Sur quelques généralisations des divergences de Bregman:

Convexité et géométrie

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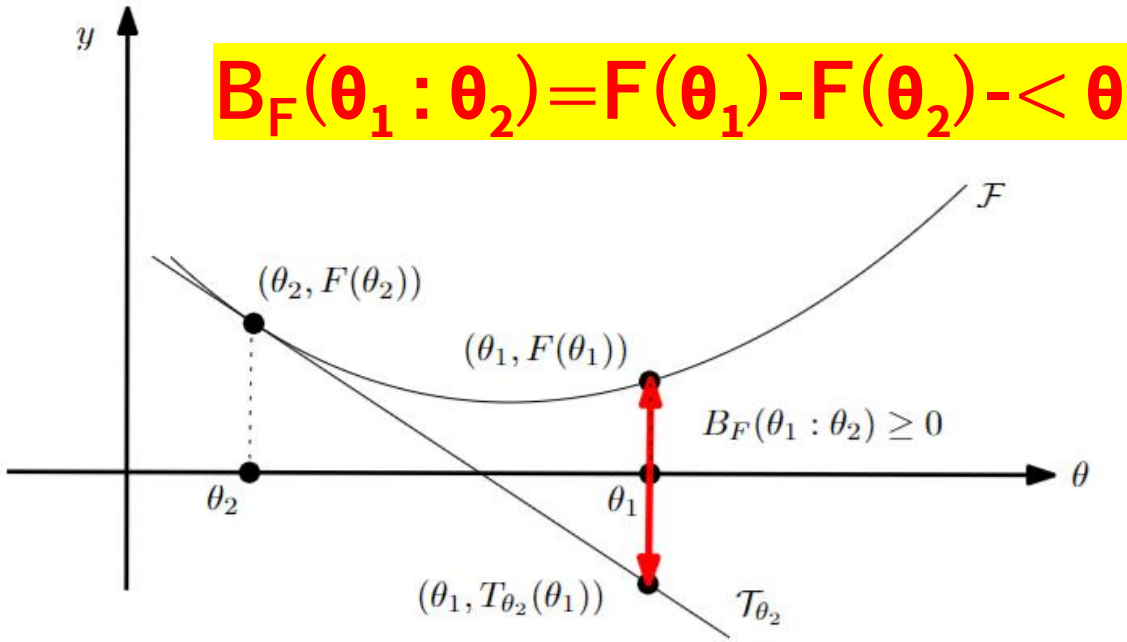
Bregman divergence (1960's)

Lev M. Bregman
(1941 - 2023)
Photo: courtesy of Alexander Fradkov

- Let $F: \Theta \subseteq \mathbb{R}^m \to \mathbb{R}$ be a strictly convex and smooth real-valued function on a Hilbert space with i. p. $<.,.>$

Bregman divergence $B_F: \Theta \times \mathrm{Int}(\Theta) \to \mathbb{R}$

$$B_F(\theta_1 : \theta_2) = F(\theta_1) - F(\theta_2) - < \theta_1 - \theta_2, \nabla F(\theta_2) >$$



BDs are popular in
- geometry,
- information theory,
- signal/sound processing

- **Unify** *squared Euclidean divergence* with *Kullback-Leibler divergence* $F_{KL}(\theta) = \Sigma_i \theta_i \log(\theta_i)$ and *Itakura-Saito divergence* $F_{IS}(\theta) = \Sigma_i -\log(\theta_i)$.
- Euclidean L22, KLD, ISD all belong to a single parametric family of **β-divergences**

Bregman divergence: Taylor remainder viewpoint

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

- BDs are non-negative because = remainder of Taylor 1st order expansion wrt θ_2:

$$F(\theta_1) = F(\theta_2) + \langle \theta_1 - \theta_2, \nabla F(\theta_2) \rangle + \mathbf{Remainder}_F(\theta_1 : \theta_2)$$

BD = exact Lagrange remainder = a *parameterized quadratic distance*:

$$\mathbf{LagrangeRemainder}_F(\theta_1 : \theta_2) = \tfrac{1}{2} (\theta_1 - \theta_2)^T \nabla^2 F(\xi) (\theta_1 - \theta_2) = \mathbf{B_F(\theta_1 : \theta_2)}$$

for some $\xi \in [\theta_1 \ \theta_2]$

- BDs are *never metrics* and
- *BDs are only symmetric for generalized quadratic distance* (proof: $\nabla^2 F$ constant)

Gen. Euclidean Divergence: $F_Q(\theta) = \frac{1}{2} \theta^T Q \theta$, Q: symmetric positive-definite matrix

Q=I, squared Euclidean distance

Bregman divergences in stats/machine learning

- **Kullback-Leibler divergence** between probability densities p(x) and q(x):

$$D_{KL}[p(x):q(x)] = \int p(x) \log (p(x)/q(x)) \, d\mu(x)$$

difficult to calculate in closed form because of the integral ∫ …

- But the Kullback-Leibler divergence between two probability densities of an **exponential family** like Gaussians, Poisson, Dirichlet, Gamma/Beta, Wishart

$$p_\lambda(x) \propto \tilde{p}_\lambda(x) = \exp(\langle \theta(\lambda), t(x) \rangle) \, h(x)$$

$p(x|\theta) \propto \exp(\langle x, \theta \rangle)$

amount to a **reverse Bregman divergence** $B_F^*(\theta_1 : \theta_2) := B_F(\theta_2 : \theta_1)$

$$D_{KL}[p(x|\theta_1) : p(x|\theta_2)] = B_F^*(\theta_1 : \theta_2) = B_F(\theta_2 : \theta_1)$$

⇒ Easy calculations

Bypass the ∫, ∇F easy!

- Notice divergence between parameters B_F vs divergence between functions KL which is a pointwise extended scalar BD

Azoury, Katy S., and Manfred K. Warmuth. "Relative loss bounds for on-line density estimation with the exponential family of distributions." ***Machine learning*** **43 (2001)**

Multivariate Bregman divergence as families of univariate Bregman divergences

- A d-variate function $F(\theta)$ can be equivalently handed as a **family** of *1D convex functions*: $\{F_{\theta_1,\theta_2}(\alpha)=F((1-\alpha)\theta_1+\alpha\theta_2)\}$

- A d-variate BD can be written as an equivalent 1D scalar BD:

Directional derivative $\nabla_{\theta_2-\theta_1} F_{\theta_1,\theta_2}(u) = (F_{\theta,\theta})'(u)$

$$\lim_{\epsilon\to 0} \frac{F(\theta_1+(\epsilon+u)(\theta_2-\theta_1))-F(\theta_1+u(\theta_2-\theta_1))}{\epsilon}$$

$$= (\theta_2-\theta_1)^\top \nabla F(\theta_1+u(\theta_2-\theta_1)).$$

Hence, write BD as equivalent scalar BDs: $B_F(\theta_1:\theta_2) := B_{F_{\theta_1,\theta_2}}(0:1)$

Gen.: write a BD wrt to anchor points as a **sub-dimensional Bregman divergence**

The chord gap divergence and a generalization of the Bhattacharyya distance." ***IEEE ICASSP, 2018***

Convex duality via Legendre-Fenchel transform

- Legendre-Fenchel transform of a convex function F aka slope transform:

$$F^*(\eta) = \sup_{\theta \in \Theta} \{ < \theta, \eta > - F(\theta) \}$$

- Consider "nice" convex functions = **Legendre-type functions** $(\Theta, F(\theta))$:

(i) Θ open, and (ii) $\lim_{\theta \to \partial\Theta} \| \nabla F(\theta) \| = \infty$

Then we get:

❶ **reciprocal gradient maps** $\eta = \nabla F(\theta)$ and $\theta = \nabla F^*(\eta)$, $\nabla F^* = (\nabla F)^{-1}$

❷ conjugation yields **dual** $(H, F^*(\eta))$ **of Legendre type**

❸ biconjugation is an **involution**: $(H, F^*(\eta))^* = (H^* = \Theta, F^{**} = F(\theta))$

- Convex conjugate: $F^*(\eta) = < \nabla F^{-1}(\eta), \eta > - F(\nabla F^{-1}(\eta))$ since $\eta = \nabla F(\theta)$

Fenchel-Young divergence: Mixed parameterization

- Young inequality: $F(\theta_1) + F^*(\eta_2) \geq < \theta_1, \eta_2 >$ with equality iff $\eta_2 = \nabla F(\theta_1)$
- Build the Fenchel-Young divergence from the inequality: lhs-rhs ≥ 0

$$\mathbf{Y_{F,F^*}(\theta_1, \eta_2) = F(\theta_1) + F^*(\eta_2) - < \theta_1, \eta_2 >} \geq 0$$

- Mixed parameterizations θ and η : $B_F(\theta_1 : \theta_2) = \mathbf{Y_{F,F^*}(\theta_1, \eta_2)}$
- $2^2=4$ equivalent expressions of Bregman divergences:

$$B_F(\theta_1 : \theta_2) = Y_{F,F^*}(\theta_1, \eta_2) = Y_{F^*,F}(\eta_2, \theta_1) = B_{F^*}(\theta_2 : \theta_1) = D_{KL}{}^*(p_{\theta 1} : p_{\theta 2})$$

Amari, Shun-ichi. *Differential-geometrical methods in statistics*. Vol. 28. Springer, 1985

Symmetrized Bregman divergences are not Bregman divergences except for generalized quadratic distances

- **Symmetrized Bregman divergence**:

$$S_F(\theta_1;\theta_2) := B_F(\theta_1 : \theta_2) + B_F(\theta_2 : \theta_1) = (\theta_2 - \theta_1)^\top (\eta_2 - \eta_1) = S_{F^*}(\eta_1;\eta_2)$$

- We may *double the dimension*, and write:

$$S_F(\theta_1,\theta_2) = B_{\hat{F}}(\theta_1^\uparrow : \theta_2^\uparrow) \qquad \xi = \begin{bmatrix} \theta \\ \eta \end{bmatrix} \quad \hat{F}(\xi) = F(\theta) + F^*(\eta) \qquad \theta^\uparrow = \begin{bmatrix} \theta \\ \nabla F(\theta) \end{bmatrix}$$

- But parameter space $\Theta^\uparrow$ is **not convex** in general! **Curved Bregman divergence**

$$\Theta^\uparrow = \left\{ \theta^\uparrow = \begin{bmatrix} \theta \\ \nabla F(\theta) \end{bmatrix} : \theta \in \Theta \right\} \subset \Xi \qquad \Xi = \left\{ \xi = \begin{bmatrix} \theta \\ \eta \end{bmatrix} : (\theta,\eta) \in \Theta \times H \right\}$$

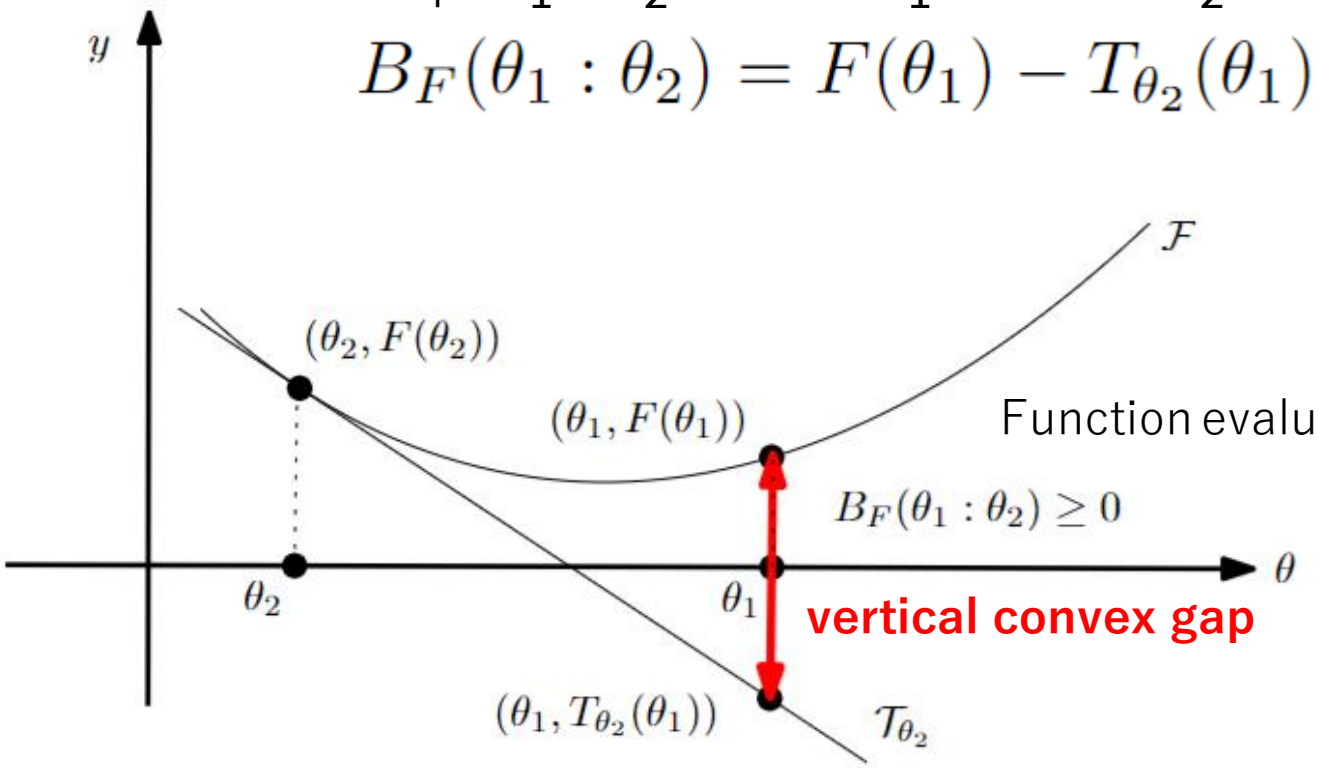
- Except for generalized quadratic distances (Mahalanobis), SBDs are not BDs. SBDs are **curved Bregman divergences.** Update B_F: θ x Int(θ) to θ x RelInt(θ)
- Bregman divergence restricted to a linear subspace is **sub-dimensional Bregman divergence** : For example, extended KLD vs KLD on simplex Δ

N+Nock., Sided and symmetrized Bregman centroids." *IEEE transactions on Information Theory* (2009)

How can we measure other convexity gaps in graphs?

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

$$B_F(\theta_1 : \theta_2) = F(\theta_1) - T_{\theta_2}(\theta_1)$$



Function evaluated at θ_1

Tangent line at θ_2 evaluated at θ_1

Bregman divergence as a **vertical convex gap**

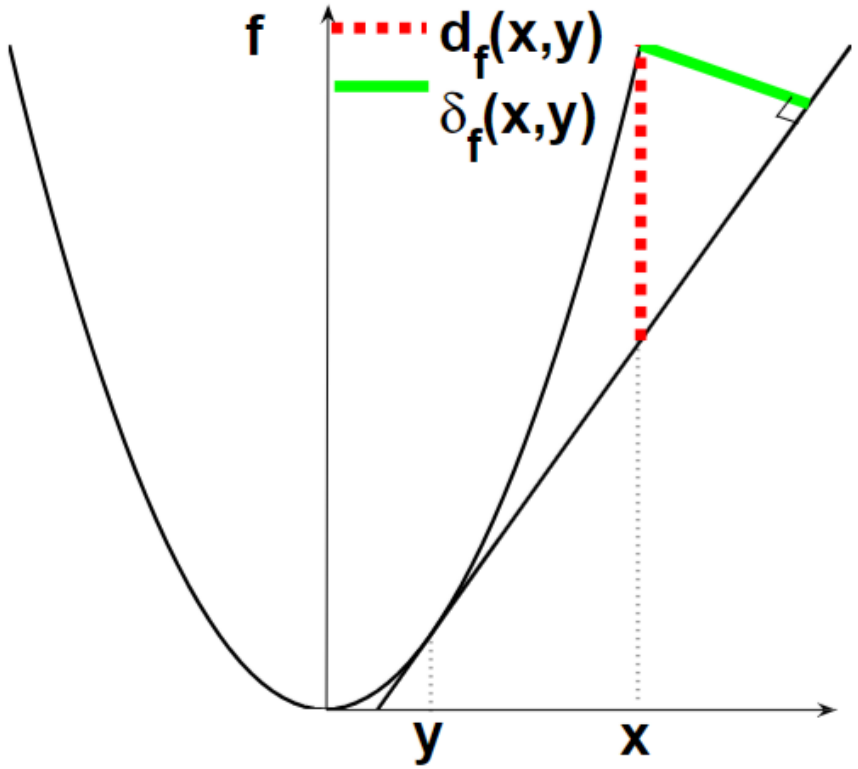
?

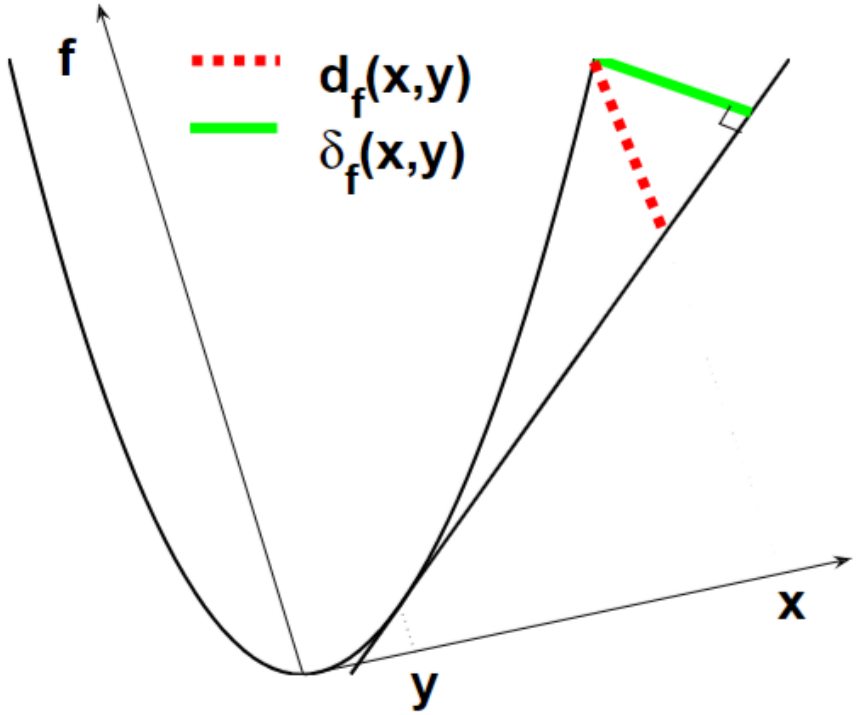
Generalize BDs by measuring other various convex gaps?

Wlog, consider univariate: $B_F(\theta_1 : \theta_2) = F(\theta_1) - F(\theta_2) - (\theta_1 - \theta_2) F'(\theta_2)$

Total Bregman divergences

$$\delta_f(x,y) = \frac{f(x) - f(y) - \langle x - y, \nabla f(y) \rangle}{\sqrt{1 + \|\nabla f(y)\|^2}}$$





"total" by analogy to total least squares vs ordinary least squares

- tBD: invariant to rotation
- tBD yields robust clustering wrt outliers
- tBD = conformal Bregman divergence

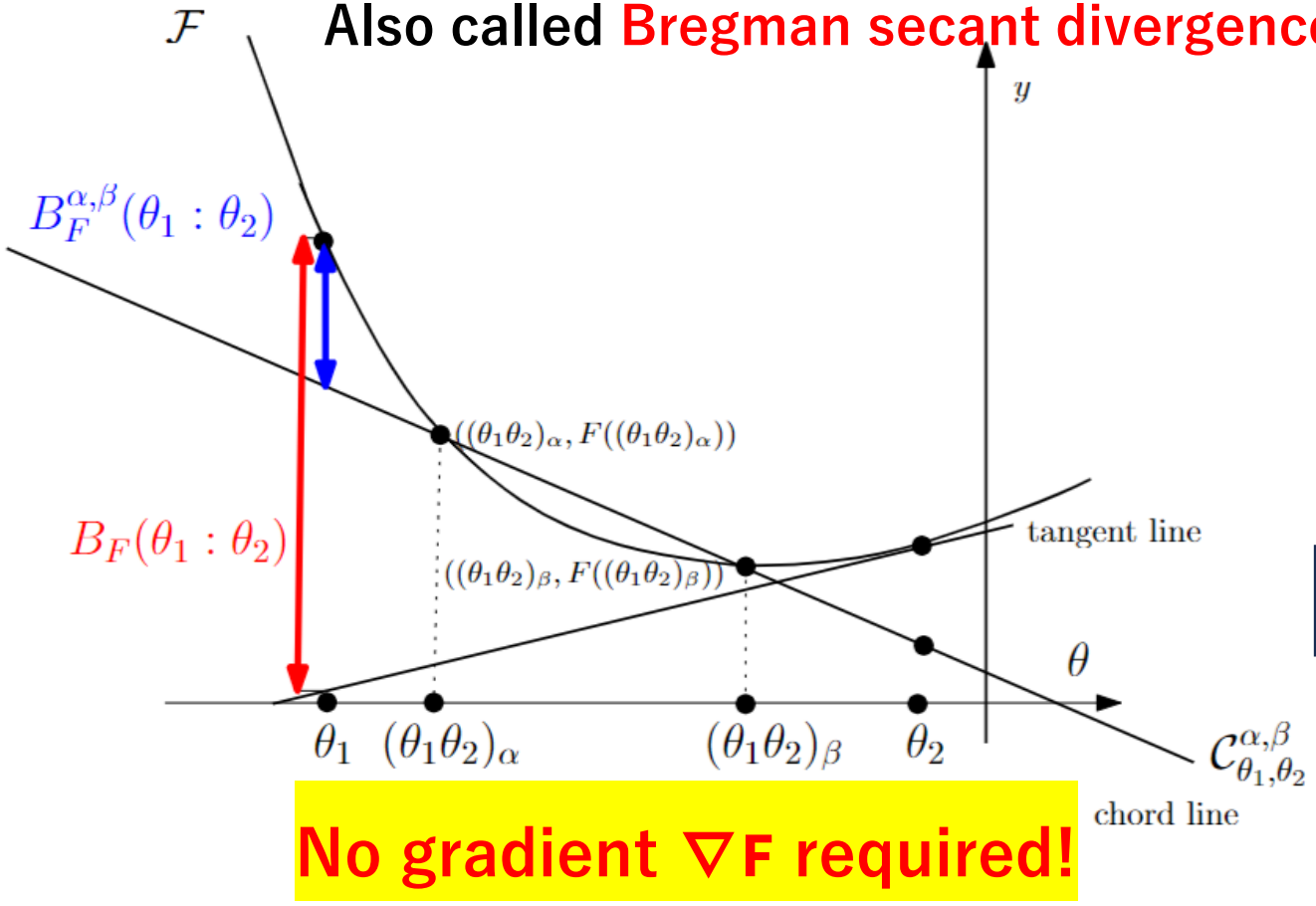
$$\mathrm{tB}(p:q) = \frac{B(p:q)}{\sqrt{1 + \langle \nabla F(q), \nabla F(q) \rangle}} = \rho_B(q) B(p:q)$$

$$\rho_B(q) = \frac{1}{\sqrt{1 + \langle \nabla F(q), \nabla F(q) \rangle}}.$$

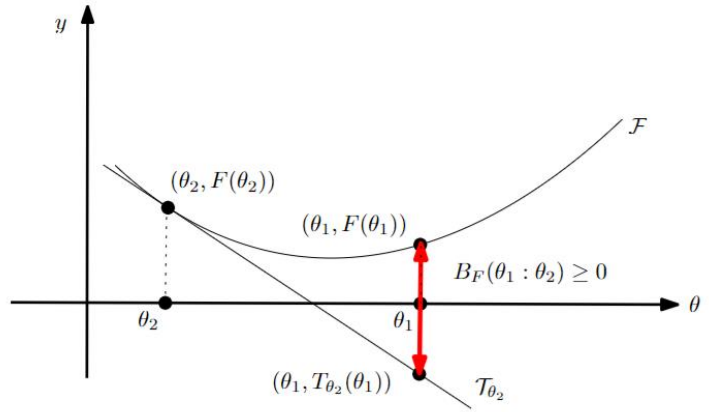
Total Bregman Divergence and its Applications to Shape Retrieval, 2010

Bregman-type divergences measuring convexity gaps

Bregman chord divergences
Also called Bregman secant divergences

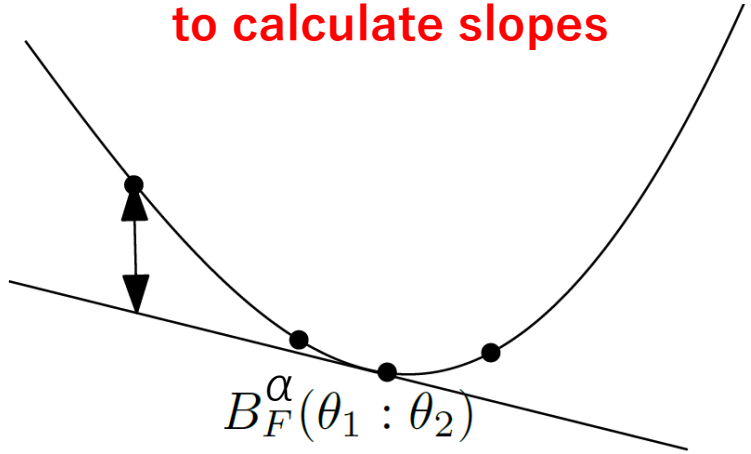


No gradient ∇F required!



gradient ∇F required to calculate slopes

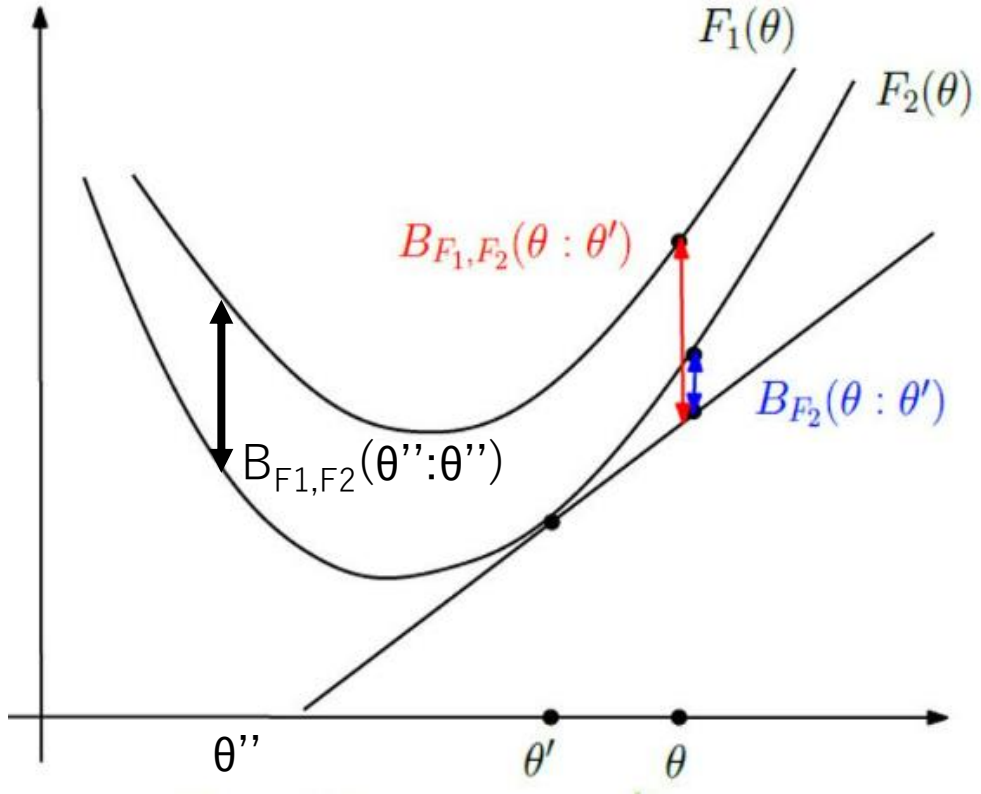
$\alpha \rightarrow \beta$



When $\alpha \rightarrow \beta$, Bregman chord divergences $\rightarrow$ **Bregman tangent divergences**

The Bregman chord divergence, 1810.09113

Duo Bregman divergences: Generalize BDs with a pair of generators



Generator F_1 **majorizes** generator F_2:

$$\mathbf{F_1(\theta) \geq F_2(\theta)}$$

Then

$$B_{F_1,F_2}(\theta : \theta') = F_1(\theta) - F_2(\theta') - (\theta - \theta')^\top \nabla F_2(\theta')$$

$$\geq B_F(\theta : \theta')$$

- Recover Bregman divergence when $\mathbf{F_1(\theta) = F_2(\theta) = F(\theta)}$

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

- Only **pseudo-divergence** because $B_{F1,F2}(\theta'' : \theta'')$ positive but not zero

KLD between nested exponential families amount to duo Bregman divergences

$q(x|\theta) \gg p(x|\theta)$

$\frac{p(x|\theta)}{q(x|\theta)}$ X_1 / X_2

- Consider an exponential family on support X_1:

$$p(x|\theta) = \exp(<x, \theta> - F_1(\theta)) \, d\mu(x)$$

with cumulant function $F_1(\theta) = \log \int_{X1} \exp(<x, \theta>) \, d\mu(x)$

$D_{KL}[p(x):q(x)] = \int p(x) \log (p(x)/q(x)) \, d\mu(x)$

$0 \log(0/0) = 0$

- Another exponential family with **nested supports: $X_1 \subseteq X_2$**

$$q(x|\theta) = \exp(<x, \theta> - F_2(\theta)) \, d\mu(x)$$

is an exponential family with $F_2(\theta) = \log \int_{X2} \exp(<x, \theta>) \, d\mu(x) \geq F_1(\theta)$

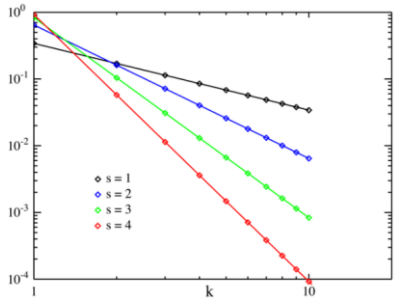
$$X_1 \subseteq X_2 \Rightarrow F_2 \geq F_1$$

- Then KL divergence amounts to a reverse duo Bregman pseudo-divergence:

$$D_{KL}[p(x|\theta_1) : q(x|\theta_2)] = B_{F2,F1}^*(\theta_1 : \theta_2) = B_{F2,F1}(\theta_2 : \theta_1)$$

"Statistical divergences between densities of truncated exponential families with nested supports: Duo Bregman and duo Jensen divergences." *Entropy* 24.3 (2022)

Application of duo Bregman divergences: Clustering distributions with different supports



- Consider *n truncated densities* $p(x|\theta_i) = \exp(\langle x, \theta_i \rangle - F_i(\theta_i))\, d\mu(x)$ with potentially different supports $X_i \subseteq X$: e.g., Zipf's distributions

$$f(k; N, s) = \frac{1}{H_{N,s}} \frac{1}{k^s} \qquad H_{N,s} = \sum_{k=1}^{N} \frac{1}{k^s}$$

- Cluster those distributions using **full support X prototypes**: e.g., Zeta distributions

$$\zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s}$$

This ensures that $q(x|\lambda_j) \gg p(x|\theta_i)$

- Objective is "k-means" type : minimize $\Sigma_i D_{KL}[p(x|\theta_i) : \{q(x|\lambda_j) : j \text{ in } \{1,\cdots,k\}\}]$

- **Duo Bregman k-means** algorithm as an extension of Bregman k-means
- Example: Cluster Zipf's distributions from word frequencies in a collection of translations of a renown book. Find similarities of word frequency in languages

MaxEnt'22, arXiv:2104.10548

Ordinary and duo Fenchel-Young divergences

- Young inequality: $F(\theta_1)+F^*(\eta_2) \geq < \theta_1, \eta_2 >$ with equality iff $\eta_2 = \nabla F(\theta_1)$
- Build the Fenchel-Young divergence from the inequality: lhs-rhs ≥0

$$\mathbf{Y_{F,F^*}(\theta_1, \eta_2) = F(\theta_1)+F^*(\eta_2) - < \theta_1, \eta_2 > \geq 0}$$

- Legendre transform reverses majorization order:

$$F_1(\theta) \geq F_2(\theta) \Leftrightarrow F_1^*(\eta) \leq F_2^*(\eta)$$

- **Duo Fenchel-Young divergence**:

$$\begin{aligned} Y_{F_1,F_2^*}(\theta,\eta') &:= F_1(\theta) + F_2^*(\eta') - \theta^\top \eta', \\ &\geq F_1(\theta) + F_1^*(\eta') - \theta^\top \eta' = Y_{F_1,F_1^*}(\theta,\eta') \geq 0 \end{aligned}$$

Larger than ordinary YFD

Biduality reference/representation

Legendre-Fenchel transformation * induces **two functions**:

❶ a convex conjugate function F*(.) : $\eta \rightarrow F^*(\eta)$

❷ a gradient map function: $\eta = \nabla F(.)$: $\theta \rightarrow \eta(\theta) = \nabla F(\theta)$

This yields the *interplay of two dualities in information geometry*:

❶ **Reference duality** of divergences: $D^*(p_1:p_2):=D(p_2:p_1)$, $(D^*)^*=D$

❷ **Representation duality**: $\theta^* = \nabla F(\theta)$, and $(\theta^*)^* = \theta$

Fenchel-Young divergence demonstrates the bi-duality interaction:

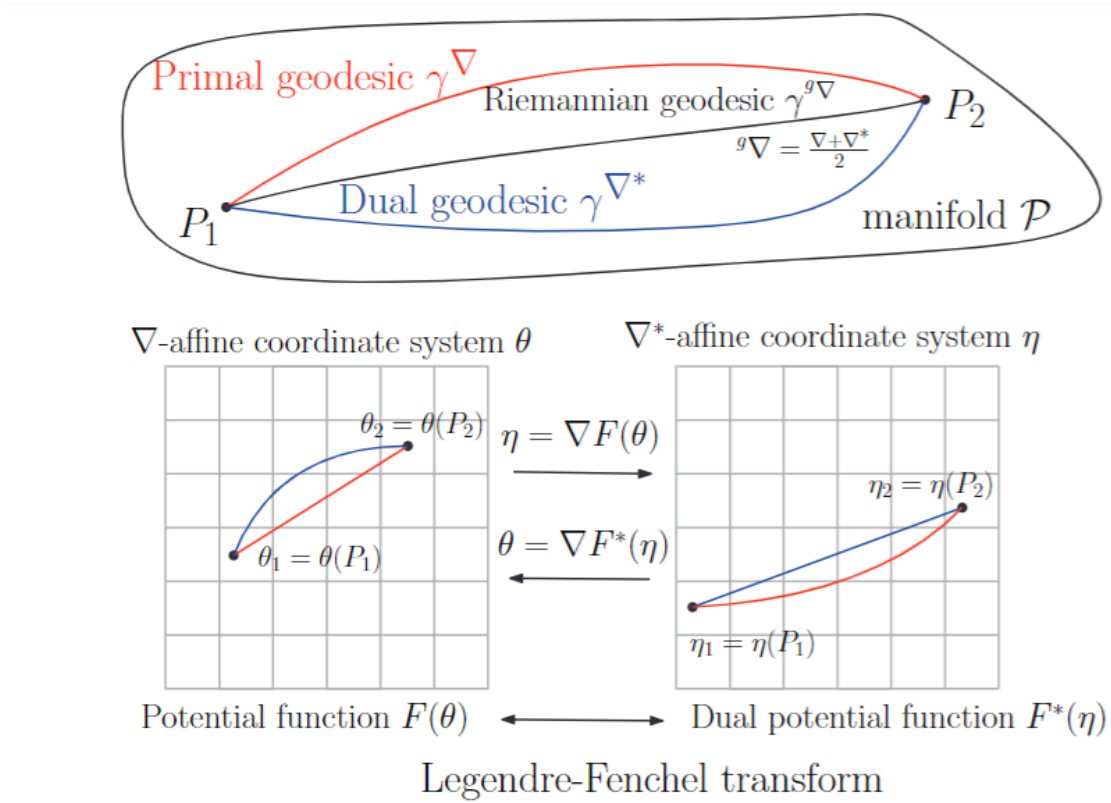
$$(Y_F)^*(\theta_1:\theta_2^*) = Y(\theta_2^*:\theta_1) = Y_{F^*}(\theta_2^*:\theta_1)$$

Functional divergences on densities as pointwise scalar BD can use general monotone (ρ,τ)-embedding dualities

Brekelmans+, Variational representations of annealing paths: Bregman information under monotonic embedding, *Information Geometry* (2024)

Information geometry of Bregman manifolds: Convex conjugates (F, F*) yield dual flat connections

A geodesic is defined with respect to a connection ∇



- A connection ∇ is **flat** if there exists a coordinate system θ such that all Christoffel symbols vanish: $\Gamma(\theta)=0$.
- θ is called **∇-affine coordinate system**
- **∇-geodesic** solves as **line segments**

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

$$(M, F \rightarrow g(\theta) = \nabla^2 F(\theta), F \rightarrow \nabla, F^* \rightarrow \nabla^*)$$

"The many faces of information geometry." *Not. Am. Math. Soc* 69.1 (2022): 36-45.

Example: Bregman manifold of multivariate normal pdfs

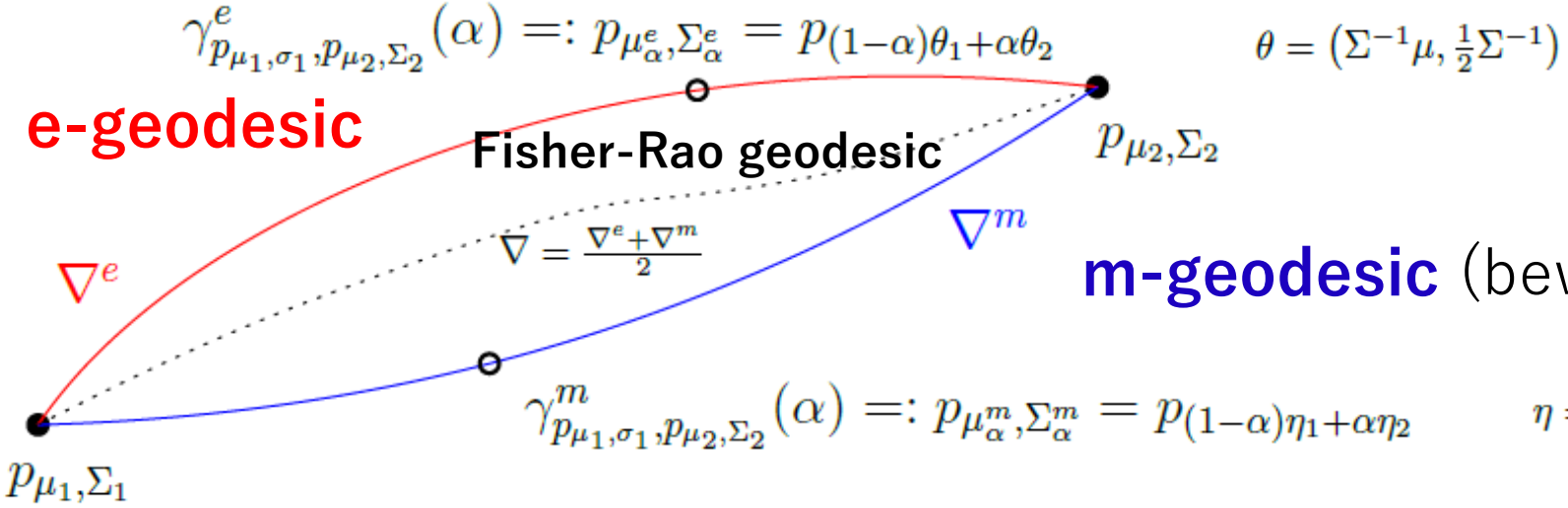
Cumulant function, convex:

$$F_\theta(\theta) = \frac{1}{2}\left(d\log\pi - \log|\theta_M| + \frac{1}{2}\theta_v^\top \theta_M^{-1}\theta_v\right)$$

Natural parameters:

$$\theta = (\theta_v, \theta_M) = \left(\Sigma^{-1}\mu, \frac{1}{2}\Sigma^{-1}\right)$$

$$\begin{aligned}\mu_\alpha^e &= \Sigma_\alpha^e\left((1-\alpha)\Sigma_1^{-1}\mu_1 + \alpha\Sigma_2^{-1}\mu_2\right)\\ \Sigma_\alpha^e &= \left((1-\alpha)\Sigma_1^{-1} + \alpha\Sigma_2^{-1}\right)^{-1}\end{aligned}$$



m-geodesic (beware: not mixture of Gaussians)

$$\begin{aligned}\mu_\alpha^m &= (1-\alpha)\mu_1 + \alpha\mu_2 =: \bar{\mu}_\alpha\\ \Sigma_\alpha^m &= (1-\alpha)\Sigma_1 + \alpha\Sigma_2 + (1-\alpha)\mu_1\mu_1^\top + \alpha\mu_2\mu_2^\top - \bar{\mu}_\alpha\bar{\mu}_\alpha^\top\end{aligned}$$

(M, g, ∇, ∇^*)

Kullback-Leibler divergence = reverse Bregman divergence

$$\frac{1}{2}\left(\mathrm{tr}(\Sigma_2^{-1}\Sigma_1) - \log\frac{\det(\Sigma_2)}{\det(\Sigma_1)} - d + (\mu_2-\mu_1)^\top\Sigma_2^{-1}(\mu_2-\mu_1)\right)$$

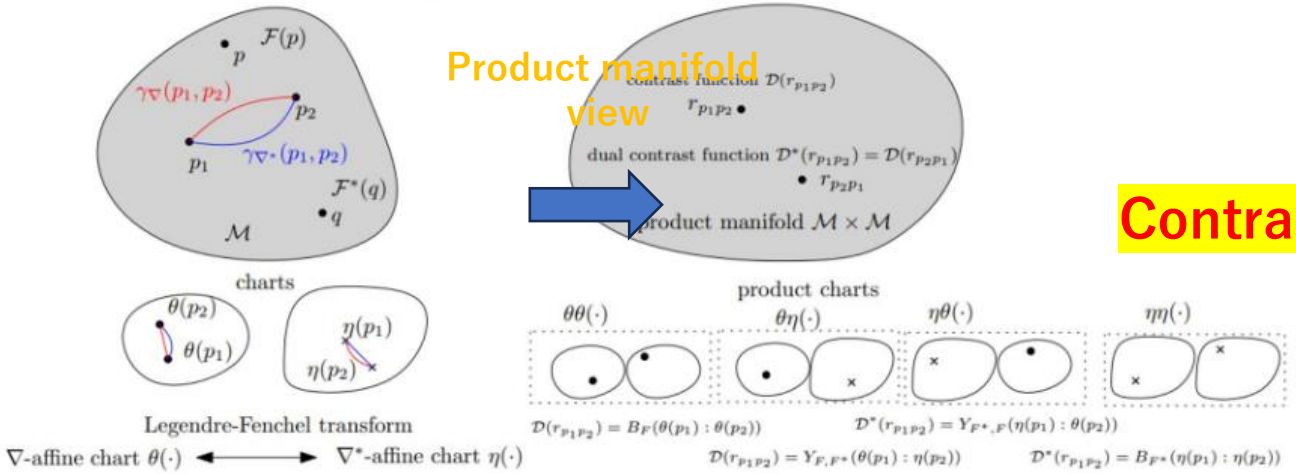
Geometric Jensen-Shannon divergence, 2019

Bregman manifolds: contrast functions on product manifolds

- A strictly convex and smooth Legendre-type function induces a **dually flat space** also called a global Hessian manifold in diff. geo.

Dually flat divergence $D_{\nabla,\nabla^*}(p:q) = B_F(\theta(p):\theta(q)) = Y_{F,F*}(\theta(p):\eta(q))$

$$\begin{aligned}\mathcal{D}(r_{pq}) &= B_F(\theta(p):\theta(q)) = Y_{F,F^*}(\theta(p):\eta(q)),\\ &= \mathcal{D}^*(r_{qp}) = B_{F^*}(\eta(q):\eta(p)) = Y_{F^*,F}(\eta q:\theta(p))\end{aligned}$$



Divergence = Contrast function on product manifold

- Reciprocally, a dually flat space induces a class of equivalent pairs of Legendre-type functions with dual Bregman/Fenchel-Young divergences. Bregman divergences = canonical divergences of dually flat spaces

Non-unique reconstruction of dual potential functions/Bregman divergences from a dually flat space

- Bregman divergence B_F yields a unique dually flat space with a dually flat divergence D_{∇,∇^*}, but not the converse: A DFS yields a **class** of Legendre-type Bregman divergences (modulo affine transformations):

$$\bar{F}(\theta) = \lambda F(A\theta + b) + \langle c, \theta \rangle + d \quad \Rightarrow \quad \eta = \nabla \bar{F}(\theta) = \lambda A^\top \nabla F(A\theta + b) + c.$$

$$A \in \mathrm{GL}(d, \mathbb{R}), \text{ vectors } b, c \in \mathbb{R}^d \text{ and scalars } d \in \mathbb{R} \text{ and } \lambda \in \mathbb{R}_{>0}$$

$$\nabla \bar{G}(\eta) = A^{-1} \nabla G\left(\frac{1}{\lambda} A^{-\top}(\eta - c)\right) - b \quad \Rightarrow \quad \bar{G}(\eta) = \langle \eta, \nabla \bar{G}(\eta) \rangle - F(\nabla \bar{G}(\eta))$$

$$B_F(\theta_1 : \theta_1) = \frac{1}{\lambda} B_{\bar{F}}(\bar{\theta}_1 : \bar{\theta}_2) \quad \text{with} \quad \bar{\theta} = A^{-1}(\theta - b)$$

$$D_{\nabla,\nabla^*}(p_1 : p_2) = B_F(\theta_1 : \theta_1) = \frac{1}{\lambda} B_{\bar{F}}(\bar{\theta}_1 : \bar{\theta}_2)$$

Affine Legendre Invariance + Divergence unit

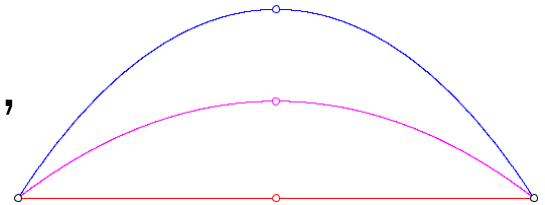
2301.10980

Fisher-Rao geodesics for d-variate normal pdfs

When d>1, some sectional curvatures of (M, g_{Fisher}) are positive,

MVN Fisher-Rao manifold is not Hadamard manifold.

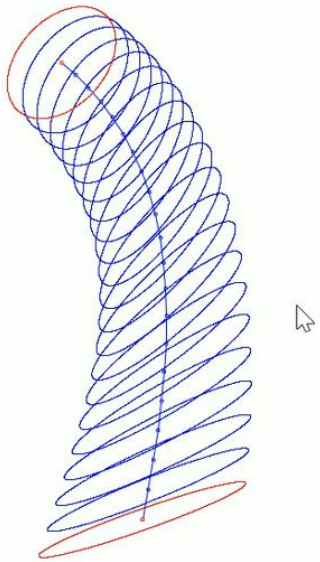
… But centered normal submanifold is Hadamard

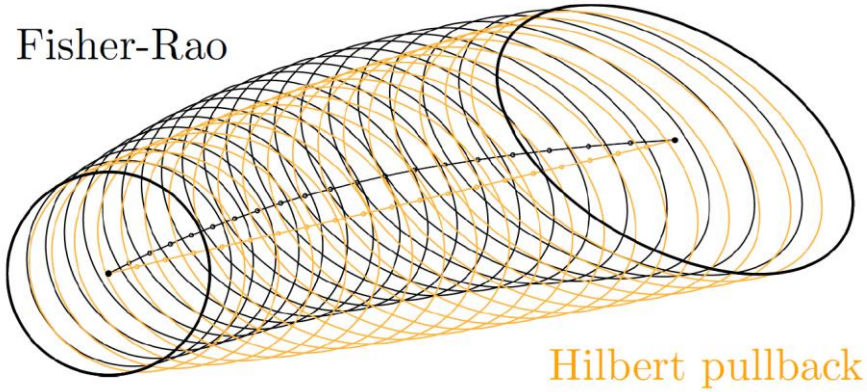


∇^*-geodesic (m-geodesic)

∇^g-geodesic (length minimizing geodesic)

∇-geodesic (e-geodesic)





Embed in SPD of dimension 2d+1, submersion

Geodesic in closed form same-mean centered normal:

$$\gamma_{\mathcal{P}}(P,Q;t) = P^{\frac{1}{2}}\left(P^{-\frac{1}{2}}Q^{\frac{1}{2}}P^{-\frac{1}{2}}\right)^{t}P^{\frac{1}{2}}, \quad t\in[0,1]$$

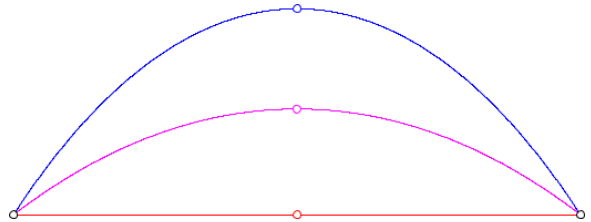
t=1/2 yields matrix geometric mean G(X,Y)= $X^{\frac{1}{2}}(X^{-\frac{1}{2}}YX^{-\frac{1}{2}})^{\frac{1}{2}}X^{\frac{1}{2}}$

Kobayashi, Geodesics of multivariate normal distributions and a Toda lattice type Lax pair, Physica Scripta 98.11 (2023)
Fisher-Rao and pullback Hilbert cone distances on the multivariate Gaussian manifold with applications to simplification and quantization of mixtures, ICML TAG 2023.

Bregman manifolds and Bregman divergences

- Any Legendre-type function $(\Theta, F(\theta))$ generates DFS (M, g, ∇, ∇^*) where $F(\theta)$ defines flat connection ∇ via Christoffel symbols $\Gamma(\theta)=0$, and $F^*(\eta)$ defines flat connection ∇^* via Christoffel symbols $\Gamma^*(\eta)=0$

- **Duality in information geometry**: $(\nabla + \nabla^*)/2$ is Levi-Civita connection ∇^g



Example of convex functions from statistical models:

- The **cumulant functions** of exponential families

$F(\theta)=\log \int \exp(<x, \theta>) \, d\mu(x)$. In that case, the Bregman divergence amounts to a reverse Kullback-Leibler divergence

- The **partition functions** $Z(\theta)= \int \exp(<x, \theta>) \, d\mu(x)=\exp(F(\theta))$ is log-convex and log-convex functions are convex. Hence, we can build a Bregman manifold from $Z(\theta)$ too!
- **Question: What is the reconstructed statistical divergence from Bregman divergence B_Z?**

"Divergences Induced by the Cumulant and Partition Functions of Exponential Families and Their Deformations Induced by Comparative Convexity." *Entropy* 26.3 (2024)

Answer: Kullback-Leibler divergence between non-normalized exponential family densities

- Kullback-Leibler divergence between **two *positive* measures**:

$$D_{KL}^{+}[p_1(x):p_2(x)] = \int \{ p_1(x) \log (p_1(x)/p_2(x)) + p_2(x) - p_1(x) \} \, d\mu(x)$$

- Exponential family density:
  - Normalized: $p(x|\theta) = \exp(<x, \theta> - F(\theta)) \, d\mu(x)$
  - Vs non-normalized: $q(x|\theta) = \exp(<x, \theta>) \, d\mu(x)$
- Hence, $p(x|\theta) = q(x|\theta)/Z(\theta)$ with **partition function** $Z(\theta) = \exp(F(\theta))$ and cumulant function $F(\theta) = \log Z(\theta)$
- **F is convex** and **Z is log-convex** and **log-convex functions are convex functions**

- Widely used in ML : KLD between normalized densities = reverse Bregman wrt F:

$$D_{KL}[p_{\theta 1}(x):p_{\theta 2}(x)] = B_F^{*}[\theta_1 : \theta_2] = B_F[\theta_2 : \theta_1]$$

- New: KLD between non-normalized densities = reverse Bregman wrt Z:

$$D_{KL}^{+}[p_{\theta 1}(x):p_{\theta 2}(x)] = B_Z^{*}[\theta_1 : \theta_2] = B_Z[\theta_2 : \theta_1]$$

2312.12849

Bregman divergences and Jensen divergences
Cumulant functions/Partition functions

$F(\theta)=\log Z(\theta) \leftrightarrow Z(\theta)=\exp(F(\theta))$

$$Z(\theta) = \int \tilde{p}_\theta(x)\mathrm{d}\mu(x)$$

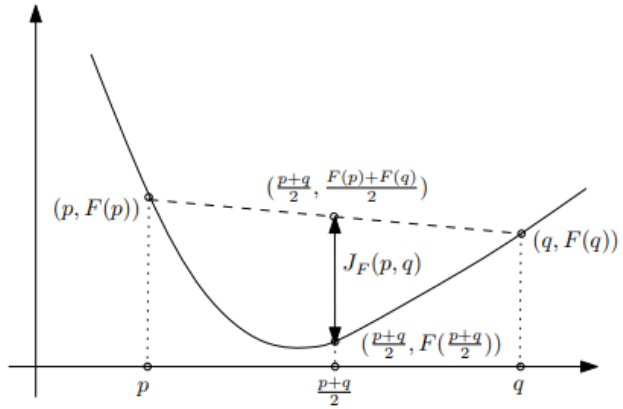
① $$B_Z(\theta_1 : \theta_2) = Z(\theta_1) - Z(\theta_2) - \langle \theta_1 - \theta_2, \nabla Z(\theta_2) \rangle \geq 0,$$

② $$B_{\log Z}(\theta_1 : \theta_2) = \log\left(\frac{Z(\theta_1)}{Z(\theta_2)}\right) - \left\langle \theta_1 - \theta_2, \frac{\nabla Z(\theta_2)}{Z(\theta_2)} \right\rangle \geq 0,$$

And furthermore, we can define **skewed Jensen divergences** from the convex generators as convexity gaps:

① $$J_{Z,\alpha}(\theta_1 : \theta_2) = \alpha Z(\theta_1) + (1-\alpha)Z(\theta_2) - Z(\alpha\theta_1 + (1-\alpha)\theta_2) \geq 0,$$

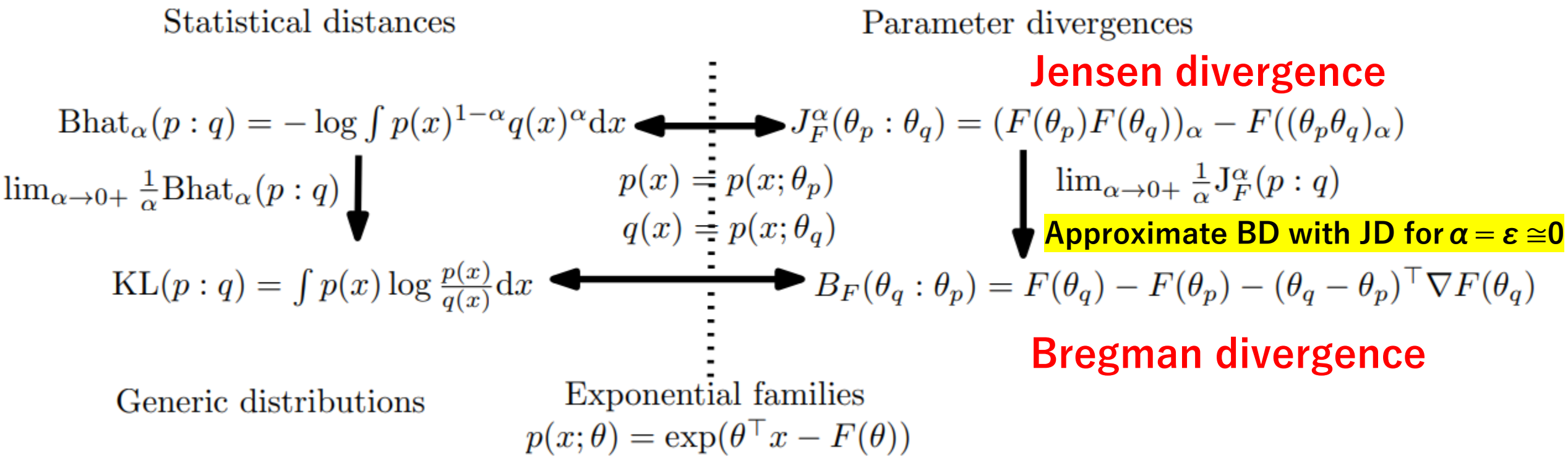
② $$J_{\log Z,\alpha}(\theta_1 : \theta_2) = \log \frac{Z(\theta_1)^\alpha Z(\theta_2)^{1-\alpha}}{Z(\alpha\theta_1 + (1-\alpha)\theta_2)} \geq 0.$$



Including the **symmetric Jensen divergence** when α=1/2:

$$J_F(\theta_1, \theta_2) = J_{F,\frac{1}{2}}(\theta_1 : \theta_2) = \frac{F(\theta_1) + F(\theta_2)}{2} - F\left(\frac{\theta_1 + \theta_2}{2}\right)$$

KLD/ α -Bhattacharyya $\Leftrightarrow$ Bregman/Jensen divergences
when considering exponential families, F cumulant function



Question: What are the reconstructed statistical divergences from Jensen-Bregman divergence J_Z / B_Z? When Z is partition function instead of F cumulant function?

Zhang, Divergence function, duality, and convex analysis, *Neural computation* 16.1 (2004)
N + Boltz. "The Burbea-Rao and Bhattacharyya centroids." *IEEE Transactions on Information Theory* (2011)

Bregman divergences corresponding to partition functions

$$\begin{aligned} D_{\mathrm{KL}}(\tilde{p}:\tilde{q}) &= H^{\times}(\tilde{p}:\tilde{q}) - H(\tilde{p}), \\ &= \int \left(\tilde{p} \log \frac{\tilde{p}}{\tilde{q}} + \tilde{q} - \tilde{p} \right) \mathrm{d}\mu \end{aligned}$$

Question: What is the reconstructed statistical divergence from Bregman divergence B_Z?

$$D_\alpha(\tilde{p}:\tilde{q}) = \begin{cases} \frac{1}{\alpha(1-\alpha)} \int \left(\alpha\tilde{p} + (1-\alpha)\tilde{q} - \tilde{p}^\alpha \tilde{q}^{1-\alpha}\right) \mathrm{d}\mu, & \alpha \notin \{0,1\} \\ D^*_{\mathrm{KL}}(\tilde{p}:\tilde{q}) = D_{\mathrm{KL}}(\tilde{q}:\tilde{p}) & \alpha = 0, \\ 4\, D^2_H(\tilde{p},\tilde{q}) & \alpha = \frac{1}{2}, \\ D_{\mathrm{KL}}(\tilde{p}:\tilde{q}) & \alpha = 1. \end{cases} \quad \Longleftrightarrow \quad \mathrm{J}^s_{Z,\alpha}(\theta_1:\theta_2) = \begin{cases} \frac{1}{\alpha(1-\alpha)} J_{Z,\alpha}(\theta_1:\theta_2), & \alpha \in \backslash\{0,1\}, \\ B_Z(\theta_1:\theta_2), & \alpha = 0, \\ 4\, J_Z(\theta_1,\theta_2), & \alpha = \frac{1}{2}, \\ B^*_Z(\theta_1:\theta_2) = B_Z(\theta_2:\theta_1), & \alpha = 1. \end{cases}$$

Amari α-divergences extended to positive measures $\Longleftrightarrow$ **Scaled skewed Jensen divergence for partition function Z**

J_Z corresponds to the **extended α-divergences**

B_Z corresponds to the reverse **extended Kullback-Leibler divergence**

"Divergences Induced by the Cumulant and Partition Functions of Exponential Families and Their Deformations Induced by Comparative Convexity." *Entropy* 26.3 (2024)

Monte Carlo Bregman divergences

- In some cases, integral Bregman generators are not available in closed-form or **computationally intractable**. Examples:

  $F(\theta)=\log \int \exp(<\text{Polynomial}(x), \theta>) \, d\mu(x)$ or $F(\theta)=\log \sum \exp(<x, \theta>)$

- By MC importance sampling on the integral, get *with high probability a convex function approximating the generator*. Perform algorithms on this **randomized Bregman manifolds** to get consistent algorithms.

$$G(\eta) = -h(m(x;\eta)) = \int_{x\in\mathcal{X}} m(x;\eta)\log m(x;\eta)\mathrm{d}\mu(x).$$

Monte Carlo
Information geometry

$$G(\eta) \simeq \tilde{G}_{\mathcal{S}}(\eta) := \frac{1}{m}\sum_{i=1}^{m}\frac{1}{q(x_i)} m(x_i;\eta)\log m(x_i;\eta).$$

Stochastic Bregman generator

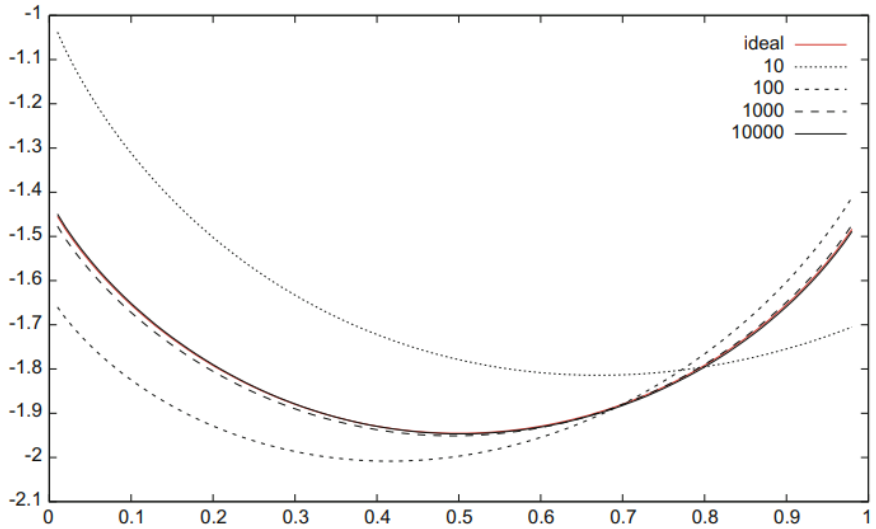


Fig. 2 A series $G_{\mathcal{S}}(\eta)$ of Bregman Monte Carlo Mixture Family generators (for $m = |\mathcal{S}| \in \{10, 100, 1000, 10000\}$) approximating the untractable ideal negentropy generator $G(\eta) = -h(m(x;\eta))$ (red) of a mixture family with prescribed Gaussian distributions $m(x;\eta) = (1-\eta)p(x;0,3) + \eta p(x;2,1)$ for the proposal distribution $q(x) = m(x;\frac{1}{2})$

Monte Carlo information-geometric structures
***Geometric Structures of Information* (2019): 69-103.**

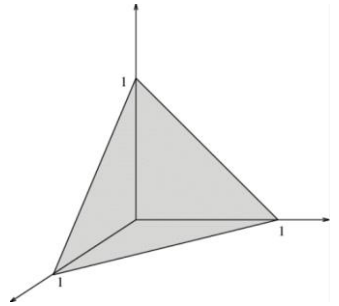
An example of Information Geometry in action

- Set of categorical distributions form a **mixture family M**, a Bregman manifold for the negentropy generator

$$\mathcal{M} = \left\{ m_\theta(x) = \sum_{i=1}^{D} \theta_i \delta(x - x_i) + \left(1 - \sum_{i=1}^{D} \theta_i\right) \delta(x - x_0) \right\}$$

$$F(\theta) = -h(m_\theta) = \sum_{i=1}^{D} \theta_i \log \theta_i + \left(1 - \sum_{i=1}^{D} \theta_i\right) \log \left(1 - \sum_{i=1}^{D} \theta_i\right).$$

A mixture family is closed under mixture operations



- Given a set of n discrete distributions (categorical distributions, normalized histograms), calculate its **Jensen-Shannon centroid**

$$\mathrm{JS}(p,q) := \frac{1}{2}\left(\mathrm{KL}\left(p : \frac{p+q}{2}\right) + \mathrm{KL}\left(q : \frac{p+q}{2}\right)\right)$$

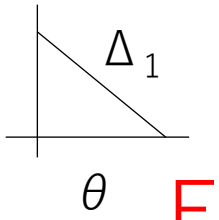
$$\mathrm{JS}(p,q) = h\left(\frac{p+q}{2}\right) - \frac{h(p)+h(q)}{2}$$

$$h(p) = -\int p \log p \, \mathrm{d}\mu$$

On a generalization of the Jensen–Shannon divergence and the Jensen–Shannon centroid, *Entropy* 22.2 (2020)

Dual e/m geodesics and Fisher-Rao geodesics on the categorical manifold

Mixture parameter space

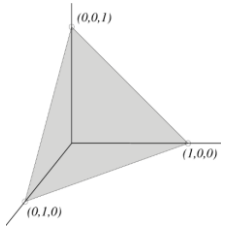


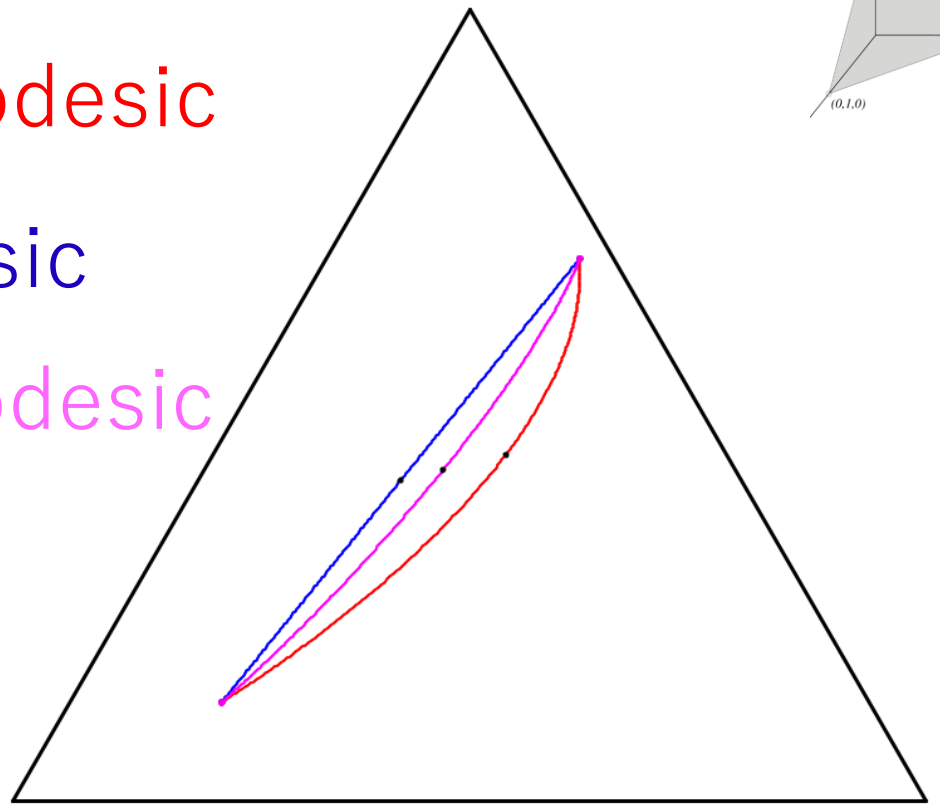
Exponential ∇-geodesic

Mixture ∇^*-geodesic

Fisher-Rao ∇^g-geodesic (Levi-Civita)

Probability simplex/Categorical manifold





Exponential ∇-geodesic
Mixture ∇^*-geodesic
Fisher-Rao ∇^g-geodesic (Levi-Civita)

Jensen-Shannon centroid for mixtures

- **Jensen-Shannon divergence between two mixtures amounts to a Jensen divergence**: $\mathrm{JS}(p_1, p_2) = J_F(\theta_1, \theta_2)$ for $p_1 = m_{\theta_1}$ and $p_2 = m_{\theta_2}$, where

$$J_F(\theta_1 : \theta_2) = \frac{F(\theta_1) + F(\theta_2)}{2} - F\left(\frac{\theta_1 + \theta_2}{2}\right).$$

- Task: Given a set of discrete distributions (categorical distributions, normalized histograms), calculate its Jensen-Shannon centroid:

$$\min_p \sum_i \mathrm{JS}(p_i, p),$$

$$\min_\theta \sum_i J_F(\theta_i, \theta),$$

$$\min_\theta \sum_i \frac{F(\theta_i) + F(\theta)}{2} - F\left(\frac{\theta_i + \theta}{2}\right),$$

$$\equiv \min_\theta \frac{1}{2}F(\theta) - \frac{1}{n}\sum_i F\left(\frac{\theta_i + \theta}{2}\right) := E(\theta)$$

Need to minimize a difference of convex functions DCA or **ConCave Convex algorithm**!

Jensen-Bregman divergence

$$\min_p \sum_i \mathrm{JS}(p_i, p),$$
$$\min_\theta \sum_i J_F(\theta_i, \theta),$$
$$\min_\theta \sum_i \frac{F(\theta_i)+F(\theta)}{2} - F\left(\frac{\theta_i+\theta}{2}\right)$$

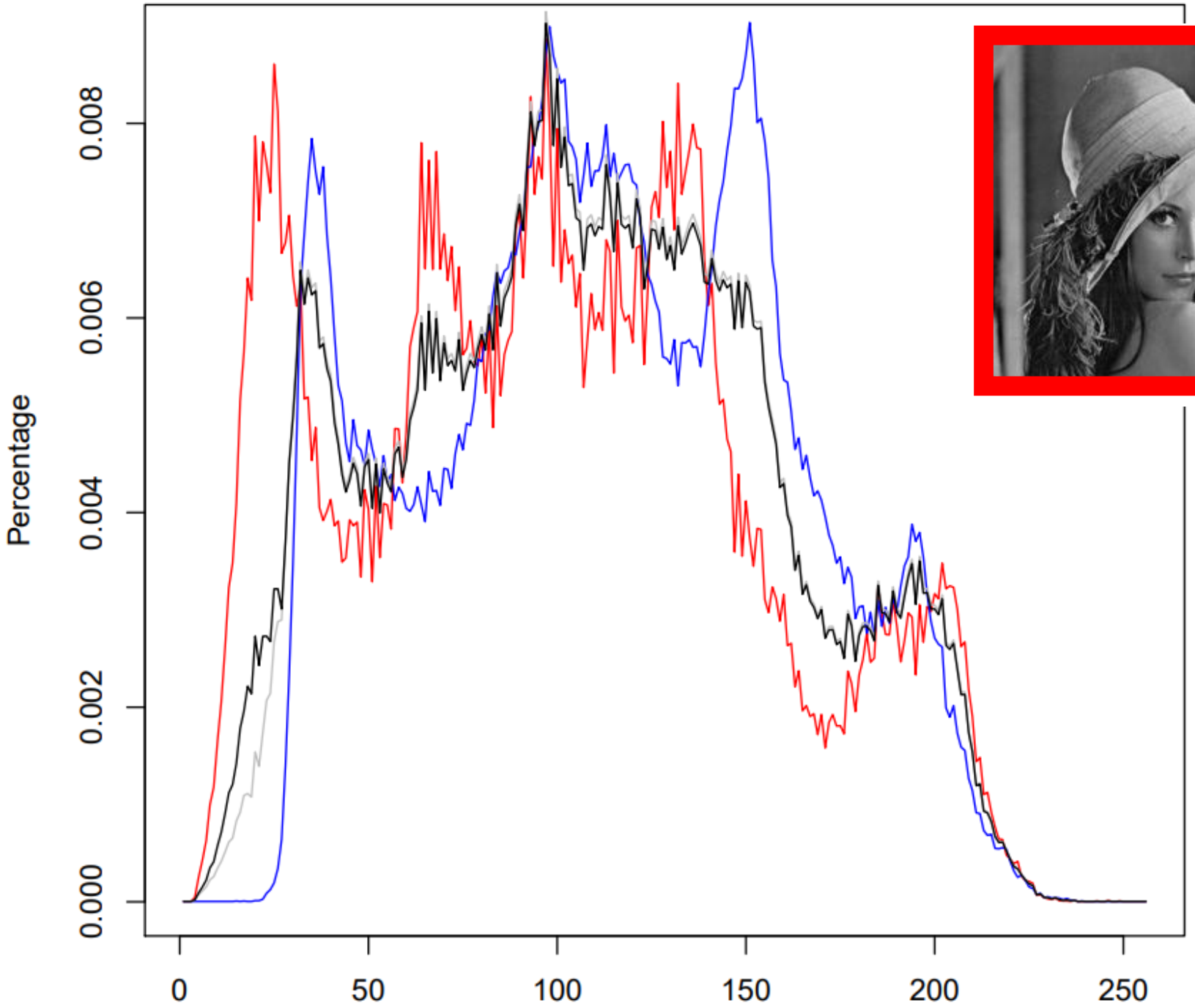
- Jensen-Bregman divergence is Jensen-Shannon symmetrization of Bregman divergence:

$$\begin{aligned}\mathrm{JB}_F(\theta:\theta') &:= \frac{1}{2}\left(B_F\left(\theta:\frac{\theta+\theta'}{2}\right)+B_F\left(\theta':\frac{\theta+\theta'}{2}\right)\right)\\ &= \frac{F(\theta)+F(\theta')}{2}-F\left(\frac{\theta+\theta'}{2}\right) =: J_F(\theta:\theta')\end{aligned}$$

amounts to a Jensen divergence (also called Burbea-Rao divergence).

- Jensen-Shannon centroid of a mixture family = Jensen-Bregman centroid = Jensen centroid

Skew Jensen-Bregman Voronoi diagrams." *Transactions Voronoi Diagrams and Delaunay Triangulation* (2011)
On the Jensen–Shannon symmetrization of distances relying on abstract means. *Entropy* 21.5 (2019)



Jensen–Shannon centroid

Jeffreys SKL centroid

Jensen–Shannon centroid do not require same support

Comparative convexity: (M,N)-convexity

Ordinary convexity of a function: $f\left(tx_1 + (1-t)x_2\right) \leq tf\left(x_1\right) + (1-t)f\left(x_2\right)$
for all t in [0,1]

- *Definition*: A function Z is **(M,N)-convex** iff for in α in [0,1]:

$$Z(M(x,y;\alpha,1-\alpha)) \leq N(Z(x),Z(y);\alpha,1-\alpha)$$

- Ordinary convexity = (A,A)-convexity wrt to arithmetic weighted mean

$$A(x,y;\alpha,1-\alpha) = \alpha x + (1-\alpha)y \qquad f\left(tx_1 + (1-t)x_2\right) \leq tf\left(x_1\right) + (1-t)f\left(x_2\right)$$
for all t in [0,1]

- **Log-convexity**: **(A,G)-convexity** wrt to A/geometric weighted means:

$$G(x,y;\alpha,1-\alpha) = x^{\alpha}y^{1-\alpha} \qquad f(tx_1 + (1-t)x_2) \leq f(x_1)^t f(x_2)^{1-t}$$
for all t in [0,1]

Comparative convexity wrt quasi-arithmetic means

- **quasi-arithmetic mean** for a strictly monotone generator h(u):

$$M_h(x,y;\alpha,1-\alpha) = h^{-1}(\alpha h(x) + (1-\alpha)h(x)).$$

- Includes **power means** which are *homogeneous means*:

$$M_p(x,y;\alpha,1-\alpha) = (\alpha x^p + (1-\alpha)y^p)^{\frac{1}{p}} = M_{h_p}(x,y;\alpha,1-\alpha), \quad p \neq 0$$

$$h_p(u) = \frac{u^p - 1}{p} \qquad h_p^{-1}(u) = (1+up)^{\frac{1}{p}}$$

Include the **geometric mean** in the limit case p→0

Proposition 6 ([1, 34]). *A function $Z(\theta)$ is strictly (M_ρ, M_τ)-convex with respect to two strictly increasing smooth functions ρ and τ if and only if the function $F = \tau \circ Z \circ \rho^{-1}$ is strictly convex.*

Generalizing Bregman divergences with (M,N)-convexity: (M,N)-Bregman divergences

- Skew Jensen divergence from (M,N) comparative convexity:

Definition:

$$J_{F,\alpha}^{M,N}(p:q) = N_\alpha(F(p),F(q)) - F(M_\alpha(p,q)).$$

Non-negative for **(M,N)-convex generators** F, provided regular means M and N (e.g. power means)

Definition 5 (Bregman Comparative Convexity Divergence, BCCD) *The Bregman Comparative Convexity Divergence (BCCD) is defined for a strictly (M,N)-convex function $F : I \to \mathbb{R}$ by*

$$B_F^{M,N}(p:q) = \lim_{\alpha\to 1^-} \frac{1}{\alpha(1-\alpha)} J_{F,\alpha}^{M,N}(p:q) = \lim_{\alpha\to 1^-} \frac{1}{\alpha(1-\alpha)} \left(N_\alpha(F(p),F(q))) - F(M_\alpha(p,q))\right) \quad (31)$$

By analogy to limit of skewed Jensen divergences amount to forward/reverse Bregman divergences.

Generalizing Bregman divergences with quasi-arithmetic mean convexity

Theorem 1 (Quasi-arithmetic Bregman divergences, QABD) *Let $F : I \subset \mathbb{R} \to \mathbb{R}$ be a real-valued (M_ρ, M_τ)-convex function defined on an interval I for two strictly monotone and differentiable functions ρ and τ. The quasi-arithmetic Bregman divergence (QABD) induced by the comparative convexity is:*

$$B_F^{\rho,\tau}(p:q) = \frac{\tau(F(p)) - \tau(F(q))}{\tau'(F(q))} - \frac{\rho(p) - \rho(q)}{\rho'(q)} F'(q). \quad (45)$$

Amounts to a **conformal Bregman divergence** on **monotonic representations**:

$$B_F^{\rho,\tau}(p:q) = \frac{1}{\tau'(F(q))} B_G(\rho(p):\rho(q))$$

With generator:

$$G(x) = \tau(F(\rho^{-1}(x)))$$

Conformal factor

Remark: Conformal Bregman divergences may yield **robustness** in applications

Shape retrieval using hierarchical total Bregman soft clustering, IEEE Transactions on pattern analysis and machine intelligence (2012)

(M,N)-convexity for convex-preserving deformations

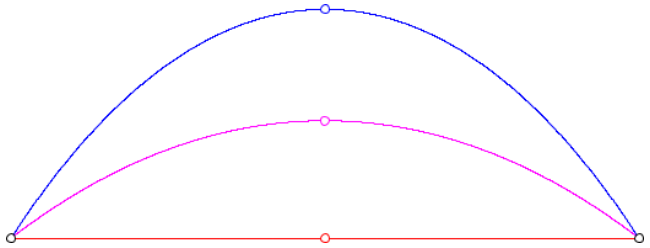
- Recall that for exponential families, we had "two" convex functions:

Cumulant function F ↔ Partition function Z

Convex $F(\theta)=\log Z(\theta)$ ↔ Log-convex $Z(\theta)=\exp(F(\theta))$, hence convex

Proposition 6 ([1, 34]). *A function $Z(\theta)$ is strictly (M_ρ, M_τ)-convex with respect to two strictly increasing smooth functions ρ and τ if and only if the function $F = \tau \circ Z \circ \rho^{-1}$ is strictly convex.*

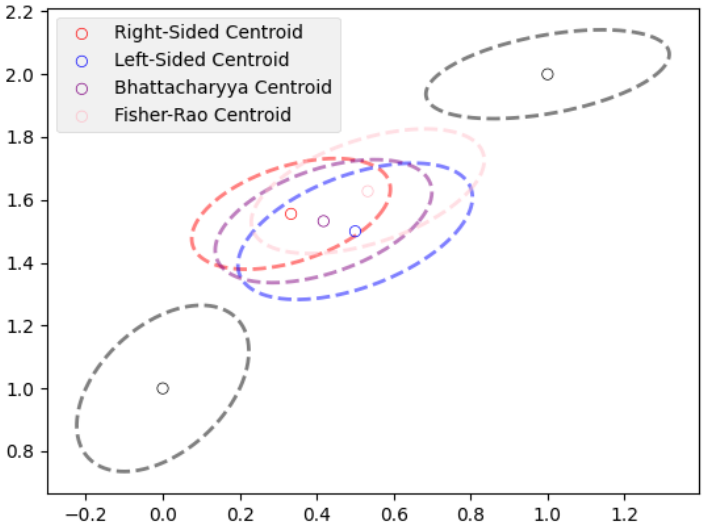
- We may thus **deform F with (ρ, τ)-quasi-arithmetic means** and seek the (ρ, τ)-convex functions which also remain ordinary convex
- For those convex-preserving (ρ, τ)-deformations, we get new Bregman divergences and Bregman manifolds to play with!



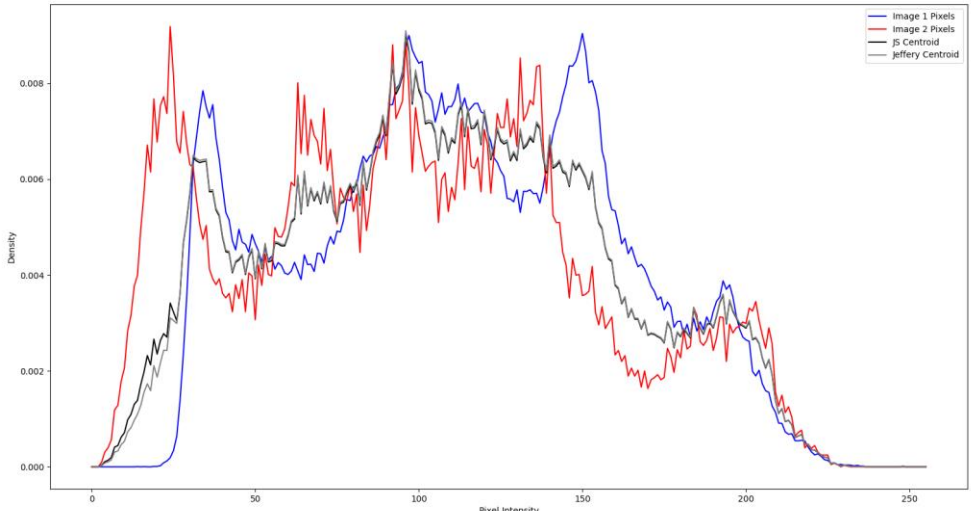
A Python library for geometric computing on Bregman Manifolds

pyBregMan

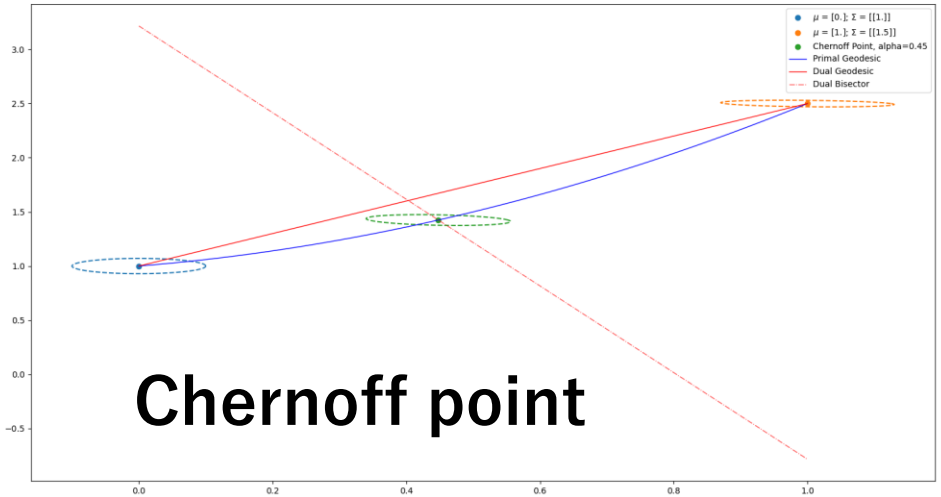
https://franknielsen.github.io/pyBregMan/



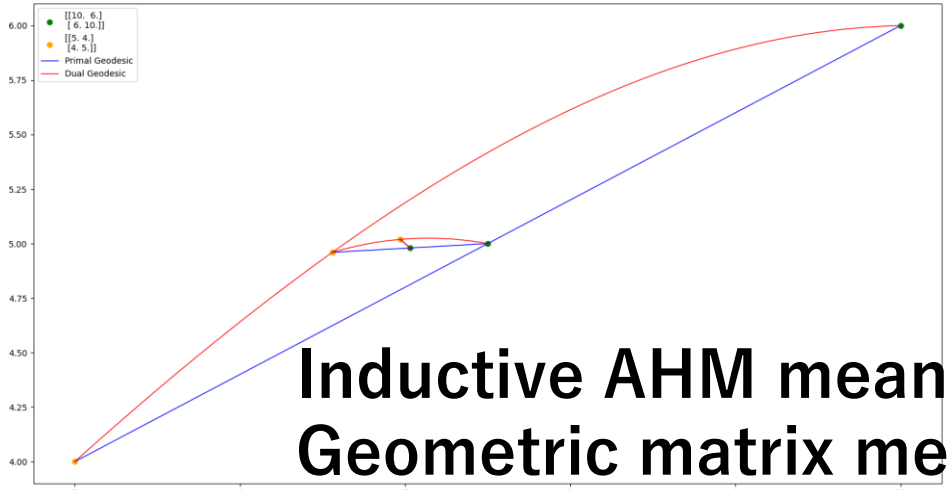
centroids for bivariate normals



Jensen-Shannon centroid



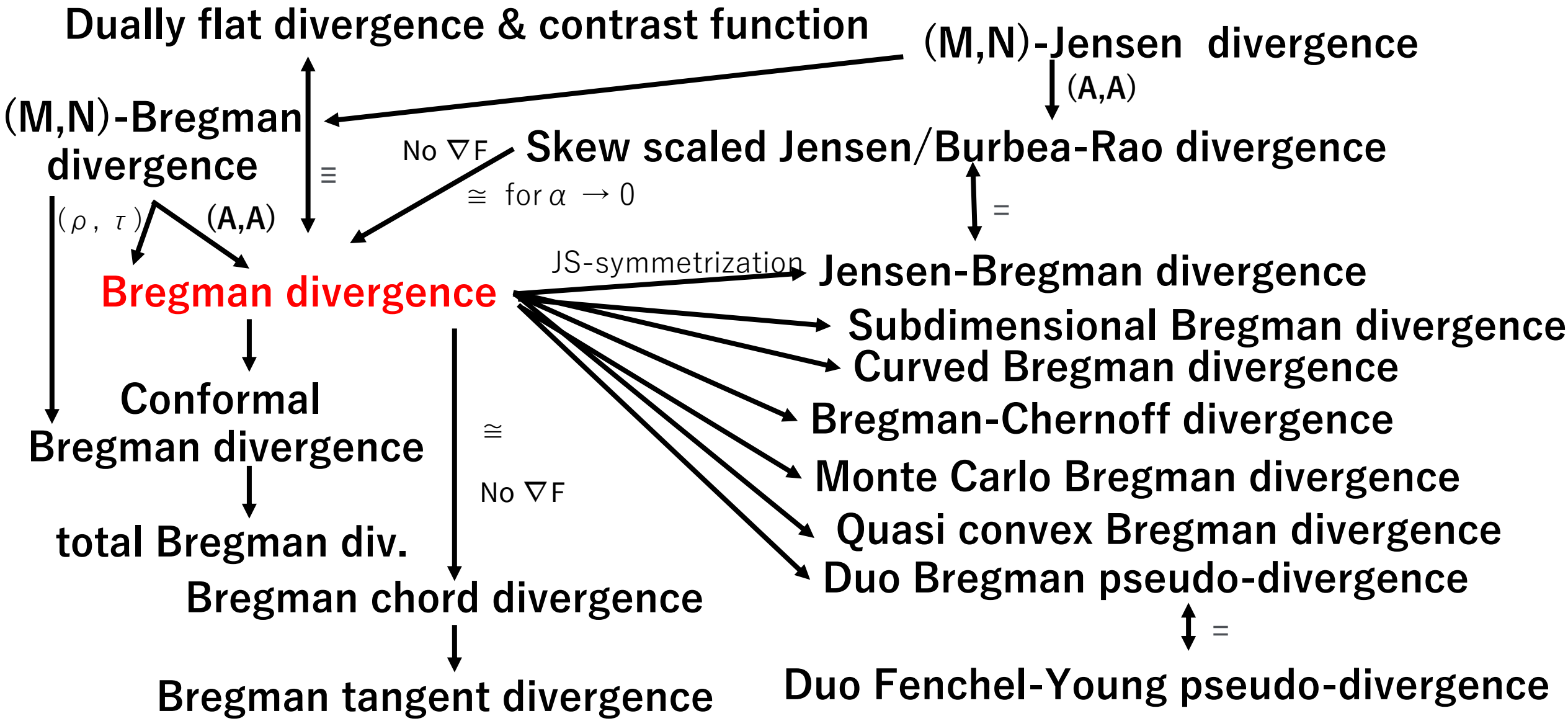
Chernoff point



Inductive AHM mean
Geometric matrix mean

Joint work of Frank Nielsen and Alexander Soen

Some generalizations of Bregman divergences in this talk



But also matrix Bregman divergence, functional Bregman divergence, submodular Bregman divergence, etc.

MEMOIRE
THEORIE DES DEBLAIS ET DES REMBLAIS.

Par M. Monge

Un des théorèmes de Monge permet d'étudier les courbures des surfaces par l'étude du comportement d'une fonction de plusieurs variables au niveau d'un point critique (point où les dérivées particulières premières existent et sont nulles).

$$\frac{d^2f}{dx^2}(x_0, y_0) = R$$

$$\frac{d^2f}{\quad}(x_0, y_0) = S$$

...ONS

...ÉCOLES NORMALES

...RÉPUBLIQUE,

...Comité de Salut ...République

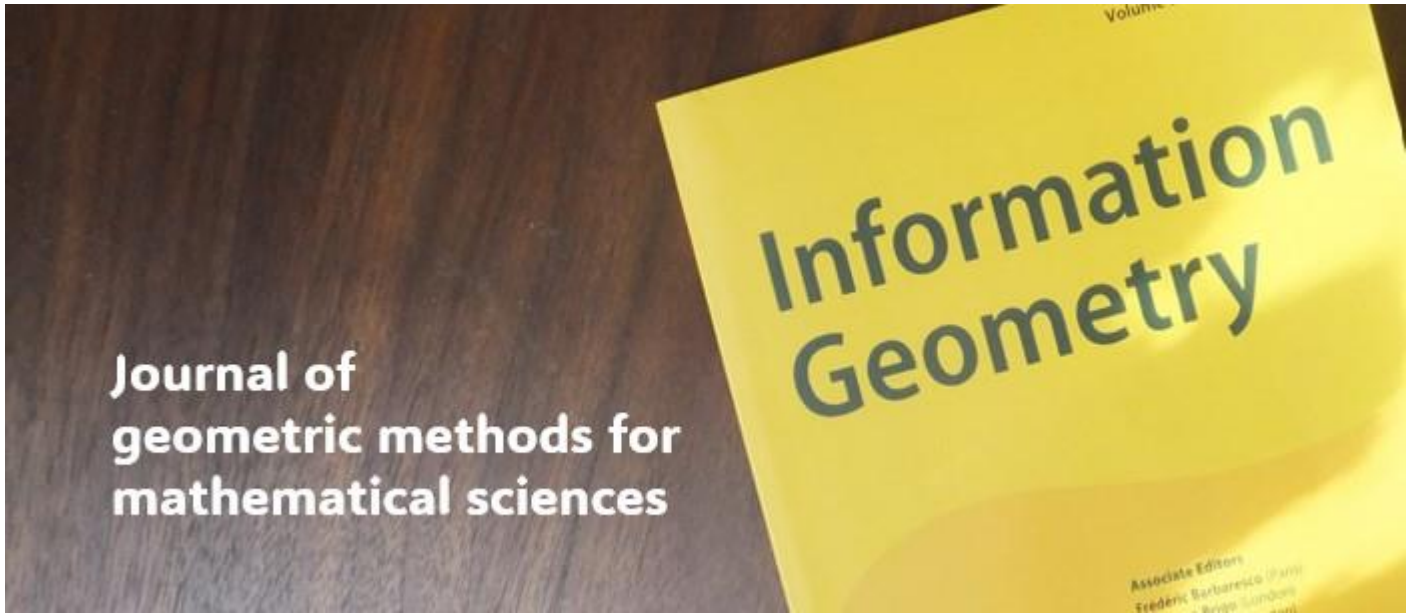
...par M. Monge

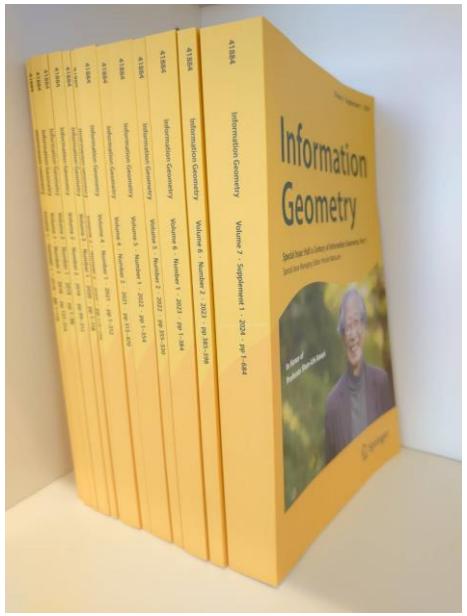
...EMBLAIS.

Thank you!

Many thanks to all my inspiring collaborators.

with special thanks to Richard Nock, Ke Sun, Ehsan Amid, and Alexander Soen





https://link.springer.com/journal/41884

https://franknielsen.github.io/

Inductive matrix arithmetic-harmonic mean (AHM)

- Consider the cone of symmetric positive-definite matrices (SPD cone), and extend the Arithmetic Harmonic Mean to SPD matrices:

[Nakamura 2001]

$$A_{t+1} = \frac{A_t + H_t}{2} = A(A_t, H_t) \quad \leftarrow \text{arithmetic mean}$$

$$H_{t+1} = 2\left(A_t^{-1} + H_t^{-1}\right)^{-1} = H(A_t, H_t) \quad \leftarrow \text{harmonic mean}$$

- Sequences with $A_0=X$ & $H_0=Y$ converge quadratically to **matrix geometric mean**:

$$\mathrm{AHM}(X,Y) = \lim_{t\to+\infty} A_t = \lim_{t\to+\infty} H_t.$$

$$\mathrm{AHM}(X,Y) = X^{\frac{1}{2}}\left(X^{-\frac{1}{2}}\,Y\,X^{-\frac{1}{2}}\right)^{\frac{1}{2}}X^{\frac{1}{2}} = G(X,Y)$$

which is also the **Riemannian center of mass** wrt the trace metric:

$$G(X,Y) = \arg\min_{M\in\mathbb{P}(d)} \frac{1}{2}\rho^2(X,M) + \frac{1}{2}\rho^2(Y,M).$$

$$\rho(P_1,P_2) = \sqrt{\sum_{i=1}^{d} \log^2\lambda_i\left(P_1^{-\frac{1}{2}}\,P_2\,P_1^{-\frac{1}{2}}\right)}$$ Riemannian distance

What is… an Inductive Mean? *Notices of the American Mathematical Society* 2023

Geometric interpretation of the AHM matrix mean

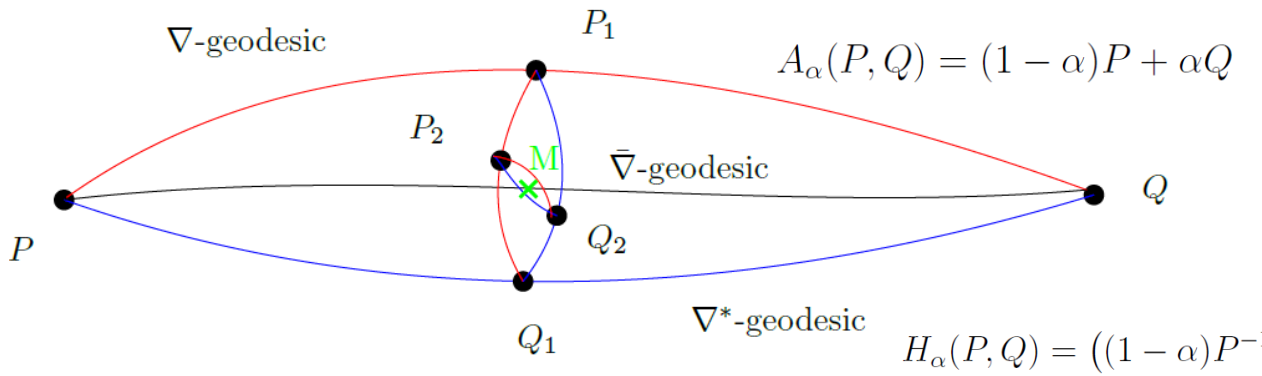
Repeat:

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

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

$(\mathrm{SPD}, g^G, \nabla^A, \nabla^H)$ 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 $(\mathrm{SPD}, g^G, \nabla^A, \nabla^H)$

Primal geodesic midpoint is the arithmetic center wrt Euclidean metric

Dual geodesic midpoint = harmonic center wrt an isometric Eucl. metric

Levi-Civita geodesic midpoint is geometric Karcher mean

$$g_P^A(X,Y) = \mathrm{tr}(X^\top Y)$$

$$g_P^H(X,Y) = \mathrm{tr}(P^{-2} X P^{-2} Y)$$

$$g_P^G(X,Y) = \mathrm{tr}(P^{-1} X P^{-1} Y)$$

[Nakamura 2001]

Here, all three connections are metric connections

Information geometry in action! (2/2)

- The **Chernoff information** between two distributions is defined by

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

$$\rho_\alpha[P:Q] := \int p^\alpha q^{1-\alpha} \mathrm{d}\mu = \rho_{1-\alpha}[Q:P].$$

- Chernoff information is the maximal **skew Bhattacharrya distance** (not metric!):

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

- α-Bhattacharrya distances related to **Rényi α-divergences**:

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

$$D_{B,\alpha}[P:Q] = (1-\alpha)\, D_{R,\alpha}[P:Q]$$

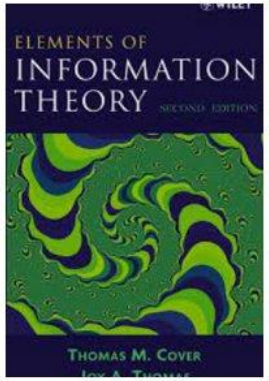
- CI is often used in **Bayesian hypothesis testing & information fusion**

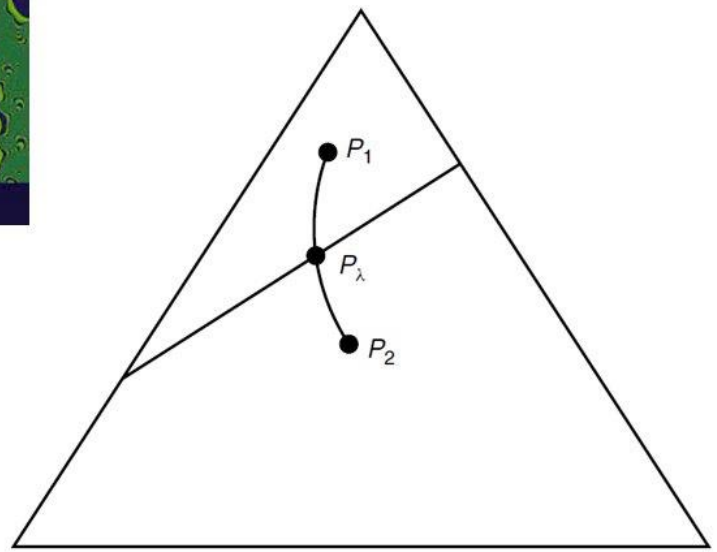
- An information-geometric characterization of Chernoff information, *IEEE Signal Processing Letters* (2013)
- Revisiting Chernoff information with likelihood ratio exponential families, *Entropy* 24.10 (2022)
- Julier, An empirical study into the use of Chernoff information for robust, distributed fusion of Gaussian mixture models , IEEE *Information Fusion* 2006.

Chernoff information: A geometric characterization

$$C(P_1, P_2) \overset{\Delta}{=} -\min_{0\le\lambda\le 1} \log\left(\sum_x P_1^{\lambda}(x) P_2^{1-\lambda}(x)\right)$$

$$= D(P_{\lambda^*}||P_1) = D(P_{\lambda^*}||P_2)$$





$$P_\lambda = \frac{P_1^{\lambda}(x) P_2^{1-\lambda}(x)}{\sum_{a\in\mathcal{X}} P_1^{\lambda}(a) P_2^{1-\lambda}(a)}$$

Probability simplex

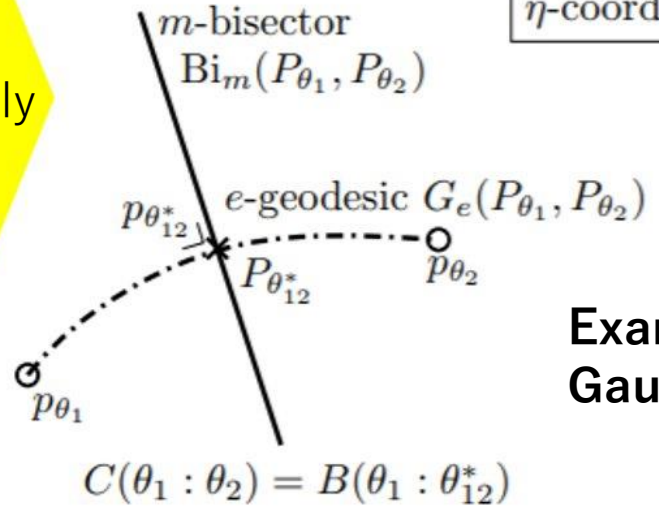
Generalized
to
exponential family
manifold

$$C(P, Q) = -\log \min_{\alpha\in(0,1)} \int p^{\alpha}(x) q^{1-\alpha}(x) \mathrm{d}\nu(x).$$

$$C(P_{\theta_1} : P_{\theta_2}) = B(\theta_1 : \theta_{12}^{(\alpha^*)}) = B(\theta_2 : \theta_{12}^{(\alpha^*)})$$

$$P^* = P_{\theta_{12}^*} = G_e(P_1, P_2) \cap \mathrm{Bi}_m(P_1, P_2)$$

η-coordinate system



Example:
Gaussian manifold

$p(x|\theta) \propto \exp(\langle x, \theta \rangle)$

Exponential family manifold

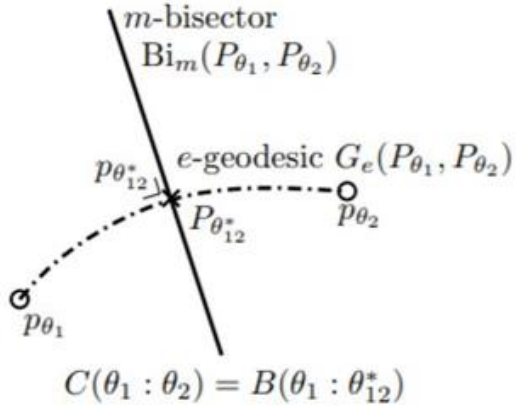
Chernoff-Bregman divergence

- Chernoff information: $C(P_{\theta_1} : P_{\theta_2}) = B(\theta_1 : \theta_{12}^{(\alpha^*)}) = B(\theta_2 : \theta_{12}^{(\alpha^*)})$
- Chernoff-Bregman is another way to symmetrize a Bregman divergence by maximizing the skew Jensen divergence:

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

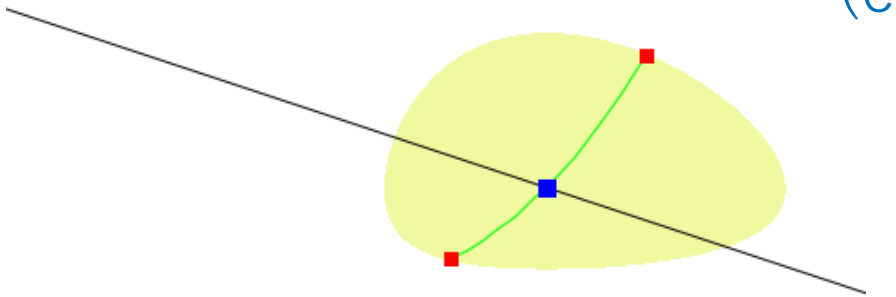
- This amounts to

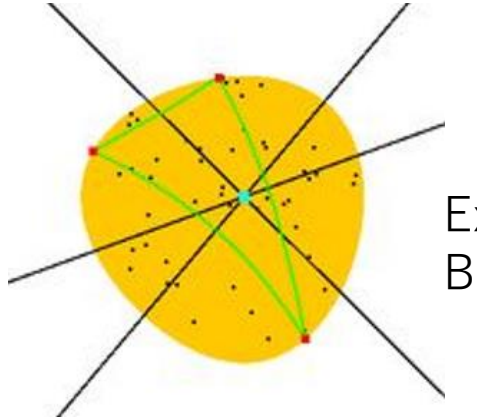
$$C_F(\theta_1, \theta_2) = \min_{\theta} \{B_F(\theta_1 : \theta), B_F(\theta_2 : \theta)\}$$



- Chernoff-Bregman divergence is the radius of a right-sided Bregman ball of two points

Chernoff point r*
(eKLD)





Exact smallest enclosing Bregman ball of n points

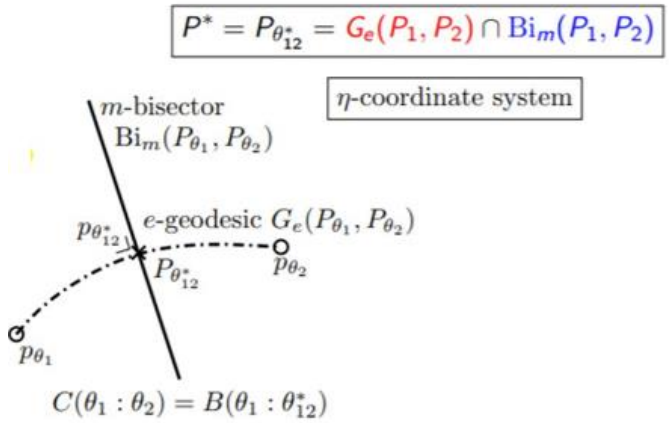
Fitting the smallest enclosing Bregman ball, ECML'05

Categorical distributions: Both an exponential and a mixture family!

	Exponential Family	*	**Mixture Family**
pdf	$p_\theta(x) = \prod_{i=1}^d p_i^{t_i(x)}, p_i = \Pr(x = e_i), t_i(x) \in \{0,1\}, \sum_{i=1}^d t_i(x) = 1$		$m_\theta(x) = \sum_{i=1}^d p_i \delta_{e_i}(x)$
primal θ	$\theta_i = \log \frac{p_i}{p_d}$		$\theta_i = p_i$
$F(\theta)$	$\log(1 + \sum_{i=1}^D \exp(\theta_i))$		$\theta_i \log \theta_i + (1 - \sum_{i=1}^D \theta_i) \log(1 - \sum_{i=1}^D \theta_i)$
dual $\eta = \nabla F(\theta)$	$\frac{e^{\theta_i}}{1+\sum_{j=1}^D \exp(\theta_j)}$		$\log \frac{\theta_i}{1-\sum_{j=1}^D \theta_j}$
primal $\theta = \nabla F^*(\eta)$	$\log \frac{\eta_i}{1-\sum_{j=1}^D \eta_j}$		$\frac{e^{\theta_i}}{1+\sum_{j=1}^D \exp(\theta_j)}$
$F^*(\eta)$	$\sum_{i=1}^D \eta_i \log \eta_i + (1 - \sum_{j=1}^D \eta_j) \log(1 - \sum_{j=1}^D \eta_j)$		$\log(1 + \sum_{i=1}^D \exp(\eta_i))$
Bregman divergence	$B_F(\theta : \theta') = \mathrm{KL}^*(p_\theta : p_{\theta'})$ $= \mathrm{KL}(p_{\theta'} : p_\theta)$		$B_F(\theta : \theta') = \mathrm{KL}(m_\theta : m_{\theta'})$

Dual of categorical exponential family is categorical mixture family, and vice verse

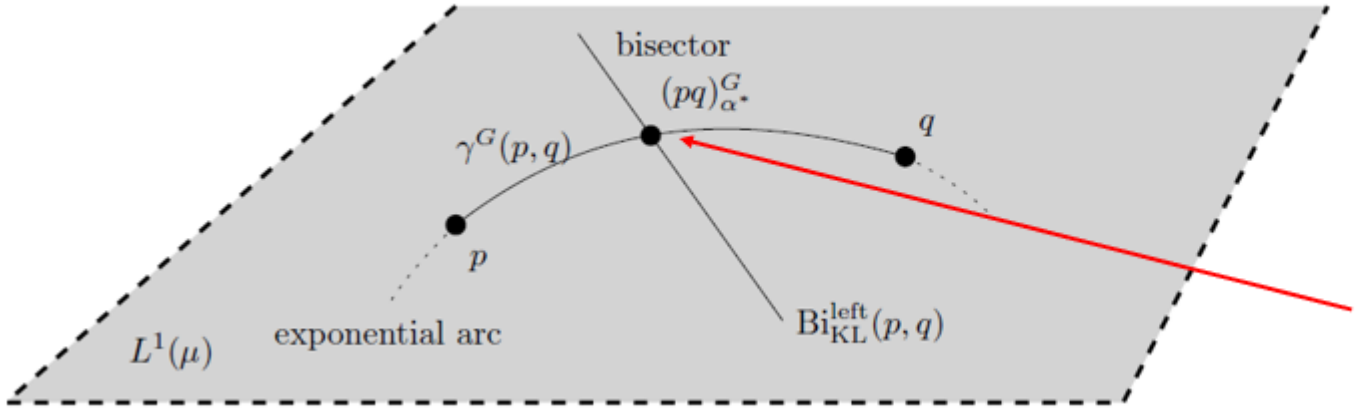
Revisiting Chernoff information/Point



$p(x|\,\theta) \propto \exp(\langle x, \theta \rangle)$

Exponential family manifold

Consider p and q arbitrary probability densities:



Geometric mixture arc

$$(pq)^G_\alpha(x) \propto p(x)^\alpha q(x)^{1-\alpha}$$

Chernoff point: $(pq)^G_{\alpha^*}$

Geometric mixture arc is a 1D likelihood ratio exponential family

- Geometric mixture Bhattacharyya / exponential arc) $(pq)_\alpha^G(x) \propto p(x)^\alpha q(x)^{1-\alpha}$ between two densities p, q of Lebesgue Banach space $L_1(\mu)$

- Set of **geometric mixtures**:

$$\mathcal{E}_{pq} := \left\{ (pq)_\alpha^G(x) := \frac{p(x)^\alpha q(x)^{1-\alpha}}{Z_{pq}(\alpha)} \ : \ \alpha \in \Theta \right\}$$

with **normalization factor**:

$$Z_{pq}(\alpha) = \int_{\mathcal{X}} p(x)^\alpha q(x)^{1-\alpha} \mathrm{d}\mu(x) = \rho_\alpha[p:q]$$

- geometric mixture interpreted as a **1D exponential family**: LREF

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

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

$k(x)=\log q(x)$

$-D_{B,\alpha}[p:q]$

Natural parameter space:

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

LREFs: EF cumulant function is always analytic

- Cumulant function of EF is **strictly convex**

- Cumulant function is neg-Bhattacharyya distance:

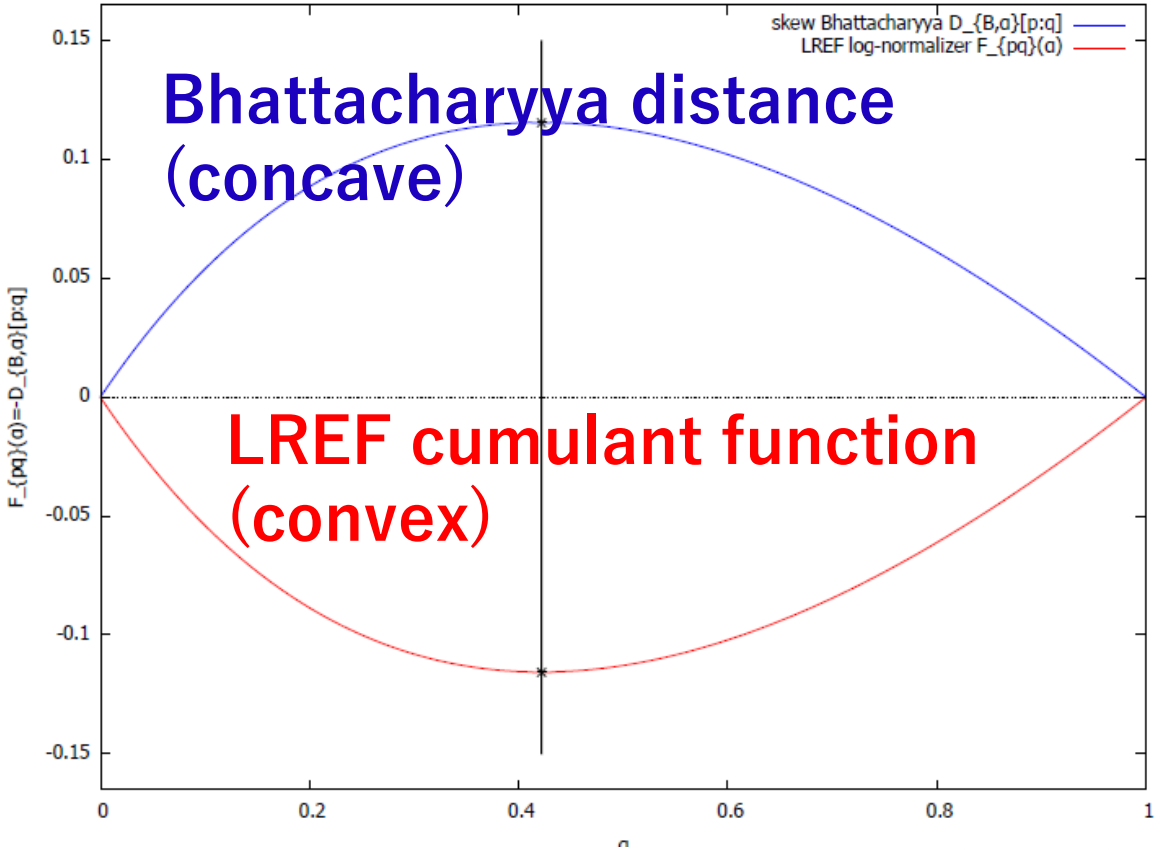
$$F_{pq}(\alpha) = \log Z_{pq}(\alpha) = -D_{B,\alpha}[p:q] < 0$$

⇒ Bhattacharyya. distance is **strictly concave**

- Theorem:

Chernoff exponent exists and is unique

$$D_C[p,q] = D_{B,\alpha^*(p:q)}(p:q) = D_{B,\alpha^*(q:p)}(q:p) = D_C[q,p].$$



p=N(0,1) q=N(1,2)

$$(pq)_\alpha^G(x) \propto p(x)^\alpha q(x)^{1-\alpha}$$

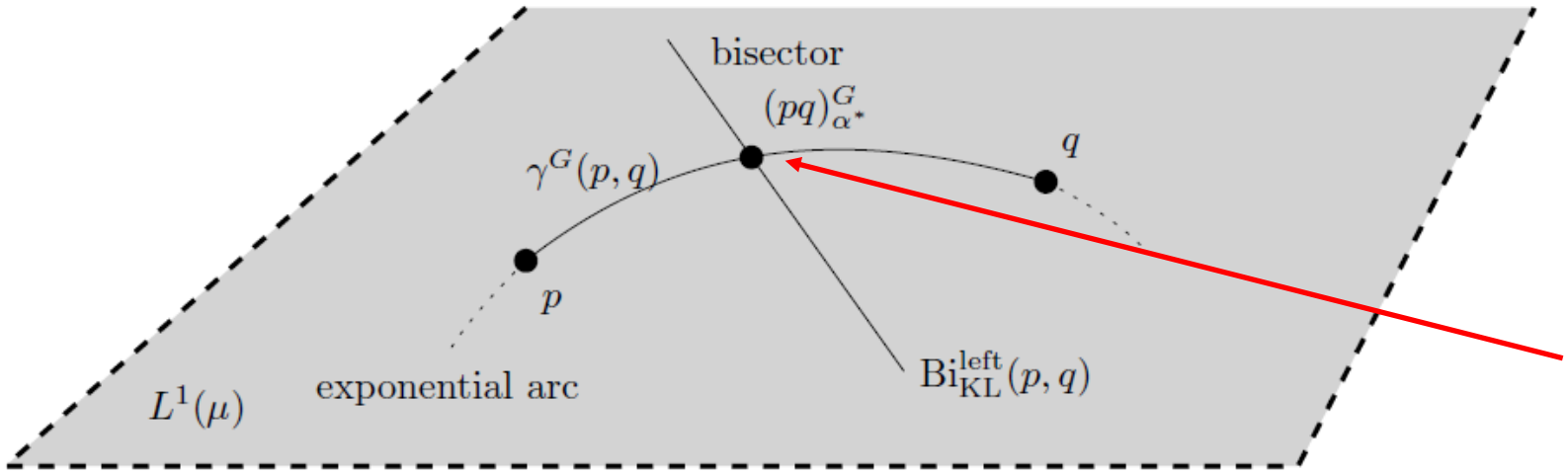
Geometric interpretation for densities on $L_1(\mu)$

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

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

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

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



Chernoff point: $(pq)^G_{\alpha^*}$

Outline

- Bregman divergences with a single generator and a pair of generators

- Bregman manifolds

  -Normalized/unnormalized exponential families and Bregman divergences

  -Fisher-Rao distance and arithmetic-harmonic mean on the SPD manifold

- Further information geometry in action!

  - Jensen-Shannon centroid on a mixture family manifold

  - Chernoff information and 1D exponential family geometric arc manifolds

- **Bregman divergence with respect to comparative convexity**

Summary

- Bregman divergences: arbitrarily well approximated by **Bregman chord divergences** or **skewed Jensen divergences** without using gradient ∇F
- **Jensen-Shannon centroid** on **mixture family manifold** using ConCave-Convex procedure
- Chernoff information on **exponential family manifold** using exact geometric characterization ``**Chernoff point**'' = unique intersection of primal geodesic with dual bisector
- Define Bregman divergences with respect to (M,N)-convexity:

  (M,N)-Bregman divergences as **conformal Bregman divergences**

  Convex-preserving (ρ, τ)-deformations
- **Duality:** biduality reference/representation from convex duality

Bregman manifolds have Hessian metrics

- The metric g of a Bregman manifold (M, g, ∇, ∇^*) is **Hessian**:

$\mathbf{g(\theta) = \nabla^2 F(\theta)}$ and $\mathbf{g(\eta) = \nabla^2 F^*(\eta)}$

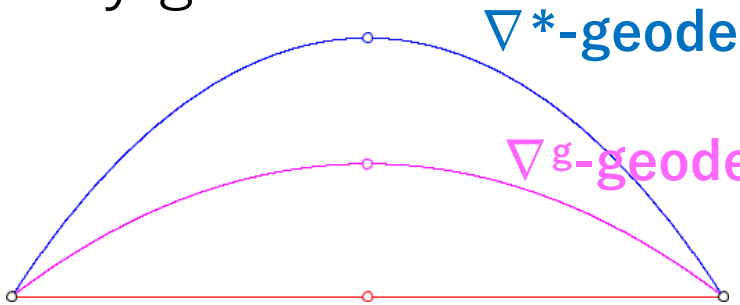
Hessian $\nabla^2 = \nabla\nabla^\top$

- The dual basis e(p) and e*(p) in tangent planes T_p are reciprocal:

$g(e_i, e^{*j}) = \delta_i^j$.

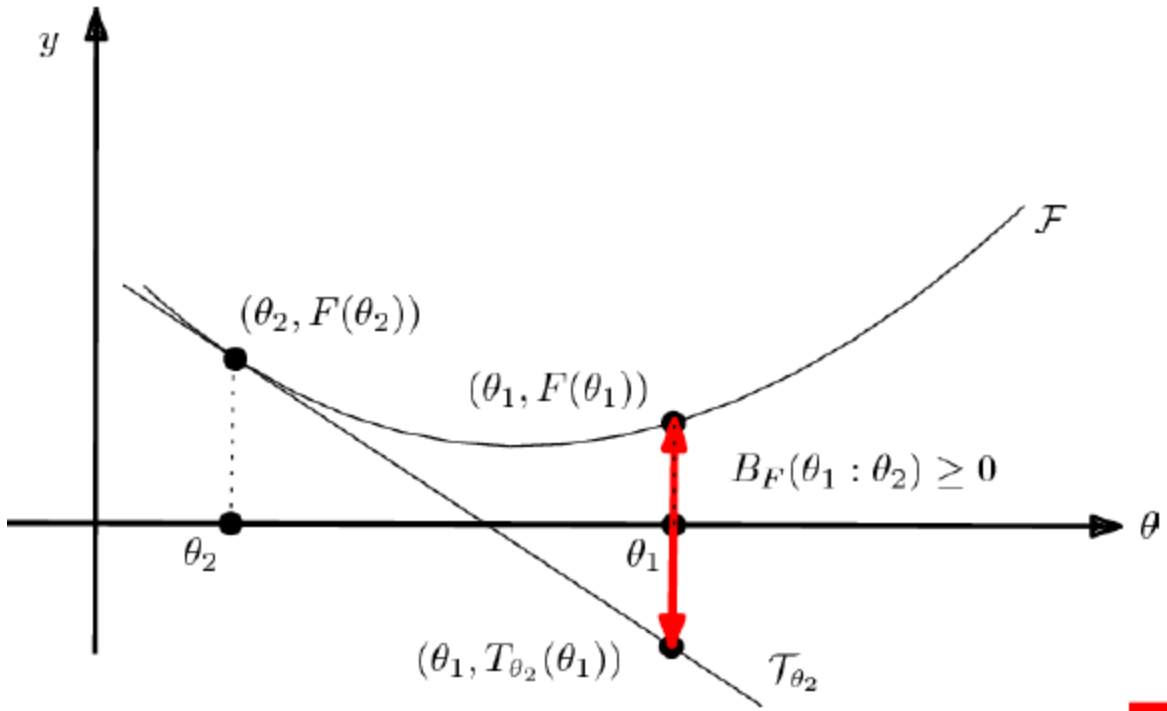
Crouzeix identity: $\nabla^2 F(\theta)\ \nabla^2 F^*(\eta(\theta)) = \nabla^2 F(\theta(\eta))\ \nabla^2 F^*(\eta) = I$

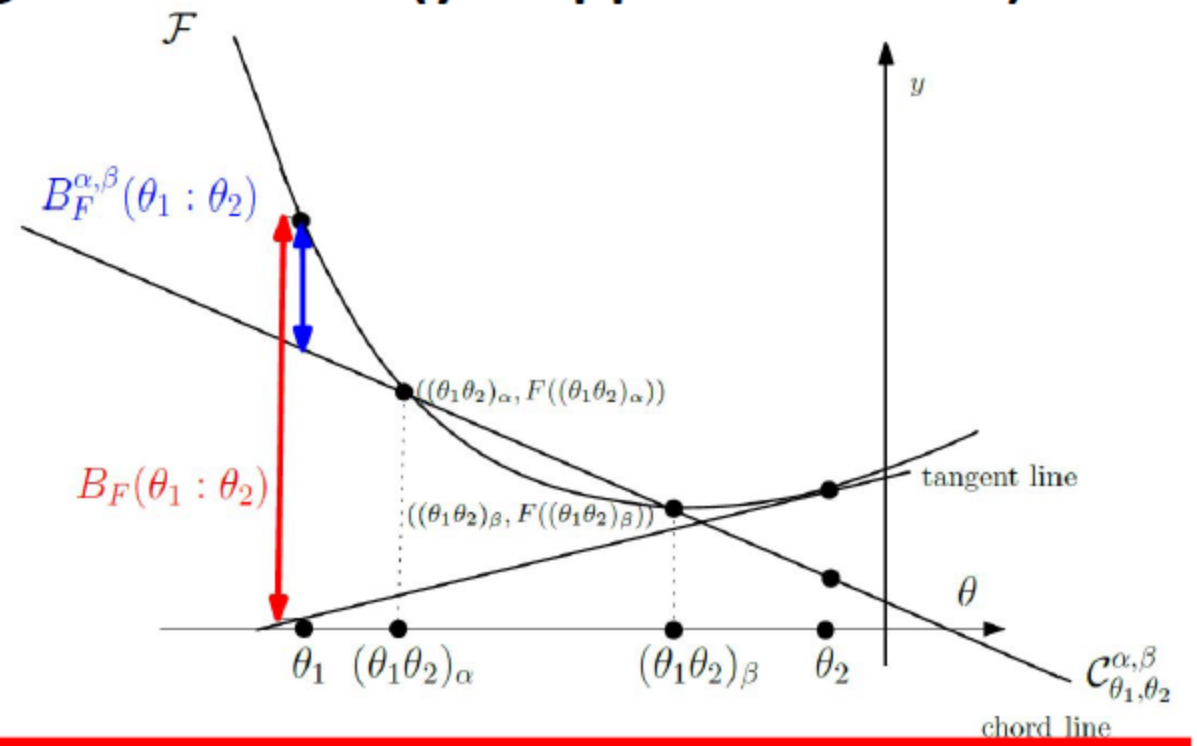
- Riemannian manifold (M,g) is not flat with respect to the Levi-Civita connection ∇^g induced by g



Scalar Bregman chord divergences

Idea: *Get rid of the gradient* in the Bregman formula (yet approximate BD)





$$B_F(\theta_1 : \theta_2) = F(\theta_1) - T_{\theta_2}(\theta_1)$$

$$T_\theta(\omega) := F(\theta) + (\omega - \theta)F'(\theta)$$

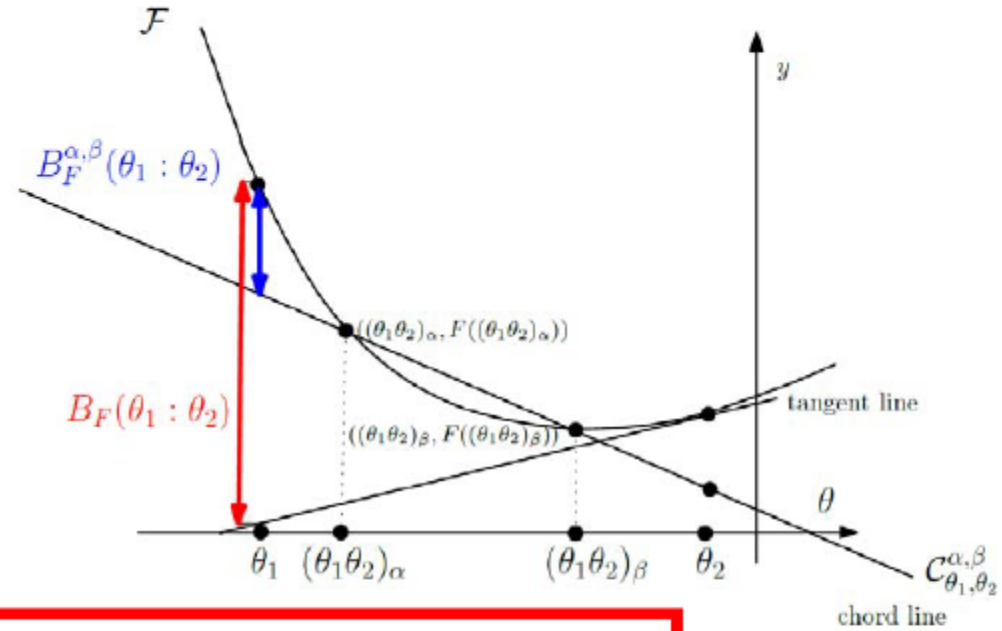
$$B_F^{\alpha,\beta}(\theta_1 : \theta_2) := F(\theta_1) - C_F^{(\theta_1\theta_2)_\alpha,(\theta_1\theta_2)_\beta}(\theta_1)$$

$$B_F^{\alpha,\beta}(\theta_1 : \theta_2) \leq B_F(\theta_1 : \theta_2)$$

Linear interpolation (LERP): $(pq)_\lambda := (1-\lambda)p + \lambda q$

Scalar Bregman chord divergences

$$B_F^{\alpha,\beta}(\theta_1 : \theta_2) := F(\theta_1) - C_F^{(\theta_1\theta_2)_\alpha,(\theta_1\theta_2)_\beta}(\theta_1)$$



$$\begin{aligned} B_F^{\alpha,\beta}(\theta_1 : \theta_2) &:= F(\theta_1) - \Delta_F^{\alpha,\beta}(\theta_1,\theta_2)(\theta_1 - (\theta_1\theta_2)_\alpha) - F((\theta_1\theta_2)_\alpha), \\ &= F(\theta_1) - F((\theta_1\theta_2)_\alpha) + \frac{\alpha\{F((\theta_1\theta_2)_\alpha) - F((\theta_1\theta_2)_\beta)\}}{\beta - \alpha} \end{aligned}$$

where the *slope of the chord* is $\Delta_F^{\alpha,\beta}(\theta_1,\theta_2) := \frac{F((\theta_1\theta_2)_\alpha) - F((\theta_1\theta_2)_\beta)}{(\theta_1\theta_2)_\alpha - (\theta_1\theta_2)_\beta}$

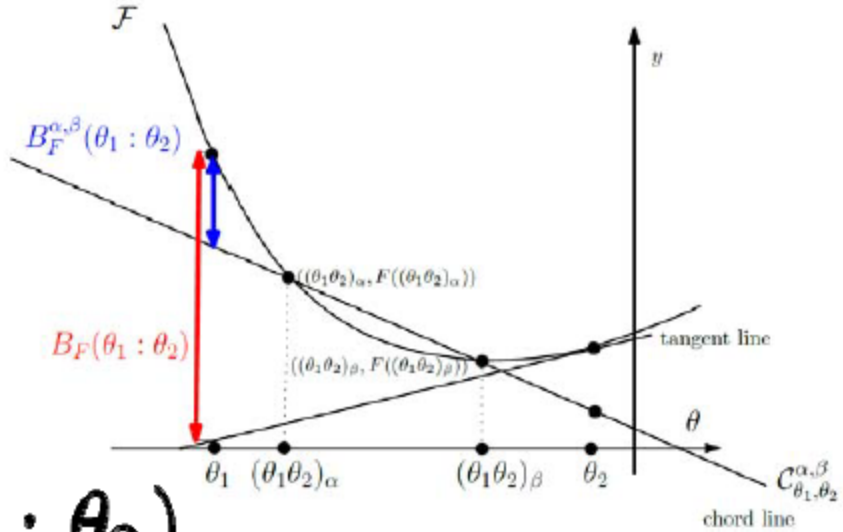
Scalar Bregman chord divergences: Properties

- Symmetry:

$$B_F^{\alpha,\beta}(\theta_1 : \theta_2) = B_F^{\beta,\alpha}(\theta_1 : \theta_2)$$

- Generalization of BD:

$$\lim_{\alpha\to 0,\beta\to 1} B_F^{\alpha,\beta}(\theta_1 : \theta_2) = B_F(\theta_1 : \theta_2).$$



- Subfamily of **Bregman tangent divergences**:

$$B_F^{\alpha}(\theta_1 : \theta_2) = \lim_{\beta\to\alpha} B_F^{\alpha,\beta}(\theta_1 : \theta_2) \leq B_F(\theta_1 : \theta_2)$$

$$\begin{aligned} B_F^{\alpha}(\theta_1 : \theta_2) &:= F(\theta_1) - F((\theta_1\theta_2)_\alpha) - (\theta_1 - (\theta_1\theta_2)_\alpha)^\top \nabla F((\theta_1\theta_2)_\alpha), \\ &= F(\theta_1) - F((\theta_1\theta_2)_\alpha) - \alpha(\theta_1 - \theta_2)^\top \nabla F((\theta_1\theta_2)_\alpha), \end{aligned}$$

Summary

- Bregman divergences induce dually flat spaces for **any** Legendre-type C^3 strictly convex generator
- When the generator is an integral from statistical models, we can **reconstruct a statistical divergence**:

  -Reverse KLD from cumulant function of exponential families, rev ext KLD from partition function

  -KLD from negentropy of mixture families

- Jensen-Shannon centroid on **mixture family manifold** using concave-convex algorithm
- Chernoff information on **exponential family manifold** using exact geometric characterization ``Chernoff point'' = unique intersection of primal geodesic with dual bisector

- Define Bregman divergences with respect to **(M,N)-convexity**:

(M,N)- Bregman divergences as conformal Bregman divergences

- **Duality and conjugacies** (convex duality, reference/representation biduality, connection duality) are at the heart of information geometry!

Jensen-Shannon centroid of categorical distributions

Input: A set $\{p_i = (p_i^1, \ldots, p_i^d)\}_{i \in [n]}$ of n categorical distributions belonging to the $(d-1)$-dimensional probability simplex Δ_{d-1}

Input: T: The number of CCCP iterations

Output: An approximation ${}^{(T)}\bar{p}$ of the Jensen–Shannon centroid $\bar{p}$ minimizing $\sum_i D_{\mathrm{JS}}(c, p_i)$

/* Convert the categorical distributions to their natural parameters by dropping the last coordinate */

$\theta_i^j = p_i^j$ for $j \in \{1, \ldots, d-1\}$;

/* Initialize the JS centroid */

$t \leftarrow 0$;

${}^{(0)}\bar{\theta} = \frac{1}{n} \sum_{i=1} \theta_i$;

/* Convert the initial natural parameter of the JS centroid to a categorical distribution */

${}^{(0)}\bar{p}^j = {}^{(0)}\bar{\theta}^j$ for $j \in \{1, \ldots, d-1\}$;

${}^{(0)}\bar{p}^d = 1 - \sum_{i=1}^{d} {}^{(0)}\bar{p}^j$;

/* Perform the ConCave-Convex Procedure (CCCP) */

while $t \leq T$ **do**

  /* Use $\nabla F(\theta) = \left[\log \frac{\theta_i}{1 - \sum_{j=1}^{D} \theta_i}\right]_i$ and $\nabla F^{-1}(\eta) = \frac{1}{1 + \sum_{j=1}^{D} \exp(\eta_j)} [\exp(\eta_i)]_i$ */

  ${}^{(t+1)}\theta = (\nabla F)^{-1}\left(\frac{1}{n} \sum_i \nabla F\left(\frac{\theta_i + {}^{(t)}\theta}{2}\right)\right)$;

  $t \leftarrow t + 1$;

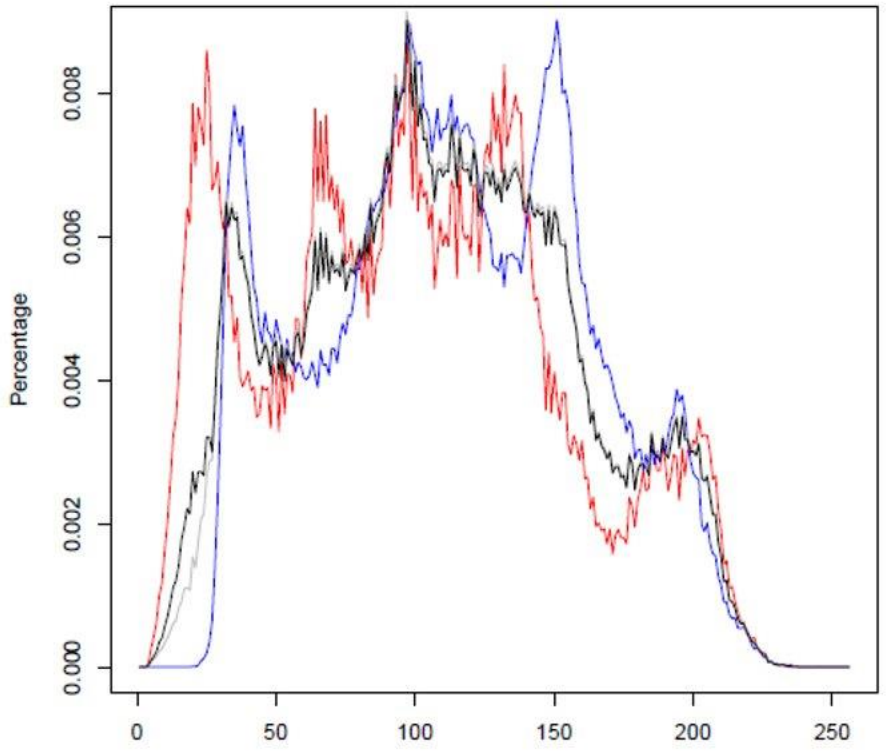
end

/* Convert back the natural parameter to the categorical distribution of the approximated Jensen-Shannon centroid */

${}^{(T)}\bar{p}^j = {}^{(T)}\bar{\theta}^j$ for $j \in \{1, \ldots, d-1\}$;

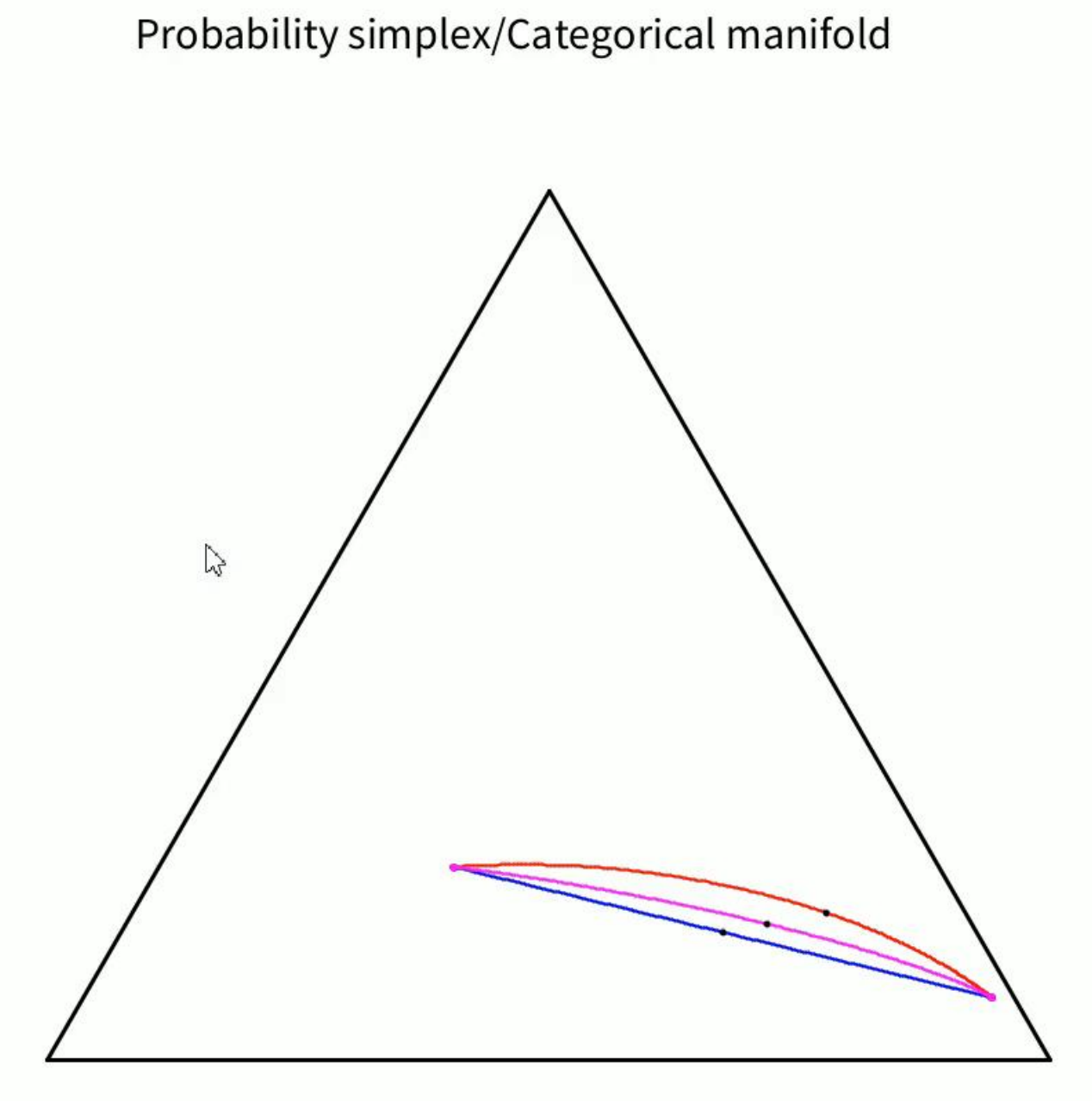
${}^{(T)}\bar{p}^d = 1 - \sum_{i=1}^{d} {}^{(T)}\bar{p}^j$;

return ${}^{(T)}\bar{p}$;

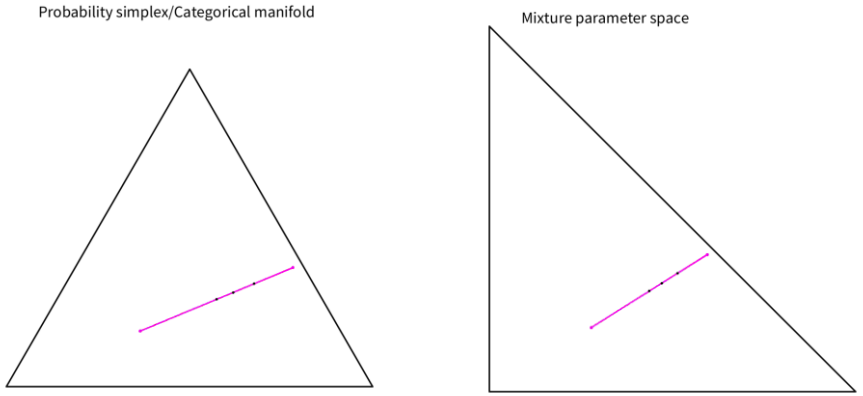


- Use the fact that the set of categorical distributions is a **mixture family** in information geometry

JSD centroid = Jensen centroid



Geodesics coincide when passing through a simplex vertex but not the midpoints



Exponential ∇-geodesic

Mixture ∇^*-geodesic

Fisher-Rao ∇^g-geodesic
(Levi-Civita)

Proof: KLD non-normalized EFs = BD wrt Z

$$D_{KL}^{+}[q_{\theta 1}(x):q_{\theta 2}(x)]=\int \{ q_{\theta 1}(x) \log (q_{\theta 1}(x)/q_{\theta 2}(x))+ q_{\theta 2}(x)-q_{\theta 1}(x) \} d\mu(x)$$
$$= Z(\theta_2)-Z(\theta_1) + E_{q\theta 1}[<(\theta_1- \theta_2),x>]$$

Recall "moment parameter": $E_{p\theta}[x]= \eta = \nabla F(\theta_1)$

But $E_{q\theta 1}[x] = Z(\theta_1)\ E_{p\theta 1}[x] = Z(\theta_1)\ \eta_1 = Z(\theta_1)\ \nabla F(\theta_1)$

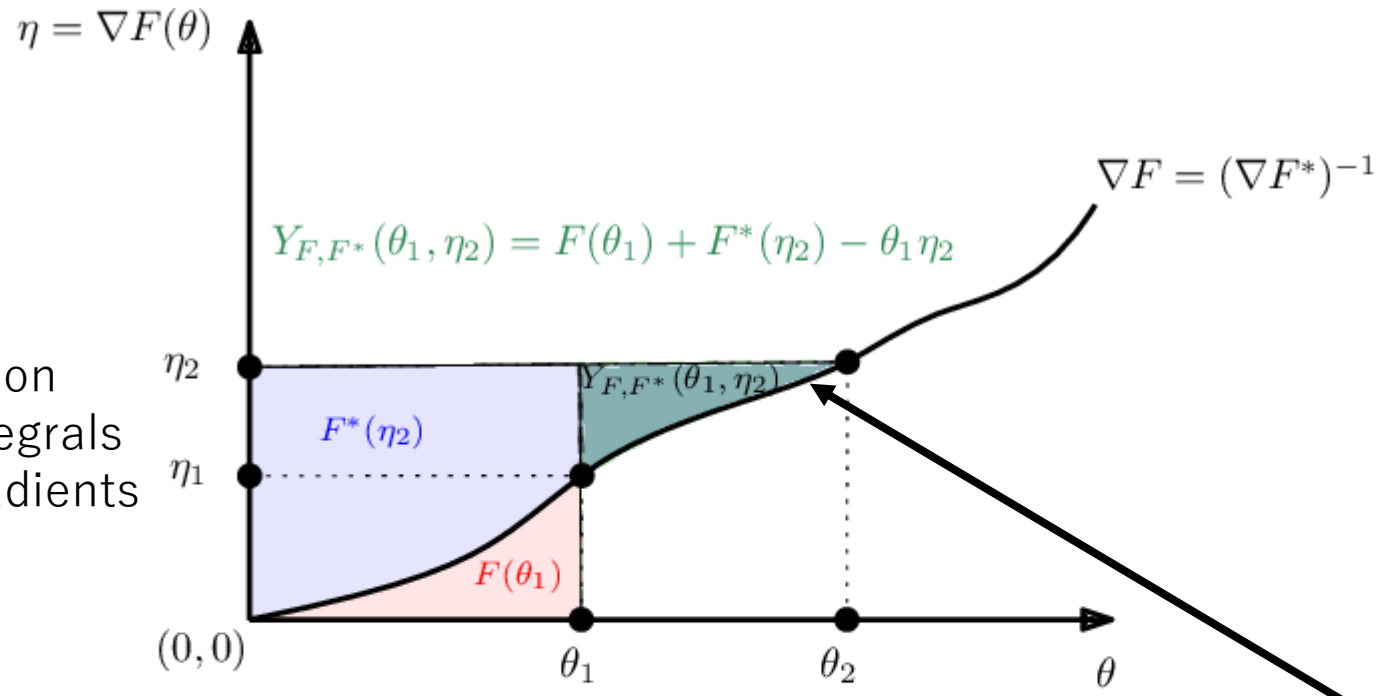
Since $F(\theta) = \log Z(\theta)$, we have $\nabla F(\theta) = \nabla Z(\theta)/Z(\theta)$

Hence, $\mathbf{E_{q\theta 1}[x]} = Z(\theta_1)\ \nabla F(\theta_1) = Z(\theta_1)\ \nabla Z(\theta_1)/Z(\theta_1) = \mathbf{\nabla Z(\theta_1)}$

$$\mathbf{D_{KL}^{+}[q_{\theta 1}(x):q_{\theta 2}(x)] = Z(\theta_2) - Z(\theta_1) - < \theta_2 - \theta_1, \nabla Z(\theta_1)> = B_Z(\theta_2: \theta_1)}$$

Visual interpretation of Fenchel-Young divergences

Area interpretation derived from integrals of monotone gradients



F strictly convex
F''>0
F' ↗ strictly increasing