Information geometry:

A short introduction with some recent advances

Frank Nielsen

Sony Computer Science Laboratories Inc

Tokyo, Japan



Talk outline

- Information geometry from the pure viewpoint of geometry:
 - → Geometry of dual structures
- Dual multivariate quasi-arithmetic averages:
 - → Information geometry yielding a generalization of quasi-arithmetic means
- Chernoff information and its purely geometric counterpart:
 - → Geometry likelihood ratio exponential families
- Duo Bregman pseudo-divergences:
 - → Application to KLD between truncated densities of an exponential family

Information geometry:

A short introduction to the geometry of dual structures

Geometry defines the architecture of spaces

Information geometry (IG): Rationale and scope

- IG field originally born by investigating **geometric structures** of statistical/probability models (e.g, space of Gaussians, space of multinomials)
- Statistical models: parametric vs nonparametric models, regular vs singular (ML) models, hierarchical (ML) or simple models, ...
- Define statistical invariance, use language of geometry (e.g., ball, projection, bisector) to design algorithms in statistics, information theory, statistical machine learning, etc.
- IG study interplays of statistical/parameter divergences with geometric structures
- Relationships between many types of dualities in IG: dual connections, reference duality (dual f-divergences), Legendre duality, duality of representations/monotone embeddings, etc

Geometric science of information (GSI)

Further extend broadly the original scope of information geometry by unravelling **connections** of information geometry (IG) with **other domains of geometry** like:

- geometry of domains and cones (e.g., Siegel/Vinberg/Koszul)
- geometric mechanics for dynamic models (symplectic/contact geometry)

franknielsen.github.io/GSI

- thermodynamics/thermostatistics and deformed statistical models
- geometric statistics (eg, computational anatomy/medical imaging)
- shape space analysis and deformation (computer vision)
- algebraic statistics (manifolds versus algebraic surfaces/varieties)
- dynamics of learning (singularity, plateau)
- neurogeometry (neuroscience)
- etc.



GSI: Biannual conference since 2013



GSI'23 Conference FROM CLASSICAL TO QUANTUM INFORMATION GEOMETRY 6th Conference Edition Palais du Grand Large, Saint-Malo August 30th - September 1st, 2023



Eva Miranda Polytechnic University of Catalonia, Spain From Alan Turing to Contact geometry: towards a "Fluid computer"



Bernd STURMFELS MPI-MiS Leipzig Germany Algebraic Statistics and Gibbs Manifolds



<u>S</u> see

Diarra FALL Institut Denis Poisson, Université d'Orléans & Université de Tours, France Statistics Methods for Medical Image Processing and Reconstruction



Hervé SABOURIN Poitiers University, France Transverse Poisson Structures to adjoint orbits in a complex semi-simple Lie algebra



Nanyang Technological University, Singapore Learning of Dynamic Processes

Random ordering of keynote speakers

https://conference-gsi.org/

Include 500+ GSI video talks: <u>franknielsen.github.io/GSI/</u>

https://gsi2023.org

https://franknielsen.github.io/GSI/



Inria, Ecole Normale Supérieure, France Information Theory with Kernel Methods Information geometry: Geometry of dual structures

Build your own information geometry in three steps Choose

(1) manifold M

Examples: Gaussians SPD cone Probability simplex



Concepts: local coordinates locally Euclidean

② metric tensor g



Examples: Fisher information metric metric g^D from divergence trace metric

Concepts:

vector length vector orthogonality Riemannian geodesic Riemannian distance Levi-Civita connection ∇^g

Examples:

(M,g,
abla

exponential connection mixture connection metric connection ∇^{g} divergence connection ∇^{D} α -connection

(3) affine connection ∇

Concepts:

covariant derivative ∇
∇-geodesic
∇-parallel transport
curvature

Get dual IG manifold (M,g,∇,∇^{*})



Concepts:

dual connections coupled to metric g dual parallel transport preserve metric g

From dual information geometry to $\pm \alpha$ -geometry, $\alpha \in \mathbb{R}$

Choose

- 1 manifold M
- ② metric tensor g
- (3) affine connection ∇by defining Christoffel symbols $\Gamma_{ijk}^{∇}$

(4) choose α

Examples:

Amari-Chentsov cubic tensor Cubic tensor from divergence $T_{ijk}(\theta) = E[\partial_i l \partial_j l \partial_k l]$ $T_{ijk}(\theta) = \partial_i \partial_j \partial_k F(\theta)$





Information geometry from statistical models: $(M,g^{F},\nabla^{-\alpha},\nabla^{\alpha})$

- Consider a parametric statistical/probability model: $\mathcal{P} := \{p_{\theta}(x)\}_{\theta \in \Theta}$
- Define metric tensor g from Fisher information = Fisher metric g^F

 ${}_{\mathcal{P}}I(\theta) := E_{\theta} \left[\partial_i l \partial_j l\right]_{ij} \succeq 0 \qquad \partial_i l := :\frac{\partial}{\partial \theta_i} l(\theta; x) \qquad l(\theta; x) := \log L(\theta; x) = \log p_{\theta}(x).$ covariance of the score $s_{\theta} = \nabla_{\theta} l = (\partial_i l)_i \qquad$ log-likelihood

• Model is regular if partial derivatives of $I_{\theta}(x)$ smooth and Fisher metric is well-defined and positive-definite

Fisher-Rao geometry when α=0, get geodesic distance called Rao distance

 $D_{\rho}(p,q) := \int_{0}^{1} \|\gamma'(t)\|_{\gamma(t)} dt = \int_{0}^{1} \sqrt{g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t))} dt$

[Hotelling 1930] [Rao 1945] [Amari Nagaoka 1982]

Rao distance on the Fisher-Rao manifold

In practice:

- Need to calculated geodesics which are curves locally minimizing the length linking two endpoints (equivalently minimize the energy of squared length elements)
- Finding Fisher-Rao geodesics is a non-trivial tasks.
- Good news 2023: closed-form geodesics with boundary conditions for MultiVariate Normals

Fisher-Rao and pullback Hilbert cone distances on the multivariate Gaussian manifold with applications to simplification and quantization of mixtures, ICML ws TAGML 2023

Information geometry from divergences: (M,g^D, ∇^{D} , ∇^{D})

• A statistical divergence like the Kullback-Leibler divergence is a smooth nonmetric distance between probability measures

$$\mathrm{KL}[p:q] = \int p(x) \log \frac{p(x)}{q(x)} \mathrm{d}\mu(x)$$

A statistical divergence between two densities of a statistical model is a **parametric divergence** (e.g., KLD between two normal distributions)

$$D_{\mathrm{KL}}^{\mathcal{P}}(\theta_1:\theta_2) := D_{\mathrm{KL}}[p_{\theta_1}:p_{\theta_2}]$$

[Eguchi 1983]

Construction of dual geometry from asymmetric parametric divergence $D(\theta_1:\theta_2)$

Dual divergence is $D^*(\theta_1:\theta_2)=D(\theta_2:\theta_1)$, reverse divergence

Dual structure:

 D^*

$$\begin{array}{rcl} {}^{D}g & := & -\partial_{i,j}D(\theta:\theta')|_{\theta=\theta'} = {}^{D^{*}}g, \\ {}^{D}\Gamma_{ijk} & := & -\partial_{ij,k}D(\theta:\theta')|_{\theta=\theta'}, \\ {}^{D^{*}}\Gamma_{ijk} & := & -\partial_{k,ij}D(\theta:\theta')|_{\theta=\theta'}. \end{array}$$

$$\begin{array}{rcl} Cubic tensor: \\ {}^{D}C_{ijk} = {}^{D^{*}}\Gamma_{ijk} - {}^{D}\Gamma_{ijk} \\ {}^{D}C_{ijk} = {}^{D^{*}}\Gamma_{ijk} - {}^{D}\Gamma_{ijk} \\ {}^{\partial_{i,jk}f(x,y) = \frac{\partial}{\partial x^{i}}\frac{\partial^{2}}{\partial y^{j}\partial y^{k}}f(x,y)} \\ {}^{\partial_{i,jk}f(x,y) = \frac{\partial}{\partial x^{i}}f(x,y) \\ {}^{\partial_{i,jk}f(x,y) = \frac{\partial}{\partial x^{i}}f(x,y) = \frac{\partial}{\partial y^{j}}f(x,y), \\ {}^{\partial_{i,jk}f(x,y) = \frac{\partial^{2}}{\partial x^{i}\partial x^{j}}\frac{\partial}{\partial y^{k}}f(x,y)} \end{array}$$

Realizations of dual information geometry (stat mfd)

• Realize (M,g,∇,∇) as a divergence information geometry $(M,g^{D},\nabla^{D},\nabla^{D^{*}})$: always exists a divergence D such that $(M,g,\nabla,\nabla)=(M,g^{D},\nabla^{D},\nabla^{D^{*}})$

Matumoto, "Any statistical manifold has a contrast function—On the C3-functions taking the minimum at the <u>diagonal of the product manifold</u>." *Hiroshima Math. J* 23.2 (1993)

• Realize (M,g,∇,∇) as a model information geometry $(M,g^{F},\nabla^{-\alpha},\nabla^{\alpha})$ always exists a statistical model M such that $(M,g,\nabla,\nabla)=(M,_{P}g^{F},_{P}\nabla^{-\alpha},_{P}\nabla^{\alpha})$

Lê, Hông Vân. "Statistical manifolds are statistical models." *Journal of Geometry* 84 (2006): 83-93.

Equivalence: model α -IG \leftrightarrow divergence IG for f-divergences

- Let $\mathsf{P}{=}\{p_{\theta}\}$ be a statistical model of probability distributions dominated by μ
- Consider the f-divergence for a convex generator f(u) with f(1)=0, f'(1)=1, f''(1)=1 ← standard f-divergence (can always rescale g(u)=f(u)/f''(1))

$$I_f[p(x;\theta):p(x;\theta')] = \int_{\mathcal{X}} p(x;\theta) f\left(\frac{p(x;\theta')}{p(x;\theta)}\right) d\mu(x)$$

$$I_{f}^{*}[p(x;\theta):p(x;\theta')] = I_{f}[p(x;\theta'):p(x;\theta)] = I_{f^{\diamond}}[p(x;\theta):p(x;\theta')]$$

Dual reverse f-divergence is a f-divergence for $f^{\diamond}(u) := uf\left(\frac{1}{u}\right)$

• The f-divergence between $p_{\theta 1}$ and $p_{\theta 2}$ is a parameter divergence $D(\theta_1:\theta_2)$

$$D_{\mathcal{P}}(\theta_1:\theta_2) := I_f[p_{\theta_1}:p_{\theta_2}]$$

from which we can build the divergence information geometry (M,g^D, ∇^{D} , ∇^{D^*})

• Then model α -geometry for α =2 f''(1)+3 coincide with divergence IG:

 $(M,g^{D},\nabla^{D},\nabla^{D^{*}}) = (M,g^{F},\nabla^{-\alpha},\nabla^{\alpha})$ for $\alpha=2$ f'''(1)+3

metric tensor g^D and cubic tensor T^D coincides with Fisher metric g^F and Amari-Chentsov tensor T

Curvature is associated to affine connection $\boldsymbol{\nabla}$

- For Riemannian structure (M,g), use default Levi-Civita connection ∇=∇^g
- Riemannian manifolds of dim d can always be embedded into Euclidean spaces E^D of dim D=O(d²)
- Euclidean spaces have a natural affine connection $\nabla = \nabla^{E}$



Cylinder is flat, 0 curvature: Parallel transport along a loop of a vector preserves the orientation



© CNRS

Sphere has positive constant curvature: Parallel transport along a loop exhibits an angle defect related to curvature

Dually flat spaces (M,g, ∇ , ∇^*)

- Fundamental theorem of information geometry: If torsion-free affine connection ∇ is of constant curvature κ , then curvature of dual torsion-free affine connection ∇^* is also constant κ
- <u>Corollary</u>: if ∇ is flat (κ =0) then ∇^* is flat: **Dually flat space (M,g,\nabla, \nabla^*)**
- A connection ∇ is flat if there exists a local coordinate system θ such that $\Gamma(\theta)=0$
- In ∇ -affine coordinate system $\theta(.)$, ∇ -geodesics are visualized as line segments

$$\Gamma(\theta) = 0$$

$$\frac{d^2\theta_k}{dt^2} + \sum_{i=1}^p \sum_{j=1}^p \Gamma_{ij}^k \frac{d\theta_i}{dt} \frac{d\theta_j}{dt} = 0, \quad k = 1, \dots, p,$$

geodesics=line segments in θ

Canonical divergences of DFSs: Bregman divergences

- Dually flat structure (M,g,∇,∇^*) can be realized by a Bregman divergence $(M,g,\nabla,\nabla^*) \leftarrow (M,g^{B_F},\nabla^{B_F},\nabla^{B_F^*})$
- Let $F(\theta)$ be a strictly convex and differentiable function defined on an open convex domain Θ
- Bregman divergence interpreted as the vertical gap between point (θ_1 , F(θ_1)) and the linear approximation of F(θ) at θ_2 evaluated at θ_1 :



$$B_F(\theta_1:\theta_2) = F(\theta_1) - \underbrace{\left(F(\theta_2) + (\theta_2 - \theta_1)^\top \nabla F(\theta_2)\right)}_{L_{F,\theta_2}(\theta_1)}$$
$$= F(\theta_1) - F(\theta_2) - (\theta_1 - \theta_2)^\top \nabla F(\theta_2)$$

[Bregman 1967]

Legendre-Fenchel transformation: Slope transformation

 Consider a Bregman generator of Legendre-type (proper, lower semicontinuous). Then its convex conjugate obtained from the Legendre-Fenchel transformation is a Bregman generator of Legendre type.



- Analogy of the Halfspace/Vertex representation of the epigraph of F
- Fenchel-Moreau's biconjugation theorem for F of Legendre-type: $F = (F^*)^*$

[Touchette 2005] Legendre-Fenchel transforms in a nutshell [2010] Legendre transformation and information geometry

Mixed coordinates and the Legendre-Fenchel divergence

- Dual <u>Legendre-type</u> functions
- Convex conjugate of F is
- Fenchel-Young inequality :

$$\theta = \nabla F^*(\eta) \qquad \qquad \eta = \nabla F(\theta)$$
$$F^*(\eta) = \eta^\top \nabla F^*(\eta) - F(\nabla F^*(\eta))$$

$$F(\theta_1) + F^*(\eta_2) \ge \theta_1^\top \eta_2$$

 $abla F^* = (
abla F)^{-1}$ Gradient
are inverse
of each other

with equality holding if and only if $\eta_2 = \nabla F(\theta_1)$

• Fenchel-Young divergence make use of the mixed coordinate systems θ et η to express a Bregman divergence as $B_F(\theta_1 : \theta_2) = Y_{F,F^*}(\theta_1 : \eta_2)$

$$Y_{F,F^*}(\theta_1:\eta_2) := F(\theta_1) + F^*(\eta_2) - \theta_1^\top \eta_2 = Y_{F^*,F}(\eta_2,\theta_1)$$

Generalized Pythagoras theorem in dually flat spaces In general, **Identity of Bregman divergence with three parameters** = law of cosines $B_F(\theta_1:\theta_2) = B_F(\theta_1:\theta_3) + B_F(\theta_3:\theta_2) - (\theta_1 - \theta_3)^\top (\nabla F(\theta_2) - \nabla F(\theta_3)) \ge 0$ Generalized Pythagoras' theorem Pythagoras' theorem in the Euclidian geometry orthogonality condition: (Self-dual) $(\eta(p) - \eta(q))^{\top}(\theta(r) - \theta(q)) = 0$ $F_{\text{Eucl}}(\theta) = \frac{1}{2} \theta^{\top} \theta$ $g_{F_{\text{Euc}}} = I$ $\gamma_{pq}(t)$ $B_{F_{\text{Eucl}}}(\theta_1:\theta_2) = \frac{1}{2}\rho_{\text{Eucl}}^2(\theta_1,\theta_2)$ b $\gamma_{pq} \perp_q \gamma_{qr}^*$ а $\gamma_{ar}^{*}(t')$ $a^2 + b^2 = c^2$ $D_F(\gamma_{pq}(t):\gamma_{qr}(t')) = D_F(\gamma_{pq}(t):q) + D_F(q:\gamma_{qr}^*(t')), \quad \forall t, t' \in (0,1).$

 $||P - Q||^2 + ||Q - R||^2 = ||P - R||^2$

Triples of points (p,q,r) with dual Pythagorean^{*} theorems holding simultaneously at q

$$\gamma_{pq} \perp_q \gamma_{qr}^* \qquad (\theta(p) - \theta(q))^\top (\eta(r) - \eta(q)) = 0 \qquad D_F(p:q) + D_F(q:r) = D_F(p:r)$$

$$\gamma_{pq}^* \perp_q \gamma_{qr} \qquad (\eta(p) - \eta(q))^\top (\theta(r) - \theta(q)) = 0 \qquad D_F(r:q) + D_F(q:p) = D_F(r:p)$$



Two blue-red geodesic pairs orthogonal at q <u>https://arxiv.org/abs/1910.03935</u>

Dually flat space from a smooth strictly convex function $F(\theta)$

• A smooth strictly convex function $F(\theta)$ define a Bregman divergence and hence a dually flat space via Eguchi's divergence-based IG

$$(\Theta, F(\theta)) \longrightarrow (M, g^{B_F}, \nabla^{B_F}, \nabla^{B_F^*}) = (M, g^F, \nabla^F, \nabla^{F^*})$$

Domain

dual Bregman divergences

 $(\nabla^F)^* = \nabla^{(F^*)}$

• Examples of DFSs induced by convex functions:





dual contrast functions

dual potential functions

dual f-representations (±α-representations) Quasi-arithmetic centers, quasi-arithmetic mixtures, and the Jensen-Shannon ∇-divergences



Outline and contributions

<u>Goals</u>:

- I. Generalize scalar quasi-arithmetic means to multivariate cases
- II. Show that the dually flat spaces of information geometry yields a natural framework for defining and studying this generalization

Weighted quasi-arithmetic means (QAMs)

Standard (n-1)-dimensional simplex: $\Delta_{n-1} = \{(w_1, \ldots, w_n) : w_i \ge 0, \sum_i w_i = 1\}$

Definition (Weighted quasi-arithmetic mean (1930's)). Let $f : I \subset \mathbb{R} \to \mathbb{R}$ be a strictly monotone and differentiable real-valued function. The weighted quasi-arithmetic mean (QAM) $M_f(x_1, \ldots, x_n; w)$ between n scalars $x_1, \ldots, x_n \in I \subset \mathbb{R}$ with respect to a normalized weight vector $w \in \Delta_{n-1}$, is defined by

$$M_f(x_1, \dots, x_n; w) := f^{-1}\left(\sum_{i=1}^n w_i f(x_i)\right).$$

QAMs enjoy the in-betweenness property:

$$\min\{x_1,\ldots,x_n\} \le M_f(x_1,\ldots,x_n;w) \le \max\{x_1,\ldots,x_n\}$$

[Kolmogorov 1930] [Nagumo 1930] [De Finetti 1931]

Quasi-arithmetic means (QAMs)

• **Classes of generators** [f]=[g] with $f \equiv g$ yieldings the same QAM:

$$M_g(x,y) = M_f(x,y)$$
 if and only if $g(t) = \lambda f(t) + c$ for $\lambda \in \mathbb{R} \setminus \{0\}$

- So let us fix wlog. strictly increasing and differentiable f since we can always either consider either f or -f (i.e., λ =-1, c=0).
- QAMs include **p-power means** for the smooth family of generators $f_p(t)$:

$$M_p(x,y) := M_{f_p}(x,y) \qquad f_p(t) = \begin{cases} \frac{t^p - 1}{p}, \ p \in \mathbb{R} \setminus \{0\}, \\ \log(t), \ p = 0. \end{cases}, \quad f_p^{-1}(t) = \begin{cases} (1+tp)^{\frac{1}{p}}, \ p \in \mathbb{R} \setminus \{0\}, \\ \exp(t), \ p = 0. \end{cases}$$

- Pythagoras means: Harmonic (p=-1), Geometric (p=0), Arithmetic (p=1)
- Homogeneous QAMs $M_f(\lambda x, \lambda y) = \lambda M_f(x, y)$ for all $\lambda > 0$ are exactly p-power means

Quasi-Arithmetic Centers (QACs) = Multivariate QAMs: Univariate QAMs: $M_f(x_1, ..., x_n; w) := f^{-1}\left(\sum_{i=1}^n w_i f(x_i)\right)$

Two problems we face when going from univariate to multivariate cases:

- 1. Define the proper notion of *"multivariate increasing"* function F and its equivalent class of functions
- 2. In general, the implicit function theorem only proves locally and inverse function F^{-1} of F: $R^d \rightarrow R^d$ provided its Jacobian matrix is not singular

Information geometry provides the right framework to generalize QAMs to quasi-arithmetic centers (QACs) and study their properties. Consider the dually flat spaces of information geometry

Legendre-type functions

 $Γ_0(E)$: Cone of lower semi-continuous (lsc) convex functions from E into $\mathbb{R} \cup \{+\infty\}$ Legendre-Fenchel transformation of a convex function: $F^*(\eta) := \sup_{\theta \in \Theta} \{\theta^\top \eta - F(\theta)\}$ Problem: Domain H of η may not be convex... $F^* \in Γ_0(E)$ $F^{**} = F$

Counterexample with $h(\xi_1, \xi_2) = [(\xi_1^2/\xi_2) + \xi_1^2 + \xi_2^2]/4$ [Rockafeller 1967] To by pass this problem:

Definition Legendre type function . (Θ, F) is of Legendre type if the function $F: \Theta \subset \mathbb{X} \to \mathbb{R}$ is strictly convex and differentiable with $\Theta \neq \emptyset$ an open convex set and

$$\lim_{\lambda \to 0} \frac{d}{d\lambda} F(\lambda \theta + (1 - \lambda)\bar{\theta}) = -\infty, \quad \forall \theta \in \Theta, \forall \bar{\theta} \in \partial \Theta.$$
(1)

Convex conjugate of a Legendre-type function (Θ , F(θ)) is of Legendre-type:

Given by the Legendre function: $F^*(\eta) = \langle \nabla F^{-1}(\eta), \eta \rangle - F(\nabla F^{-1}(\eta))$ Gradient map ∇F is globally invertible: $\nabla F^{-1}(\eta)$

Comonotone functions in inner product spaces

• Comonotone functions: $\forall \theta_1, \theta_2 \in \mathbb{X}, \theta_1 \neq \theta_2, \quad \langle \theta_1 - \theta_2, G(\theta_1) - G(\theta_2) \rangle > 0$

(i.e., **co**monotone = monotone with respect to the **identity function**)

Proposition (Gradient co-monotonicity). The gradient functions $\nabla F(\theta)$ and $\nabla F^*(\eta)$ of the Legendre-type convex conjugates F and F^* in \mathcal{F} are strictly increasing co-monotone functions.

Proof using symmetrization of Bregman divergences = Jeffreys-Bregman divergence:

 $B_{F}(\theta_{1}:\theta_{2}) + B_{F}(\theta_{2}:\theta_{1}) = \langle \theta_{2} - \theta_{1}, \nabla F(\theta_{2}) - \nabla F(\theta_{1}) \rangle > 0, \quad \forall \theta_{1} \neq \theta_{2}$ $B_{F^{*}}(\eta_{1}:\eta_{2}) + B_{F^{*}}(\eta_{2}:\eta_{1}) = \langle \eta_{2} - \eta_{1}, \nabla F^{*}(\eta_{2}) - \nabla F^{*}(\eta_{1}) \rangle > 0, \quad \forall \eta_{1} \neq \eta_{2}$

because Bregman divergences (and sums thereof) are always non-negative

 $B_F(\theta_1:\theta_2) = F(\theta_1) - F(\theta_2) - \langle \theta_1 - \theta_2, \nabla F(\theta_2) \rangle \ge 0,$

 $B_{F^*}(\eta_1:\eta_2) = F^*(\eta_1) - F^*(\eta_2) - \langle \eta_1 - \eta_2, \nabla F^*(\eta_2) \rangle \ge 0$

Remark: Generalization of monotonicity because when d=1, f(x) is strictly monotone iff $f(x_1)-f(x_2)$ is of same sign of x_1-x_2 that is, $(f(x_1)-f(x_2))(x_1-x_2)>0$

Quasi-arithmetic centers: Definition generalizing QAMs

Definition (Quasi-arithmetic centers, QACs)). Let $F : \Theta \to \mathbb{R}$ be a strictly convex and smooth real-valued function of Legendre-type in \mathcal{F} . The weighted quasi-arithmetic average of $\theta_1, \ldots, \theta_n$ and $w \in \Delta_{n-1}$ is defined by the gradient map ∇F as follows:

$$M_{\nabla F}(\theta_1, \dots, \theta_n; w) := \nabla F^{-1} \left(\sum_i w_i \nabla F(\theta_i) \right),$$
$$= \nabla F^* \left(\sum_i w_i \nabla F(\theta_i) \right),$$

where $\nabla F^* = (\nabla F)^{-1}$ is the gradient map of the Legendre transform F^* of F.

This definition generalizes univariate quasi-arithmetic means : $M_f(x_1, \ldots, x_n; w) := f^{-1}\left(\sum_{i=1}^n w_i f(x_i)\right)$

Let
$$F(t) = \int_a^t f(u) du$$

Then we have $M_f = M_{F'}$

An illustrating example: The matrix harmonic mean

- Consider the real-value minus logdet function $F(\theta) = -\log \det(\theta)$
- Domain F: $Sym_{++}(d) \rightarrow \mathbb{R}$ the cone of symmetric positive-definite matrices
- Inner product: $\langle A, B \rangle := \operatorname{tr}(AB^{\top})$

• We have: $F(\theta) = -\log \det(\theta),$ \leftarrow Legendre-type function $\nabla F(\theta) = -\theta^{-1} =: \eta(\theta),$ $\nabla F^{-1}(\eta) = -\eta^{-1} =: \theta(\eta)$ $F^*(\eta) = \langle \theta(\eta), \eta \rangle - F(\theta(\eta)) = -d - \log \det(-\eta)$ \leftarrow Legendre-type function

The quasi-arithmetic center with respect to F: $M_{\nabla F}(\theta_1, \theta_2) = 2(\theta_1^{-1} + \theta_2^{-1})^{-1}$ The quasi-arithmetic center with respect to F*: $M_{\nabla F^*}(\eta_1, \eta_2) = 2(\eta_1^{-1} + \eta_2^{-1})^{-1}$ Generalize univariate harmonic mean with F(x)= log x, f(x)=F'(x)=1/x: $H(a,b) = \frac{2ab}{a+b}$ for a, b > 0A Legendre-type function F gives rise to a pair of dual quasi-arithmetic centers $M_{\nabla F}$ and $M_{\nabla F^*}$: dual operators

Dually flat structures of information geometry

- A Legendre-type Bregman generator F() induces a dually flat space structure: $(\Theta, g(\theta) = \nabla_{\theta}^{2} F(\theta), \nabla, \nabla^{*})$
- A point P can be either parameterized by θ -coordinate and dual η -coordinate



IAMS 20221

Quasi-arithmetic barycenters and dual geodesics

• The **dual geodesics** induced by the dual flat connections can be expressed using **dual weighted quasi-arithmetic centers**:



n-Variable Quasi-arithmetic centers as centroids in dually flat spaces

Consider *n* points P_1, \ldots, P_n on the DFS (M, g, ∇, ∇^*) (canonical divergence = Bregman divergence)

Reterenc

duality

Right-sided centroid:

$$\bar{C}_R = \arg\min_{P \in M} \sum_{i=1}^n \frac{1}{n} D_{\nabla,\nabla^*}(P_i : P)$$
$$\bar{\theta}_R = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^n B_F(\theta_i : \theta)$$

$$\bar{\theta}_R = \theta(\bar{C}_R) = \frac{1}{n} \sum_{i=1}^n \theta_i = M_{id}(\theta_1, \dots, \theta_n)$$

 $\bar{\eta}_R = \nabla F(\bar{\theta}_R) = M_{\nabla F^*}(\eta_1, \dots, \eta_n).$ $\leftarrow \text{dual QAC}$



Left-sided centroid:

$$\bar{C}_L = \arg \min_{P \in M} \sum_{i=1}^n \frac{1}{n} D_{\nabla, \nabla^*}(P : P_i)$$

$$\bar{\theta}_L = \arg \min_{\theta} \frac{1}{n} \sum_{i=1}^n B_F(\theta : \theta_i)$$

$$\bar{\theta}_L = M_{\nabla F}(\theta_1, \dots, \theta_n), \quad \leftarrow \text{primal QAC}$$

$$\bar{\eta}_L = \nabla F(\bar{\theta}_L) = M_{\text{id}}(\eta_1, \dots, \eta_n)$$

Notice that when n=2, weighted dual quasi-arithmetic barycenters define the dual geodesics

Invariance/equivariance of quasi-arithmetic centers

Information geometry is well-suited to study the properties of QACs: A dually flat space (DFS) can be realized by a class of Bregman generators:

 $(M, q, \nabla, \nabla^*) \leftarrow \mathrm{DFS}([\theta, F(\theta); \eta, F^*(\eta)])$

Affine Legendre invariance of dually flat spaces:

• By adding an affine term...

Same DFS with $\overline{F}(\theta) = F(\theta) + \langle c, \theta \rangle + d$.

Invariance of quasi-arithmetic center: $M_{\nabla \bar{F}}(\theta_1, \dots; \theta_n; w) = M_{\nabla F}(\theta_1, \dots; \theta_n; w)$

• By an affine change of coordinate...

Same DFS with $\theta = A\theta + b$ such that $\overline{F}(\overline{\theta}) = F(\theta)$ Equivariance of quasi-arithmetic center: $\nabla \bar{F}(x) = (A^{-1})^{\top} \nabla F(A^{-1}(x-b)) \longrightarrow M_{\nabla \bar{F}}(\bar{\theta}_1, \dots, \bar{\theta}_n; w) = A M_{\nabla F}(\theta_1, \dots, \theta_n; w) + b$ Same canonical divergence of the DFS $B_{\bar{F}(\overline{\theta_1}:\overline{\theta_2})} = B_F(\theta_1:\theta_2)$ (= constrast function on the diagonal of the product manifold)

Canonical divergence versus Legendre-Fenchel/Bregman divergences

- Canonical divergence induced by dual flat connections is between points
- dual Bregman divergences ${\rm B}_{\rm F}$ and ${\rm B}_{\rm F^*}$ between dual coordinates
- Legendre-Fenchel divergence Y_F between mixed coordinates

 $F(\theta) + F^*(\eta) - \langle \theta, \eta \rangle = 0$ $\eta = \nabla F(\theta)$

$$B_F(\theta_1:\theta_2) := F(\theta_1) - \underbrace{F(\theta_2)}_{=\langle \theta_2, \eta_2 \rangle - F^*(\eta_2)} - \langle \theta_1 - \theta_2, \nabla F(\eta_2) \rangle$$
$$= F(\theta_1) + F^*(\eta_2) - \langle \theta_1, \eta_2 \rangle =: Y_F(\theta_1:\eta_2)$$

 $\begin{array}{rcl} (M,g,\nabla,\nabla^*) & \leftarrow & \mathrm{DFS}([\Theta,F(\theta),H,F^*(\eta)]) \\ & \leftarrow & \mathrm{DFS}([\bar{\Theta},\bar{F}(\bar{\theta}),\bar{H},\bar{F}^*(\bar{\eta})]) \end{array}$

 $D_{\nabla,\nabla^*}(P_1:P_2) = B_F(\theta_1:\theta_2) = B_{F^*}(\eta_1,\eta_2) = Y_F(\theta_1:\eta_2) = Y_{F^*}(\eta_2:\theta_1)$ $= B_{\bar{F}}(\overline{\theta_1}:\overline{\theta_2}) = B_{\bar{F}^*}(\overline{\eta_1},\overline{\eta_2}) = Y_F(\overline{\theta_1}:\overline{\eta_2}) = Y_{F^*}(\overline{\eta_2}:\overline{\theta_1})$

Affine Legendre invariance of dually flat spaces plus setting the unit scale of divergences

• Affine Legendre invariance: $\bar{F}(\bar{\theta}) = F(A\theta + b) + \langle c, \theta \rangle + d$

$$F(\theta) = F(A\theta + b) + \langle c, \theta \rangle + d$$

$$\bar{F}^*(\bar{\eta}) = F^*(A^*\eta + b^*) + \langle c^*, \eta \rangle + d^*$$

• Set the unit scale of canonical divergence (DFS differ here, rescaled): (does not change the quasi-arithmetic center) $D_{\lambda, \nabla, \nabla^*} := \lambda D_{\nabla, \nabla^*}$

amount to scale the potential function $\lambda F(\theta)$ vs $F(\theta)$

Proposition (Invariance and equivariance of QACs). Let $F(\theta)$ be a function of Legendre type. Then $\overline{F}(\overline{\theta}) := \lambda(F(A\theta+b) + \langle c, \theta \rangle + d)$ for $A \in GL(d)$, $b, c \in \mathbb{R}^d$, $d \in \mathbb{R}^d$ and $\lambda \in \mathbb{R}_{>0}$ is a Legendre-type function, and we have

$$M_{\nabla \bar{F}} = A M_{\nabla F} + b.$$

Illustrating example: Mahalanobis divergence

Mahalanobis divergence = squared Mahalanobis metric distance

$$\Delta^2(\theta_1, \theta_2) = B_{F_Q}(\theta_1 : \theta_2) = \frac{1}{2}(\theta_2 - \theta_1)^\top Q(\theta_2 - \theta_1)$$

fails triangle inequality of metric distances

Primal potential function: $F_O(\theta)$

 $F^*(\eta)$ Dual potential function:

$$(\theta) = \frac{1}{2}\theta^{\dagger}Q\theta + c\theta + \kappa$$
$$) = \frac{1}{2}\eta^{\top}Q^{-1}\eta = F_{Q^{-1}}(\eta),$$

 The dual QACs induced by the dual Mahalanobis generators F and F* coincide to weighted arithmetic mean M_{id}:

$$M_{\nabla F_Q}(\theta_1, \dots, \theta_n; w) = Q^{-1} \left(\sum_{i=1}^n w_i Q \theta_i \right) = \sum_{i=1}^n w_i \theta_i = M_{\mathrm{id}}(\theta_1, \dots, \theta_n; w),$$
$$M_{\nabla F_Q^*}(\eta_1, \dots, \eta_n; w) = Q \left(\sum_{i=1}^n w_i Q^{-1} \eta_i \right) = M_{\mathrm{id}}(\eta_1, \dots, \eta_n; w).$$

Quasi-arithmetic mixtures (QAMixs), and α -mixtures

Definition . The M_f -mixture of n densities p_1, \ldots, p_n weighted by $w \in \Delta_n^\circ$ is defined by

$$(p_1, \dots, p_n; w)^{M_f}(x) := \frac{M_f(p_1(x), \dots, p_n(x); w)}{\int M_f(p_1(x), \dots, p_n(x); w) d\mu(x)}.$$

Centroid of n densities with respect to the α -divergences yields a QAMix:

$$(p_1,\ldots,p_n;w)^{M_{\alpha}} = \arg\min_p \sum_i w_i D_{\alpha}(p_i,p)_i$$

 $D_{m}[m(s) \cdot l(s)]$

 D_{α} denotes the α -divergences:

$$= \begin{cases} \int m(s)ds - \int l(s)ds + \int m(s)\log\frac{m(s)}{l(s)}ds & \alpha = \\ \int l(s)ds - \int m(s)ds + \int l(s)\log\frac{l(s)}{m(s)}ds + \int l(s)\log\frac{l(s)}{m(s)}ds & \alpha = \\ \frac{2}{1+\alpha}\int m(s)ds + \frac{2}{1-\alpha}\int l(s)ds - \frac{4}{1-\alpha^2}\int m(s)^{\frac{1-\alpha}{2}}l(s)^{\frac{1+\alpha}{2}}ds, \quad \alpha \neq \alpha \end{cases}$$

[arXiv:2209.07481]

 $\pm 1.$

-1

α-families of probability distributions [Amari 2007]

k=2 QAMixs and the ∇**-Jensen-Shannon divergence** • Jensen-Shannon divergence is bounded symmetrization of KL divergence: $D_{\rm JS}(p,q) = \frac{1}{2} \left(D_{\rm KL} \left(p : \frac{p+q}{2} \right) + D_{\rm KL} \left(q : \frac{p+q}{2} \right) \right) \leq \log(2)$

- Interpret arithmetic mixture as the midpoint of a mixture geodesic (wrt to the flat non-parametric mixture connection ∇^m in information geometry).
- Generalize Jensen-Shannon divergence with arbitrary **∇-connections**:

Definition (Affine connection-based ∇ -Jensen-Shannon divergence). Let ∇ be an affine connection on the space of densities \mathcal{P} , and $\gamma_{\nabla}(p,q;t)$ the geodesic linking density $p = \gamma_{\nabla}(p,q;0)$ to density $q = \gamma_{\nabla}(p,q;1)$. Then the ∇ -Jensen-Shannon divergence is defined by:

$$D_{\nabla}^{\mathrm{JS}}(p,q) := \frac{1}{2} \left(D_{\mathrm{KL}}\left(p : \gamma_{\nabla}\left(p,q;\frac{1}{2} \right) \right) + D_{\mathrm{KL}}\left(q : \gamma_{\nabla}\left(p,q;\frac{1}{2} \right) \right) \right).$$

Inductive Means: Geodesics/quasi-arithmetic centers

- Gauss and Lagrange independently studied the following convergence of pairs of iterations:
- $a_{t+1} = \frac{a_t + b_t}{2}$ and proves quadratic convergence to $b_{t+1} = \sqrt{a_t b_t}$ the arithmetic-geometric mean AGM

 $AGM(a_0, b_0) = \frac{\pi}{4} \frac{a_0 + b_0}{K\left(\frac{a_0 - b_0}{a_0 + b_0}\right)}$

where K is complete elliptic integral of the first kind AGM also used to approximate ellipse perimeter and π

- In general, choosing two strict means M and M' with interness property will converge but difficult to *analytically express the common limits of iterations*
- When M=Arithmetic and M'=Harmonic, the arithmetic-harmonic mean AHM yields the geometric mean:

$$a_{t+1} = A(a_t, h_t)$$
$$h_{t+1} = H(a_t, h_t)$$

$$AHM(x, y) = \lim_{t \to \infty} a_t = \lim_{t \to \infty} h_t = \sqrt{xy} = G(x, y)$$

Inductive matrix arithmetic-harmonic mean

• Consider the cone of symmetric positive-definite matrices (SPD cone), and extend the AHM to SPD matrices:

$$\begin{aligned} A_{t+1} &= \frac{A_t + H_t}{2} = A(A_t, H_t) & \leftarrow \text{arithmetic mean} \\ H_{t+1} &= 2\left(A_t^{-1} + H_t^{-1}\right)^{-1} = H(A_t, H_t) & \leftarrow \text{harmonic mean} \end{aligned}$$

• Then the sequences converge quadratically to the matrix geometric mean:

$$AHM(X,Y) = \lim_{t \to +\infty} A_t = \lim_{t \to +\infty} H_t.$$
$$AHM(X,Y) = X^{\frac{1}{2}} \left(X^{-\frac{1}{2}} Y X^{-\frac{1}{2}} \right)^{\frac{1}{2}} X^{\frac{1}{2}} = G(X,Y)$$

which is also the **Riemannian center of mass** with respect to the trace metric:

Geometric interpretation of the AHM matrix mean

$$A_{t+1} = \frac{A_t + H_t}{2} = A(A_t, H_t) \qquad P_{t+1} = \gamma \left(P_t, Q_t : \frac{1}{2} \right)$$

$$H_{t+1} = 2 \left(A_t^{-1} + H_t^{-1} \right)^{-1} = H(A_t, H_t) \qquad Q_{t+1} = \gamma^* \left(P_t, Q_t : \frac{1}{2} \right)$$

(SPD, g^G , ∇^A , ∇^H) is a dually flat space, ∇^G is Levi-Civita connection $G_{\alpha}(P,Q) = P^{\frac{1}{2}} \left(P^{-\frac{1}{2}} Q P^{-\frac{1}{2}} \right)^{\alpha} P^{\frac{1}{2}}$



Dually flat space (SPD, g^G , ∇^A , ∇^H) in information geometry defines quasi-arithmetic centers as geodesic midpoints

1 \

 $H_{\alpha}(P,Q) = \left((1-\alpha)P^{-1} + \alpha Q^{-1}\right)^{-1}$

 $g_P^A(X,Y) = \operatorname{tr}(X^\top Y)$ Primal geodesic midpoint is the arithmetic center wrt Euclidean metric Dual geodesic midpoint = harmonic center wrt an isometric Eucl. metric $g_P^H(X, Y) = tr(P^{-2}XP^{-2}Y)$ $g_P^G(X,Y) = \operatorname{tr}(P^{-1}XP^{-1}Y)$ Levi-Civita geodesic midpoint is geometric Karcher mean (not QAC) $g_P(V_1, V_2) = \operatorname{tr} \left(P^{-1} V_1 P^{-1} V_2 \right)$ A balanced metric [Nakamura 2001, Thanwerdas & Pennec 2019]

Revisiting Chernoff information with Likelihood Ratio Exponential Families



Chernoff information: Definition & Background A symmetric statistical divergence

• Originally introduced by Chernoff (1952) to *upper bound the probability of error* (Bayes' error) in statistical hypothesis testing.

Definition:

$$D_{C}[P,Q] := \max_{\alpha \in (0,1)} -\log \rho_{\alpha}[P:Q] = D_{C}[Q,P],$$

$$p_{\alpha}[P:Q] := \int p^{\alpha} q^{1-\alpha} d\mu = \rho_{1-\alpha}[Q:P] \qquad 0 < \rho_{\alpha}[P:Q] \le 1$$
(via Hölder inequality)

Herman Chernoff (1923-)

• skewed Bhattacharyya coefficient ρ_{α} (similarity coefficient)

- Synonyms: Chernoff divergence, Chernoff information number, Chernoff index...
- Found later many applications in information fusion, radar target detection, generative adversarial networks (GANs), etc. due to its <u>empirical robustness</u>



Chernoff information = <u>Maximally skewed Bhattacharyya distance</u>

• skewed Bhattacharyya distance (a Ali-Silvey f-divergence):

$$D_{B,\alpha}[p:q] := -\log \rho_{\alpha}[P:Q] = D_{B,1-\alpha}[q:p],$$

- Chernoff information: $D_C[p,q] = \max_{\alpha \in (0,1)} D_{B,\alpha}[p:q].$
- scaled skewed Bhattacharyya distance = Rényi divergence (extends KLD)

$$D_{R,\alpha}[P:Q] = \frac{1}{\alpha - 1} \log \int p^{\alpha} q^{1-\alpha} d\mu = \frac{1}{1-\alpha} D_{B,\alpha}[P:Q] \qquad \alpha \in [0,\infty] \setminus \{1\}$$

 Optimal values of α is called ``Chernoff (error) exponent'' (due to its seminal use in statistical hypothesis testing)

Rationale for CI: Statistical hypothesis testing



Statistical mixture: m(x)=0.5*N(0,1)+0.5*N(5,2)Hypothesis task: Decides whether x emanates from p1 or p2? Classification rule: **Maximum a posteriori** (MAP) if p1(x)>p2(x) classify as p1 else classify as p2

Error at x: min(p1(x),p2(x)) Histogram intersection similarity:

$$P_e = \int \min(p_1(x), p_2(x)) \mathrm{d}x$$

Rewriting and bounding the probability of error

• Use rewriting trick min(a,b)=(a+b)/2 + |b-a|/2 for a,b>0

express the probability of error using the total variation distance:

$$P_{e} = \int \min(p_{1}(x), p_{2}(x)) dx \implies P_{e} = \frac{1}{2} \left(1 - D_{\text{TV}}[p_{1}, p_{2}] \right)$$
$$D_{\text{TV}}[p_{1}, p_{2}] = \frac{1}{2} \int (p_{1}(x) - p_{2}(x)) dx$$

• Use a **generic (weighted) mean** which necessarily falls inbetween its extrema (e.g., **geometric mean**):

$$\min(a,b) \le M(a,b) \le \max(a,b) \longrightarrow \min(a,b) \le M_{\alpha}(a,b) \le \max(a,b), \forall \alpha \in [0,1]$$
$$P_e = \int \min(p_1(x), p_2(x)) \mathrm{d}x \le \min_{\alpha \in [0,1]} \int M_{\alpha}(p_1(x), p_2(x)) \mathrm{d}x \xrightarrow{M_{\alpha}(a,b) = a^{\alpha}b^{1-\alpha}}_{\text{geometric weighted mean}} P_e \le \rho_{\alpha}(p_1, p_2)$$

"Generalized Bhattacharyya and Chernoff upper bounds on Bayes error using quasi-arithmetic means." *Pattern Recognition Letters* 42 (2014): 25-34.

Likelihood ratio exponential families (LREFs)

- Geometric mixture (Bhattacharyya /exponential arc) between two densities p, q of Lebesgue Banach space $L_1(\mu)$ $(pq)^G_{\alpha}(x) \propto p(x)^{\alpha}q(x)^{1-\alpha}$
- Set of **geometric mixtures**: with **normalization factor**:

$$\mathcal{E}_{pq} := \left\{ (pq)^G_{\alpha}(x) := \frac{p(x)^{\alpha}q(x)^{1-\alpha}}{Z_{pq}(\alpha)} : \alpha \in \Theta \right\}$$
$$Z_{pq}(\alpha) = \int_{\mathcal{X}} p(x)^{\alpha}q(x)^{1-\alpha} \mathrm{d}\mu(x) = \rho_{\alpha}[p:q]$$

geometric mixture interpreted as a <u>1D exponential family</u>: LREF

$$pq)_{\alpha}^{G}(x) = \exp\left(\alpha \log \frac{p(x)}{q(x)} - \log Z_{pq}(\alpha)\right) q(x),$$

$$\stackrel{*}{=:} \exp\left(\alpha t(x) - F_{pq}(\alpha) + k(x)\right).$$

$$\Theta := \{\alpha \in \mathbb{R} : Z_{pq}(\alpha) < \infty\}$$

LREFs: EF cumulant function is always analytic C^{ω}



Geometric mixtures and LREFs: <u>Regular EFs</u>

- Natural parameter space: $\Theta_{pq} = \{ \alpha \in \mathbb{R} : \rho_{\alpha}(p:q) < +\infty \}$ always contains (0,1) since $0 < \rho_{\alpha}[P:Q] \le 1$.
- What happens at extremities and when extrapolating (depends on support):

$$\operatorname{supp}\left((pq)_{\alpha}^{G}\right) = \begin{cases} \operatorname{supp}(p) \cap \operatorname{supp}(q), & \alpha \in \Theta_{pq} \setminus \{0, 1\} \\ \operatorname{supp}(p), & \alpha = 1 \\ \operatorname{supp}(q), & \alpha = 0. \end{cases}$$

Exponential family is said regular when the natural parameter space Θ is open (e.g., normal family, Dirichlet family, Wishart family, etc.)

Definition: regular EF
$$\Theta = \Theta^{\circ}$$

When (0,1) is strictly included in regular LREFs

Proposition (Finite sided Kullback-Leibler divergences). When the LREF \mathcal{E}_{pq} is a regular exponential family with natural parameter space $\Theta \supseteq [0,1]$, both the <u>forward Kullback-Leibler</u> divergence $D_{KL}[p:q]$ and the reverse Kullback-Leibler divergence $D_{KL}[q:p]$ are finite.

$$D_{\mathrm{KL}}[P:Q] = D_{\mathrm{KL}}[p:q] = \int_{\mathcal{X}} p \log\left(\frac{p}{q}\right) \mathrm{d}\mu.$$

• KLD between two densities of a regular EF = <u>reverse</u> Bregman divergence:

$$D_{\mathrm{KL}}[p_{\theta_1}:p_{\theta_2}] = E_{p_{\theta_1}}\left[\log\frac{p_{\theta_1}}{p_{\theta_2}}\right],$$

= $F(\theta_2) - F(\theta_1) - (\theta_1 - \theta_2)^\top E_{p_{\theta_1}}[t(x)]$ steep $\Rightarrow E_{p_{\theta_1}}[t(x)] = \nabla F(\theta_1)$
regular EF \Rightarrow steep EF

 $D_{\mathrm{KL}}[p_{\theta_1}:p_{\theta_2}] = F(\theta_2) - F(\theta_1) - (\theta_1 - \theta_2)^\top \nabla F(\theta_1) =: B_F(\theta_2:\theta_1) = (B_F)^*(\theta_1:\theta_2).$

Venn diagram: Regular & steepness of (LR)EFs

• Steepness implies duality between natural θ and moment η parameters



Proposition (Finite sided Kullback-Leibler divergences). When the LREF \mathcal{E}_{pq} is a regular exponential family with natural parameter space $\Theta \supseteq [0,1]$, both the forward Kullback-Leibler divergence $D_{KL}[p:q]$ and the reverse Kullback-Leibler divergence $D_{KL}[q:p]$ are finite. **PROOF**

Remember KLD=Bregman divergence between densities of a regular (LR)EF

$$\begin{split} D_{\mathrm{KL}}[p:q] &= (B_F)^*(\alpha_p:\alpha_q) = B_{Fpq}(\alpha_q:\alpha_p) = B_{Fpq}(0:1)\\ \text{Scalar Bregman divergence } B_{Fpq}:\Theta\times\mathrm{ri}(\Theta)\to[0,\infty)\\ B_{Fpq}(\alpha_1:\alpha_2) &= F_{pq}(\alpha_1) - F_{pq}(\alpha_2) - (\alpha_1-\alpha_2)F'_{pq}(\alpha_2).\\ F_{pq}(0) &= F_{pq}(1) = 0\\ \hline D_{\mathrm{KL}}[p:q] &= B_{Fpq}(\alpha_q:\alpha_p) = B_{Fpq}(0:1) = F'_{pq}(1) < \infty\\ \text{idem for } D_{\mathrm{KL}}[q:p] &= B_{Fpq}(\alpha_p:\alpha_q) = B_{Fpq}(1:0) = -F'_{pq}(0) < \infty \end{split}$$

Chernoff information (for densities of a LREF)

• Proposition: $D_{C}[p:q] = D_{KL}[(pq)_{\alpha^{*}}^{G}:p] = D_{KL}[(pq)_{\alpha^{*}}^{G}:q] = D_{B,\alpha^{*}}[p:q]$

PROOF

First, skew Bhattacharyya distance = skew Jensen divergence $D_{B,\alpha}[p:q] := -\log \rho_{\alpha}[P:Q]$ $D_{B,\alpha}(p_{\theta_1}:p_{\theta_2}) = J_{F,\alpha}(\theta_1:\theta_2)$ $J_{F,\alpha}(\theta_1:\theta_2) = \alpha F(\theta_1) + (1-\alpha)F(\theta_2) - F(\alpha \theta_1 + (1-\alpha)\theta_2).$ Thus we have: $D_{B,\alpha}((pq)_{\alpha_1}^G:(pq)_{\alpha_2}^G) = J_{F_{pq},\alpha}(\alpha_1:\alpha_2),$

 $= \alpha F_{pq}(\alpha_1) + (1 - \alpha) F_{pq}(\alpha_2) - F_{pq}(\alpha \alpha_1 + (1 - \alpha) \alpha_2)$

At the optimal value α^* , we have $F'_{pq}(\alpha^*) = 0$ $D_{KL}[(pq)_{\alpha^*}^G : p] = B_{F_{pq}}(1 : \alpha^*) = -F(\alpha^*)$ $D_{KL}[(pq)_{\alpha^*}^G : q] = B_{F_{pq}}(0 : \alpha^*) = -F(\alpha^*)$ $D_{C}[p:q] = -\log \rho_{\alpha^*}(p:q) = J_{F_{pq},\alpha^*}(1:0) = -F_{pq}(\alpha^*)$



$$J_F^C(\theta_1:\theta_2) := \max_{\alpha \in (0,1)} J_{F,\alpha}(\theta_1:\theta_2)$$

 $(pq)^G_{\alpha}$

Geometric interpretation for densities p, q on $L_1(\mu)$

Proposition (Geometric characterization of the Chernoff information). On the vector space $L^{1}(\mu)$, the Chernoff information distribution is the unique distribution

 $(pq)^G_{\alpha^*} = \gamma^G(p,q) \cap \operatorname{Bi}_{\operatorname{KL}}^{\operatorname{left}}(p,q).$

Left KL Voronoi bisector: $\operatorname{Bi}_{\mathrm{KL}}^{\mathrm{left}}(p,q) := \left\{ r \in L^{1}(\mu) : D_{\mathrm{KL}}[r:p] = D_{\mathrm{KL}}[r:q] \right\}$

Geodesic = exponential arc: $\gamma^G(p,q) := \left\{ (pq)^G_{\alpha} : \alpha \in [0,1] \right\}$ 2209.07481



Special case of LREF: p,q are densities of a same EF! EF includes Gaussians, Beta, Dirichlet, Wishart, etc.

$$\mathcal{E} = \left\{ P_{\lambda} : \frac{\mathrm{d}P_{\lambda}}{\mathrm{d}\mu} = p_{\lambda}(x) = \exp(\theta(\lambda)^{\top} t(x) - F(\theta(\lambda))), \quad \lambda \in \Lambda \right\}$$

$$p_{\theta_1}(x)^{\alpha} p_{\theta_2}(x)^{1-\alpha} \propto \exp(\langle \alpha \theta_1 + (1-\alpha)\theta_2, t(x) \rangle - \alpha F(\theta_1) - (1-\alpha)F(\theta_2)),$$

= $p_{\alpha \theta_1 + (1-\alpha)\theta_2}(x) \exp(F(\alpha \theta_1 + (1-\alpha)\theta_2) - \alpha F(\theta_1) - (1-\alpha)F(\theta_2)))$
= $p_{\alpha \theta_1 + (1-\alpha)\theta_2}(x) \exp(-J_{F,\alpha}(\theta_1:\theta_2)),$

 $(p_{\theta_1} p_{\theta_2})^G_{\alpha} = p_{\alpha \theta_1 + (1-\alpha)\theta_2} \qquad D_{\mathrm{KL}}[p_{\theta_1} : p_{\theta_2}] = B_F(\theta_2 : \theta_1),$ $OC_{\mathrm{EF}} : \quad B_F(\theta_1 : \theta_{\alpha^*}) = B_F(\theta_2 : \theta_{\alpha^*})$

Proposition Let p_{λ_1} and p_{λ_2} be two densities of a regular exponential family \mathcal{E} with natural parameter $\theta(\lambda)$ and log-normalizer $F(\theta)$. Then the Chernoff information is

$$D_C[p_{\lambda_1}:p_{\lambda_2}]=J_{F,\alpha^*}(\theta(\lambda_1):\theta(\lambda_2))=B_F(\theta_1:\theta_{\alpha^*})=B_F(\theta_2:\theta_{\alpha^*}),$$

where $\theta_1 = \theta(\lambda_1)$, $\theta_2 = \theta(\lambda_2)$, and the optimal skewing parameter α^* is unique and satisfies the following optimality condition:

$$OC_{EF}: \quad (\theta_2 - \theta_1)^\top \eta_{\alpha^*} = F(\theta_2) - F(\theta_1),$$



Interpreting the uniqueness of Chernoff exponent from pure information geometry point of view

 Since the Chernoff point is unique, we can also interpret more generally this property in a general dually flat space (not necessarily an EF) as known as a Bregman manifold

Proposition Let $(\mathcal{M}, g, \nabla, \nabla^*)$ be a dually flat space with corresponding canonical divergence a Bregman divergence B_F . Let $\gamma_{pq}^e(\alpha)$ and $\gamma_{pq}^m(\alpha)$ be a e-geodesic and m-geodesic passing through the points p and q of \mathcal{M} , respectively. Let $\operatorname{Bi}^m(p,q)$ and $\operatorname{Bi}^e(p,q)$ be the right-sided ∇^m -flat and left-sided ∇^e -flat Bregman bisectors, respectively. Then the intersection of $\gamma_{pq}^e(\alpha)$ with $\operatorname{Bi}^m(p,q)$ and the intersection of $\gamma_{pq}^m(\alpha)$ with $\operatorname{Bi}^e(p,q)$ are unique. The point $\gamma_{pq}^e(\alpha) \cap \operatorname{Bi}^m(p,q)$ is called the Chernoff point and the point $\gamma_{pq}^m(\alpha) \cap \operatorname{Bi}^e(p,q)$ is termed the reverse or dual Chernoff point.

> "On geodesic triangles with right angles in a dually flat space." Progress in Information Geometry. Springer, 2021. 153-190.

Duo Bregman pseudo-divergences: Applications to the KL divergence between truncated densities

Legendre transformation reverses majorization order Legendre-Fenchel transformation: $F^*(\eta) := \sup\{\eta^\top \theta - F(\theta)\}$ $\theta \in \Theta$ F Legendre-type function, Moreau **biconjugation theorem**: $(F^*)^* = F$ proper+lower semi-continuous+convex $F_2(\theta)$ $F_1(\theta)$ $\theta_1 \theta_2$ (0, 0)Legendre-Fenchel transform reverses ordering: $H_1(\eta) = \eta^{\mathsf{T}}\theta - F_1^*(\eta)$ $F_1^*(\eta)$ $\forall \theta \in \Theta, \quad F_1(\theta) \ge F_2(\theta) \Leftrightarrow \forall \eta \in H, \quad F_1^*(\eta) \le F_2^*(\eta)$ $H_2(\eta) = \eta^\top \theta - F_2^*(\eta)$ $-F_{2}^{*}(\eta)$ 1.2 **Proof:** theta^2 eta^2/4 theta^4 (3*eta^(4/3))/4^(4/3) 0.8 0.8 $F_1^*(\eta) := \sup_{\theta \in \Theta} \{\eta^\top \theta - F_1(\theta)\},$ 0.6 0.6 0.4 0.4 $= \eta^{\mathsf{T}} \theta_1 - F_1(\theta_1) \qquad (\text{with } \eta = \nabla F_1(\theta_1))$ 0.2 0.2 $\leq \eta^{\mathsf{T}} \theta_1 - F_2(\theta_1),$ 0 0.2 0.6 0.8 0.5 1.5 0.4 0 2 theta eta $\leq \sup\{\eta^{\mathsf{T}}\theta - F_2(\theta)\} =: F_2^*(\eta).$ Convex functions $F_1(\theta) \ge F_2(\theta)$ Conjugate functions $F_1^*(\eta) \leq F_2^*(\eta)$ $\theta \in \Theta$



Kullback-Leibler divergence $D_{KL}[P:Q] = \int_{\mathcal{X}} \log \frac{dP}{dQ} dP = E_P \left[\log \frac{dP}{dQ} \right]$ between exponential family densities

 $B_{F}(\theta_{1}:\theta_{2}) := F(\theta_{1}) - F(\theta_{2}) - (\theta_{1} - \theta_{2})^{\top} \nabla F(\theta_{2})$ $B_{F_{1},F_{2}}(\theta:\theta') := Y_{F_{1},F_{2}^{*}}(\theta,\eta') = F_{1}(\theta) - F_{2}(\theta') - (\theta - \theta')^{\top} \nabla F_{2}(\theta')$ $Y_{F_{1},F_{2}^{*}}(\theta,\eta') := F_{1}(\theta) + F_{2}^{*}(\eta') - \theta^{\top}\eta'.$

- Same exponential family: KLD = reverse Bregman divergence or reverse Fenchel-Young divergence $D_{\text{KL}}[P_{\theta_1}: P_{\theta_2}] = Y_{F,F^*}(\theta_2: \eta_1) = B_F(\theta_2: \theta_1) = B_{F^*}(\eta_1: \eta_2) = Y_{F^*,F}(\eta_1: \eta_2).$
- Different exponential families (mutually absolutely continuous): $D_{\text{KL}}[P_{\theta}:Q_{\theta'}] = F_{\mathcal{Q}}(\theta') - F_{\mathcal{P}}(\theta) + \theta^{\top} E_{P_{\theta}}[t_{\mathcal{P}}(x)] - {\theta'}^{\top} E_{P_{\theta}}[t_{\mathcal{Q}}(x)]$
- Same truncated exponential family: reverse duo Bregman divergence or reverse duo Fenchel-Young divergence (nested supports)

$$D_{\mathrm{KL}}[p_{\theta_1}:q_{\theta_2}] = Y_{F_2,F_1^*}(\theta_2:\eta_1) = B_{F_2,F_1}(\theta_2:\theta_1) = B_{F_1^*,F_2^*}(\eta_1:\eta_2) = Y_{F_1^*,F_2}(\eta_1:\theta_2).$$

KL divergence between truncated normal densities

PDF of truncated normal on (a,b):

$$p_{m,s}^{a,b}(x) = \frac{1}{\sqrt{2\pi}s \ (\Phi_{m,s}(b) - \Phi_{m,s}(a))} \exp\left(-\frac{(x-m)^2}{2s^2}\right)$$
$$\Phi_{m,s}(x) = \frac{1}{2}\left(1 + \operatorname{erf}\left(\frac{x-m}{\sqrt{2}s}\right)\right), \quad \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} \mathrm{d}t.$$

Truncated normal PDFs form an exponential family with log-normalizer :

$$F_{a,b}(m,s) = \frac{m^2}{2s^2} + \frac{1}{2}\log 2\pi s^2 + \log\left(\Phi_{m,s}(b) - \Phi_{m,s}(a)\right)$$

Kullback-Leibler divergence between nested truncated normal distributions:

$$D_{\mathrm{KL}}[p_{m_{1},s_{1}}^{a_{1},b_{1}}:p_{m_{2},s_{2}}^{a_{2},b_{2}}] = \frac{m_{2}}{2s_{2}^{2}} - \frac{m_{1}}{2s_{1}^{2}} + \log \frac{Z_{a_{2},b_{2}}(m_{2},s_{2})}{Z_{a_{1},b_{1}}(m_{1},s_{1})} - \left(\frac{m_{2}}{s_{2}^{2}} - \frac{m_{1}}{s_{1}^{2}}\right) \eta_{1}(m_{1},s_{1};a_{1},b_{1}) \\ - \left(\frac{1}{2s_{1}^{2}} - \frac{1}{2s_{2}^{2}}\right) \eta_{2}(m_{1},s_{1};a_{1},b_{1}) \quad \text{if nested distributions} \quad (a_{1},b_{1}) \subseteq (a_{2},b_{2}) \\ D_{\mathrm{KL}}[p_{m_{1},s_{1}}^{a_{1},b_{1}}:p_{m_{2},s_{2}}^{a_{2},b_{2}}] = +\infty, (a_{1},b_{1}) \not\subseteq (a_{2},b_{2}) \quad \text{otherwise}$$

Paper references

- "An elementary introduction to information geometry." *Entropy* 22.10 (2020): 1100.
- "Beyond scalar quasi-arithmetic means: Quasi-arithmetic averages and quasiarithmetic mixtures in information geometry." *arXiv preprint arXiv:2301.10980* (2023).
- "Revisiting Chernoff Information with Likelihood Ratio Exponential Families." *Entropy* 24.10 (2022): 1400.
- "Statistical divergences between densities of truncated exponential families with nested supports: Duo Bregman and duo Jensen divergences." *Entropy* 24.3 (2022): 421.