Computational information geometry on Bregman manifolds and submanifolds

Frank Nielsen

Sony Computer Science Laboratories, Inc.

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Outline of the talk

- Bregman divergences with some extensions
- Geometry of Bregman balls
- Two applications on Bregman manifolds:
  - Jensen-Shannon centroid on a mixture family manifold
  - Chernoff information/point on an exponential family manifold

Bregman divergences (1960's)

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

- $F: \Theta \subseteq \mathbb{R}^m \to \mathbb{R}$ a strictly convex and smooth

real-valued function on a finite dim. Hilbert space $\langle .,. \rangle$

Bregman divergence $B_F: \Theta \times \mathrm{RelInt}(\Theta) \to \mathbb{R}_{\geq 0}$

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

Smooth measure of discrepancy, not a metric distance because it violates the triangle inequality, and is asymmetric when F is not quadratic function. Hence the delimiter notation ":" instead of $B_F(\theta_1, \theta_2)$

BD interpreted as **remainder** of a first order Taylor expression of $F(\theta_1)$ around θ_2:

$$F(\theta_1) = F(\theta_2) + \langle \theta_1 - \theta_2, \nabla F(\theta_2) \rangle + \underbrace{B_F(\theta_1 : \theta_2)}_{\text{Taylor remainder}}$$

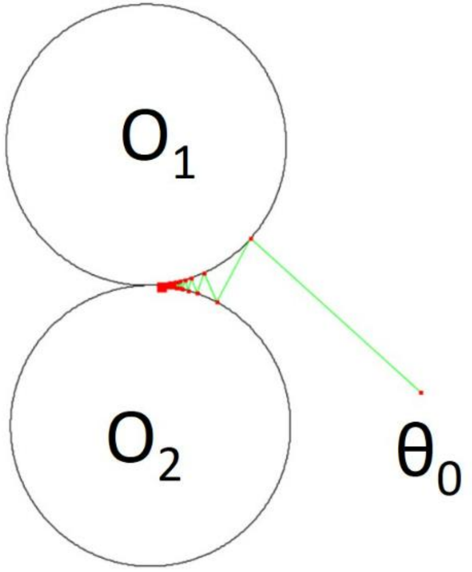
Example of remainder: **Lagrange remainder** (smooth C^2 generators): $\nabla^2 F$ **SPD** $\Rightarrow B_F(\theta_1 : \theta_2) \geq 0$

$$B_F(\theta_1 : \theta_2) = \tfrac{1}{2} (\theta_2 - \theta_1)^T \nabla^2 F(\theta) (\theta_2 - \theta_1) \geq 0, \ \theta \in [\theta_1 \theta_2]$$

BDs: Versatile and popular in OR, ML, IT, signal processing

Originally motivated for finding an intersection point in a set of convex objects using **Bregman projections**.
(ex. of convex objects: halfspaces, balls, etc.)

convex feasibility of
Bregman cyclic projections



$\theta_0 \in \Theta, t \leftarrow 0$

$$\boxed{\theta_{t+1} = \arg \min_{\theta \in O_{1+(t \mod n)}} B_F(\theta_t : \theta)}$$

BDs unify:

- *squared Euclidean divergence* $F(\theta) = \frac{1}{2} \sum_i \langle \theta, \theta \rangle$
- *Kullback-Leibler divergence* $F(\theta) = \sum_i \theta_i \log(\theta_i)$ (relative Shannon entropy)
- *Itakura-Saito divergence* $F(\theta) = \sum_i -\log(\theta_i)$ (relative Burg entropy)

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

L22 (β =2), KLD ($\beta \to 0$), ISD (β =1), belong to a *family* of **β-divergences**, learn ad hoc $\beta \geq 0$

x,y>0, $\beta \geq 0$

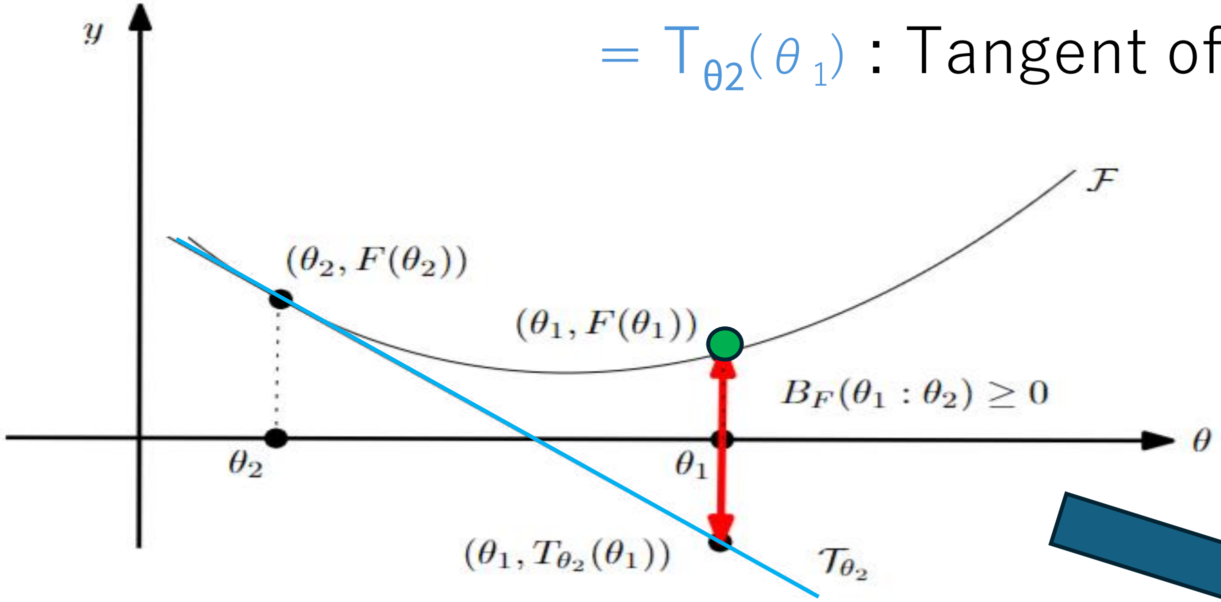
$$d_\beta(x|y) = \begin{cases} \frac{x}{y} - \log(\frac{x}{y}) - 1 & \beta = 0 \\ x(\log x - \log y) + (y - x) & \beta = 1 \\ \frac{x^\beta + (\beta-1)y^\beta - \beta x y^{\beta-1}}{\beta(\beta-1)} & \beta \in \mathbb{R}\backslash\{0,1\} \end{cases}$$

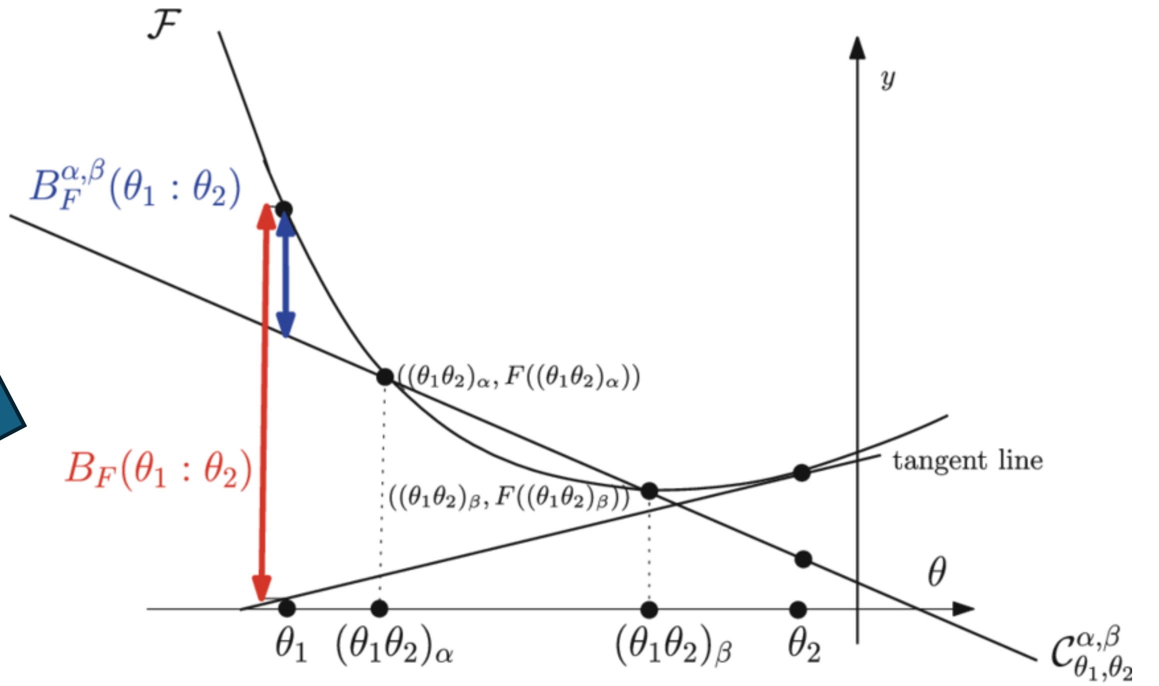
Bregman Generator: $$\phi_\beta(x) = \begin{cases} -\log x + x - 1 & \beta = 0 \\ x \log x - x + 1 & \beta = 1 \\ \frac{x^\beta}{\beta(\beta-1)} - \frac{x}{\beta-1} + \frac{1}{\beta} & \text{otherwise.} \end{cases}$$

Geometric interpretation as a **vertical gap** using the graph $(\theta, F(\theta))$:

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

$= T_{\theta_2}(\theta_1)$: Tangent of the function graph at θ_2 evaluated at θ_1





Design novel divergences from graph of convex functions···

Example: **Bregman chord divergence**, **application**: zero-order optimization in ML

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

Bregman divergences in machine learning…

- Kullback-Leibler divergence between two probability densities:

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

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

- But Kullback-Leibler divergence between two probability densities of a **natural exponential family** with densities $p(x|\theta) \propto \exp(\langle x, \theta \rangle)$ amount to a **reverse Bregman divergence** $B_F^{rev}(\theta_1 : \theta_2) := B_F(\theta_2 : \theta_1)$

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

Bypass the ∫, ∇F in BD easy to calculate! ⇒ Easy calculations of KLDs

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)

Representational Bregman divergences (2009)

- Use a **representation function** R :

$$B_{F,R}(\lambda_1 : \lambda_2) := B_F(R(\lambda_1) : R(\lambda_2))$$
$$= F(R(\lambda_1)) - F(R(\lambda_2)) - \langle R(\lambda_1) - R(\lambda_2), \nabla F(R(\lambda_2)) \rangle$$

Note that $F \circ R$ may not be a Bregman generator, i.e., not be strictly convex.

For example, consider the KLD between two densities of a **generic exponential family (natural parameter from representation function)**

$$p_\lambda(x) \propto \tilde{p}_\lambda(x) = \exp(\langle \theta(\lambda), t(x) \rangle)\, h(x)$$ include normal, Gamma/Beta, Wishart, Poisson, etc.

$\theta(\lambda)$: natural parameter corresponding to λ, representation function $R(.) = \theta(.)$

$$D_{KL}[p(x|\lambda_1) : p(x|\lambda_2)] = B_F^{rev}(\theta(\lambda_1) : \theta(\lambda_2)) = B_F(\theta(\lambda_2) : \theta(\lambda_1))$$

NEF density $p(x|\theta) \propto \exp(\langle x, \theta \rangle)$ $\quad D_{KL}[p(x|\theta_1) : p(x|\theta_2)] = B_F^{rev}(\theta_1 : \theta_2) = B_F(\theta_2 : \theta_1)$

Extended α -divergences are representational BDs

α -divergences extended to m-dimensional positive measures are **representational Bregman divergences**:

$$D_\alpha^+(q_1:q_2) = \begin{cases} \frac{4}{1-\alpha^2}\sum_{i=1}^m\left(\frac{1-\alpha}{2}q_1+\frac{1+\alpha}{2}q_2-q_1^{\frac{1-\alpha}{2}}q_2^{\frac{1+\alpha}{2}}\right), & \alpha\in\mathbb{R}\backslash\{-1,1\} \\ {D_{\mathrm{KL}}^*}^+(q_1:q_2) = D_{\mathrm{KL}}^+(q_2:q_1) = \sum_{i=1}^m q_2^i\log\frac{q_2^i}{q_1^i}+q_1^i-q_2^i & \alpha=1 \\ D_{\mathrm{KL}}^+(q_1:q_2) = \sum_{i=1}^m q_1^i\log\frac{q_1^i}{q_2^i}+q_2^i-q_1^i & \alpha=-1. \end{cases}$$

$$\boxed{D_\alpha^+(q_1:q_2) = B_{F_\alpha}(R_\alpha(q_1):R_\alpha(q_2))}$$

Bregman generator: $F_\alpha(r)=\sum_{i=1}^m f_\alpha(r_i), \quad f_\alpha(x)=\begin{cases}\frac{2}{1+\alpha}\left(\frac{1-\alpha}{2}x\right)^{\frac{2}{1-\alpha}}, & \alpha\neq 1\\ \log x, & \alpha=1.\end{cases}$

Representation function: $R_\alpha(q)=(r_\alpha(q_1),\ldots,r_\alpha(q_m)), \quad r_\alpha(x)=\frac{2}{1-\alpha}x^{\frac{1-\alpha}{2}}$

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

"The dual Voronoi diagrams with respect to representational Bregman divergences." IEEE ISVD *2009*

Convex duality via Legendre-Fenchel transform

- Legendre-Fenchel transform of a convex function F:

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

- Problem: some *tricky functions* with gradient map ∇F domain not convex…

  Example: $h(\xi_1,\xi_2)=[(\xi_1^2/\xi_2)+\xi_1^2+\xi_2^2]/4$ on upper plane domain $\Xi=(\xi_1,\xi_2)$

- Thus, we consider "**nice convex functions**" = **Legendre-type functions $(\Theta, F(\theta))$**

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

Then we get:

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

❷ conjugation yields $(H,F^*(\eta))$ 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 divergences & convex duality

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

$$Y_{F,F^*}(\theta_1, \eta_2) = F(\theta_1)+F^*(\eta_2) - \langle \theta_1, \eta_2 \rangle \geq 0$$

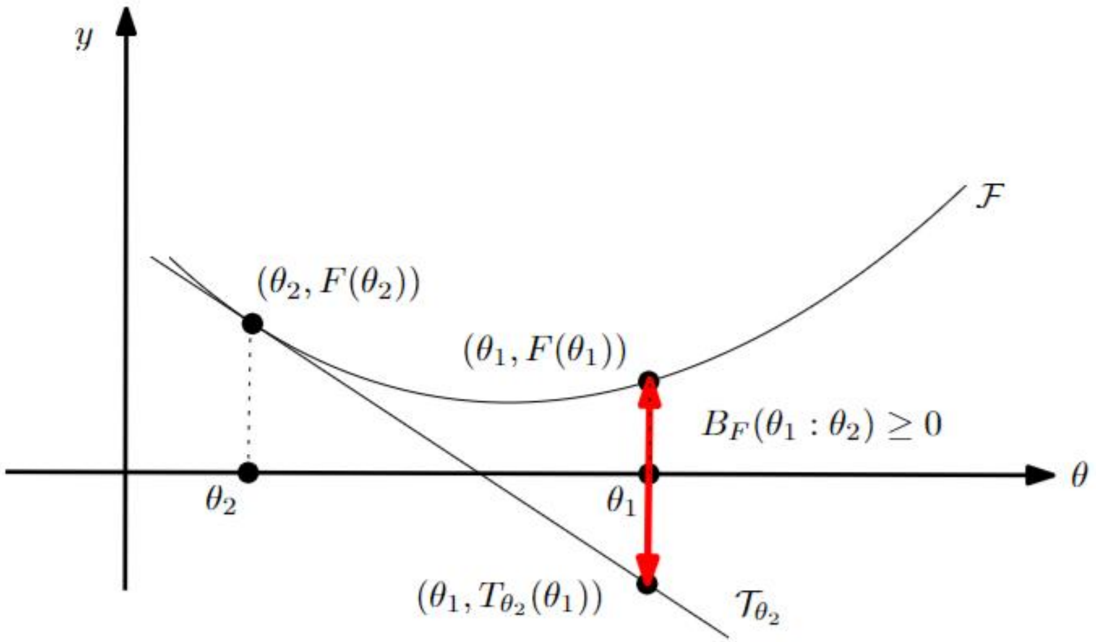
- **Mixed parameterizations** θ and η : $B_F(\theta_1 : \theta_2) = Y_{F,F^*}(\theta_1, \eta_2)$
- Duality: $\mathbf{B_F(\theta_1 : \theta_2)} = \mathbf{Y_{F,F^*}(\theta_1, \eta_2)} = \mathbf{Y_{F^*,F}(\eta_2, \theta_1)} = \mathbf{B_{F^*}(\eta_2, \eta_1)}$
- Dual BDs + Dual FYs from involution $F^{**}=F$
- Note : $B_F(\theta_1 : \theta_2)=0 \Leftrightarrow \theta_1 = \theta_2 \Leftrightarrow \eta_1 = \eta_2$ i.e., $\nabla F(\theta_1) = \nabla F(\theta_2)$

(FY initially called Legendre-Fenchel divergences…)

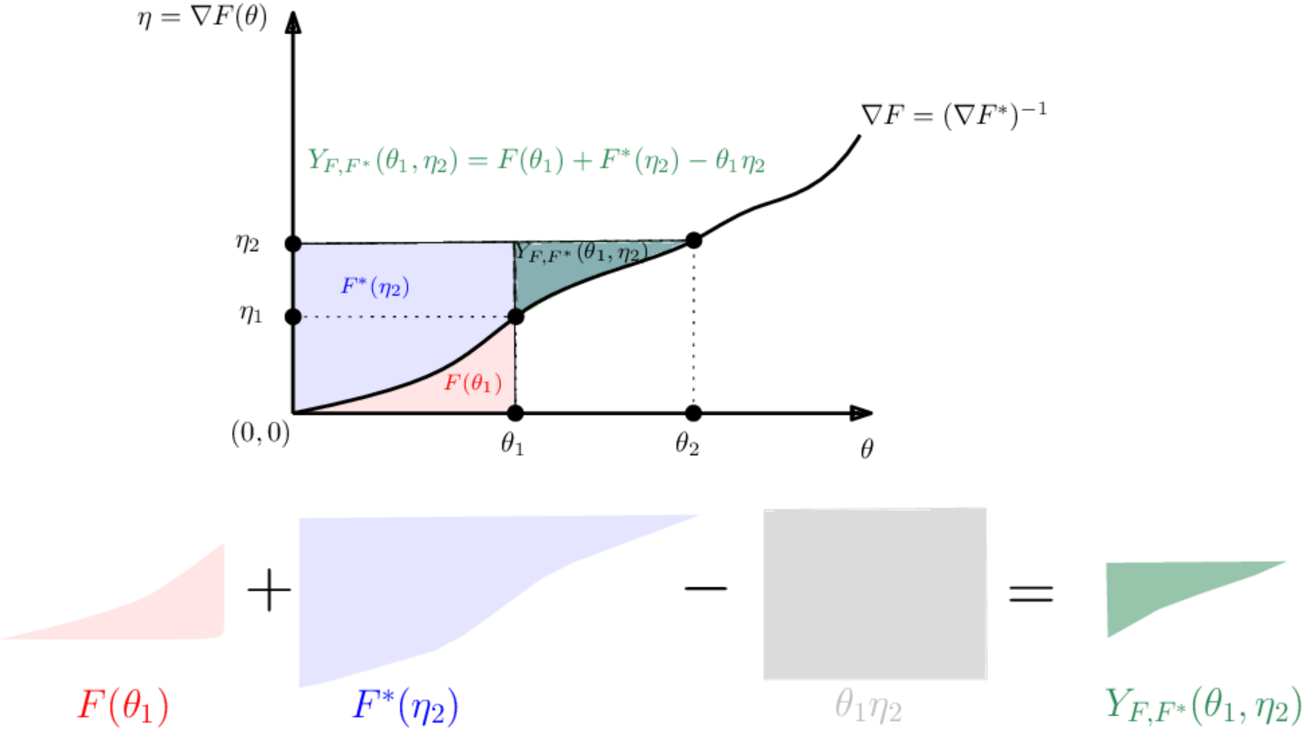
Bregman divergence vs Fenchel-Young divergence

Same parameterization $B_F(\theta_1 : \theta_2) = Y_{F,F^*}(\theta_1, \eta_2)$ **mixed parameterization**

F strictly convex and differentiable



F' ↗ strictly increasing



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

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

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: $p(x|\theta) = \exp(\langle x, \theta\rangle - F(\theta)) \, d\mu(x)$
  - Non-normalized: $q(x|\theta) = \exp(\langle x, \theta\rangle) \, d\mu(x)$
- Hence, $p(x|\theta) = q(x|\theta)/Z(\theta)$ with **partition function** $Z(\theta)=\exp(F(\theta))$ and **cumulant function** $F(\theta)=\log Z(\theta)$
- When F is convex, Z=exp(F) is log-convex
- log-convex functions are convex functions: So **both F and Z are convex functions**

- KLD between normalized densities = reverse Bregman wrt F:

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

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

$$D_{KL}^{+}[q_{\theta_1}(x):q_{\theta_2}(x)] = B_Z^*[\theta_1:\theta_2] = B_Z[\theta_2:\theta_1]$$

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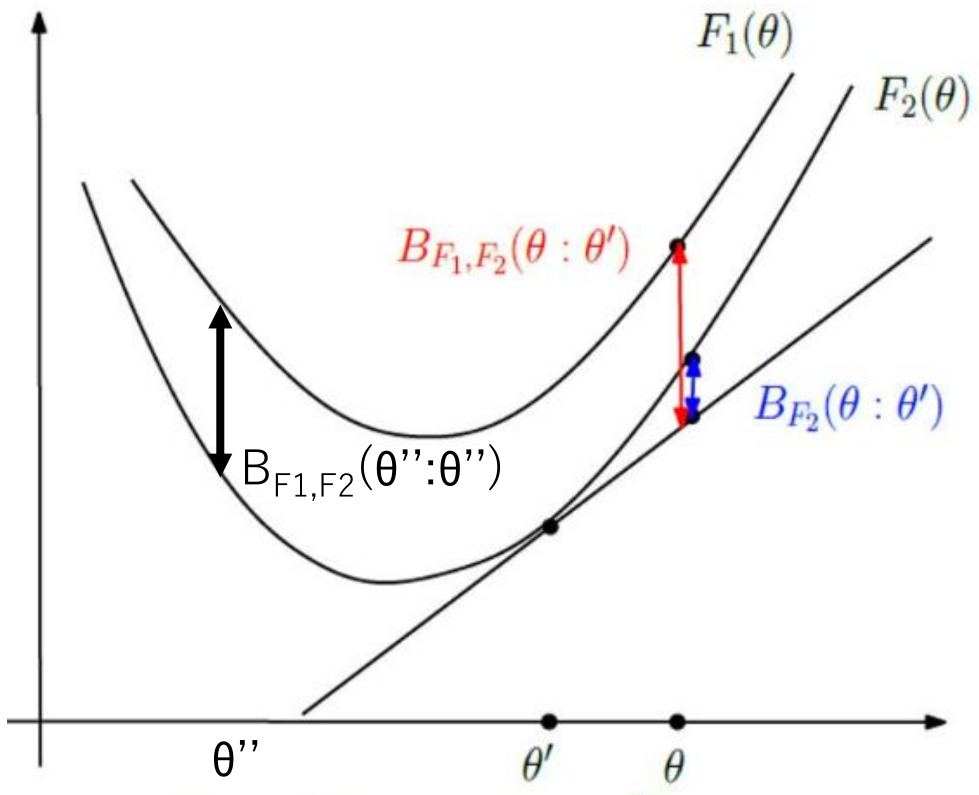
Duo Bregman divergences: Generalize BDs with a pair of generators



One generator **majorizes** the other one:

$$F_1(\theta) \geq F_2(\theta)$$

Then

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

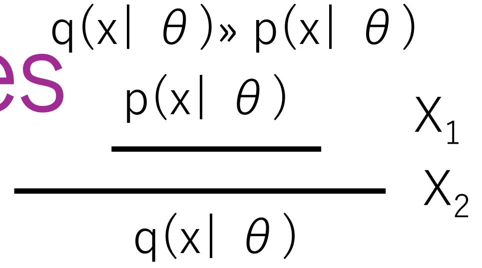
$$\geq B_{F2}(\theta:\theta')$$

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

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

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

KLD between nested exponential families amount to duo Bregman pseudo-divergences



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

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

- Consider an exponential family on support X_1:

$$p(x|\theta) = \exp(\langle x, \theta\rangle - F_1(\theta)) \, d\mu(x)$$

with cumulant function $F_1(\theta)=\log \int_{X_1} \exp(\langle x, \theta\rangle) \, d\mu(x)$

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

$$q(x|\theta) = \exp(\langle x, \theta\rangle - F_2(\theta)) \, d\mu(x)$$

is an exponential family with $F_2(\theta)=\log \int_{X_2} \exp(\langle x, \theta\rangle) \, d\mu(x) \geq F_1(\theta)$

- Then KLD amounts to a **reverse duo Bregman pseudo-divergence**:

$$D_{KL}[p(x|\theta_1) : q(x|\theta_2)] = B_{F_2,F_1}^{rev}(\theta_1 : \theta_2) = B_{F_2,F_1}(\theta_2 : \theta_1)$$

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

Curved Bregman divergences

Consider a domain U which maps to a subset of Θ by $\theta = c(u)$ with $\dim(U) < \dim(\Theta)$:

$B_{F,u}(u_1 : u_2) := B_F(c(u_1) : c(u_2))$ is not Bregman when $\{c(u) \mid u \in U\}$ not convex

usually not a Bregman divergence unless c(.) is affine

Example: Symmetrized Bregman divergences (Jeffreys-Bregman div.) are curved Bregman divergences: $S_F(\theta_1, \theta_2) = \langle \theta_1 - \theta_2, \eta_1 - \eta_2 \rangle$

$$\begin{aligned} S_F(\theta_1 : \theta_2) &= B_F(\theta_1 : \theta_2) + B_F(\theta_2 : \theta_1), \\ &= B_F(\theta_1 : \theta_2) + B_{F^*}(\nabla F(\theta_1) : \nabla F(\theta_2)) \\ &= \breve{B}_{F_\xi}(\xi(\theta_1) : \xi(\theta_2)), \end{aligned}$$

$$F^*(\eta) = \langle \theta, \eta \rangle - F(\theta) \qquad F_\xi(\theta, \eta) := F(\theta) + F^*(\eta) \qquad \xi(\theta) = (\theta, \nabla F(\theta))$$

$$\mathcal{U} = \{(\theta, \nabla F(\theta)) : \theta \in \Theta\}$$

m-dimensional submanifold in 2m-dimensional space

Curved Bregman centroid is the Bregman projection of the full Bregman centroid

Theorem:

$$\arg\min_{u\in\mathcal{U}} \sum_{i=1}^{n} w_i\, B_F(\theta_i : \theta(u)) = \arg\min_{u\in\mathcal{U}} B_F(\bar\theta : \theta(u))$$

[Bregman projection]

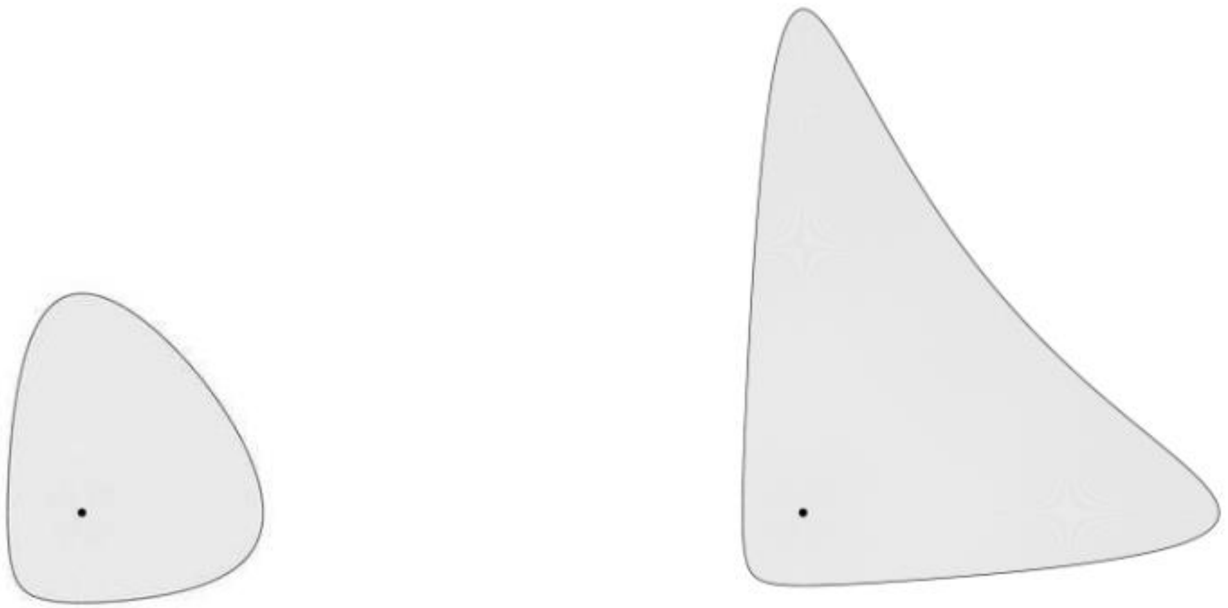
$$\theta_i = \theta(u_i) \qquad \bar\theta = \textstyle\sum_i w_i\theta_i$$

Proof.

$$\begin{aligned}
\min_{u\in\mathcal{U}} \sum_{i=1}^{n} w_i\, B_F(\theta_i : \theta(u)) &= \sum_{i=1}^{n} w_i(F(\theta_i) - F(\theta(u)) - \langle \theta_i - \theta(u), \nabla F(\theta(u))\rangle),\\
&\equiv -F(\theta(u)) - \langle \bar\theta - \theta(u), \nabla F(\theta(u))\rangle,\\
&\equiv F(\bar\theta) - F(\theta(u)) - \langle \bar\theta - \theta(u), \nabla F(\theta(u))\rangle\\
&= B_F(\bar\theta : \theta(u)).
\end{aligned}$$

"What is... an information projection?" Notices of the AMS 65.3 (2018): 321-324.

Space of Bregman balls



Example:
Itakura-Saito right and left spheres

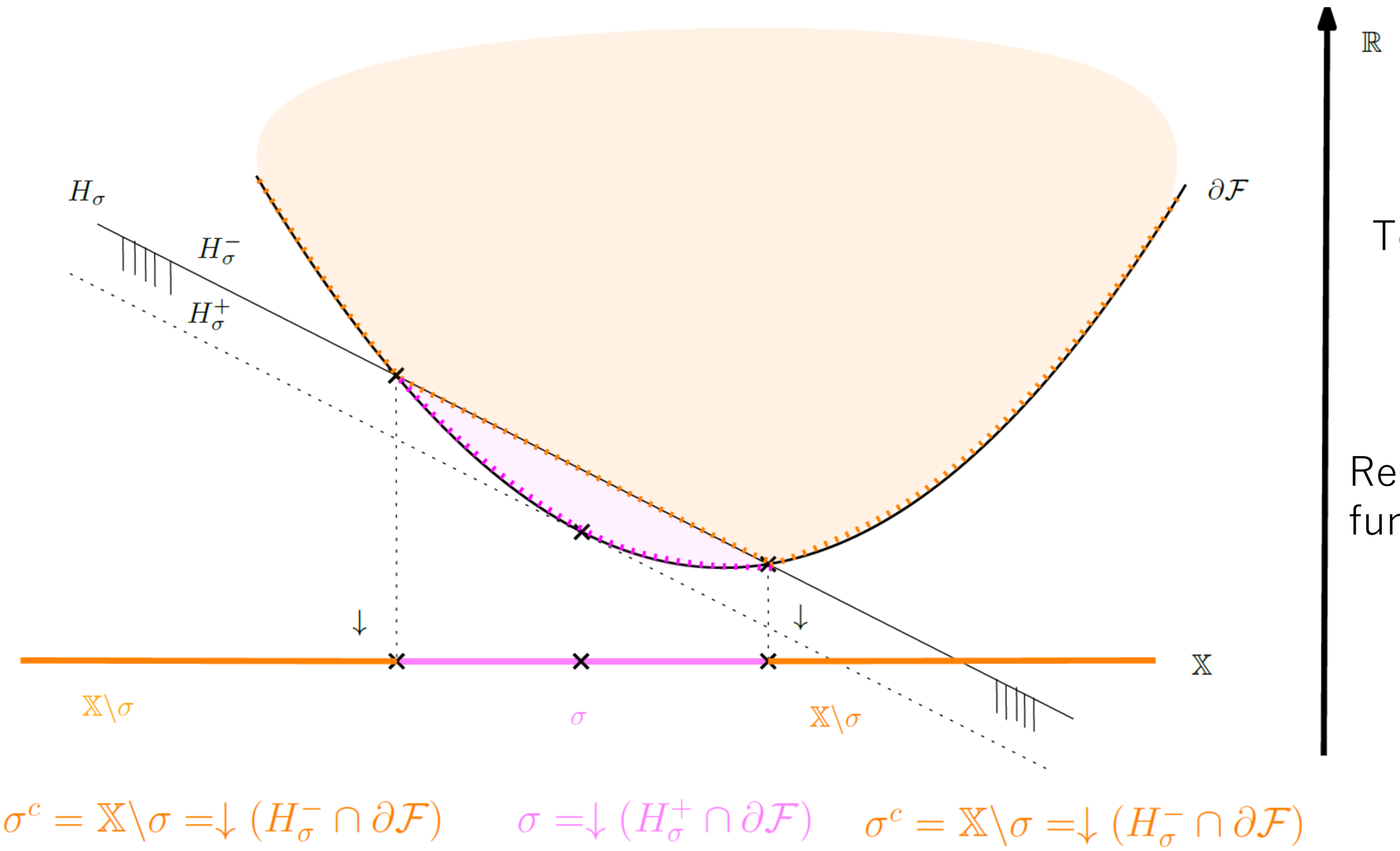
Right-sided Bregman ball: $$\sigma_F(\theta, r) = \{\theta' \in \Theta : B_F(\theta' : \theta) \leq r\}$$

Left-sided Bregman ball: $$\sigma_F^{\star}(\theta, r) = \{\theta' \in \Theta : B_F(\theta : \theta') \leq r\}$$

Application: Boolean algebra of unions & intersections of Bregman balls

Right Bregman ball and its complement

$$\mathcal{F} := \{(\theta, y \geq F(\theta)) \ : \ \theta \in \Theta \subset \mathbb{R}^m\} \subset \mathbb{R}^{m+1}$$



↓ means vertical projection

S^c: complement of set S

To any sphere, associate an hyperplane:

$$H_{\theta,r} : y = \langle \theta' - \theta, \nabla F(\theta) \rangle + F(\theta) + r$$

Reciprocally, to an hyperplane cutting the function graph, associate a sphere

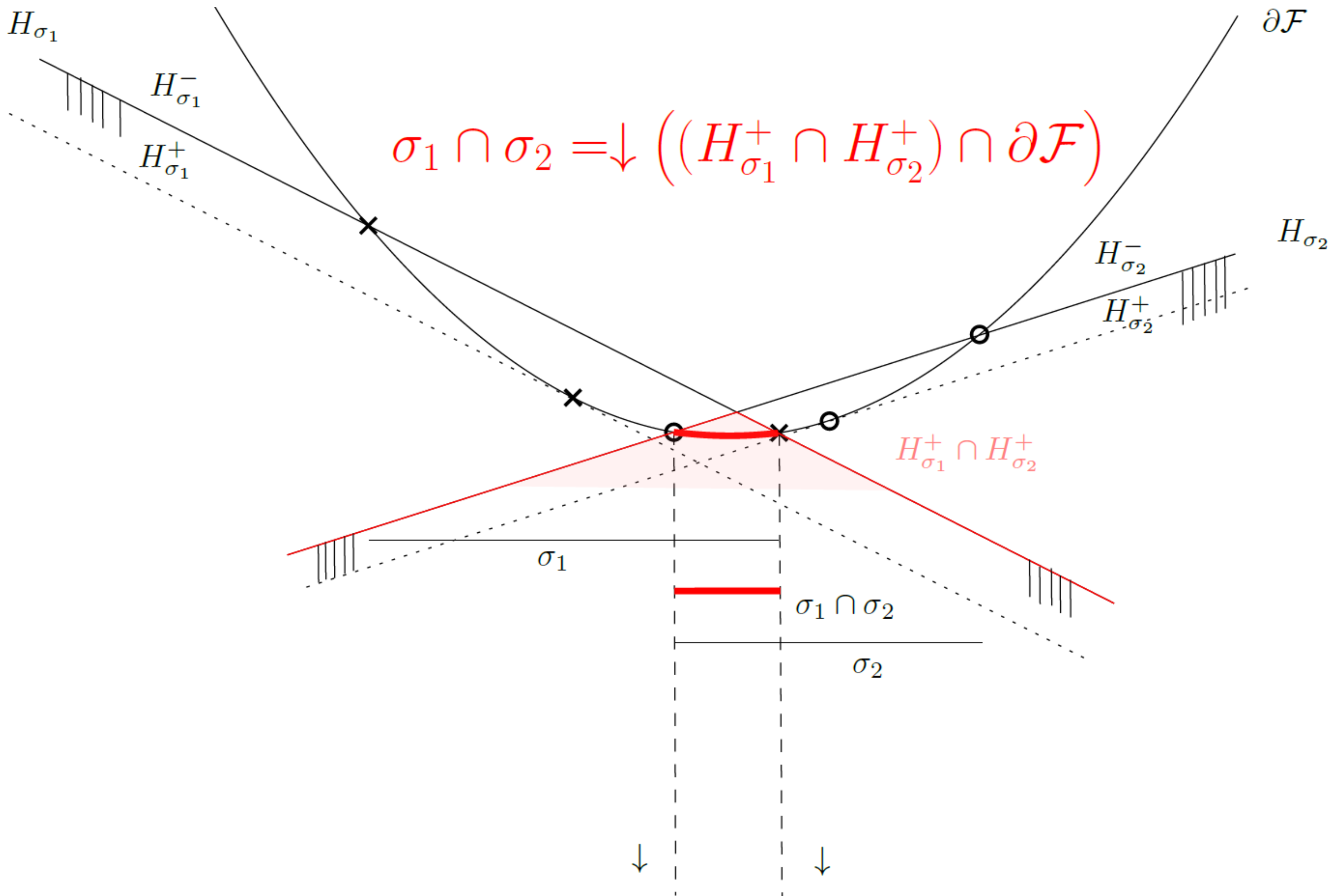
$$z = \langle \mathbf{x}, \mathbf{a} \rangle + b$$

Center: $\mathbf{c} = \nabla^{-1} F(\mathbf{a})$

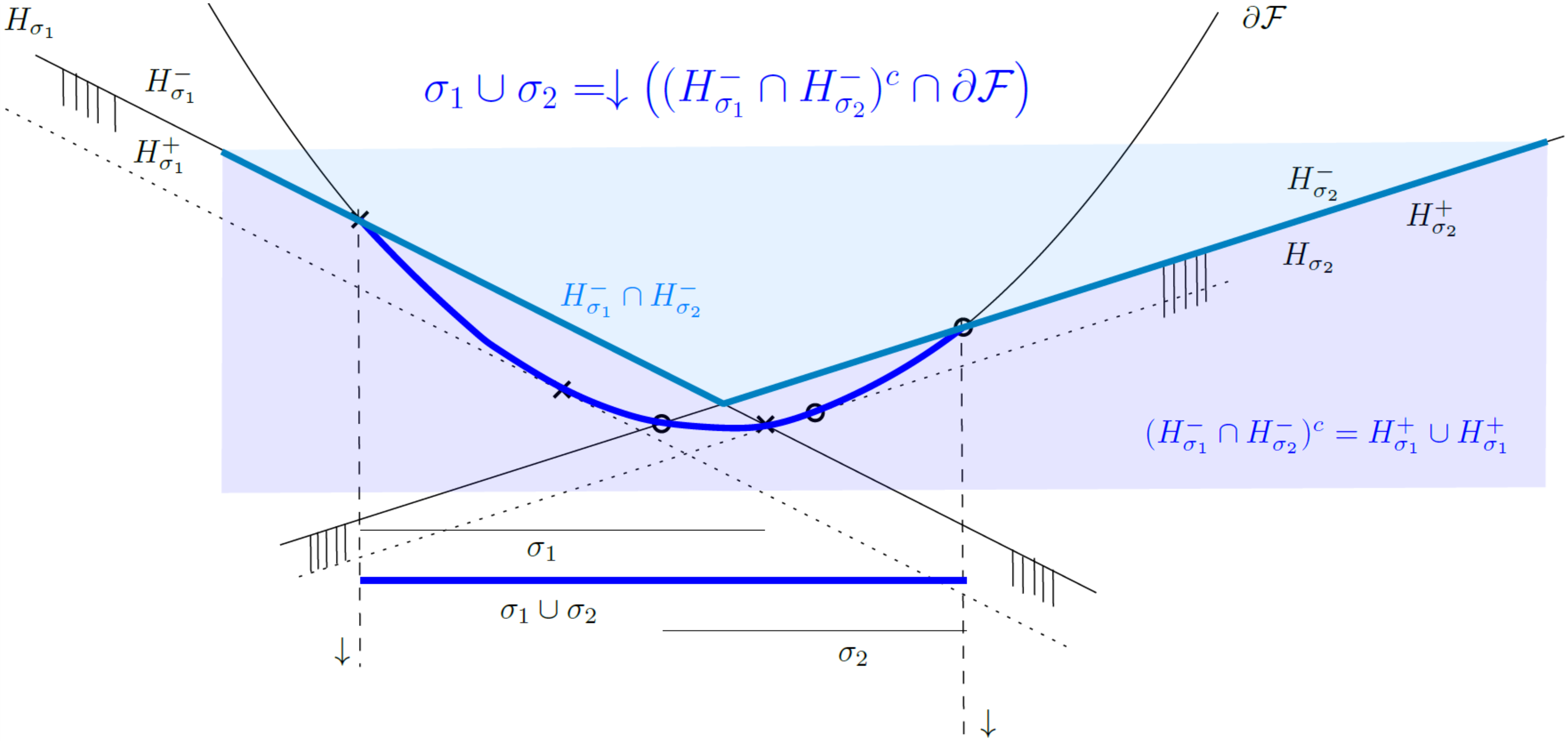
Radius: $\langle \mathbf{a}, \mathbf{c} \rangle - F(\mathbf{c}) + b$

Lifting to potential Bregman generator graph

Intersection of two right Bregman balls



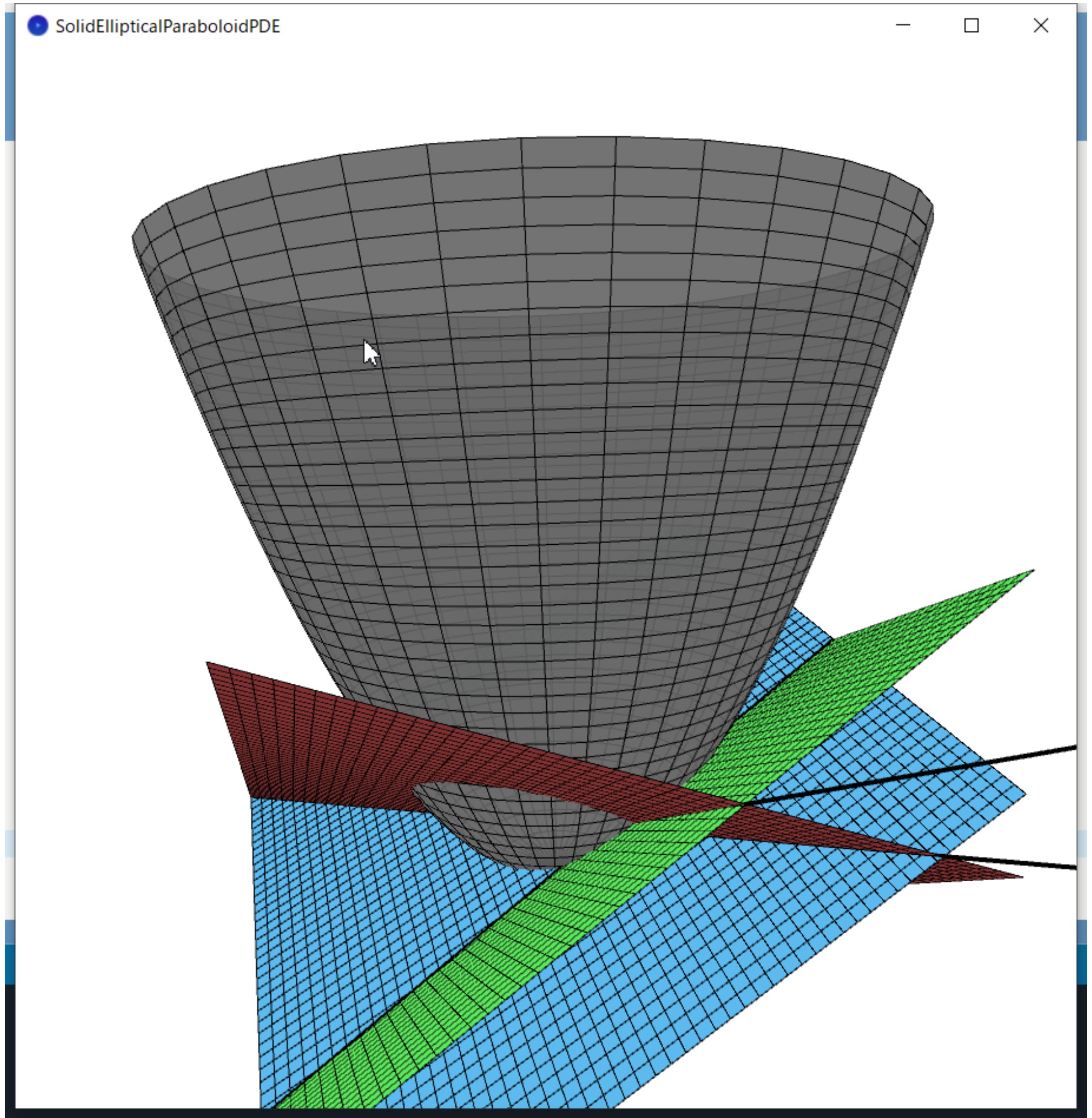
Union of two right Bregman balls



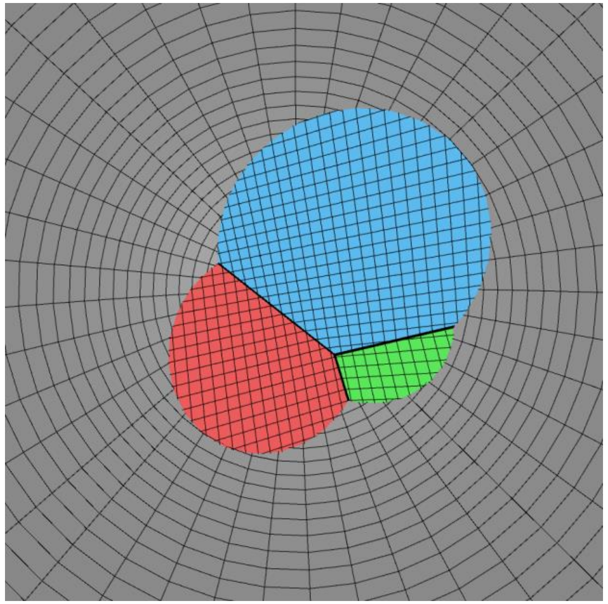
Set Morgan's law: $(A \cup B)^c = A^c \cap B^c$

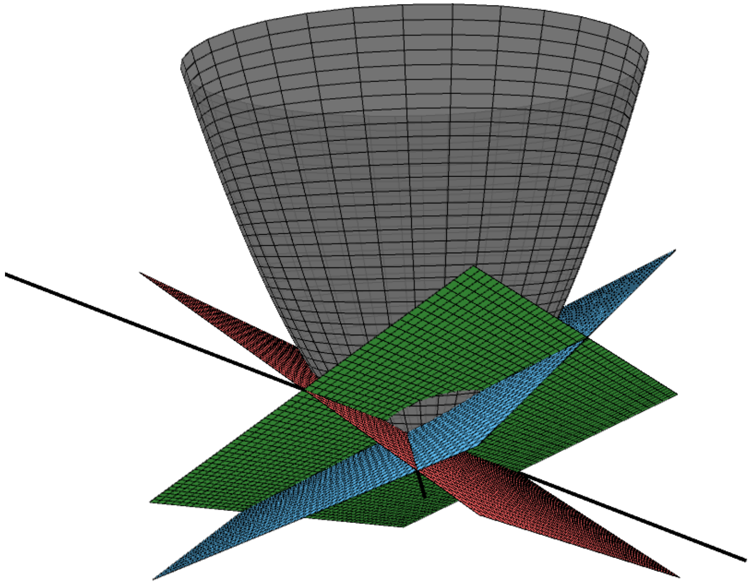
Complement of halfspace $(H^+)^c = H^-$

Example: Euclidean spheres potential function: Paraboloid, L22



Top view displays the union of disks





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

Bregman manifolds:
Geometry of convex conjugates

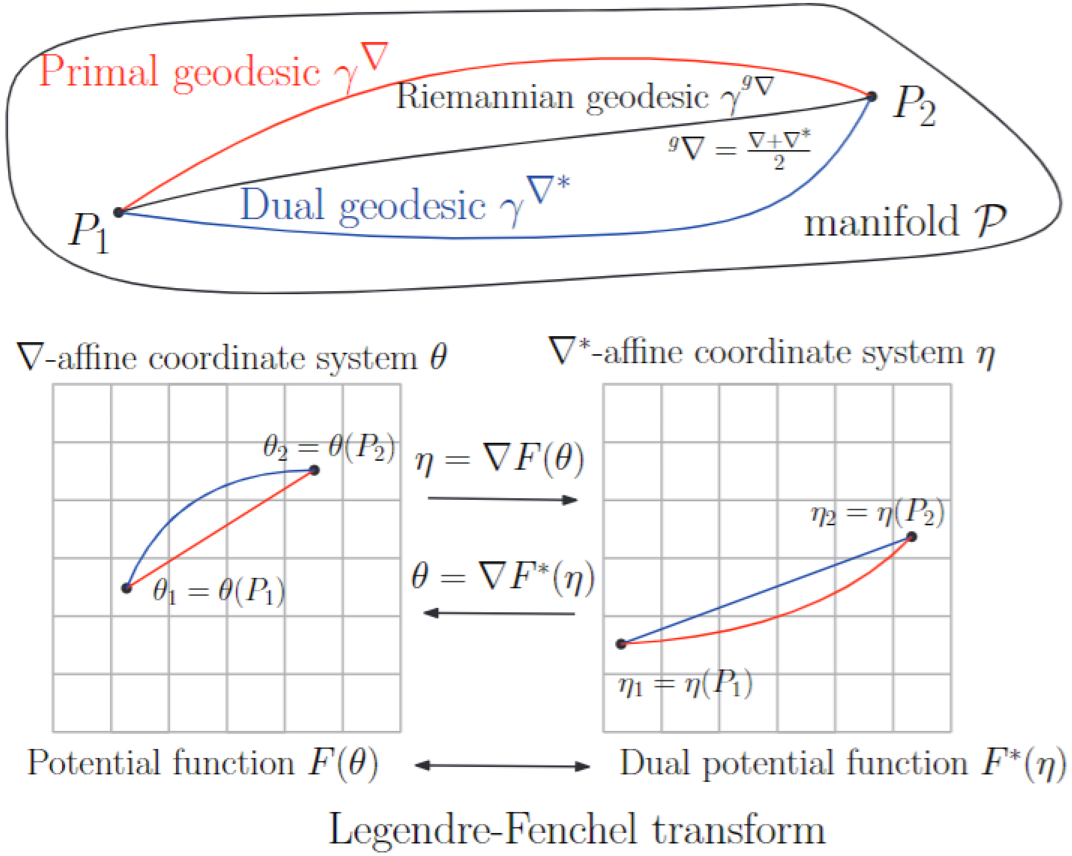
Dual Hessian geometry

[Koszul'64, Shima'70's, Amari&Nagaoka'80's]

On geodesic triangles with right angles in a dually flat space,
Progress in Information Geometry: Theory and Applications, Springer 2021

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

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



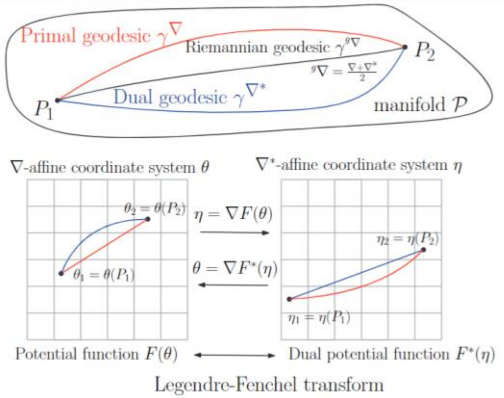
$D(P_1,P_2) = B_F(\theta_1 : \theta_2) = Y_{F,F^*}(\theta_1, \eta_2) = Y_{F^*,F}(\eta_2, \theta_1) = B_{F^*}(\eta_2, \eta_1)$

- 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**

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

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

Dual geometry of smooth Legendre-type functions



Legendre-Fenchel transform

$$(\Theta, F(\theta)) \longleftrightarrow (H, F^*(\eta))$$

$\eta = \nabla F(\theta), \eta = \nabla F^*(\theta)$

Riemannian Hessian metric g

$$g(\theta) = \nabla^2 F(\theta)$$

$$g(\eta) = \nabla^2 F^*(\eta)$$

$$\partial_i = \frac{\partial}{\partial \theta_i}$$

$$\partial^i = \frac{\partial}{\partial \eta_i}$$

flat ∇ torsion-free affine connection

$\Gamma_{ijk}(\theta) = 0, \Gamma^{ijk}(\eta) = \partial^i \partial^j \partial^k F^*(\eta)$

torsion-free affine connection ∇^* flat

$\Gamma^{*ijk}(\eta) = 0, \Gamma^{*ijk}(\theta) = \partial_i \partial_j \partial_k F(\theta)$

Levi-Civita connection

$$\bar{\nabla} = \frac{\nabla + \nabla^*}{2}$$

g-conjugate connections

$\bar{\Gamma}_{ijk}(\theta) = \frac{1}{2} \partial_i \partial_j \partial_k F(\theta)$ $\quad$ $\bar{\Gamma}^{ijk}(\eta) = \partial^i \partial^j \partial^k F^*(\eta)$

Example: Bregman manifold of multivariate Gaussians

(M, g, ∇, ∇^*)

Cumulant function is convex:

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

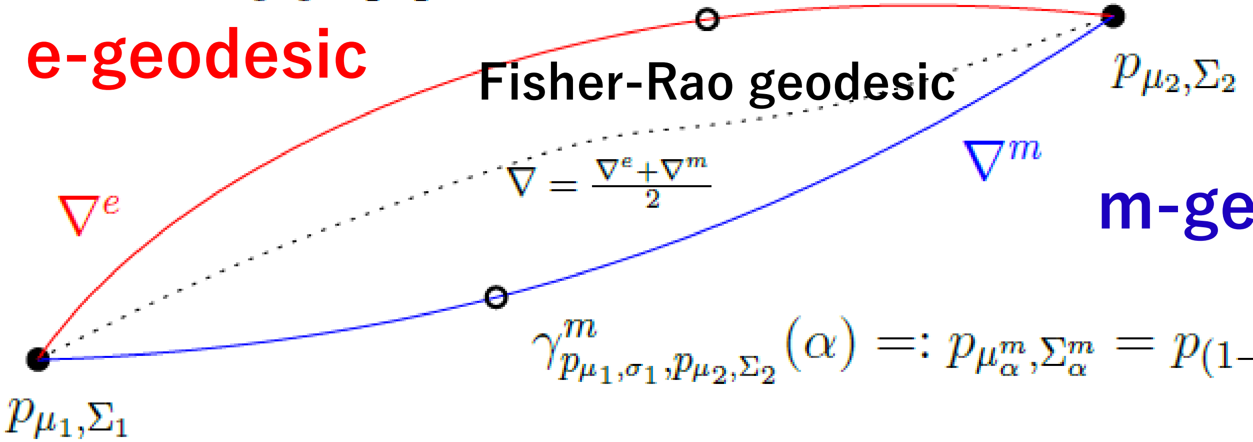
with respect to natural parameters:

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

…but not convex wrt（μ Σ）parameters

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

$$\gamma^e_{p_{\mu_1,\sigma_1},p_{\mu_2,\Sigma_2}}(\alpha) =: p_{\mu_\alpha^e,\Sigma_\alpha^e} = p_{(1-\alpha)\theta_1+\alpha\theta_2} \qquad \theta = (\Sigma^{-1}\mu, \tfrac{1}{2}\Sigma^{-1})$$



m-geodesic beware not mixture of Gaussians!

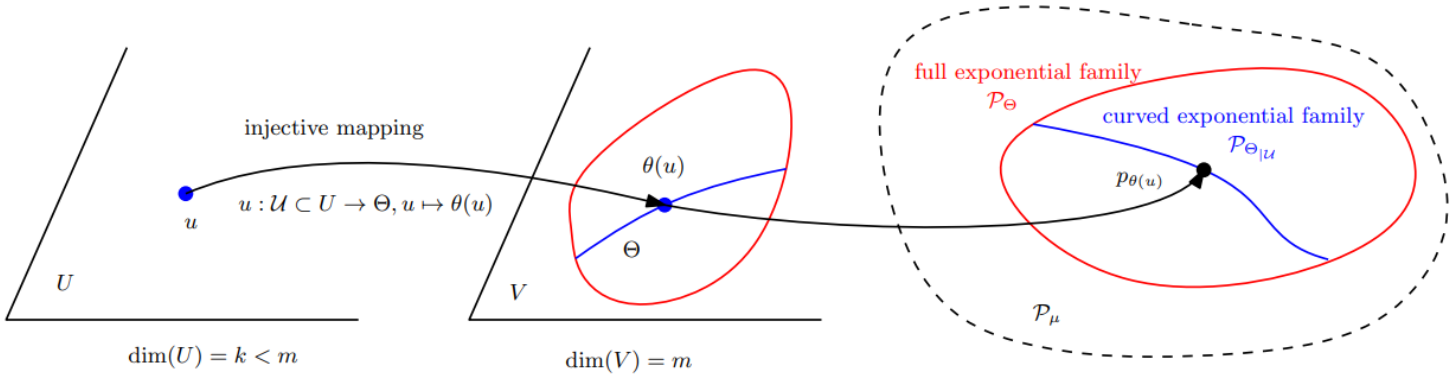
$$\gamma^m_{p_{\mu_1,\sigma_1},p_{\mu_2,\Sigma_2}}(\alpha) =: p_{\mu_\alpha^m,\Sigma_\alpha^m} = p_{(1-\alpha)\eta_1+\alpha\eta_2} \qquad \eta = (\mu, -\Sigma - \mu\mu^\top)$$

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

Bregman divergence = reverse Kullback-Leibler divergence

$$\frac{1}{2}\left(\operatorname{tr}(\Sigma_2^{-1}\Sigma_1) - \log\frac{\det(\Sigma_2)}{\det(\Sigma_1)} - d + (\mu_2-\mu_1)^\top\Sigma_2^{-1}(\mu_2-\mu_1)\right)(5$$

Curved exponential families: Submanifolds



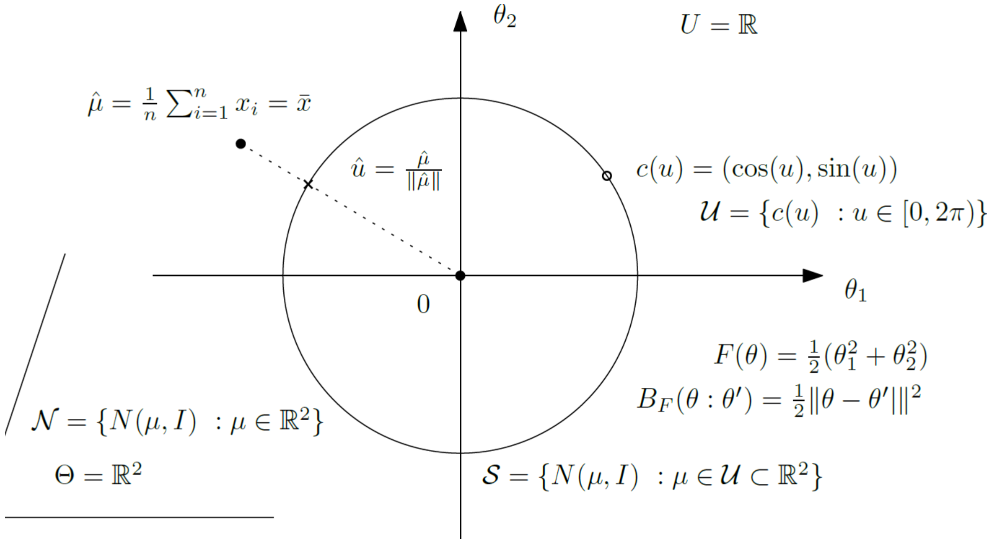
Constraint space

Parameter space

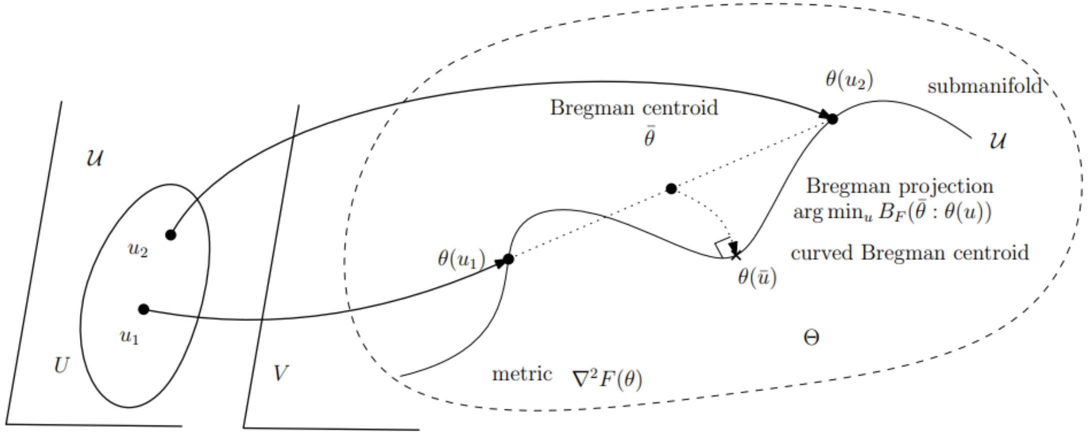
Theorem (Curved Bregman centroid/barycenter) *Let $\theta_i = \theta(u_i)$'s be n weighted parameters of $\mathcal{U}$ with weight vector $w \in \Delta_{n-1}$ (the $(n-1)$-dimensional standard simplex). Then the barycenter in $\mathcal{U}$ with respect to the curved Bregman divergence amounts to the Bregman projection of the center of mass $\bar{\theta} = \sum_i w_i \theta_i$ (right Bregman barycenter) onto $\mathcal{U}$:*

$$\arg\min_{u \in \mathcal{U}} \sum_{i=1}^{n} w_i B_F(\theta_i : \theta(u)) = \arg\min_{u \in \mathcal{U}} B_F(\bar{\theta} : \theta(u)).$$

Example: Fisher circle model



Note: submanifold topology can be non-trivial



Bijection between regular exponential families and regular Bregman divergences:

$$\log p_F(x;\theta) = -B_{F^*}(t(x) : \eta) + F^*(t(x))$$

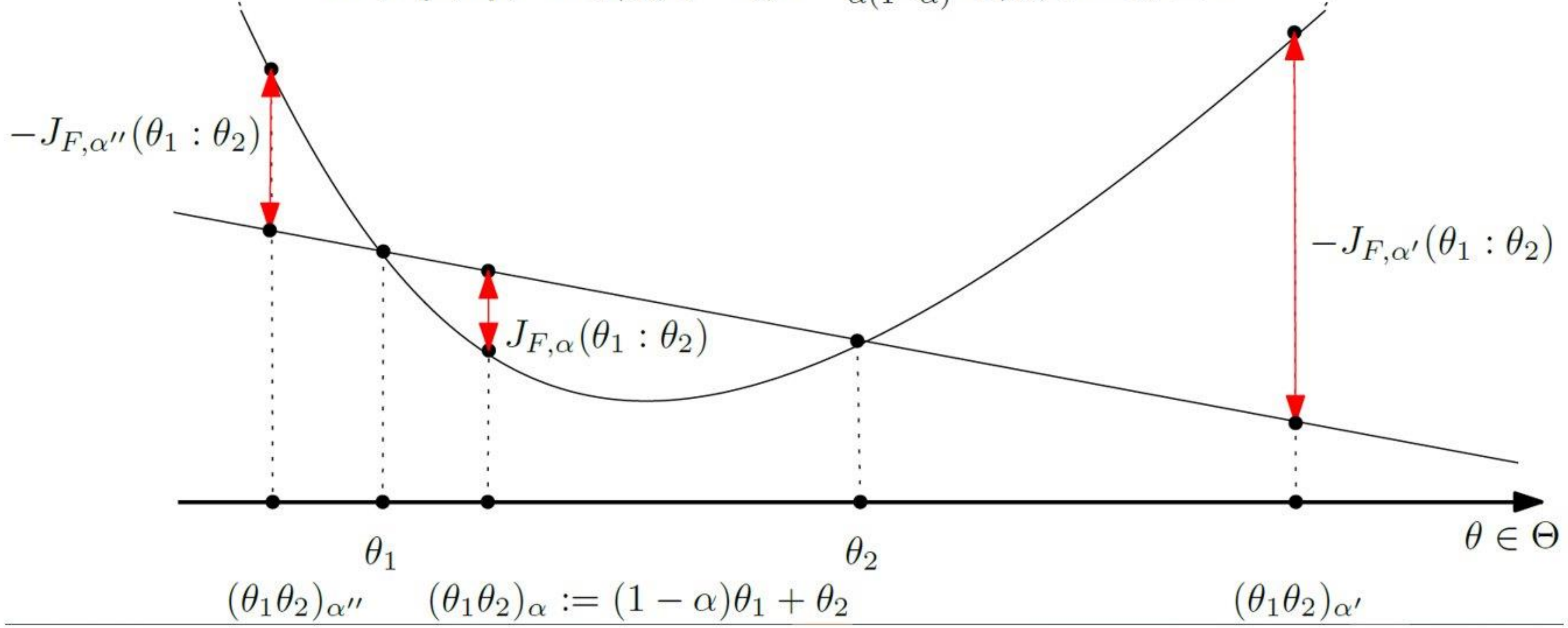
Curved BD centroid $\leftrightarrow$ MLE of curved exp. fam.

k-MLE: A fast algorithm for learning statistical mixture models, IEEE ICASSP 2012

Scaled skewed Jensen divergences & Bregman divergences

$$\forall \alpha \in (0,1), \quad J_{F,\alpha}(\theta_1 : \theta_2) := (1-\alpha)F(\theta_1) + \alpha F(\theta_2) - F((1-\alpha)\theta_1 + \alpha\theta_2)$$

Rescale: $$\forall \alpha \notin \{0,1\}, \quad \mathrm{sJ}_{F,\alpha}(\theta_1 : \theta_2) := \frac{1}{\alpha(1-\alpha)} J_{F,\alpha}(\theta_1 : \theta_2) \geq 0$$



Jensen divergences measures the vertical gap induced by a strictly convex function

$$\lim_{\alpha \to 0} \mathrm{sJ}_{F,\alpha}(\theta_1 : \theta_2) = B_F(\theta_1 : \theta_2)$$ (Bregman divergence) $$\lim_{\alpha \to 1} \mathrm{sJ}_{F,\alpha}(\theta_1 : \theta_2) = B_F(\theta_2 : \theta_1)$$ (reverse BD)

The Burbea-Rao and Bhattacharyya centroids, IEEE Transactions on Information Theory 57.8 (2011)

Example 1 of Bregman manifolds:

Mixture family manifolds
(F=-S is Shannon negentropy)

Jensen-Shannon centroid for mixture families

Jensen-Shannon divergence
Bounded symmetrization of KLD

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

- **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:

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

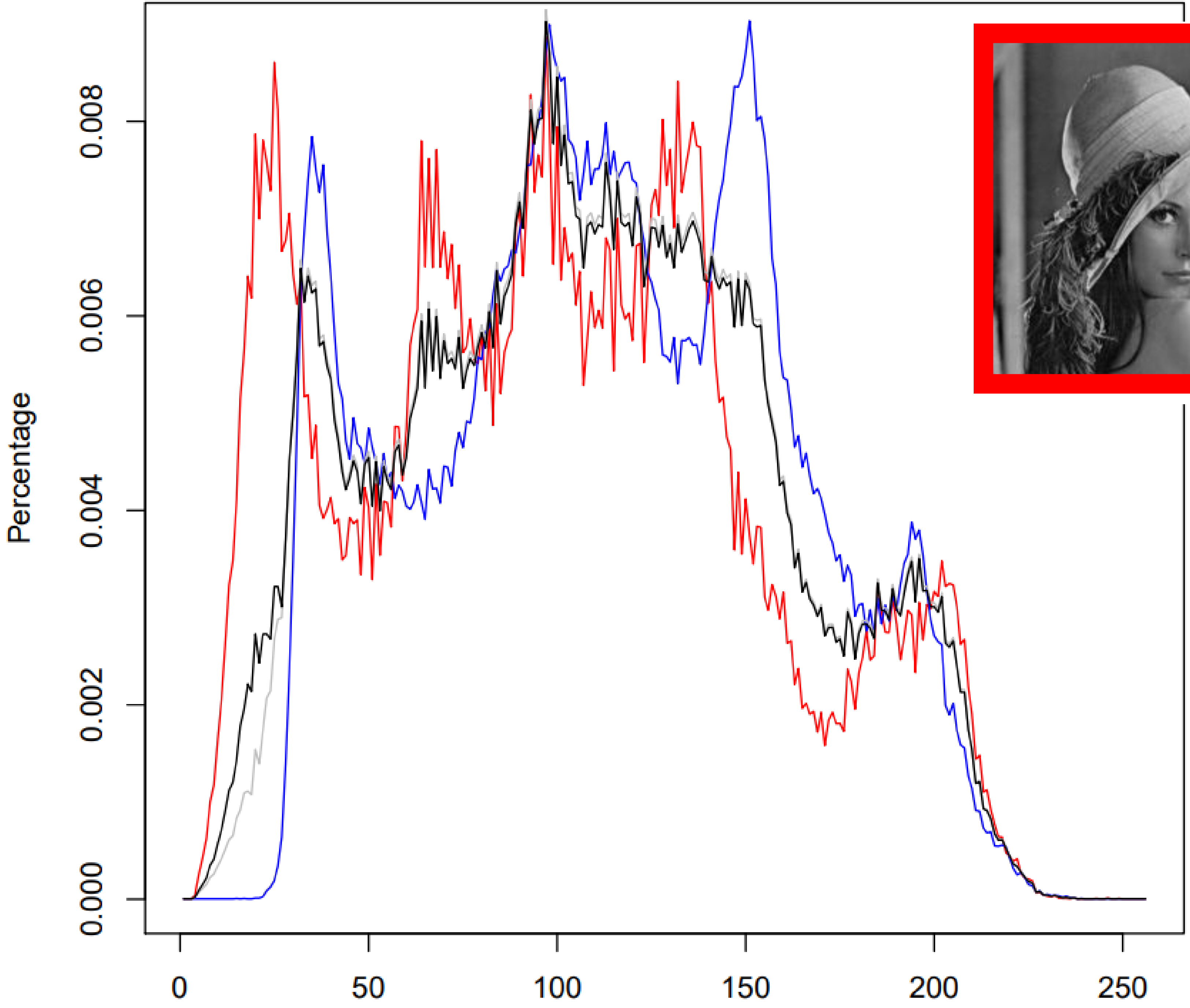
$$\min_\theta \sum_i J_F(\theta_i,\theta),$$

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

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

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

F is Shannon negentropy (convex)



Jensen–Shannon centroid

Jeffreys/SKL centroid

Jensen–Shannon centroid do not require same support

Example 2 of Bregman manifolds:

Exponential family manifolds

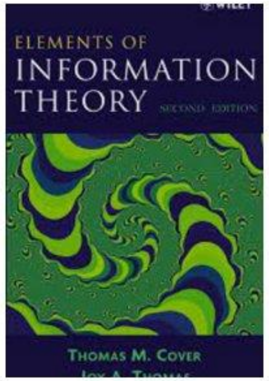
(F is cumulant function aka log-partition function)

Chernoff information: A geometric characterization

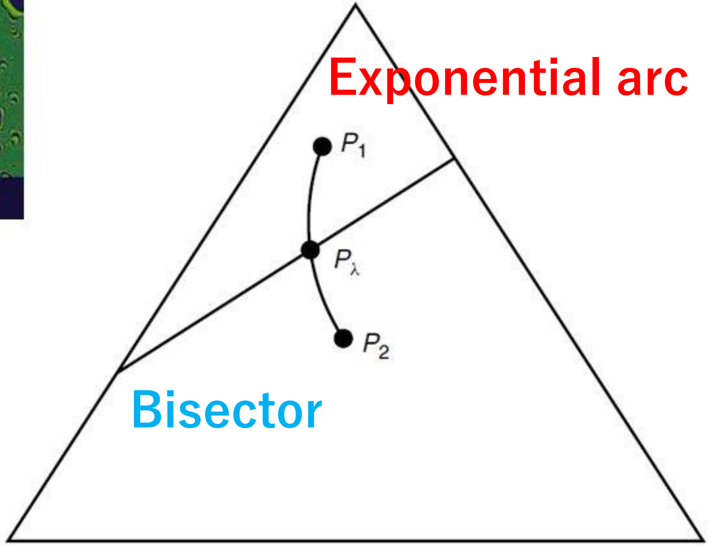
Exponential arc

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

Bisector



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



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

Probability simplex

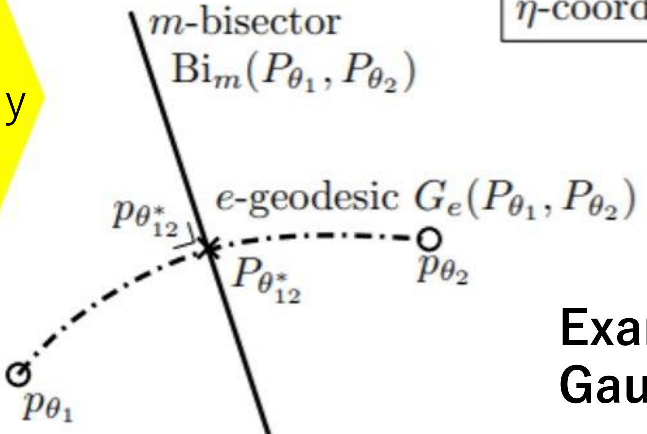
Generalized to exponential family manifold

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

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

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

$\boxed{\eta\text{-coordinate system}}$



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

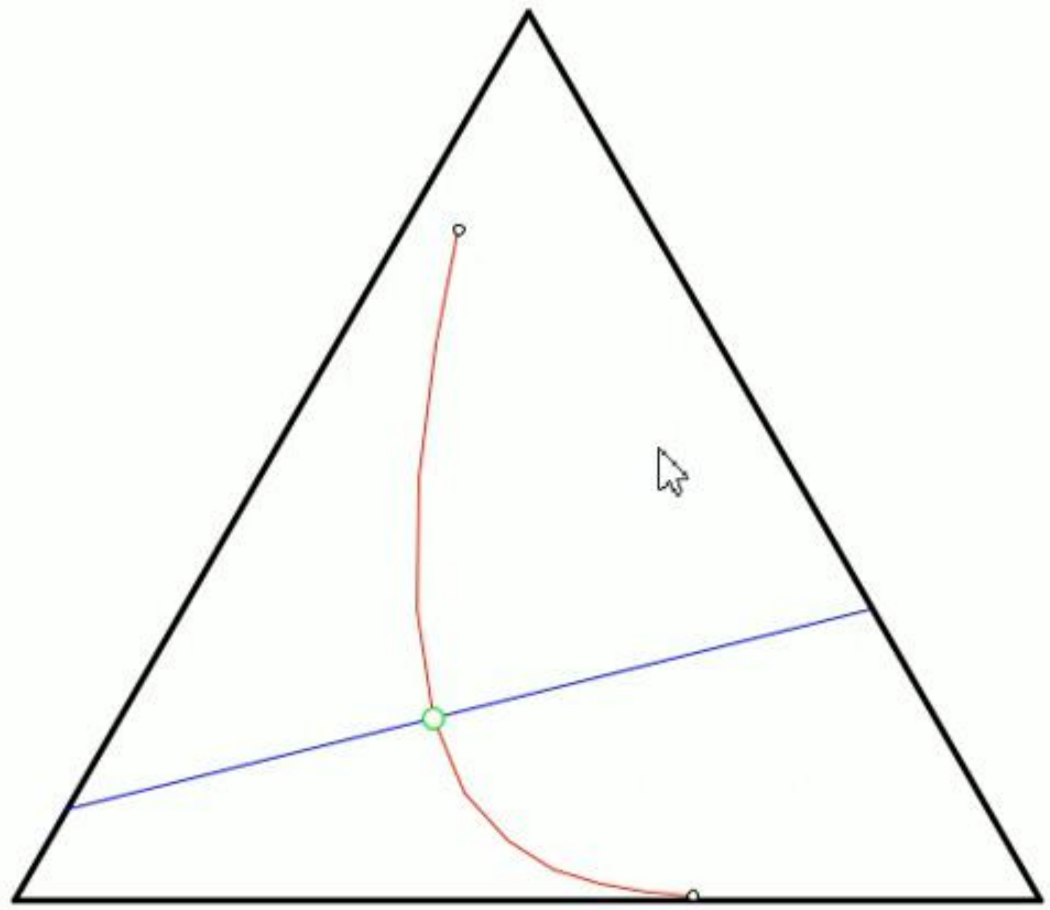
Example:
Gaussian manifold

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

Exponential family manifold

Chernoff point & information-geometry

Unique intersection point of
the exponential geodesic
with
the dual mixture bisector



Here 2D probability simplex of the family of categorical distributions with 3 choices

In the beginning of IG···

[Hotelling 1930, Rao 1945]

$$I(\theta) = [I_{ij}(\theta)], \quad I_{ij}(\theta) = \mathrm{Cov}(X_i, X_j) = E_\theta\left[\frac{\partial}{\partial_{\theta_i}} \log p_\theta(x) \, \frac{\partial}{\partial_{\theta_j}} \log p_\theta(x)\right] = -E_\theta\left[\frac{\partial^2}{\partial\theta_i \partial\theta_j} \log p_\theta(x)\right]$$

Fisher-Rao manifolds

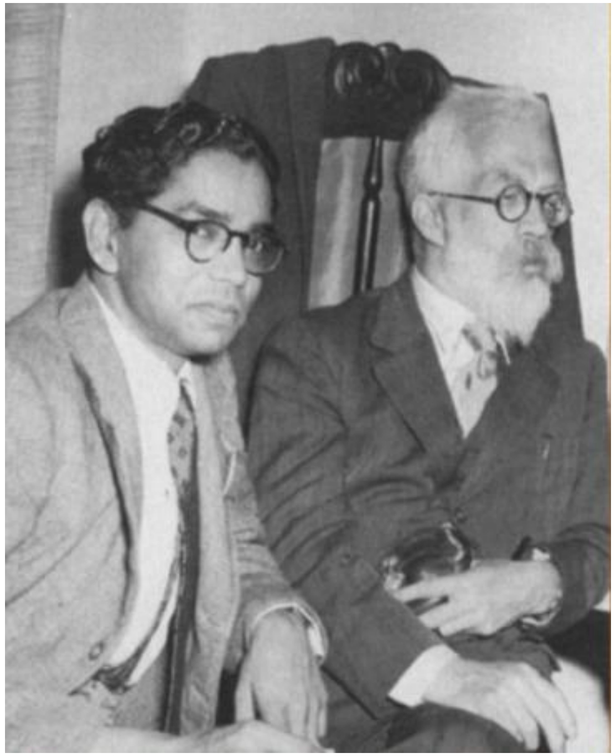
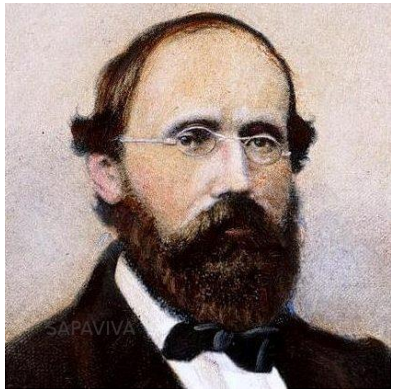


Photo 1956

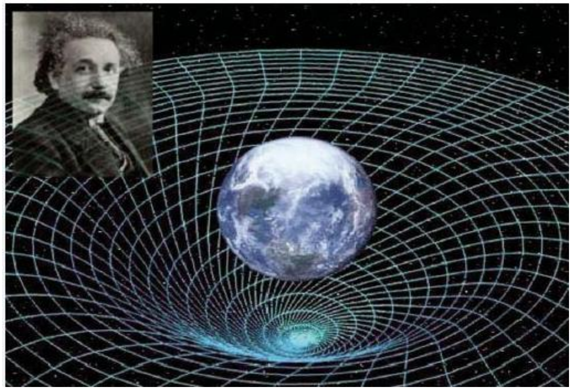
Riemannian geometry

Length element
ds

1854



``Killer''
application



1915, GR

Tractability of Fisher-Rao distance: Yet the open case of the multivariate normal family!

$$I_{ij}(\theta) = \left(\frac{\partial\mu}{\partial\theta_i}\right)^\top \Sigma^{-1}\frac{\partial\mu}{\partial\theta_j} + \frac{1}{2}\mathrm{tr}\left(\Sigma^{-1}\frac{\partial\mu}{\partial\theta_i}\Sigma^{-1}\frac{\partial\mu}{\partial\theta_j}\right)$$

Fisher length:

$$\mathrm{d}s^2_{\mathcal{N}}(\mu,\Sigma) = \mathrm{d}\mu^\top\Sigma^{-1}\mathrm{d}\mu + \frac{1}{2}\mathrm{tr}\left(\left(\Sigma^{-1}\mathrm{d}\Sigma\right)^2\right)$$

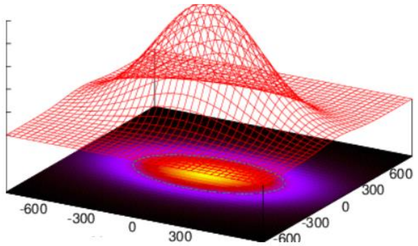
Geodesic ODE:

$$\begin{cases} \ddot{\mu} - \dot{\Sigma}\Sigma^{-1}\dot{\mu} & = & 0, \\ \ddot{\Sigma} + \dot{\mu}\dot{\mu}^\top - \dot{\Sigma}\Sigma^{-1}\dot{\Sigma} & = & 0. \end{cases}$$

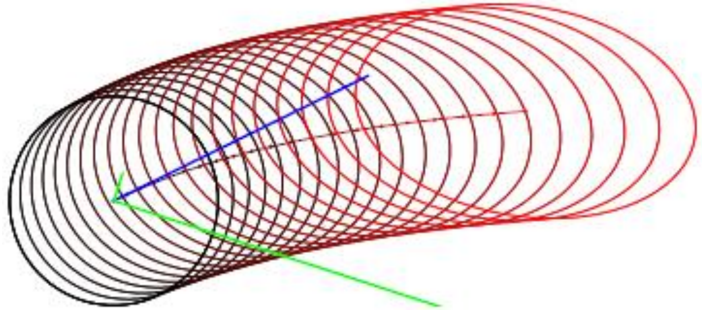
Solve ODE with initial values (IV) or boundary values (BV)

Non-constant sectional curvatures which can also be positive!
(geodesics are always unique when negative sectional curvatures)

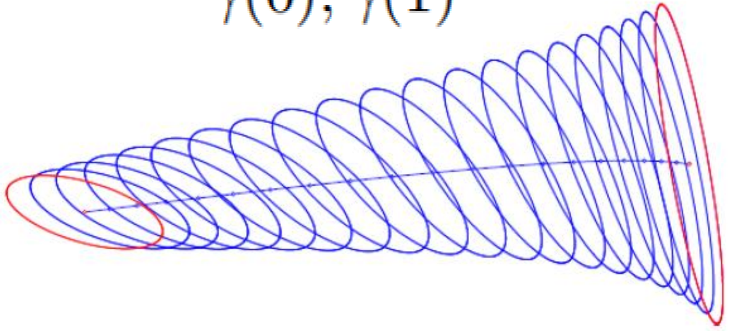
Bivariate normal (represented by ellipsoids)



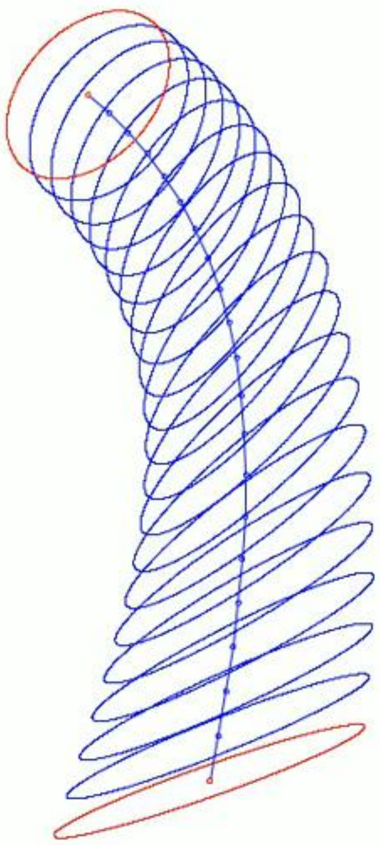
[IV: Eriksen 1987]
$\gamma(0), \dot{\gamma}(0) \in T_{\gamma(0)}$



[BV: Kobayashi 2023]
$\gamma(0), \gamma(1)$



Fisher-Rao geodesics with boundary



$\gamma(0), \gamma(1)$

$$\begin{cases} \ddot{\mu} - \dot{\Sigma}\Sigma^{-1}\dot{\mu} & = & 0, \\ \ddot{\Sigma} + \dot{\mu}\dot{\mu}^\top - \dot{\Sigma}\Sigma^{-1}\dot{\Sigma} & = & 0. \end{cases}$$

Red ellipsoids are the boundary conditions:
That is bivariate normal distributions
(μ_0, Σ_0) and (μ_1, Σ_1)

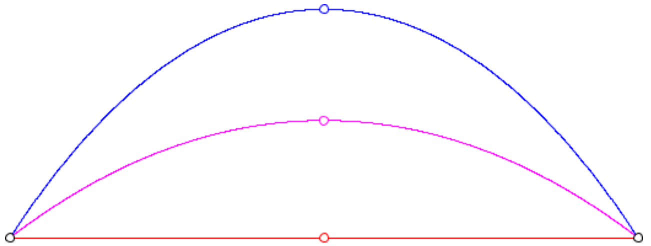
[BV: Kobayashi 2023]

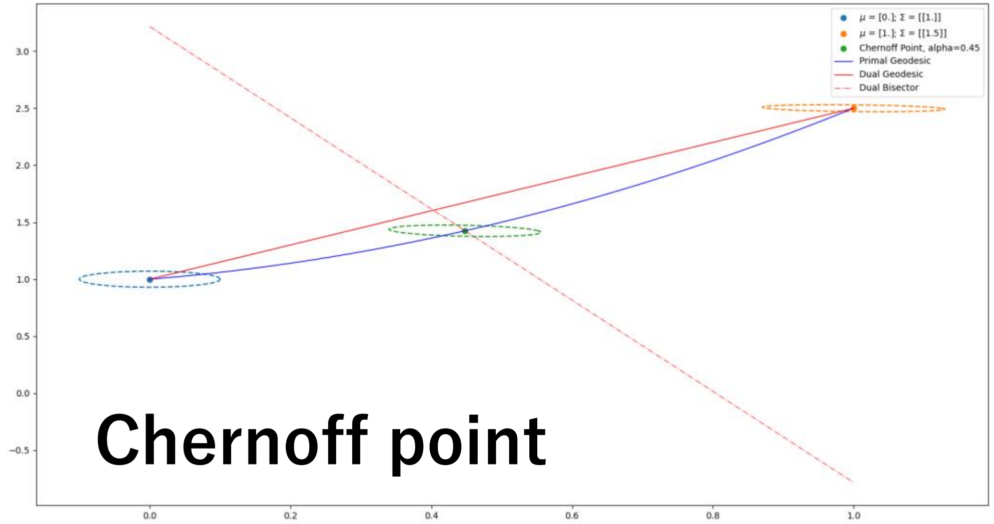
Technically, MVN Fisher-Rao geodesic:
Riemannian submersion of a horizontal geodesic
of a Riemannian symmetric space in 2d+1 dimension

A Python library for geometric computing on Bregman Manifolds

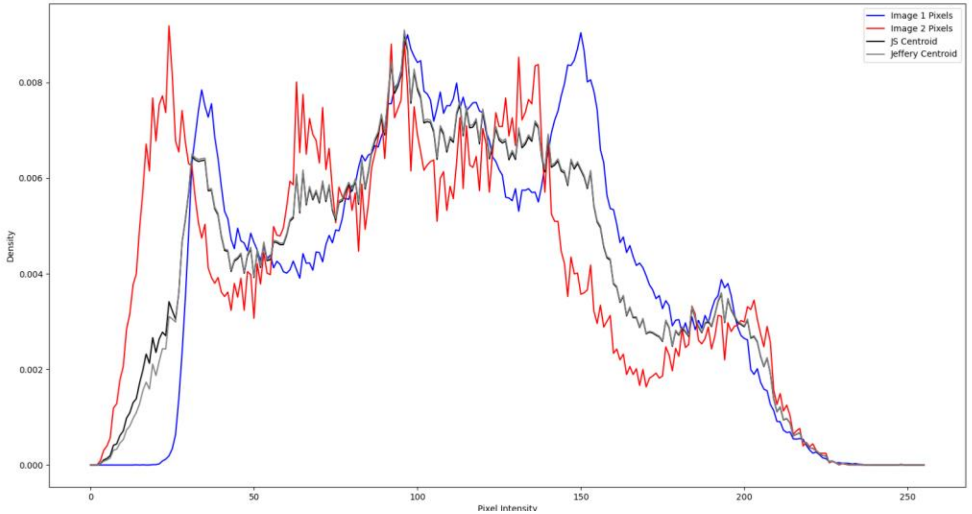
pyBregMan

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

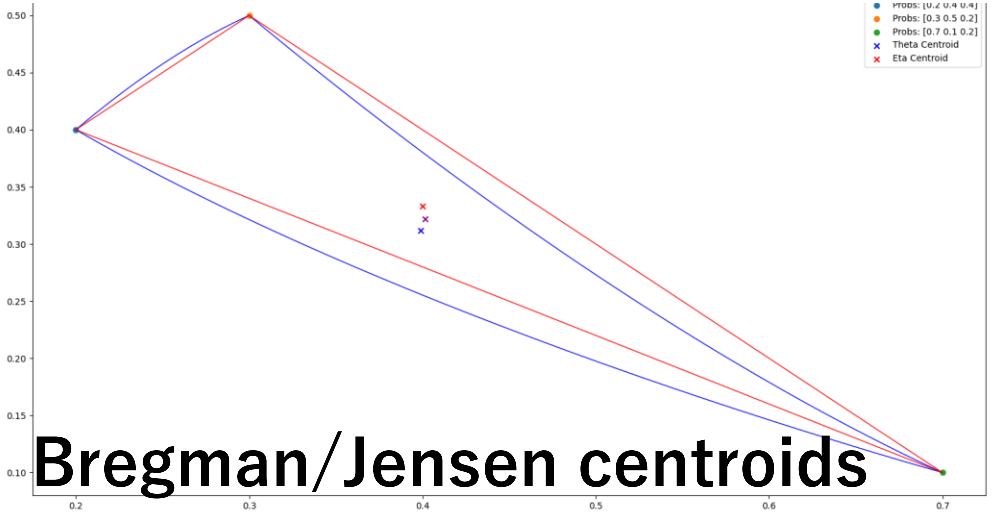




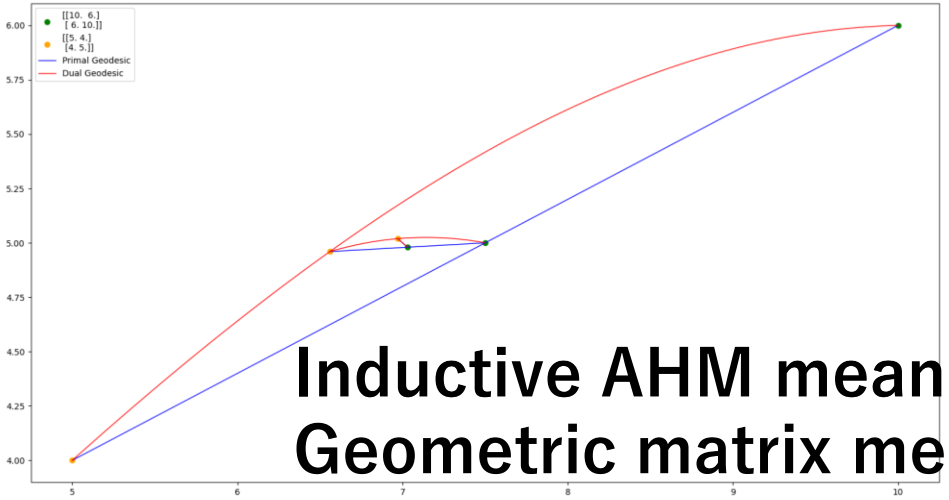
Chernoff point



Jensen-Shannon centroid



Bregman/Jensen centroids



Inductive AHM mean
Geometric matrix mean

Joint work of Frank Nielsen and Alexander Soen

Thank you! Some references

- NF and Richard Nock. "**The dual Voronoi diagrams with respect to representational Bregman divergences**." *Sixth International Symposium on Voronoi Diagrams*. IEEE, 2009.
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- NF. "**Statistical divergences between densities of truncated exponential families with nested supports: Duo Bregman and duo Jensen divergences**." *Entropy* 24.3 (2022
- NF and Richard Nock. "**Generalizing skew Jensen divergences and Bregman divergences with comparative convexity**." *IEEE Signal Processing Letters* 24.8 (2017)
- NF. "**Curved representational Bregman divergences and their applications**." *arXiv preprint arXiv:2504.05654*