## Information geometry:

# A short introduction with some recent advances 

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## Talk outline

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


## Information geometry:

## A short introduction to the geometry of dual structures

Geometry defines the architecture of spaces

## Information geometry (IG): Rationale and scope

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


## Geometric science of information (GSI)

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

- geometry of domains and cones (e.g., Siegel/Vinberg/Koszul)
- geometric mechanics for dynamic models (symplectic/contact geometry)
- thermodynamics/thermostatistics and deformed statistical models
- geometric statistics (eg, computational anatomy/medical imaging)
- shape space analysis and deformation (computer vision)
- algebraic statistics (manifolds versus algebraic surfaces/varieties)
- dynamics of learning (singularity, plateau)
- neurogeometry (neuroscience)
- etc.

GSI: Biannual conference since 2013


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


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


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


Francis BACH
Inria, Ecole Normale Supérieure, France Information Theory with Kernel Methods


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

Juan-Pablo ORTEGA
Nanyang Technological University, Singapore Learning of Dynamic Processes

## https://conference-gsi.org/

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

## Information geometry: Geometry of dual structures

## Build your own information geometry in three steps

## Choose

(1) manifold M


Examples:
Gaussians
SPD cone
Probability simplex

chart

## Concepts:

local coordinates
locally Euclidean
(2) metric tensorg


Examples:
Fisher information metric metric $g^{D}$ from divergence trace metric

## Concepts:

vector length
vector orthogonality
Riemannian geodesic
Riemannian distance
Levi-Civita connection $\nabla^{\mathrm{g}}$
(3) affine connection $\nabla$


## Examples:

exponential connection mixture connection metric connection $\nabla \mathrm{g}$ divergence connection $\nabla^{\text {D }}$ $\alpha$-connection

## Concepts:

covariant derivative $\nabla$
$\nabla$-geodesic
$\nabla$-parallel transport
curvature

Get dual IG manifold ( $\left.M, g, \nabla, \nabla^{*}\right)$

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

## Concepts:

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

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

## Choose

(1) manifold M
(2) metric tensor g
(3) affine connection $\nabla$ by defining Christoffel symbols $\Gamma_{i j k}^{\nabla}$
(4) choose $\alpha$

Examples:
Amari-Chentsov cubic tensor

$$
T_{i j k}(\theta)=E\left[\partial_{i} l \partial_{j} l \partial_{k} l\right]
$$

Cubic tensor from divergence

Get dual IG manifold ( $\mathbf{M}, \mathbf{g}, \nabla, \nabla^{*}$ )


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



$$
\begin{aligned}
T_{i j k} & =\Gamma_{i j k}^{*}-\Gamma_{i j k} \\
T_{i j k} & =\nabla_{i} g_{j k}
\end{aligned}
$$

Get a family of dual connections/IG
(M,g, $\nabla^{\alpha}, \nabla^{-\alpha}$ )

$$
\begin{aligned}
& \quad \nabla^{\alpha}=\bar{\Gamma}_{i j k}-\frac{\alpha}{2} T_{i j k} \\
& \quad \nabla^{-\alpha}=\bar{\Gamma}_{i j k}+\frac{\alpha}{2} T_{i j k} \\
& \text { l-geometry } \\
& \left(M, g, \nabla^{\alpha}, \nabla^{-\alpha}\right)
\end{aligned}
$$

$\pm \alpha$-geometry

0-geometry
= Riemannian geometry
with geodesic distance

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

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

$$
\begin{array}{cc}
\mathcal{P} I(\theta):=E_{\theta}\left[\partial_{i} l \partial_{j} l\right]_{i j} \succeq 0 & \partial_{i} l:=: \frac{\partial}{\partial \theta_{i}} l(\theta ; x)
\end{array} \quad l(\theta ; x):=\log L(\theta ; x)=\log p_{\theta}(x) .
$$

- Model is regular if partial derivatives of $\mathrm{I}_{\theta}(\mathrm{x})$ smooth and Fisher metric is well-defined and positive-definite
- Amari-Chentsov cubic tensor: $C_{i j k}:=E_{\theta}\left[\partial_{i} l \partial_{j} l \partial_{k} l\right]$

```
{(\mathcal{P},\mathcal{P}g,\mathcal{P}\mp@subsup{\nabla}{}{-\alpha},\mp@subsup{\mathcal{P}}{}{\prime}\mp@subsup{\nabla}{}{+\alpha})\mp@subsup{}}{\alpha\in\mathbb{R}}{}
```

- $\boldsymbol{\alpha}$-connections $\nabla^{\alpha}=\frac{1+\alpha}{2} \nabla^{e}+\frac{1-\alpha}{2} \nabla^{m} \quad \alpha=1 \quad$ exponential connection

$$
\begin{aligned}
& { }_{\mathcal{P}} \Gamma^{\alpha}{ }_{i j, k}(\theta):=E_{\theta}\left[\partial_{i} \partial_{j} l \partial_{k} l\right]+\frac{1-\alpha}{2} C_{i j k}(\theta), \\
& { }_{\mathcal{P}}^{e} \nabla:=E_{\theta}\left[\left(\partial_{i} \partial_{j} l\right)\left(\partial_{k} l\right)\right],
\end{aligned}
$$

- Fisher-Rao geometry when $\alpha=0$, get geodesic distance called Rao distance

$$
D_{\rho}(p, q):=\int_{0}^{1}\left\|\gamma^{\prime}(t)\right\|_{\gamma(t)} \mathrm{d} t=\int_{0}^{1} \sqrt{g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t))} \mathrm{d} t
$$

## Rao distance on the Fisher-Rao manifold

$$
\begin{aligned}
D_{\text {Rao }}\left[p_{\theta_{1}}, p_{\theta_{2}}\right] & =\rho_{g}\left(\theta_{1}, \theta_{2}\right)=\int_{0}^{1} \sqrt{g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t))} \mathrm{d} t, \gamma(0)=\theta_{1}, \gamma(1)=\theta_{2} \\
& =\int_{0}^{1} d s_{\theta}(\gamma(t)) \mathrm{d} t \quad \begin{array}{l}
\text { Here, } \boldsymbol{\gamma} \text { is the Riemannian geodesic } \\
\text { (or add a minimizer on all paths } \gamma \text { ) }
\end{array}
\end{aligned}
$$



$$
\mathrm{d} s_{\theta}^{2}(t)=\sum_{i=1}^{D} \sum_{j=1}^{D} g_{i j}(\theta) \dot{\theta}_{i}(t) \dot{\theta}_{j}(t)
$$

In practice:

$\left(\mathcal{P}, g_{F}\right)$

- Need to calculated geodesics which are curves locally minimizing the length linking two endpoints (equivalently minimize the energy of squared length elements)
- Finding Fisher-Rao geodesics is a non-trivial tasks.

Good news 2023: closed-form geodesics with boundary conditions for MultiVariate Normals

## Information geometry from divergences: ( $\left.M, \mathrm{~g}^{\mathrm{D}}, \nabla^{\mathrm{D}}, \nabla^{D^{*}}\right)$

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

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

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

$$
D_{\mathrm{KL}}^{P}\left(\theta_{1}: \theta_{2}\right):=D_{\mathrm{KL}}\left[p_{\theta_{1}}: p_{\theta_{2}}\right]
$$

- Construction of dual geometry from asymmetric parametric divergence $D\left(\theta_{1}: \theta_{2}\right)$
- Dual divergence is $D^{*}\left(\theta_{1}: \theta_{2}\right)=D\left(\theta_{2}: \theta_{1}\right)$, reverse divergence

$$
\begin{aligned}
D_{g} & :=-\left.\partial_{i, j} D\left(\theta: \theta^{\prime}\right)\right|_{\theta=\theta^{\prime}}=D^{*} g: \\
{ }^{D^{*}} \Gamma_{i j k} & :=-\left.\partial_{i j, k} D\left(\theta: \theta^{\prime}\right)\right|_{\theta=\theta^{\prime}}, \\
{ }^{*} \Gamma_{i j k} & :=-\left.\partial_{k, i j} D\left(\theta: \theta^{\prime}\right)\right|_{\theta=\theta^{\prime}} .
\end{aligned}
$$

Cubic tensor:

$$
\begin{aligned}
& { }^{D} C_{i j k}={ }^{D^{*}} \Gamma_{i j k}-{ }^{D} \Gamma_{i j k} . \\
& \quad \partial_{i, j k} f(x, y)=\frac{\partial}{\partial x^{i}} \frac{\partial^{2}}{\partial y^{2} \partial y^{k}} f(x, y)
\end{aligned}
$$

$$
{ }^{D} \nabla^{*}={ }^{D^{*}} \nabla
$$

$$
\partial_{i,} f(x, y)=\frac{\partial}{\partial x^{i}} f(x, y): \quad \partial_{\cdot, j} f(x, y)=\frac{\partial}{\partial y y^{j}} f(x, y), \partial_{i j, k} f(x, y)=\frac{\partial^{2}}{\partial x^{i} \partial x^{j}} \frac{\partial}{\partial y^{k}} f(x, y)
$$

## Realizations of dual information geometry (stat mfd)

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

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

- Realize ( $M, g, \nabla, \nabla$ ) as a model information geometry ( $M, g^{\mathrm{F}}, \nabla^{-\alpha}, \nabla^{\alpha}$ ) always exists a statistical model $M$ such that $(M, g, \nabla, \nabla)=\left(M,{ }^{\prime} g^{\mathrm{F}}{ }^{\mathrm{p}} \nabla^{-\alpha},{ }_{, \mathrm{p}} \nabla^{\alpha}\right)$

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

## Equivalence: model $\alpha$-IG $\leftrightarrow$ divergence IG for f-divergences

- Let $\mathrm{P}=\left\{\mathrm{p}_{\theta}\right\}$ be a statistical model of probability distributions dominated by $\mu$
- Consider the $f$-divergence for a convex generator $f(u)$ with $f(1)=0, f^{\prime}(1)=1$, $\mathrm{f}^{\prime \prime}(1)=1 \leftarrow$ standard f -divergence (can always rescale $\mathrm{g}(\mathrm{u})=\mathrm{f}(\mathrm{u}) / \mathrm{f}^{\prime \prime}(1)$ )

$$
\begin{array}{r}
I_{f}\left[p(x ; \theta): p\left(x ; \theta^{\prime}\right)\right]=\int_{\mathcal{X}} p(x ; \theta) f\left(\frac{p\left(x ; \theta^{\prime}\right)}{p(x ; \theta)}\right) \mathrm{d} \mu(x) \quad I_{f^{*}}\left[p(x ; \theta): p\left(x ; \theta^{\prime}\right)\right]=I_{f}\left[p\left(x ; \theta^{\prime}\right): p(x ; \theta)\right]=I_{f^{\circ}}\left[p(x ; \theta): p\left(x ; \theta^{\prime}\right)\right. \\
\text { Dual reverse f-divergence is a f-divergence for } f^{\circ}(u):=u f\left(\frac{1}{u}\right)
\end{array}
$$

- The f-divergence between $p_{\theta 1}$ and $p_{\theta 2}$ is a parameter divergence $D\left(\theta_{1}: \theta_{2}\right)$

$$
D_{\mathcal{P}}\left(\theta_{1}: \theta_{2}\right):=I_{f}\left[p_{\theta_{1}}: p_{\theta_{2}}\right]
$$

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

- Then model $\alpha$-geometry for $\alpha=2 \mathrm{f}^{\prime \prime \prime}(1)+3$ coincide with divergence IG:

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

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

## Curvature is associated to affine connection $\nabla$

- For Riemannian structure ( $\mathrm{M}, \mathrm{g}$ ), use default Levi-Civita connection $\nabla=\nabla^{\mathrm{g}}$
- Riemannian manifolds of dim d can always be embedded into Euclidean spaces $E^{D}$ of dim $D=O\left(d^{2}\right)$
- Euclidean spaces have a natural affine connection $\nabla=\nabla^{\mathrm{E}}$


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

© CNRS

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

## Dually flat spaces (M,g, $\left.\nabla, \nabla^{*}\right)$

- Fundamental theorem of information geometry: If torsion-free affine connection $\nabla$ is of constant curvature к, then curvature of dual torsion-free affine connection $\nabla^{*}$ is also constant k
- Corollary: if $\nabla$ is flat $(\mathrm{k}=0)$ then $\nabla^{*}$ is flat: Dually flat space $\left(\mathrm{M}, \mathrm{g}, \nabla, \nabla^{*}\right)$
- A connection $\nabla$ is flat if there exists a local coordinate system $\theta$ such that $\Gamma(\theta)=0$
- In $\nabla$-affine coordinate system $\theta(),. \nabla$-geodesics are visualized as line segments

$$
\begin{gathered}
\Gamma(\theta)=0 \\
\frac{d^{2} \theta_{k}}{d t^{2}}+\sum_{i=1}^{p} \sum_{j=1}^{p} \Gamma^{k} \frac{d \theta}{d t} \frac{d \theta_{j}}{d t}=0, \quad k=1, \ldots, p, \quad \square \quad \text { geodesics=line segments in } \theta
\end{gathered}
$$

## Canonical divergences of DFSs: Bregman divergences

- Dually flat structure ( $\mathrm{M}, \mathrm{g}, \nabla, \nabla^{*}$ ) can be realized by a Bregman divergence

$$
\left(M, g, \nabla, \nabla^{*}\right) \longleftarrow\left(M, g^{B_{F}}, \nabla^{B_{F}}, \nabla^{B_{F^{*}}}\right)
$$

- Let $F(\theta)$ be a strictly convex and differentiable function defined on an open convex domain $\Theta$
- Bregman divergence interpreted as the vertical gap between point $\left(\theta_{1}, F\left(\theta_{1}\right)\right)$ and the linear approximation of $F(\theta)$ at $\theta_{2}$ evaluated at $\theta_{1}$ :


$$
\begin{aligned}
B_{F}\left(\theta_{1}: \theta_{2}\right) & =F\left(\theta_{1}\right)-\underbrace{\left(F\left(\theta_{2}\right)+\left(\theta_{2}-\theta_{1}\right)^{\top} \nabla F\left(\theta_{2}\right)\right)}_{L_{F, \theta_{2}}\left(\theta_{1}\right)} \\
& =F\left(\theta_{1}\right)-F\left(\theta_{2}\right)-\left(\theta_{1}-\theta_{2}\right)^{\top} \nabla F\left(\theta_{2}\right)
\end{aligned}
$$

## Legendre-Fenchel transformation: Slope transformation

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

- Analogy of the Halfspace/Vertex representation of the epigraph of $F$
- Fenchel-Moreau's biconjugation theorem for F of Legendre-type: $\quad F=\left(F^{*}\right)^{*}$
[Touchette 2005] Legendre-Fenchel transforms in a nutshell [2010] Legendre transformation and information geometry


## Mixed coordinates and the Legendre-Fenchel divergence

- Dual Legendre-type functions

$$
\theta=\nabla F^{*}(\eta) \quad \eta=\nabla F(\theta)
$$

- Convex conjugate of F is
$F^{*}(\eta)=\eta^{\top} \nabla F^{*}(\eta)-F\left(\nabla F^{*}(\eta)\right)$
- Fenchel-Young inequality :

$$
F\left(\theta_{1}\right)+F^{*}\left(\eta_{2}\right) \geq \theta_{1}^{\top} \eta_{2}
$$

$$
\text { with equality holding if and only if } \eta_{2}=\nabla F\left(\theta_{1}\right)
$$

$$
\nabla F^{*}=(\nabla F)^{-1}
$$

Gradient are inverse of each other

- Fenchel-Young divergence make use of the mixed coordinate systems $\theta$ et $\eta$ to express a Bregman divergence as $\quad B_{F}\left(\theta_{1}: \theta_{2}\right)=Y_{F, F^{*}}\left(\theta_{1}: \eta_{2}\right)$

$$
Y_{F, F^{*}}\left(\theta_{1}: \eta_{2}\right):=F\left(\theta_{1}\right)+F^{*}\left(\eta_{2}\right)-\theta_{1}^{\top} \eta_{2}=Y_{F^{*}, F}\left(\eta_{2}, \theta_{1}\right)
$$

## Generalized Pythagoras theorem in dually flat spaces

 In general, Identity of Bregman divergence with three parameters = law of cosines$$
B_{F}\left(\theta_{1}: \theta_{2}\right)=B_{F}\left(\theta_{1}: \theta_{3}\right)+B_{F}\left(\theta_{3}: \theta_{2}\right)-\left(\theta_{1}-\theta_{3}\right)^{\top}\left(\nabla F\left(\theta_{2}\right)-\nabla F\left(\theta_{3}\right)\right) \geq 0
$$

Generalized Pythagoras' theorem

## $p$



$$
D_{F}\left(\gamma_{p q}(t): \gamma_{q r}\left(t^{\prime}\right)\right)=D_{F}\left(\gamma_{p q}(t): q\right)+D_{F}\left(q: \gamma_{q r}^{*}\left(t^{\prime}\right)\right), \quad \forall t, t^{\prime} \in(0,1)
$$

Pythagoras' theorem in
the Euclidian geometry (Self-dual)
$F_{\text {Eucl }}(\theta)=\frac{1}{2} \theta^{\top} \theta \quad g_{F_{\text {Euc }}}=I$
$B_{F_{\text {Eucl }}}\left(\theta_{1}: \theta_{2}\right)=\frac{1}{2} \rho_{\text {Eucl }}^{2}\left(\theta_{1}, \theta_{2}\right)$


## Triples of points (p,q,r) with dual Pythagorean' theorems holding simultaneously at q



$$
\begin{aligned}
& \gamma_{p q} \perp_{q} \gamma_{q r}^{*} \leadsto(\theta(p)-\theta(q))^{\top}(\eta(r)-\eta(q))=0 \Leftrightarrow D_{F}(p: q)+D_{F}(q: r)=D_{F}(p: r) \\
& \gamma_{p q}^{*} \perp_{q} \gamma_{q r} \leadsto(\eta(p)-\eta(q))^{\top}(\theta(r)-\theta(q))=0 \leadsto D_{F}(r: q)+D_{F}(q: p)=D_{F}(r: p)
\end{aligned}
$$



Itakura-Saito
Manifold
(solve quadratic system)

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

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

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

$$
\begin{array}{cc}
(\Theta, F(\theta)) \longrightarrow\left(M, g^{B_{F}}, \nabla^{B_{F}}, \nabla^{B_{F}^{*}}\right)=\left(M, g^{F}, \nabla^{F}, \nabla^{F^{*}}\right) \\
\text { Domain } \quad \text { dual Bregman divergences } & \left(\nabla^{F}\right)^{*}=\nabla^{\left(F^{*}\right)}
\end{array}
$$

- Examples of DFSs induced by convex functions:



# Dual geometry of information geometry: Information geometry as a tool to geometrize duality 

A pair of (torsion-free) affine connections $\left(\nabla, \nabla^{*}\right)$ with $\left(\nabla^{*}\right)^{*}=\nabla$


dual contrast functions

## Quasi-arithmetic centers,

 quasi-arithmetic mixtures, and the Jensen-Shannon $\nabla$-divergences
## Outline and contributions

## Goals:

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

## Weighted quasi-arithmetic means (QAMs)

Standard (n-1)-dimensional simplex: $\quad \Delta_{n-1}=\left\{\left(w_{1}, \ldots, w_{n}\right): w_{i} \geq 0, \sum_{i} w_{i}=1\right\}$
Definition (Weighted quasi-arithmetic mean (1930's)). Let f:I $\subset$ $\mathbb{R} \rightarrow \mathbb{R}$ be a strictly monotone and differentiable real-valued function. The weighted quasi-arithmetic mean (QAM) $M_{f}\left(x_{1}, \ldots, x_{n} ; w\right)$ between $n$ scalars $x_{1}, \ldots, x_{n} \in I \subset \mathbb{R}$ with respect to a normalized weight vector $w \in \Delta_{n-1}$, is defined by

$$
M_{f}\left(x_{1}, \ldots, x_{n} ; w\right):=f^{-1}\left(\sum_{i=1}^{n} w_{i} f\left(x_{i}\right)\right) .
$$

QAMs enjoy the in-betweenness property:

$$
\min \left\{x_{1}, \ldots, x_{n}\right\} \leq M_{f}\left(x_{1}, \ldots, x_{n} ; w\right) \leq \max \left\{x_{1}, \ldots, x_{n}\right\}
$$

## Quasi-arithmetic means (QAMs)

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

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

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

$$
M_{p}(x, y):=M_{f_{p}}(x, y) \quad f_{p}(t)=\left\{\begin{array}{l}
\frac{t^{p}-1}{p}, p \in \mathbb{R} \backslash\{0\}, \\
\log (t), p=0 .
\end{array}, \quad f_{p}^{-1}(t)= \begin{cases}(1+t p)^{\frac{1}{p}}, p \in \mathbb{R} \backslash\{0\}, \\
\exp (t), & p=0 .\end{cases}\right.
$$

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


## Quasi-Arithmetic Centers (QACs) = Multivariate QAMs:

Univariate QAMs: $\quad M_{f}\left(x_{1}, \ldots, x_{n} ; w\right):=f^{-1}\left(\sum_{i=1}^{n} w_{i} f\left(x_{i}\right)\right)$
Two problems we face when going from univariate to multivariate cases:

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

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

## Legendre-type functions

$\Gamma_{0}(E)$ : Cone of lower semi-continuous (lsc) convex functions from $E$ into $\mathbb{R} \cup\{+\infty\}$
Legendre-Fenchel transformation of a convex function: $\quad F^{*}(\eta):=\sup _{\theta \in \Theta}\left\{\theta^{\top} \eta-F(\theta)\right\}$
Problem: Domain H of $\eta$ may not be convex... $\quad F^{*} \in \Gamma_{0}(E) \quad F^{* *}=F$ counterexample with $h\left(\xi_{1}, \xi_{2}\right)=\left[\left(\xi_{1}{ }^{2} / \xi_{2}\right)+\xi_{1}{ }^{2}+\xi_{2}{ }^{2}\right] / 4$
To by pass this problem:
Definition Legendre type function . $(\Theta, F)$ is of Legendre type if the function $F: \Theta \subset \mathbb{X} \rightarrow \mathbb{R}$ is strictly convex and differentiable with $\Theta \neq \emptyset$ an open convex set and

$$
\begin{equation*}
\lim _{\lambda \rightarrow 0} \frac{d}{\mathrm{~d} \lambda} F(\lambda \theta+(1-\lambda) \bar{\theta})=-\infty, \quad \forall \theta \in \Theta, \forall \bar{\theta} \in \partial \Theta \tag{1}
\end{equation*}
$$

Convex conjugate of a Legendre-type function $(\theta, F(\theta))$ is of Legendre-type:
Given by the Legendre function: $\quad F^{*}(\eta)=\left\langle\nabla F^{-1}(\eta), \eta\right\rangle-F\left(\nabla F^{-1}(\eta)\right)$
Gradient map $\nabla F$ is globally invertible: $\nabla F^{-1}$

## Comonotone functions in inner product spaces

- Comonotone functions: $\forall \theta_{1}, \theta_{2} \in \mathbb{X}, \theta_{1} \neq \theta_{2}, \quad\left\langle\theta_{1}-\theta_{2}, G\left(\theta_{1}\right)-G\left(\theta_{2}\right)\right\rangle>0$ (i.e., comonotone $=$ monotone with respect to the identity function)

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

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

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

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

$$
\begin{aligned}
B_{F}\left(\theta_{1}: \theta_{2}\right) & =F\left(\theta_{1}\right)-F\left(\theta_{2}\right)-\left\langle\theta_{1}-\theta_{2}, \nabla F\left(\theta_{2}\right)\right\rangle \geq 0, \\
B_{F^{*}}\left(\eta_{1}: \eta_{2}\right) & =F^{*}\left(\eta_{1}\right)-F^{*}\left(\eta_{2}\right)-\left\langle\eta_{1}-\eta_{2}, \nabla F^{*}\left(\eta_{2}\right)\right\rangle \geq 0 .
\end{aligned}
$$

Remark: Generalization of monotonicity because when $d=1, f(x)$ is strictly monotone iff $f\left(x_{1}\right)-f\left(x_{2}\right)$ is of same sign of $x_{1}-x_{2}$ that is, $\left(f\left(x_{1}\right)-f\left(x_{2}\right)\right)\left(x_{1}-x_{2}\right)>0$

## Quasi-arithmetic centers: Definition generalizing QAMs

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

$$
\begin{aligned}
M_{\nabla F}\left(\theta_{1}, \ldots, \theta_{n} ; w\right) & :=\nabla F^{-1}\left(\sum_{i} w_{i} \nabla F\left(\theta_{i}\right)\right), \\
& =\nabla F^{*}\left(\sum_{i} w_{i} \nabla F\left(\theta_{i}\right)\right),
\end{aligned}
$$

where $\nabla F^{*}=(\nabla F)^{-1}$ is the gradient map of the Legendre transform $F^{*}$ of $F$.
This definition generalizes univariate quasi-arithmetic means : $\quad M_{f}\left(x_{1}, \ldots, x_{n} ; w\right):=f^{-1}\left(\sum_{i=1}^{n} w_{i} f\left(x_{i}\right)\right)$

$$
\text { Let } F(t)=\int_{a}^{t} f(u) \mathrm{d} u
$$

$$
\text { Then we have } \quad M_{f}=M_{F^{\prime}}
$$

## An illustrating example: The matrix harmonic mean

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

$$
\begin{aligned}
F(\theta) & =-\log \operatorname{det}(\theta), \\
\nabla F(\theta) & =-\theta^{-1}=: \eta(\theta), \\
\nabla F^{-1}(\eta) & =-\eta^{-1}=: \theta(\eta)
\end{aligned}
$$

$$
\leftarrow \text { Legendre-type function }
$$

$$
F^{*}(\eta)=\langle\theta(\eta), \eta\rangle-F(\theta(\eta))=-d-\log \operatorname{det}(-\eta) \quad \leftarrow \text { Legendre-type function }
$$

The quasi-arithmetic center with respect to $\mathbf{F}: \quad M_{\nabla F}\left(\theta_{1}, \theta_{2}\right)=2\left(\theta_{1}^{-1}+\theta_{2}^{-1}\right)^{-1}$ The quasi-arithmetic center with respect to $\mathrm{F}^{*}: \quad M_{\nabla F^{*}}\left(\eta_{1}, \eta_{2}\right)=2\left(\eta_{1}^{-1}+\eta_{2}^{-1}\right)^{-1}$ Generalize univariate harmonic mean with $\mathrm{F}(\mathrm{x})=\log \mathrm{x}, \mathrm{f}(\mathrm{x})=\mathrm{F}^{\prime}(\mathrm{x})=1 / \mathrm{x}: \quad H(a, b)=\frac{2 a b}{a+b}$ for $a, b>0$

## A Legendre-type function $F$ gives rise to a pair of dual quasi-arithmetic centers

 $\mathrm{M}_{\nabla \mathrm{F}}$ and $\mathrm{M}_{\nabla \mathrm{F}^{*}}$ : dual operators
## Dually flat structures of information geometry

- A Legendre-type Bregman generator F() induces a dually flat space structure:

$$
\left(\Theta, g(\theta)=\nabla_{\theta}^{2} F(\theta), \nabla, \nabla^{*}\right)
$$

- A point P can be either parameterized by $\theta$-coordinate and dual $\eta$-coordinate



## Quasi-arithmetic barycenters and dual geodesics

- The dual geodesics induced by the dual flat connections can be expressed using dual weighted quasi-arithmetic centers:
$\nabla$-geodesic $\gamma_{\nabla}(P, Q ; t)=(P Q)^{\nabla}(t)$



## n-Variable Quasi-arithmetic centers as centroids in duallv flat spaces

Consider $n$ points $P_{1}, \ldots, P_{n}$ on the $\operatorname{DFS}\left(M, g, \nabla, \nabla^{*}\right) \quad$ (canonical divergence $=$ Bregman divergence)

## Right-sided centroid:

$\bar{C}_{R}=\arg \min _{P \in M} \sum_{i=1}^{n} \frac{1}{n} D_{\nabla, \nabla^{*}}\left(P_{i}: P\right)$

$$
\bar{\theta}_{R}=\arg \min _{\theta} \frac{1}{n} \sum_{i=1}^{n} B_{F}\left(\theta_{i}: \theta\right)
$$

$\bar{\theta}_{R}=\theta\left(\bar{C}_{R}\right)=\frac{1}{n} \sum_{i=1}^{n} \theta_{i}=M_{\mathrm{id}}\left(\theta_{1}, \ldots, \theta_{n}\right)$
$\bar{\eta}_{R}=\nabla F\left(\bar{\theta}_{R}\right)=M_{\nabla F^{*}}\left(\eta_{1}, \ldots, \eta_{n}\right) . \leftarrow$ dual QAC
$P_{i}\binom{\theta_{i}}{\eta_{i}}$

$\left(M, g, \nabla, \nabla^{*}\right)$

## D Left-sided centroid:

$\bar{C}_{L}=\arg \min _{P \in M} \sum_{i=1}^{n} \frac{1}{n} D_{\nabla, \nabla^{*}}\left(P: P_{i}\right)$

$$
\bar{\theta}_{L}=\arg \min _{\theta} \frac{1}{n} \sum_{i=1}^{n} B_{F}\left(\theta: \theta_{i}\right)
$$

$$
\begin{aligned}
\bar{\theta}_{L} & =M_{\nabla F}\left(\theta_{1}, \ldots, \theta_{n}\right), \quad \leftarrow \text { primal QAC } \\
\bar{\eta}_{L} & =\nabla F\left(\bar{\theta}_{L}\right)=M_{\mathrm{id}}\left(\eta_{1}, \ldots, \eta_{n}\right)
\end{aligned}
$$

Notice that when $\mathrm{n}=2$, weighted dual quasi-arithmetic barycenters define the dual geodesics

## Invariance/equivariance of quasi-arithmetic centers

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

$$
\left(M, g, \nabla, \nabla^{*}\right) \leftarrow \operatorname{DFS}\left(\left[\theta, F(\theta) ; \eta, F^{*}(\eta)\right]\right)
$$

## Affine Legendre invariance of dually flat spaces:

- By adding an affine term...

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

Invariance of quasi-arithmetic center:

$$
M_{\nabla \bar{F}}\left(\theta_{1}, \ldots ; \theta_{n} ; w\right)=M_{\nabla F}\left(\theta_{1}, \ldots ; \theta_{n} ; w\right)
$$

- By an affine change of coordinate... Same DFS with $\quad \bar{\theta}=A \theta+b$ such that $\bar{F}(\bar{\theta})=F(\theta)$

$$
\begin{aligned}
& \nabla \bar{F}(x)=\left(A^{-1}\right)^{\top} \nabla F\left(A^{-1}(x-b)\right) \square M_{\nabla \bar{F}}\left(\bar{\theta}_{1}, \ldots, \bar{\theta}_{n} ; w\right)=A M_{\nabla F}\left(\theta_{1}, \ldots, \theta_{n} ; w\right)+b \\
& B_{\bar{F}\left(\overline{\theta_{1}}: \overline{\theta_{2}}\right)}=B_{F}\left(\theta_{1}: \theta_{2}\right) \quad \begin{array}{l}
\text { Same canonical divergence of the DFS } \\
\text { (= constrast function on the diagonal of the product manifold) }
\end{array}
\end{aligned}
$$

## Canonical divergence versus Legendre-Fenchel/Bregman divergences

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

$$
\begin{gathered}
F(\theta)+F^{*}(\eta)-\langle\theta, \eta\rangle=0 \quad \eta=\nabla F(\theta) \\
B_{F}\left(\theta_{1}: \theta_{2}\right):=F\left(\theta_{1}\right)-\underbrace{F\left(\theta_{2}\right)}_{=\left\langle\theta_{2}, \eta_{2}\right\rangle-F^{*}\left(\eta_{2}\right)}-\left\langle\theta_{1}-\theta_{2}, \nabla F\left(\eta_{2}\right)\right\rangle \\
=F\left(\theta_{1}\right)+F^{*}\left(\eta_{2}\right)-\left\langle\theta_{1}, \eta_{2}\right\rangle=: Y_{F}\left(\theta_{1}: \eta_{2}\right)
\end{gathered}
$$

$$
\begin{aligned}
&\left(M, g, \nabla, \nabla^{*}\right) \leftarrow \operatorname{DFS}\left(\left[\Theta, F(\theta), H, F^{*}(\eta)\right]\right) \\
& \leftarrow \operatorname{DFS}\left(\left[\bar{\Theta}, \bar{F}(\bar{\theta}), \bar{H}, \bar{F}^{*}(\bar{\eta})\right]\right) \\
&=D_{\nabla, \nabla^{*}}\left(P_{1}: P_{2}\right)
\end{aligned} \begin{aligned}
& =B_{F}\left(\theta_{1}: \theta_{2}\right)=B_{F^{*}}\left(\eta_{1}, \eta_{2}\right)=Y_{F}\left(\theta_{1}: \eta_{2}\right)=Y_{F^{*}}\left(\eta_{2}: \theta_{1}\right) \\
& =B_{\bar{F}}\left(\overline{\theta_{1}}: \overline{\theta_{2}}\right)=B_{\bar{F}^{*}}\left(\overline{\eta_{1}}, \overline{\eta_{2}}\right)=Y_{F}\left(\overline{\theta_{1}}: \overline{\eta_{2}}\right)=Y_{F^{*}}\left(\overline{\eta_{2}}: \overline{\theta_{1}}\right)
\end{aligned}
$$

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

- Affine Legendre invariance:

$$
\begin{aligned}
& \bar{F}(\bar{\theta})=F(A \theta+b)+\langle c, \theta\rangle+d \\
& \bar{F}^{*}(\bar{\eta})=F^{*}\left(A^{*} \eta+\dot{b}^{*}\right)+\left\langle c^{*}, \eta\right\rangle+\dot{d}^{*}
\end{aligned}
$$

- Set the unit scale of canonical divergence (DFS differ here, rescaled): (does not change the quasi-arithmetic center) $\quad D_{\lambda, \nabla, \nabla^{*}}:=\lambda D_{\nabla, \nabla^{*}}$ amount to scale the potential function $\lambda F(\theta)$ vs $F(\theta)$

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

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

## Illustrating example: Mahalanobis divergence

- Mahalanobis divergence = squared Mahalanobis metric distance

$$
\Delta^{2}\left(\theta_{1}, \theta_{2}\right)=B_{F_{Q}}\left(\theta_{1}: \theta_{2}\right)=\frac{1}{2}\left(\theta_{2}-\theta_{1}\right)^{\top} Q\left(\theta_{2}-\theta_{1}\right)
$$

fails triangle inequality
of metric distances

Primal potential function: $\quad F_{Q}(\theta)=\frac{1}{2} \theta^{\top} Q \theta+c \theta+\kappa$
Dual potential function: $\quad F^{*}(\eta)=\frac{1}{2} \eta^{\top} Q^{-1} \eta=F_{Q^{-1}}(\eta)$,

- The dual QACs induced by the dual Mahalanobis generators F and $\mathrm{F}^{*}$ coincide to weighted arithmetic mean $\mathrm{M}_{\mathrm{id}}$ :

$$
\begin{aligned}
& M_{\nabla F_{Q}}\left(\theta_{1}, \ldots, \theta_{n} ; w\right)=Q^{-1}\left(\sum_{i=1}^{n} w_{i} Q \theta_{i}\right)=\sum_{i=1}^{n} w_{i} \theta_{i}=M_{\mathrm{id}}\left(\theta_{1}, \ldots, \theta_{n} ; w\right) \\
& M_{\nabla F_{Q}^{*}}\left(\eta_{1}, \ldots, \eta_{n} ; w\right)=Q\left(\sum_{i=1}^{n} w_{i} Q^{-1} \eta_{i}\right)=M_{\mathrm{id}}\left(\eta_{1}, \ldots, \eta_{n} ; w\right) .
\end{aligned}
$$

## Quasi-arithmetic mixtures (OAMixs), and $\alpha$-mixtures

Definition . The $M_{f}$-mixture of $n$ densities $p_{1}, \ldots, p_{n}$ weighted by $w \in \Delta_{n}^{\circ}$ is defined by

$$
\left(p_{1}, \ldots, p_{n} ; w\right)^{M_{f}}(x):=\frac{M_{f}\left(p_{1}(x), \ldots, p_{n}(x) ; w\right)}{\int M_{f}\left(p_{1}(x), \ldots, p_{n}(x) ; w\right) \mathrm{d} \mu(x)}
$$

## Centroid of n densities with respect to the $\alpha$-divergences yields a QAMix:

$$
\left(p_{1}, \ldots, p_{n} ; w\right)^{M_{\alpha}}=\arg \min _{p} \sum_{i} w_{i} D_{\alpha}\left(p_{i}, p\right)
$$

$D_{\alpha}$ denotes the $\alpha$-divergences:

$$
\begin{aligned}
& D_{\alpha}[m(s): l(s)] \\
& = \begin{cases}\int m(s) d s-\int l(s) d s+\int m(s) \log \frac{m(s)}{l(s)} d s & \alpha=-1 \\
\int l(s) d s-\int m(s) d s+\int l(s) \log \frac{l(s)}{m(s)} d s+\int l(s) \log \frac{l(s)}{m(s)} d s=1 \\
\frac{2}{1+\alpha} \int m(s) d s+\frac{2}{1-\alpha} \int l(s) d s-\frac{4}{1-\alpha^{2}} \int m(s)^{\frac{1-\alpha}{2}} l(s)^{\frac{1 m}{2}} d s, & \alpha \neq \pm 1 .\end{cases}
\end{aligned}
$$

## $\mathrm{k}=2$ QAMixs and the $\nabla$-Jensen-Shannon divergence

- Jensen-Shannon divergence is bounded symmetrization of KL divergence:

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

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

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

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

## Inductive Means: Geodesics/quasi-arithmetic centers

- Gauss and Lagrange independently studied the following convergence of pairs of iterations:

$$
\begin{aligned}
a_{t+1} & =\frac{a_{t}+b_{t}}{2} \\
b_{t+1} & =\sqrt{a_{t} b_{t}}
\end{aligned}
$$

$$
\operatorname{AGM}\left(a_{0}, b_{0}\right)=\frac{\pi}{4} \frac{a_{0}+b_{0}}{K\left(\frac{a_{0}-b_{0}}{a_{0}+b_{0}}\right)}
$$

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

- In general, choosing two strict means M and $\mathrm{M}^{\prime}$ with interness property will converge but difficult to analytically express the common limits of iterations
- When $M=A r i t h m e t i c ~ a n d ~ M '=H a r m o n i c, ~ t h e ~ a r i t h m e t i c-h a r m o n i c ~ m e a n ~ A H M ~$ yields the geometric mean:

$$
\begin{aligned}
a_{t+1} & =A\left(a_{t}, h_{t}\right) \\
h_{t+1} & =H\left(a_{t}, h_{t}\right)
\end{aligned}
$$

$$
\operatorname{AHM}(x, y)=\lim _{t \rightarrow \infty} a_{t}=\lim _{t \rightarrow \infty} h_{t}=\sqrt{x y}=G(x, y)
$$

## Inductive matrix arithmetic-harmonic mean

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

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

- Then the sequences converge quadratically to the matrix geometric mean:
$\operatorname{AHM}(X, Y)=\lim _{t \rightarrow+\infty} A_{t}=\lim _{t \rightarrow+\infty} H_{t}$.

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

which is also the Riemannian center of mass with respect to the trace metric:
$G(X, Y)=\arg \min _{M \in \mathbb{P}(d)} \frac{1}{2} \rho^{2}(X, M)+\frac{1}{2} \rho^{2}(Y, M) . \quad \rho\left(P_{1}, P_{2}\right)=\sqrt{\sum_{i=1}^{d} \log ^{2} \lambda_{i}\left(P_{1}^{-\frac{1}{3}} P_{2} P_{1}^{-\frac{1}{2}}\right)} \quad$ Riemannian distance $g_{P}\left(V_{1}, V_{2}\right)=\operatorname{tr}\left(P^{-1} V_{1} P^{-1} V_{2}\right)$

## Geometric interpretation of the AHM matrix mean

$$
\begin{aligned}
& A_{t+1}=\frac{A_{t}+H_{t}}{2}=A\left(A_{t}, H_{t}\right) \\
& H_{t+1}=2\left(A_{t}^{-1}+H_{t}^{-1}\right)^{-1}=H\left(A_{t}, H_{t}\right)
\end{aligned}
$$

$$
\begin{aligned}
& P_{t+1}=\gamma\left(P_{t}, Q_{t}: \frac{1}{2}\right) \\
& Q_{t+1}=\gamma^{*}\left(P_{t}, Q_{t}: \frac{1}{2}\right)
\end{aligned}
$$

(SPD, $\mathrm{g}^{\mathrm{G}}, \nabla^{\mathrm{A}}, \nabla^{\mathrm{H}}$ ) is a dually flat space, $\nabla^{\mathrm{G}}$ is Levi-Civita connection


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

$G_{\alpha}(P, Q)=P^{\frac{1}{2}}\left(P^{-\frac{1}{2}} Q P^{-\frac{1}{2}}\right)^{\alpha} P^{\frac{1}{2}}$
Dually flat space (SPD, $g^{G}, \nabla^{\mathrm{A}}, \nabla^{H}$ ) in information geometry defines quasi-arithmetic centers as geodesic midpoints

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

## Revisiting Chernoff information with Likelihood Ratio Exponential Families

## Chernoff information: Definition \& Background A symmetric statistical divergence

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

Definition:

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

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

$0<\rho_{\alpha}[P: Q] \leq 1$.
(via Hölder inequality)

- skewed Bhattacharyya coefficient $\rho_{\alpha}$ (similarity coefficient)


Herman Chernoff (1923-)

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


## Chernoff information = <br> Maximally skewed Bhattacharyya distance

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

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

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

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

- Optimal values of $\alpha$ is called "Chernoff (error) exponent" (due to its seminal use in statistical hypothesis testing)


## Rationale for Cl: Statistical hypothesis testing


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

## Error at $x$ : $\min (p 1(x), p 2(x))$

Histogram intersection similarity:

$$
P_{e}=\int \min \left(p_{1}(x), p_{2}(x)\right) \mathrm{d} x
$$

## Rewriting and bounding the probability of error

- Use rewriting trick $\min (a, b)=(a+b) / 2+|b-a| / 2$ for $a, b>0$
express the probability of error using the total variation distance:

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

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

$$
\min (a, b) \leq M(a, b) \leq \max (a, b) \longrightarrow \min (a, b) \leq M_{\alpha}(a, b) \leq \max (a, b), \forall \alpha \in[0,1]
$$

$$
P_{e}=\int \min \left(p_{1}(x), p_{2}(x) \mathrm{d} x \leq \min _{\alpha \in[0,1]} \int M_{\alpha}\left(p_{1}(x), p_{2}(x)\right) \mathrm{d} x \xrightarrow[\text { geometric weighted mean }]{M_{\alpha}(a, b)=a^{\alpha} b^{1-\alpha}} P_{e} \leq p_{\alpha}\left(p_{1}, p_{2}\right)\right.
$$

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

## Likelihood ratio exponential families (LREFs)

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

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

$$
\text { with normalization factor: } \quad Z_{p q}(\alpha)=\int_{\mathcal{X}} p(x)^{\alpha} q(x)^{1-\alpha} \mathrm{d} \mu(x)=\underline{\rho_{\alpha}[p: q]}
$$

- geometric mixture interpreted as a 1D exponential family:

$$
\begin{aligned}
(p q)_{\alpha}^{G}(x) & =\exp \left(\alpha \log \frac{p(x)}{q(x)}-\log Z_{p q}(\alpha)\right) q(x), \\
& \stackrel{*}{=}: \exp \left(\alpha t(x)-F_{p q}(\alpha)+k(x)\right) . \quad \text { Natural parameter space: } \\
& =\log q(\mathrm{x}) \\
& \Theta:=\left\{\alpha \in \mathbb{R}: Z_{p q}(\alpha)<\infty\right\}
\end{aligned}
$$

## LREFs: EF cumulant function is always analytic $\mathrm{C}^{\omega}$

- Cumulant function of EF is strictly convex (and smooth for regular EFs)
- Cumulant function is neg-Bhattacharyya distance:

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

$\Rightarrow$ Bhattacharyya. distance is strictly concave ${ }^{\text {ain }}$


- Theorem:

Chernoff exponent exists and is unique

$$
\left.\mathrm{p}=\mathrm{N}(0,1)_{(p q)_{\alpha}^{G}(x)} \propto p(x)^{\alpha} q(x)^{1-\alpha}\right)
$$

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

$$
\alpha^{*}(q: p)=1-\alpha^{*}(p: q)
$$

## Geometric mixtures and LREFs: Regular EFs

- Natural parameter space:

$$
\Theta_{p q}=\left\{\alpha \in \mathbb{R}: \rho_{\alpha}(p: q)<+\infty\right\}
$$ always contains $(\mathbf{0}, \mathbf{1})$ since $\quad 0<\rho_{\alpha}[P: Q] \leq 1$.

- What happens at extremities and when extrapolating (depends on support):

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

- Exponential family is said regular when the natural parameter space $\Theta$ is open (e.g., normal family, Dirichlet family, Wishart family, etc.)
Definition:
regular EF
$\Theta=\Theta^{\circ}$


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

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

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

- KLD between two densities of a regular EF = reverse Bregman divergence:

$$
\begin{array}{rlr}
D_{\mathrm{KL}}\left[p_{\theta_{1}}: p_{\theta_{2}}\right] & =E_{p_{\theta_{1}}}\left[\log \frac{p_{\theta_{1}}}{p_{\theta_{2}}}\right], \\
& =F\left(\theta_{2}\right)-F\left(\theta_{1}\right)-\left(\theta_{1}-\theta_{2}\right)^{\top} E_{p_{\theta_{1}}}[t(x)] . & \\
& \text { steep } \Rightarrow E_{p_{\theta_{1}}}[t(x)]=\nabla F\left(\theta_{1}\right) \\
& \text { regular EF } \Rightarrow \text { steep EF }
\end{array}
$$

$$
D_{\mathrm{KL}}\left[p_{\theta_{1}}: p_{\theta_{2}}\right]=F\left(\theta_{2}\right)-F\left(\theta_{1}\right)-\left(\theta_{1}-\theta_{2}\right)^{\top} \nabla F\left(\theta_{1}\right)=: B_{F}\left(\theta_{2}: \theta_{1}\right)=\left(B_{F}\right)^{*}\left(\theta_{1}: \theta_{2}\right)
$$

## Venn diagram: Regular \& steepness of (LR)EFs

- Steepness implies duality between natural $\theta$ and moment $\eta$ parameters


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

## PROOF

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

$$
D_{\mathrm{KL}}[p: q]=\left(B_{F}\right)^{*}\left(\alpha_{p}: \alpha_{q}\right)=B_{F_{p q}}\left(\alpha_{q}: \alpha_{p}\right)=B_{F_{p q}}(0: 1)
$$

Scalar Bregman divergence $B_{F_{p q}}: \Theta \times \operatorname{ri}(\Theta) \rightarrow[0, \infty)$

$$
\begin{gathered}
B_{F_{p q}}\left(\alpha_{1}: \alpha_{2}\right)=F_{p q}\left(\alpha_{1}\right)-F_{p q}\left(\alpha_{2}\right)-\left(\alpha_{1}-\alpha_{2}\right) F_{p q}^{\prime}\left(\alpha_{2}\right) \\
F_{p q}(0)=F_{p q}(1)=0
\end{gathered}
$$

$$
D_{\mathrm{KL}}[p: q]=B_{F_{p q}}\left(\alpha_{q}: \alpha_{p}\right)=B_{F_{p q}}(0: 1)=F_{p q}^{\prime}(1)<\infty
$$

idem for

$$
D_{\mathrm{KL}}[q: p]=B_{F_{p q}}\left(\alpha_{p}: \alpha_{q}\right)=B_{F_{p q}}(1: 0)=-F_{p q}^{\prime}(0)<\infty
$$

## Chernoff information (for densities of a LREF)

- Proposition: $D_{C}[p: q]=D_{\mathrm{KL}}\left[(p q)_{\alpha^{*}}^{G}: p\right]=D_{\mathrm{KL}}\left[(p q)_{\alpha^{*}}^{G}: q\right]=D_{B, \alpha^{*}}[p: q]$


## PROOF

First, skew Bhattacharyya distance $=$ skew Jensen divergence

$$
\begin{aligned}
D_{B, \alpha}[p: q]:=-\log \rho_{\alpha}[P: Q] & \square D_{B, \alpha}\left(p_{\theta_{1}}: p_{\theta_{2}}\right)=J_{F, \alpha}\left(\theta_{1}: \theta_{2}\right) \\
J_{F, \alpha}\left(\theta_{1}: \theta_{2}\right) & =\alpha F\left(\theta_{1}\right)+(1-\alpha) F\left(\theta_{2}\right)-F\left(\alpha \theta_{1}+(1-\alpha) \theta_{2}\right) .
\end{aligned}
$$

Thus we have: $D_{B, \alpha}\left((p q)_{\alpha_{1}}^{G}:(p q)_{\alpha_{2}}^{G}\right)=J_{F_{p q, \alpha}}\left(\alpha_{1}: \alpha_{2}\right)$,

$$
=\alpha F_{p q}\left(\alpha_{1}\right)+(1-\alpha) F_{p q}\left(\alpha_{2}\right)-F_{p q}\left(\alpha \alpha_{1}+(1-\alpha) \alpha_{2}\right)
$$

At the optimal value $\alpha^{*}$, we have $F_{p q}^{\prime}\left(\alpha^{*}\right)=0$
(1) $D_{\mathrm{KL}}\left[(p q)_{\alpha^{*}}^{G}: p\right]=B_{F_{p q}}\left(1: \alpha^{*}\right)=-F\left(\alpha^{*}\right)$ (2) $D_{\mathrm{KL}}\left[(p q)_{\alpha^{*}}^{G}: q\right]=B_{F_{p q}}\left(0: \alpha^{*}\right)=-F\left(\alpha^{*}\right)$
(3) $D_{C}[p: q]=-\log \rho_{\alpha^{*}}(p: q)=J_{F_{p q}, \alpha^{*}}(1: 0)=-F_{p q}\left(\alpha^{*}\right)$

## Jensen-Chernoff divergence

$$
D_{\mathrm{C}}[p: q]=D_{\mathrm{KL}}\left[(p q)_{\alpha^{*}}^{G}: p\right]=D_{\mathrm{KL}}\left[(p q)_{\alpha^{*}}^{G}: q\right]
$$

## non-parametric arguments

$$
\begin{aligned}
D_{C}[p, q] & =B_{F_{p q}}\left(1: \alpha^{*}\right)=B_{F_{p q}}\left(0: \alpha^{*}\right) \\
& =J_{F_{p q}, \alpha^{*}}(0: 1)
\end{aligned}
$$

## scalar parametric arguments



In general, define Jensen-Chernoff divergence

$$
J_{F}^{C}\left(\theta_{1}: \theta_{2}\right):=\max _{\alpha \in(0,1)} J_{F, \alpha}\left(\theta_{1}: \theta_{2}\right)
$$

## Geometric interpretation for densities $p, q$ on $L_{1}(\mu)$

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

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

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

$$
\gamma^{G}(p, q):=\left\{(p q)_{\alpha}^{G}: \alpha \in[0,1]\right\}
$$



## Special case of LREF: p,q are densities of a same EF!

EF includes Gaussians, Beta, Dirichlet, Wishart, etc.

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

$$
\begin{aligned}
p_{\theta_{1}}(x)^{\alpha} p_{\theta_{2}}(x)^{1-\alpha} & \propto \exp \left(\left\langle\alpha \theta_{1}+(1-\alpha) \theta_{2}, t(x)\right\rangle-\alpha F\left(\theta_{1}\right)-(1-\alpha) F\left(\theta_{2}\right)\right), \\
& \left.=p_{\alpha \theta_{1}+(1-\alpha) \theta_{2}}(x) \exp \left(F\left(\alpha \theta_{1}+(1-\alpha) \theta_{2}\right)-\alpha F\left(\theta_{1}\right)-(1-\alpha) F\left(\theta_{2}\right)\right)\right) \\
& =p_{\alpha \theta_{1}+(1-\alpha) \theta_{2}}(x) \exp \left(-J_{F, \alpha}\left(\theta_{1}: \theta_{2}\right)\right)
\end{aligned}
$$

$$
\left(p_{\theta_{1}} p_{\theta_{2}}\right)_{\alpha}^{G}=p_{\alpha \theta_{1}+(1-\alpha) \theta_{2}} . \quad D_{\mathrm{KL}}\left[p_{\theta_{1}}: p_{\theta_{2}}\right]=B_{F}\left(\theta_{2}: \theta_{1}\right)
$$

$$
\mathrm{OC}_{\mathrm{EF}}: \quad B_{F}\left(\theta_{1}: \theta_{\alpha^{*}}\right)=B_{F}\left(\theta_{2}: \theta_{\alpha^{*}}\right)
$$

Proposition
Let $p_{\lambda_{1}}$ and $p_{\lambda_{2}}$ be two densities of a regular exponential family $\mathcal{E}$ with natural parameter $\theta(\lambda)$ and $\log$-normalizer $F(\theta)$. Then the Chernoff information is

$$
D_{C}\left[p_{\lambda_{1}}: p_{\lambda_{2}}\right]=J_{F, \alpha^{*}}\left(\theta\left(\lambda_{1}\right): \theta\left(\lambda_{2}\right)\right)=B_{F}\left(\theta_{1}: \theta_{\alpha^{*}}\right)=B_{F}\left(\theta_{2}: \theta_{\alpha^{*}}\right)
$$

where $\theta_{1}=\theta\left(\lambda_{1}\right), \theta_{2}=\theta\left(\lambda_{2}\right)$, and the optimal skewing parameter $\alpha^{*}$ is unique and satisfies the following optimality condition:

$$
\mathrm{OC}_{\mathrm{EF}}: \quad\left(\theta_{2}-\theta_{1}\right)^{\top} \eta_{\alpha^{*}}=F\left(\theta_{2}\right)-F\left(\theta_{1}\right)
$$


$\mathcal{M}=\left(\left\{p_{\theta}\right\}, g_{F}=\nabla^{2} F(\theta), \nabla^{m}, \nabla^{e}\right)$

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

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

Proposition $\operatorname{Let}\left(\mathcal{M}, g, \nabla, \nabla^{*}\right)$ be a dually flat space with corresponding canonical divergence a Bregman divergence $B_{F}$. Let $\gamma_{p q}^{e}(\alpha)$ and $\gamma_{p q}^{m}(\alpha)$ be a e-geodesic and m-geodesic passing through the points $p$ and $q$ of $\mathcal{M}$, respectively. Let $\mathrm{Bi}^{m}(p, q)$ and $\mathrm{Bi}^{e}(p, q)$ be the right-sided $\nabla^{m_{-}}$flat and left-sided $\nabla^{e}$-flat Bregman bisectors, respectively. Then the intersection of $\gamma_{p q}^{e}(\alpha)$ with $\mathrm{Bi}^{m}(p, q)$ and the intersection of $\gamma_{p q}^{m}(\alpha)$ with $\operatorname{Bi}^{e}(p, q)$ are unique. The point $\gamma_{p q}^{e}(\alpha) \cap \operatorname{Bi}^{m}(p, q)$ is called the Chernoff point and the point $\gamma_{p q}^{m}(\alpha) \cap \mathrm{Bi}^{e}(p, q)$ is termed the reverse or dual Chernoff point.
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# Duo Bregman pseudo-divergences: Applications to the KL divergence between truncated densities 

## Legendre transformation reverses majorization order

Legendre-Fenchel transformation: $\quad F^{*}(\eta):=\sup _{\theta \in \Theta}\left\{\eta^{\top} \theta-F(\theta)\right\}$
F Legendre-type function, Moreau biconjugation theorem: $\left(F^{*}\right)^{*}=F$ proper+lower semi-continuous+convex

Legendre-Fenchel transform reverses ordering:
$\forall \theta \in \Theta, \quad F_{1}(\theta) \geq F_{2}(\theta) \Leftrightarrow \forall \eta \in H, \quad F_{1}^{*}(\eta) \leq F_{2}^{*}(\eta)$
Proof:

$$
\begin{aligned}
F_{1}^{*}(\eta) & :=\sup _{\theta \in \Theta}\left\{\eta^{\top} \theta-F_{1}(\theta)\right\}, \\
& =\eta^{\top} \theta_{1}-F_{1}\left(\theta_{1}\right) \quad\left(\text { with } \eta=\nabla F_{1}\left(\theta_{1}\right)\right) . \\
& \leq \eta^{\top} \theta_{1}-F_{2}\left(\theta_{1}\right), \\
& \leq \sup _{\theta \in \Theta}\left\{\eta^{\top} \theta-F_{2}(\theta)\right\}=: F_{2}^{*}(\eta) .
\end{aligned}
$$





Conjugate functions $F_{1}^{*}(\eta) \leq F_{2}^{*}(\eta)$


Duo Bregman divergence

$$
B_{F_{1}, F_{2}}\left(\theta: \theta^{\prime}\right)=F_{1}(\theta)-F_{2}\left(\theta^{\prime}\right)-\left(\theta-\theta^{\prime}\right)^{\top} \nabla F_{2}\left(\theta^{\prime}\right)
$$

## Duo Fenchel-Young divergence



## Duo Jensen divergence

$$
J_{F_{1}, F_{2}, \alpha}\left(\theta_{1}: \theta_{2}\right)=\alpha F_{1}\left(\theta_{1}\right)+(1-\alpha) F_{2}\left(\theta_{2}\right)-F_{1}\left(\alpha \theta_{1}+(1-\alpha) \theta_{2}\right) .
$$

$$
Y_{F_{1}, F_{2}^{*}}\left(\theta, \eta^{\prime}\right):=F_{1}(\theta)+F_{2}^{*}\left(\eta^{\prime}\right)-\theta^{\top} \eta^{\prime} .
$$

Relationship with truncated exponential families with nested supports:

$$
D_{\mathrm{KL}}\left[p_{\theta_{1}}: q_{\theta_{2}}\right]=Y_{F_{2}, F_{1}^{*}}\left(\theta_{2}: \eta_{1}\right)=B_{F_{2}, F_{1}}\left(\theta_{2}: \theta_{1}\right) \quad D_{\text {Bhat }, \alpha}[p: q]:=-\log \int_{\mathcal{X}} p(x)^{\alpha} q(x)^{1-\alpha} \mathrm{d} \mu(x)
$$

$$
D_{\text {Bhat }, \alpha}\left[p_{\theta_{1}}: q_{\theta_{2}}\right]=J_{F_{1}, F_{2}, \alpha}\left(\theta_{1}: \theta_{2}\right)
$$

Kullback-Leibler divergence $\quad D_{\text {KL }}[P: Q]=\int_{\mathcal{X}} \log \frac{\mathrm{d} P}{\mathrm{~d} Q} \mathrm{~d} P=E_{P}\left[\log \frac{\mathrm{~d} P}{\mathrm{~d} Q}\right]$ between exponential family densities

$$
\begin{array}{ll}
B_{F}\left(\theta_{1}: \theta_{2}\right):=F\left(\theta_{1}\right)-F\left(\theta_{2}\right)-\left(\theta_{1}-\theta_{2}\right)^{\top} \nabla F\left(\theta_{2}\right) \\
Y_{F, F^{*}}\left(\theta_{1}, \eta_{2}\right):=F\left(\theta_{1}\right)+F^{*}\left(\eta_{2}\right)-\theta_{1}^{\top} \eta_{2}
\end{array} \quad \begin{aligned}
& \text { Duo }
\end{aligned} \quad \begin{aligned}
& F_{F_{1}, F_{2}}\left(\theta: \theta^{\prime}\right):=Y_{F_{1}, F_{2}^{*}}\left(\theta, \eta^{\prime}\right)=F_{1}(\theta)-F_{2}\left(\theta^{\prime}\right)-\left(\theta-\theta^{\prime}\right)^{\top} \nabla F_{2}\left(\theta^{\prime}\right) \\
& Y_{F_{1}, F_{2}^{*}}\left(\theta, \eta^{\prime}\right):=F_{1}(\theta)+F_{2}^{*}\left(\eta^{\prime}\right)-\theta^{\top} \eta^{\prime} .
\end{aligned}
$$

- Same exponential family: KLD = reverse Bregman divergence or reverse Fenchel-Young divergence

$$
D_{\mathrm{KL}}\left[P_{\theta_{1}}: P_{\theta_{2}}\right]=Y_{F, F^{*}}\left(\theta_{2}: \eta_{1}\right)=B_{F}\left(\theta_{2}: \theta_{1}\right)=B_{F^{*}}\left(\eta_{1}: \eta_{2}\right)=Y_{F^{*}, F}\left(\eta_{1}: \eta_{2}\right)
$$

- Different exponential families (mutually absolutely continuous):

$$
D_{\mathrm{KL}}\left[P_{\theta}: Q_{\theta^{\prime}}\right]=F_{\mathcal{Q}}\left(\theta^{\prime}\right)-F_{\mathcal{P}}(\theta)+\theta^{\top} E_{P_{\theta}}\left[t_{\mathcal{P}}(x)\right]-\theta^{\prime \top} E_{P_{\theta}}\left[t_{\mathcal{Q}}(x)\right]
$$

- Same truncated exponential family: reverse duo Bregman divergence or reverse duo Fenchel-Young divergence (nested supports)

$$
D_{\mathrm{KL}}\left[p_{\theta_{1}}: q_{\theta_{2}}\right]=Y_{F_{2}, F_{1}^{*}}\left(\theta_{2}: \eta_{1}\right)=B_{F_{2}, F_{1}}\left(\theta_{2}: \theta_{1}\right)=B_{F_{1}^{*}, F_{2}^{*}}\left(\eta_{1}: \eta_{2}\right)=Y_{F_{1}^{*}, F_{2}}\left(\eta_{1}: \theta_{2}\right) .
$$

## KL divergence between truncated normal densities

PDF of truncated normal on ( $\mathbf{a}, \mathbf{b}$ ): $\quad p_{m, s}^{a, b}(x)=\frac{1}{\sqrt{2 \pi} s\left(\Phi_{m, s}(b)-\Phi_{m, s}(a)\right)} \exp \left(-\frac{(x-m)^{2}}{2 s^{2}}\right)$

$$
\Phi_{m, s}(x)=\frac{1}{2}\left(1+\operatorname{erf}\left(\frac{x-m}{\sqrt{2} s}\right)\right), \quad \operatorname{erf}(x)=\frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^{2}} \mathrm{~d} t .
$$

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

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

Moment parameters and mean \& variance:

$$
\underset{\mu(m, s ; a, b)}{ }=m-s \frac{\phi(\beta)-\phi(\alpha)}{\Phi(\beta)-\Phi(\alpha)}, \quad \phi(x):=\frac{1}{\sqrt{2 \pi}} \exp \left(-\frac{x^{2}}{2}\right)
$$

$\eta_{1}(m, s ; a, b)=E_{p_{m, s}^{a, b}}[x]=\mu(m, s ; a, b)$,

$$
\eta_{2}(m, s ; a, b)=E_{p_{m, s}, s}\left[x^{2}\right]=\sigma^{2}(m, s ; a, b)+\mu^{2}(m, s ; a, b) . \quad \sigma^{2}(m, s ; a, b)=s^{2}\left(1-\frac{\beta \phi(\beta)-\alpha \phi(\alpha)}{\Phi(\beta)-\Phi(\alpha)}-\left(\frac{\phi(\beta)-\phi(\alpha)}{\Phi(\beta)-\Phi(\alpha)}\right)^{2}\right)
$$

Kullback-Leibler divergence between nested truncated normal distributions:

$$
\begin{aligned}
& D_{\mathrm{KL}}\left[p_{m_{1}, s_{1}}^{a_{1}, b_{1}}: p_{m_{2}, s_{2}}^{a_{2}, b_{2}}\right]= \frac{m_{2}}{2 s_{2}^{2}}-\frac{m_{1}}{2 s_{1}^{2}}+\log \frac{Z_{a_{2}, b_{2}}\left(m_{2}, s_{2}\right)}{Z_{a_{1}, b_{1}}\left(m_{1}, s_{1}\right)}-\left(\frac{m_{2}}{s_{2}^{2}}-\frac{m_{1}}{s_{1}^{2}}\right) \eta_{1}\left(m_{1}, s_{1} ; a_{1}, b_{1}\right) \\
&-\left(\frac{1}{2 s_{1}^{2}}-\frac{1}{2 s_{2}^{2}}\right) \eta_{2}\left(m_{1}, s_{1} ; a_{1}, b_{1}\right) \text { if nested distributions }\left(a_{1}, b_{1}\right) \subseteq\left(a_{2}, b_{2}\right) \\
& D_{\mathrm{KL}}\left[p_{m_{1}, s_{1}}^{a_{1}, b_{1}}: p_{\left.m_{2}, s_{2}\right]}^{\left.a_{2}, b_{2}\right]}=+\infty,\left(a_{1}, b_{1}\right) \nsubseteq\left(a_{2}, b_{2}\right)\right. \text { otherwise }
\end{aligned}
$$

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