected value parameters** of $\mathcal{E}$.

We study a closure $\operatorname{cl}\mathcal{E}$ which is maximal, $\pi_U(\operatorname{cl}\mathcal{E})=\pi_U(\mathcal{D}_n)$, and for which analogous theorems of information geometry hold.

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Closures in Norm and rI-Topology

E. H. Wichmann's Theorem (JMP 4, 884, 1963)

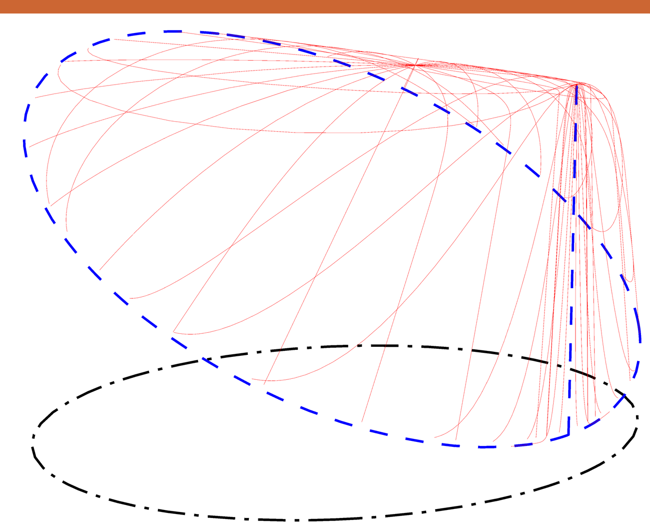
The projection $\pi_U(\mathcal{E})$ is the relative interior of $\pi_U(\mathcal{D}_n)$.

The convex set $\pi_U(\mathcal{D}_n)$ is isomorphic to the **state space** of the operator system $U+\mathrm{i}U+\mathbb{C}\mathbb{1}$ (W 2018) and to a **joint algebraic numerical range** (Müller 2010).

Transversality Fails in the Norm Closure $\overline{\mathcal{E}}$

Figure: Two-dimensional exponential family $\mathcal{E}(U)$ where U is spanned by $X\oplus 1, Y\oplus 0\in M_3$
- (+1)-geodesics in $\mathcal{E}$ (solid, red)
- components of $\overline{\mathcal{E}}$ outside of $\mathcal{E}$ (dashed, blue)
- boundary of $\pi_U(\mathcal{D}_n)$ (dot-dashed, black)

$\overline{\mathcal{E}}$ and $U^\perp$ are not transversal as π_U maps a segment (dashed, blue) to a singleton (W and Knauf 2012)



An information closure solves the problem (W, Journal of Convex Analysis **21**, 339, 2014).

The rI-Closure

- the acronym **rI** stands for **reverse information** and refers to the ordering of the arguments of the relative entropy (Csiszár and Matúš 2003)
- the open disks $\{\sigma\in\mathcal{D}_n \mid D(\rho,\sigma)<\epsilon\}$, $\rho\in\mathcal{D}_n$, $\epsilon\in(0,+\infty]$, form a base of the **rI-topology**; caution: the rI-topology has to be defined as a sequential topology for ∞-dim. von Neumann algebras (Csiszár 1964, Harremoës 2007)
- the **rI-closure** $\operatorname{cl}X := \{\rho\in\mathcal{D}_n \mid D(\rho,X)=0\}$ equals the closure in the rI-topology

The rI-Closure of an Exponential Family

Transversality

If $\rho\in\mathcal{D}_n$ then there is a unique state $\pi_{\mathcal{E}}(\rho)\in\operatorname{cl}\mathcal{E}(U)$ such that $\langle\rho-\pi_{\mathcal{E}}(\rho),U\rangle=0$.

Pythagorean Theorem

If $\rho,\sigma\in\mathcal{D}_n$ and $\sigma\in\operatorname{cl}\mathcal{E}$ then $D(\rho,\pi_{\mathcal{E}}(\rho))+D(\pi_{\mathcal{E}}(\rho),\sigma)=D(\rho,\sigma)$.

Projection Theorem

If $\rho\in\mathcal{D}_n$ then $D(\rho,\mathcal{E})=D(\rho,\operatorname{cl}\mathcal{E})=D(\rho,\pi_{\mathcal{E}}(\rho))$.

The state $\pi_{\mathcal{E}}(\rho)$ is called **rI-projection** of ρ to $\operatorname{cl}\mathcal{E}$. Proofs of Thms: W, *ibid*, 2014

Algebra of the rI-Closure

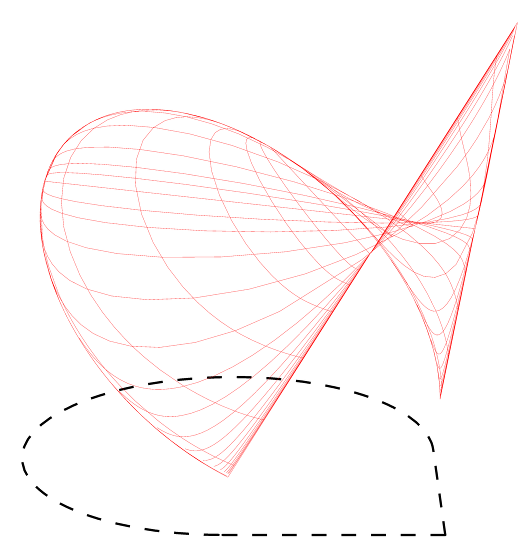
An **exposed face** of $\pi_U(\mathcal{D}_n)$ is a subset of minimizers

$$F(u) := \operatorname{argmin}\{\langle z,u\rangle \mid z\in\pi_U(\mathcal{D}_n)\},\qquad u\in U.$$

The **ground projection** $p(u)$ of $u\in U$ is the spectral projection of u corresponding to the smallest eigenvalue.

For all $u\in U$ and $p=p(u)$, the exponential family $\mathcal{E}_p(U) := \{\frac{pe^{pvp}}{\operatorname{tr}(pe^{pvp})} : v\in U\}$ lies in $\operatorname{cl}\mathcal{E}(U)$ as $\mathcal{E}_p(U)=\{\lim_{\mu\to\infty}R(v+\mu u) : v\in U\}$; the restriction $\pi_U|_{\mathcal{E}_p(U)}$ is a bijection to the (relative) interior of $F(u)$.

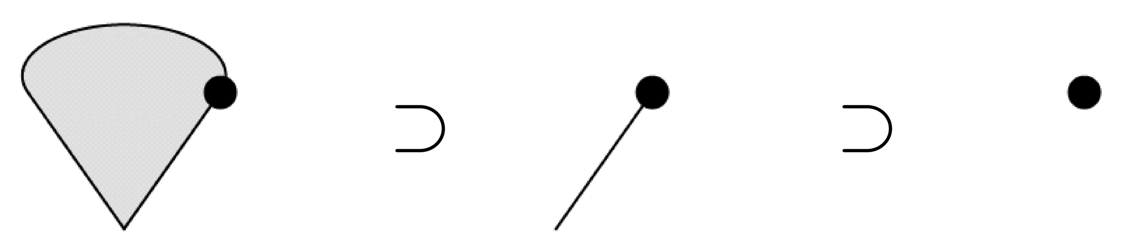
Figure: Two-dim. exponential family $\mathcal{E}(U)$, (+1)-geodesics (solid, red), boundary of $\pi_U(\mathcal{D}_n)$ (dashed, blue)



Just as relative interiors of exposed faces of $\pi_U(\mathcal{D}_n)$ do not cover $\pi_U(\mathcal{D}_n)$, $\operatorname{cl}\mathcal{E}$ is not covered by limit points of (+1)-geodesics in $\mathcal{E}$.

Exhausting the rI-Closure

A **poonem** (Grünbaum 1966) of $\pi_U(\mathcal{D}_n)$ is, recursively defined, either an exposed face of $\pi_U(\mathcal{D}_n)$ or an exposed face of a poonem of $\pi_U(\mathcal{D}_n)$. The notion of **access sequence** (Csiszár and Matúš 2005) is equivalent to poonem.



Poonems of $\pi_U(\mathcal{D}_n)$ correspond to projections $p_1\succeq p_2\succeq\cdots$ where p_1 is a ground projection of U, $p_2\in p_1M_np_1$ is a ground projection of p_1Up_1, etc. (W 2011); one has

$$\bigcup\mathcal{E}_p(U)=\operatorname{cl}\mathcal{E},$$

where the union extends over the projections p corresponding to poonems of $\pi_U(\mathcal{D}_n)$.

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