# Bregman divergences, dual information geometry, and generalized comparative convexity

### Frank Nielsen

Sony Computer Science Laboratories Inc.

Tokyo, Japan

https://franknielsen.github.io/



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• Bregman divergences

• Dual information geometry & Bregman manifolds

• Generalized convexity and designing divergences from convexity gaps

### Part I.

# Bregman divergences:

- Legendre-Fenchel transformation (dual parameterization)
- Fenchel-Young divergences (mixed parameterization)
- Statistical divergences, statistical models & Bregman divergences

# Bregman divergences

- F(θ): strictly convex and differentiable convex function on an open convex domain Θ
- Design the **Bregman divergence** as the vertical gap between  $F(\theta_1)$  and the linear approximation of  $F(\theta)$  at  $\theta_2$  evaluated at  $\theta_1$ :



# Bregman divergences: Some properties

### • Positive-definite:

- $B_F(\theta_1:\theta_2) > 0$  when  $\theta_1 \neq \theta_2$
- $B_F(\theta_1:\theta_2) = 0$  if and only if  $\theta_1 = \theta_2$
- Symmetric only for generalized squared Euclidean/Mahalanobis distance, <u>asymmetric</u> otherwise [N+ 2007]

 $Q \succ 0 \qquad D_Q^2(\theta_1, \theta_2) = B_{F_Q}(\theta_1, \theta_2) = (\theta_2 - \theta_1)^\top Q (\theta_2 - \theta_1), \quad F_Q(x) = x^\top Q x$  $D_E(\theta_1, \theta_2)^2 = \|\theta_1 - \theta_2\|_2^2 = D_I^2(\theta_1, \theta_2)$  $M_{\Sigma}^2[\mathcal{N}(\mu_1, \Sigma), \mathcal{N}(\mu_2, \Sigma)] = D_{\Sigma^{-1}}^2(\mu_1, \mu_2) = \Delta \mu^\top \Sigma^{-1} \Delta \mu$ 

- Does not satisfy the triangle inequality of metric distances
- Smooth/differentiable w.r.t. parameters ⇒ divergences (contrast functions)

[N+ 2007] Bregman Voronoi diagrams: Properties, algorithms and applications, arXiv:0709.2196

# Bregman divergences: 1<sup>st</sup> order Taylor remainder

• Bregman divergence (BD) can be interpreted as the mean-value remainder of a first-order Taylor expansion of  $F(\theta)$  at  $\theta_2$ :

$$F(\theta_1) = \underbrace{F(\theta_2) + (\theta_1 - \theta_2)^\top \nabla F(\theta_2)}_{\text{first-order Taylor expansion}} + \underbrace{R_F(\theta_1 : \theta_2)}_{\text{Taylor remainder}}$$

$$R_F(\theta_1 : \theta_2) = \frac{1}{2} (\theta_2 - \theta_1)^\top \nabla^2 F(\xi) (\theta_2 - \theta_1), \quad \xi \in [\theta_1 \theta_2]$$

$$= F(\theta_1) - F(\theta_2) - (\theta_1 - \theta_2)^\top \nabla F(\theta_2) =: B_F(\theta_1 : \theta_2)$$

• Since F is strictly convex, the Hessian is positive-definite:

$$\nabla^2 F(\theta) \succ 0 \Leftrightarrow \forall x \neq 0, x^\top \nabla^2 F(\theta) x > 0$$

• and this proves that BDs are positive-definite:

$$R_F(\theta_1:\theta_2) = \frac{1}{2}(\theta_2 - \theta_1)^\top \nabla^2 F(\xi) \left(\theta_2 - \theta_1\right) \ge 0$$

# Scalar and separable Bregman divergences

- D-variate Bregman divergence w.r.t. parameter  $\theta = (\theta^1, \dots, \theta^D)$
- Separable: Bregman generator is sum of univariate/scalar Bregman generators: D = D = D

$$F(\theta) := \sum_{i=1}^{D} F_i(\theta^i)$$
$$B_F(\theta_1 : \theta_2) = \sum_{i=1}^{D} B_{F_i}(\theta_1^i : \theta_2^i)$$

• For example, generalized square Euclidean distance with diagonal matrix Q

$$Q = \text{diag}(q_1, \dots, q_d) \qquad B_{F_Q}(\theta_1, \theta_2) = \sum_{i=1}^{D} q_i (\theta_2^i - \theta_1^i)^2 = \sum_{i=1}^{D} B_{F_{q_i}}(\theta_1^i : \theta_2^i)$$
$$F_{q_i}(x) = q_i x^2$$

# Extended Kullback-Leibler divergence

 Extended Kullback-Leibler divergence (eKL) is a D-dimensional separable Bregman divergence induced by the Shannon negentropy Bregman generator:

$$\mathcal{D}_{eKL}[p_{\theta_1}^+ : p_{\theta_2}^+] := \sum_{i=1}^{D} \theta_1^i \log \frac{\theta_1^i}{\theta_2^i} + \theta_2^i - \theta_1^i =: B_{F_{eKL}}(\theta_1 : \theta_2)$$
$$F_{eKL}(\theta) := \sum_{i=1}^{D} \theta^i \log \theta^i - \theta^i$$

- p<sup>+</sup> means a **positive measure** (not necessarily normalized to a probability)
- When p<sup>+</sup> is normalized:

$$\mathcal{D}_{\text{eKL}}[p_{\lambda_1}:p_{\lambda_2}] := \sum_{i=1}^D \theta_1^i \log \frac{\theta_1^i}{\theta_2^i}$$

 eKL divergence also called extended relative entropy in information theory

Lafferty, Lebanon, Boosting and maximum likelihood for exponential models, NeurIPS 14 (2002)

# Discrete Kullback-Leibler divergence: A non-separable Bregman divergence

 The KLD between two categorical distributions a.k.a. multinoulli amounts to a non-separable Bregman divergence on the natural parameters of the multinoulli distributions interpreted as an exponential family.

$$p_{\lambda} = (p_{\lambda}^1, \dots, p_{\lambda}^d) \in \Delta_{d-1}^{\circ}, \quad \sum_{i=1}^{d} p_{\lambda}^i = 1$$

$$\mathcal{D}_{\mathrm{KL}}[p_{\lambda_1}:p_{\lambda_2}] := \sum_{i=1}^D \lambda_1^i \log \frac{\lambda_1^i}{\lambda_2^i} =: B_{F_{\mathrm{KL}}}(\theta_1:\theta_2) \qquad \qquad \theta^i = \log \frac{\lambda^i}{\lambda^D}, i \in \{1,\ldots,D=d-1\}$$
$$F_{\mathrm{KL}}(\theta) = \log(1 + \sum_{i=1}^D \exp(\theta_i)) =: \mathrm{LogSumExp}_+(\theta_1,\ldots,\theta_D)$$

### LogSumExp is only convex but LogSumExp<sub>+</sub> is strictly convex [NH 2019]

[NH 2019] Monte Carlo information-geometric structures, Geometric Structures of Information, 2019. Guaranteed bounds on information-theoretic measures of univariate mixtures using piecewise log-sum-exp inequalities, Entropy, 18(12), 2016

# Legendre-Fenchel 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.

$$F^{*}(\eta) = \sup_{\theta \in \Theta} \{\theta^{\top} \eta - F(\theta)\}$$
  
=  $-\inf_{\theta \in \Theta} \{F(\theta) - \theta^{\top} \eta\}$   
$$F^{*}(\eta) = \sup_{\theta \in \Theta} \{\theta^{\top} \eta - F(\theta)\} = \sup_{\theta \in \Theta} \{E(\theta)\}$$

$$\nabla E(\theta) = \eta - \nabla F(\theta) = 0 \Rightarrow \eta = \nabla F(\theta)$$

Concave programming:

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

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

## **Reading the Legendre-Fenchel transformation**

Legendre-Fenchel transformation also called the slope transform



(Here, F was chosen as the cumulant function of the Poisson distributions)

# Legendre-Fenchel transform: Mixed coordinates and Fenchel-Young divergence

- **Dual parameterizations** of epigraph:  $\theta = \nabla F^*(\eta)$  and  $\eta = \nabla F(\theta)$
- Convex conjugate expressed as :  $F^*(\eta) = \eta^\top \nabla F^*(\eta) F(\nabla F^*(\eta))$
- To get in closed form the convex conjugate F<sup>\*</sup>, we need ∇F<sup>\*</sup>(η), i.e., <u>invert</u> ∇F(θ)
- Fenchel-Young inequality:  $F(\theta_1) + F^*(\eta_2) \ge \theta_1^\top \eta_2$

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

• Fenchel-Young divergence use mixed parameterization  $\theta/\eta$ :

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

## **Dual Bregman and dual Fenchel divergences**

- Identity of dual Bregman divergences:  $B_F(\theta_1 : \theta_2) = B_{F^*}(\eta_2 : \eta_1)$
- In general, dual or **reverse divergence**:  $D^*(\theta_1 : \theta_2) := D(\theta_2 : \theta_1)$
- Primal, dual or mixed parameterizations of Bregman divergences:

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

## **3-parameter identity of Bregman divergences**

• Generalize the law of cosines for the squared Euclidean distance



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

# 4-parameter identity of Bregman divergences

• Parallelogram identity



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



$$B_{F}(\theta_{1}:\theta_{2}) = \int_{\theta_{2}}^{\theta_{1}} (F'(\theta) - F'(\theta_{2})) d\theta \qquad S_{F}(\theta_{1},\theta_{2}) = B_{F}(\theta_{1}:\theta_{2}) + B_{F}(\theta_{2}:\theta_{1}) \\ = B_{F}(\theta_{1}:\theta_{2}) + B_{F*}(\eta_{1}:\eta_{2}) \\ B_{F*}(\eta_{2}:\theta_{1}) = \int_{\eta_{1}}^{\eta_{2}} (F^{*'}(\eta) - F^{*'}(\eta_{1})) d\eta \qquad = (\theta_{1} - \theta_{2})^{\top} (\eta_{1} - \eta_{2})$$

$$[arXiv:2107.059]$$

# Statistical divergences between parametric models = parameter divergences

Statistical divergences between densities of a parametric model  $\mathcal{F} = \{f_{\theta}(x)\}_{\theta}$  amount equivalently to (parameter) divergences between corresponding parameters:

$$\mathcal{D}[f_{\theta_1}:f_{\theta_2}] =: D_{\mathcal{M}}(\theta_1:\theta_2)$$

For which statistical models and statistical divergences,

do we obtain  $D_M(\theta_1 : \theta_2)$  as a Bregman divergence?

# **Example 1: Natural exponential family models**

- Parametric model  $\mathcal{E} = \{e_{\theta}(x)\}_{\theta}$  with densities  $e_{\theta}(x) = \exp\left(\sum_{i=1}^{D} t_i(x)\theta_i F(\theta) + k(x)\right)$
- Examples of **natural exponential families**:
  - Exponential distributions (continuous): p.d.f.
  - Poisson distributions (discrete): p.m.f.

$$egin{array}{lll} \lambda e^{-\lambda x} & x \geq 0 \ \Pr(X{=}k) = rac{\lambda^k e^{-\lambda}}{k!} \end{array}$$

• Examples of exponential families with density  $e_{\lambda}(x) = \exp\left(\sum_{i=1}^{D} t_i(x)\theta_i(\lambda) - F(\theta) + k(x)\right)$ Gaussian distributions once reparameterized with natural parameters  $\theta(\lambda) = \theta(\mu, \sigma^2)$ 

• We have  $\mathcal{D}_{\mathrm{KL}}[e_{\theta_1}:e_{\theta_2}] = \underbrace{B_F^*(\theta_1:\theta_2)}_{D_{\mathcal{E}}(\theta_1:\theta_2)} = B_F(\theta_2:\theta_1)$  with Bregman generator: the log-normalizer convex real-analytic function:  $F_{\mathcal{E}}(\theta) = \log\left(\int \exp(\sum_{i=1}^D t_i(x)\theta_i + k(x)) \,\mathrm{d}\mu(x)\right)$ 

On a Variational Definition for the Jensen-Shannon Symmetrization of Distances Based on the Information Radius, Entropy (2021)

# Example 2: Mixture family models

- Let 1, p<sub>0</sub>(x), ..., p<sub>D</sub>(x) be (D+2) **linearly independent** densities
- Mixture family  $\mathcal{M} = \{m_{\theta}(x)\}_{\theta}$  with densities:  $m_{\theta}(x) = \sum_{i=1}^{D} w_i p_i(x) + \left(1 \sum_{i=1}^{D} w_i\right) p_0(x)$

• We have: 
$$\mathcal{D}_{\mathrm{KL}}[m_{\theta_1}:m_{\theta_2}] = \underbrace{B_{F_{\mathcal{M}}}(\theta_1:\theta_2)}_{D_{\mathcal{M}}(\theta_1:\theta_2)} \qquad \theta = (w_1,\ldots,w_D)$$

• with the Bregman generator = **Shannon negentropy**:

$$F_{\mathcal{M}}(\theta) = \int m_{\theta}(x) \log m_{\theta}(x) \mathrm{d}\mu(x)$$

Natural parameters

Usually  $F_{M}(\theta)$  not in closed-form...

But 2-mixture family of Cauchy distributions has closed-form!

The dually flat information geometry of the mixture family of two prescribed Cauchy components, arXiv:2104.13801



# Example 3: q-Gaussians and statistical divergence

- The set of Cauchy distributions  $C:=\left\{p_{\lambda}(x):=\frac{s}{\pi(s^2+(x-l)^2)}, \lambda:=(l,s)\in\mathbb{H}:=\mathbb{R}\times\mathbb{R}_+\right\}$  form a **q-Gaussian exponential family** for q=2
- Deformed exponential family generalize exponential family with deformed log/exp functions
- Cumulant function of the Cauchy 2-Gaussian family:  $F(\theta) = -\frac{\pi^2}{\theta_2} \frac{\theta_1^2}{4\theta_2} 1.$  $(\theta_1, \theta_2) = \left(2\pi_{\overline{s}}^l, -\frac{\pi}{s}\right)$
- The following statistical divergence between 2 Cauchy distributions amount to a Bregman divergence:

$$D_{\text{flat}}[p_{\lambda_1}:p_{\lambda_2}] := \frac{1}{\int p_{\lambda_2}^2(x) dx} \left( \int \frac{p_{\lambda_2}^2(x)}{p_{\lambda_1}(x)} dx - 1 \right) = B_F(\theta_1:\theta_2)$$

• Bregman generator is the **q-free energy** for q=2

On Voronoi diagrams on the information-geometric Cauchy manifolds, Entropy 22.7 (2020)

# Information geometry & Bregman divergences

- Bregman divergences are canonical divergences of dually flat spaces (Bregman manifolds)
- Information geometry gives a principle to reconstruct the statistical divergence corresponding to a Bregman divergence for a Bregman generator  $F(f_{\theta})$ , and not the converse

Bregman generator Bregman divergence Statistical divergence

$$F_{\mathcal{E}}(\theta) = \log\left(\int \exp(\sum_{i=1}^{D} t_i(x)\theta_i + k(x)) \,\mathrm{d}\mu(x)\right) - B_F(\theta_1 : \theta_2) - \mathcal{D}_{\mathrm{KL}}^*[p_1 : p_2] = \mathcal{D}_{\mathrm{KL}}[p_2 : p_1] - \mathcal{D}_{\mathrm{KL}}^*[p_1 : \theta_2] = \mathcal{D}_{\mathrm{KL}}[p_2 : p_1] - \mathcal{D}_{\mathrm{KL}}^*[p_1 : \theta_2] = \mathcal{D}_{\mathrm{KL}}[p_2 : e_{\theta_1}]$$

An elementary introduction to information geometry." Entropy 22.10 (2020)

### Class of Bregman generators modulo affine terms & KLD between exponential family densities expressed as log-ratio

- Bregman generators are strictly convex and differentiable convex functions defined modulo affine terms: B<sub>F</sub>=B<sub>G</sub> iff. F(θ)=G(θ)+Aθ +b
- Choose for any  $\omega$  in the support of the exponential family the Bregman generator:  $F_{\omega}(\theta) := -\log(p_{\theta}(\omega)) = F(\theta) - (\theta^{\top}t(\omega) + k(\omega))$

$$\frac{\omega}{\omega} = F(\theta) - (\theta - t(\omega) + k(\omega))$$
  
affine term in  $\theta$ 

• We get: 
$$D_{\mathrm{KL}}[p_{\lambda_1}:p_{\lambda_2}] = \log\left(\frac{p_{\lambda_1}(\omega)}{p_{\lambda_2}(\omega)}\right) + (\theta(\lambda_2) - \theta(\lambda_1))^{\top}(t(\omega) - \nabla F(\theta(\lambda_1))), \quad \forall \omega \in \mathcal{X}$$

• By choosing s points:  $D_{\mathrm{KL}}[p_{\lambda_1}:p_{\lambda_2}] = \frac{1}{s} \sum_{i=1}^{s} \log\left(\frac{p_{\lambda_1}(\omega_i)}{p_{\lambda_2}(\omega_i)}\right)$  such that  $\frac{1}{s} \sum_{i=1}^{s} t(\omega_i) = \mathsf{E}_{p_{\lambda_1}}[t(x)]$ 

Computing Statistical Divergences with Sigma Points. GSI 2021 Cumulant-free closed-form formulas for some common (dis)similarities between densities of an exponential family, arXiv:2003.02469

# Part II. Information geometry & Bregman manifolds



### The **fabric** of information geometry and the **untangling** of its **geometry**, **divergence**, **statistical models**

# Motivation & history of information geometry

- Information geometry studies the <u>geometric structures</u> and <u>statistical invariance</u> principles (sufficient statistics, Markov kernels) of a family of probability distributions (=statistical model) and demonstrate their use in information sciences (statistics, ML).
- The newly revealed geometric structures (e.g., dually flat space) can *also* be used in non-statistical contexts (e.g., mathematical programming)
  - Born as a mathematical curiosity! Use Fisher information matrix as a Riemannian metric = Fisher metric [Hotelling 1930] [Rao 1945]
  - Decouple metric tensor with Levi-Civita connection, consider a family of affine connections [Chenstov 1960-1970's] : Geometrostatistics
  - Statistical curvature, Efron's e-connection, Dawid's m-connection [Efron 1975]
  - Consider dual torsion-free affine connections coupled to the metric, explicit
     α-structures [Amari 1980's] (Amari-Chentsov totally symmetric cubic tensor)
  - Non-parametric information geometry [Pistone 1990's], quantum information geometry, algebraic statistics, geometric science of information, etc.



# Part II.A - Fisher-Riemannian geometry

# Fisher information matrix (FIM)

- A parametric family of distributions  $\mathcal{P} = \{p_{\theta}\}_{\theta \in \Theta}$
- Fisher information matrix is positive-semidefinite matrix:

Score:  $s(\theta) := \nabla_{\theta} \log p_{\theta}(x)$   $I_X(\theta) = \operatorname{Cov}(s_{\theta})$   $X = (x_1, \dots, x_D)^{\mathsf{T}} \sim p_{\theta}$ 

• Under independence, Fisher information is additive:

 $Y = (Y_1, \dots, Y_n)_{\sim_{\mathrm{iid}} p_{\theta}} \quad \Rightarrow \quad I_Y(\theta) = n I_X(\theta)$ 

- Under *regularity conditions I (FIM type 1)*:  $I_1(\theta) = E_{p_{\theta}} \left[ (\nabla_{\theta} \log p_{\theta}) (\nabla_{\theta} \log p_{\theta})^{\top} \right]$
- Under *regularity conditions II (FIM type 2)*:  $I_2(\theta) = -E_{p_{\theta}} \left[ \nabla_{\theta}^2 \log p_{\theta} \right]$
- FIM can be singular (hierarchical models like mixtures, neural networks in ML)
- FIM can be infinite (irregular models, e.g., support depend on parameters )

N., Cramér-Rao lower bound and information geometry, Connected at Infinity II, 2013 Soen and Sun, On the Variance of the Fisher Information for Deep Learning, NeurIPS 2021



## Key concept: Sufficient statistics

- A statistic is a function of a random vector (e.g., mean, variance)
- A <u>sufficient statistic</u> collect and concentrate from a random sample all necessary information for estimating the parameters.

Informally, a statistical lossless compression scheme...

- <u>Definition:</u> conditional distribution of X given t $\frac{\textit{does not depend}}{\Pr(x| heta)} = \Pr(x|t)$
- Fisher-Neyman factorization theorem: Statistic t(x) sufficient iff. the density can be decomposed as:  $n(m, \lambda) = n(m)h_{1}(t(m))$

$$p(x;\lambda) = a(x)b_{\lambda}(t(x))$$

Statistical exponential families: A digest with flash cards, arXiv:0911.4863 (2009)

## Natural exponential families (NEF)

- Consider a positive measure  $\mu$  (usually counting or Lebesgue)
- A natural exponential family is a parametric family of densities that write as

$$p(x;\theta) = \exp(\theta x - F(\theta))$$

where F is **real-analytic, strictly convex and differentiable**:

$$F(\theta) = \log \int \exp(\theta x) d\mu(x)$$
Natural parameter space  $\Theta = \{\theta : \int \exp(\theta x) d\mu(x) < \infty\}$ 
F: Log-normalizer (also known as partition function, cumulant function, etc.)

Barndorff-Nielsen, Information and exponential families: in statistical theory. John Wiley & Sons, 2014 Sundberg, Statistical modelling by exponential families. Vol. 12. Cambridge University Press, 2019 N., Garcia, Statistical exponential families: A digest with flash cards." arXiv:0911.4863

# Exponential families (from Natural EFs to EFs)

- Consider a (sufficient) statistic t(x)
- Consider an additional carrier measure term k(x)
- Consider an inner product between t(x) and  $\boldsymbol{\theta}$

(usual scalar/dot product)

$$p_{ heta}(x) = \exp(\langle heta, t(x) 
angle - F( heta) + k(x))$$

Properties:

$$egin{aligned} E[t(X)] &= 
abla F( heta) \ \operatorname{Cov}[t(X)] &= 
abla^2 F( heta) = I( heta) \ ( ext{Hessian of -log p}_ heta( ext{x})) \ ( ext{FIM type 2}) \end{aligned}$$

### **Exponential families have finite moments of any order**

### Many common distributions are exponential families in disguise



Statistical exponential families: A digest with flash cards, arXiv:0911.4863 (2009) Tojo and Yoshino, On a method to construct exponential families by representation theory, GSI 2019 (Springer)

# Bhattacharyya arc: Likelihood Ratio Exponential Family

• Bhattacharyya arc or Hellinger arc induced by two mutually absolutely continuous distributions p and q (same support  $\mathcal{X}$ ):

$$\mathcal{E}(p,q) := \left\{ p_{\lambda}(x) := \frac{p^{1-\lambda}(x)q^{\lambda}(x)}{Z_{\lambda}^{G}(p,q)}, \quad \lambda \in (0,1) \right\} \quad Z_{\lambda}^{G}(p,q) := \int_{\mathcal{X}} p^{1-\lambda}(x)q^{\lambda}(x) d\mu(x)$$

- Log-normalizer  $F(\lambda)$  (aka cumulant generating function, log partition function):
- Bhattacharyya arc (geometric mixtures) = 1D exponential family:

$$p_{\lambda}(x) = \frac{p_0^{1-\lambda}(x)p_1^{\lambda}(x)}{Z_{\lambda}^G(p,q)}$$

$$= p_0(x)\exp\left(\lambda\log\left(\frac{p_1(x)}{p_0(x)}\right) - \log Z_{\lambda}^G(p,q)\right)$$

$$= \exp\left(\lambda t(x) - F(\lambda) + k(x)\right)$$

$$F(\lambda) := \log(Z_{\lambda}^G(p,q)) = \log\left(\int_{\mathcal{X}} p^{1-\lambda}(x)q^{\lambda}(x)d\mu(x)\right)$$

$$=: -D_{\lambda}^{\text{Bhat}}[p:q]$$

Log-likelihood sufficient statistics:

$$t(x) := \log\left(\frac{p_1(x)}{p_0(x)}\right)$$

Base measure is  $p_0 \quad k(x) := \log p_0(x)$ 

$$D_{\alpha}^{\text{Bhat}}[p:q] := -\log\left(\int_{\mathcal{X}} p^{1-\alpha}(x)q^{\alpha}(x)\mathrm{d}\mu(x)\right)$$

Generalizing the Geometric Annealing Path using Power Means, UAI 2021

Likelihood Ratio Exponential Families, NeurIPS Workshop on Deep Learning through Information Geometry 2020

# Rao's length distance (Riemannian distance)

(M,g) Riemannian manifold: Parameter space equipped with the Fisher information metric

$$d\left(\boldsymbol{\theta}^{1},\boldsymbol{\theta}^{2}\right) = \min_{\boldsymbol{\theta}(t)} \int_{t_{1}}^{t_{2}} \sqrt{\sum_{i=1}^{p} \sum_{j=1}^{p} g_{ij}(\boldsymbol{\theta}(t)) \frac{d\theta_{i}(t)}{dt} \frac{d\theta_{j}(t)}{dt}} dt.$$

**Invariant** under smooth & bijective reparameterization E.g., normal family:  $(\mu,\sigma)$ ,  $(\mu,\sigma^2)$ ,  $(\mu,\log\sigma)$ FIM is **covariant** under reparameterization





Rao distance in the probability simplex:

$$\rho_{\rm FHR}(p,q) = 2 \arccos\left(\sum_{i=0}^{d} \sqrt{\lambda_p^i \lambda_q^i}\right)$$



## Rao's distance between 1D normal distributions

Fisher information metric becomes the Poincare upper plane metric after scale change of variable



#### On Voronoi diagrams on the information-geometric Cauchy manifolds, Entropy 22.7 (2020)

# In practice, calculating Rao's distance may be difficult!

E.g., no closed form of Rao's distance between multivariate normals

$$d\left(\boldsymbol{\theta}^{1},\boldsymbol{\theta}^{2}\right) = \min_{\boldsymbol{\theta}(t)} \int_{t_{1}}^{t_{2}} \sqrt{\sum_{i=1}^{p} \sum_{j=1}^{p} g_{ij}(\boldsymbol{\theta}(t)) \frac{d\theta_{i}(t)}{dt} \frac{d\theta_{j}(t)}{dt}} dt$$

1. Need to solve the Ordinary Differential Equation (ODE) for find the **geodesic**:

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

$$\Gamma_{ij}^{k} = \frac{1}{2} \sum_{m=1}^{p} \left( \frac{\partial g_{im}(\theta)}{\partial \theta_{j}} + \frac{\partial g_{jm}(\theta)}{\partial \theta_{i}} - \frac{\partial g_{ij}(\theta)}{\partial \theta_{m}} \right) g^{mk}(\theta), \quad i, j, k = 1, \dots, p,$$

2. Need to **integrate** the infinitesimal length elements ds along the geodesics

## Approximating geodesics for MVNs: geodesic shooting



Minyeon Han · F.C. Park, DTI Segmentation and Fiber Tracking Using Metrics on Multivariate Normal Distributions, 2014 Calvo, Miquel, and Josep Maria Oller. "An explicit solution of information geodesic equations for the multivariate normal model." *Statistics & Risk Modeling* 9.1-2 (1991): 119-138.

# Part II.B - Dual information geometry

# Another look at Riemannian geodesics: Connections

• Riemannian geodesics are locally minimizing length curves



- The general definition of geodesics is wrt. to an affine connection: For Riemannian geodesics, the default connection = Levi-Civita connection. This special Levi-Civita connection is derived from the metric tensor g.
- A geodesic  $\gamma(t)$  with respect to a connection  $\nabla$  is an  $\underline{\nabla}$ -autoparallel curve (straight free fall particle in physics):  $\nabla_{\dot{\gamma}}\dot{\gamma} = 0, \quad \dot{\gamma} = \frac{d}{dt}\gamma(t)$

where  $\nabla_X T$  is the **covariant derivative** of a tensor T wrt. a vector field X An elementary introduction to information geometry, Entropy 22.10 (2020)

# What makes the Levi-Civita connection so special?

• A connection is described by **Christoffel symbols** (functions  $\Gamma$ ), and the geodesics is described by this ODE:  $\ddot{\gamma}(t) + \Gamma_{ij}^k \dot{\gamma}(t) \dot{\gamma}(t) = 0$ ,  $\gamma^l(t) = x^l \circ \gamma(t)$ ,

An affine connection defines how to **parallel transport** a vector from one tangent plane to another tangent plane

### • Fundamental theorem of Riemann geometry:

An elementary introduction to information geometry, Entropy 22.10 (2020)



# **∇** : Curvature, torsion, and parallel transport



Cylinder is flat Parallel transport is independent of path



Sphere has constant curvature Parallel transport is path-dependent

A connection is flat is there exists locally a coordinate system such that the Christofel symbols are all zero: Geodesics plotted in that coordinate system are line segments

Torsion tensor  $T(X,Y) := \nabla_X Y - \nabla_Y X - [X,Y]$ Connections that differ only on torsions yield same geodesics

# Dualistic information geometry: $(M, g, \nabla, \nabla^*)$

 Given an affine torsion-free connection ∇ and a metric g, we can build a unique dual affine torsion-free connection: the dual connection ∇\* such that the metric (inner product) is preserved by the primal and dual parallel transports:

$$\langle u,v\rangle_{c(0)} = \left\langle \prod_{c(0)\to c(t)}^{\nabla} u, \prod_{c(0)\to c(t)}^{\nabla^*} v \right\rangle_{c(t)}.$$

 $v_{1} \qquad v_{2} \qquad g(v_{1}, v_{2}) = g\left(\prod_{c(t)}^{\nabla} v_{1}, \prod_{c(t)}^{\nabla^{*}} v_{2}\right)$ 

• This amounts to say that  $\nabla^*$  is defined uniquely by

$$Xg(Y,Z) = g(\nabla_X Y,Z) + g(Y,\nabla_X^* Z),$$

meaning  $X_pg_p(Y_p, Z_p) = g_p((\nabla_X Y)_p, Z_p) + g_p(Y_p, (\nabla_X^* Z)_p).$ 

• The dual of a dual connection is the primal connection:  $(\nabla^*)^* = \nabla$ .

An elementary introduction to information geometry, Entropy 22.10 (2020)

# Amari/Chentsov's $\alpha$ -structures $\{(\mathcal{P}, _{\mathcal{P}}g, _{\mathcal{P}}\nabla^{-\alpha}, _{\mathcal{P}}\nabla^{+\alpha})\}_{\alpha \in \mathbb{R}}$

- Regular statistical parametric models (identifiable and finite positive-definite FIM)  $\mathcal{P}{:=}\{p_{\theta}(x)\}_{\theta\in\Theta}$
- Amari's  $\alpha$ -connections  $\mathcal{P}\Gamma^{\alpha}_{ij,k}(\theta) := E_{\theta} \left[ \left( \partial_{\alpha} \mathcal{P} \right)^{\alpha} \right]_{ij,k}(\theta) = E_{\theta} \left[ \left( \partial_{$

$${}_{\mathcal{P}}\Gamma^{lpha}{}_{ij,k}( heta)\!:=\! {}^{E_{ heta}} \! \left[ \left( \partial_i \partial_j l + rac{1-lpha}{2} \partial_i l \partial_j l 
ight) (\partial_k l) 
ight] . \ l( heta;x)\!:=\! \log L( heta;x) = \log p_{ heta}(x)$$

- O-connection is Fisher Levi-Civita connection
- 1-connection is **exponential connection** (flat for exponential families)
- -1 connection is **mixture connection** (flat for mixture families)

Amari, Differential geometry of curved exponential families-curvatures and information loss, Annals of Statistics (1982)

## Lauritzen' statistical manifolds: Cubic tensor

Beware: Apply also to non-statistical contexts too! (M, g, C)Dualistic structure with metric tensor g and cubic tensor C  $C(X, Y, Z) := \langle \nabla_X Y - \nabla_X^* Y, Z \rangle$   $C = \nabla g$  $C_{ijk} = C(\partial_i, \partial_j, \partial_k) = \langle \nabla_{\partial_i} \partial_j - \nabla_{\partial_i}^* \partial_j, \partial_k \rangle$ 

C is **totally symmetric** (= components invariant by index permutation)

In a local basis:  $C_{ijk}$ := $\Gamma^k_{ij} - \Gamma^{*k}_{ij}$ 

 ${}^{LC}\nabla q = 0$ 

Levi-Civita connection is self-dual with respect to the metric!

Lauritzen, Statistical manifolds, Differential geometry in statistical inference 10 (1987)

## Eguchi's Information geometry of divergences

• Reverse/dual parameter divergence (reference duality)

$$D^*( heta: heta') := D( heta': heta) \qquad (D^*)^* = D$$

### • Statistical manifold structures:

$$(M, {}^Dg, {}^D
abla, {}^D
abla, {}^D^*
abla) \qquad (M, {}^Dg, {}^DC)$$

$$\begin{split} {}^{D}g &:= -\partial_{i,j}D(\theta:\theta')|_{\theta=\theta'} = {}^{D^{*}}g, \qquad {}^{D}C_{ijk} = {}^{D^{*}}\Gamma_{ijk} - {}^{D}\Gamma_{ijk} \\ {}^{D}\Gamma_{ijk} &:= -\partial_{ij,k}D(\theta:\theta')|_{\theta=\theta'}, \qquad {}^{D}\nabla^{*} = {}^{D^{*}}\nabla \\ {}^{D^{*}}\Gamma_{ijk} &:= -\partial_{k,ij}D(\theta:\theta')|_{\theta=\theta'}. \qquad {}^{D}\nabla^{-\alpha}, ({}^{D}\nabla^{-\alpha})^{*} = {}^{D^{*}}\nabla \\ & \left\{ (M, {}^{D}g, {}^{D}C^{\alpha}) \equiv (M, {}^{D}g, {}^{D}\nabla^{-\alpha}, ({}^{D}\nabla^{-\alpha})^{*} = {}^{D}\nabla^{\alpha}) \right\}_{\alpha \in \mathbb{R}} \end{split}$$

Eguchi, Geometry of minimum contrast, Hiroshima Mathematical Journal 22.3 (1992)

# Part II.C - Bregman manifolds: Dually flat spaces

# Dually flat geometry from a convex function



Not necessarily related to statistical models,

but can always be realized by a regular statistical model

Vân Lê, Hông. "Statistical manifolds are statistical models." Journal of Geometry 84.1-2 (2006)

### Metric tensor using covariant/contravariant notations

2-covariant metric tensor in local coordinates:

$$g_{ij}( heta) = 
abla^2 F( heta)$$

**Dual metric tensor** in local coordinates:



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

**<u>Crouzeix's identity</u>**: x of Hessians of convex conjugates= Id:

$$abla^2 F( heta) 
abla^2 F^*(\eta) = I$$

An elementary introduction to information geometry." Entropy 22.10 (2020)

# Bregman information geometry: Bregman manifolds



$$F^*(\eta) = \sup_{ heta \in \Theta} \{ heta^ op \eta - F( heta) \}$$

- Start from a potential function F(heta)  $^{F}g=
  abla^{2}F( heta)$
- Get the dual potential function F\*( $\eta$ )  ${}^Fg^* = 
  abla^2 F^*(\eta)$
- Define the primal flat connection:  ${}^F\Gamma_{ijk}( heta)=0$
- Define the dual flat connection:  ${}^{F}\Gamma^{*\,ijk}(\eta)=0$
- Get the dual Bregman divergences or dual Fenchel-Young divergences

The many faces of information geometry, Notices of the AMS, January 2022

# Bregman manifolds vs Hessian manifolds

- Hessian metric wrt. a flat connection  $\nabla$ . function is 0-form on M: Riemannian Hessian metric when  $g = \nabla^2 F_M$
- Hessian operator:  $(\nabla^2 F_M)(X,Y) := (\nabla_X d)(F_M(Y)) = X(dF_M(Y)) dF_M(\nabla_X Y)$

 $\nabla^2 F_M\left(\partial_{x^i}, \partial_{x^j}\right) = \frac{\partial^2 F_M}{\partial x^i \partial x^j} - \Gamma_{ij}^k \frac{\partial F_M}{\partial x^k} \quad \text{vflat} \quad \nabla^2 F_M\left(\partial_{x^i}, \partial_{x^j}\right) = \frac{\partial^2 F_M}{\partial x^i \partial x^j}$ 

• **Bregman manifold**: geometry on an open convex domain:

Here,  $\nabla$  = gradient Here,  $\nabla$ ,  $\nabla^*$  = affine flat connections

$$g(\theta) = \nabla^2 F(\theta) \qquad \qquad \nabla \ : \ \Gamma_{ijk}(\theta) = 0$$
$$g^*(\eta) = \nabla^2 F^*(\eta) \qquad \qquad \nabla^* \ : \ \Gamma^{*ijk}(\eta) = 0$$

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

![](_page_48_Picture_7.jpeg)

# Part III Generalized convexity and divergences from convexity gaps

# Chordal slope lemma & Jensen/Bregman divergences

![](_page_50_Figure_1.jpeg)

# Bregman divergences wrt comparative convexity

- Two abstract means M and N, i.e.  $\min\{p,q\} \le M(p,q) \le \max\{p,q\}$ .
- Define a function F (M,N) convex if

 $F(M(p,q)) \le N(F(p), F(q)), \quad \forall p, q \in \mathcal{X},$ 

- Consider the means regular: homogeneous, symmetric continuous, and increasing in each variable
- Define skew (M,N)-Jensen divergence for a strictly convex (M,N)-function for regular means M and N:

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

• By analogy of ordinary Bregman divergences obtained as limit of scaled skew Jensen divergences, define (M,N)-Bregman divergences:

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

Generalizing skew Jensen divergences and Bregman divergences with comparative convexity, IEEE Signal Proc. Letters (2017)

# Quasi-arithmetic (rho-tau)-Bregman divergences

- For a strictly continuously monotone function  $\gamma$ , define the weighted quasi-arithmetic means  $M_{\gamma,\alpha}(x,y) = \gamma^{-1}((1-\alpha)\gamma(x) + \alpha\gamma(y))$
- Quasi-arithmetic Bregman divergence:

$$B_{F}^{\rho,\tau}(q:p) = \lim_{\alpha \to 0} \frac{1}{\alpha(1-\alpha)} \left( M_{\tau,\alpha}(F(p), F(q)) \right) - F\left( M_{\rho,\alpha}(p,q) \right)$$
$$B_{F}^{\rho,\tau}(q:p) = \lim_{\alpha \to 0} \frac{1}{\alpha(1-\alpha)} \left( M_{\tau,\alpha}(F(p), F(q)) \right) - F\left( M_{\rho,\alpha}(p,q) \right)$$

- Consider the ordinary convex function:  $G(x) = \tau(F(\rho^{-1}(x)))$
- Quasi-arithmetic (rho-tau)-Bregman divergences is a conformal regular Bregman divergence:  $B_F^{\rho,\tau}(p:q) = \frac{1}{\tau'(F(q))} B_G(\rho(p):\rho(q))$

Generalizing skew Jensen divergences and Bregman divergences with comparative convexity, IEEE Signal Proc. Letters (2017) Nock, N., Amari, On conformal divergences and their population minimizers, IEEE Transactions on Information Theory 62.1 (2015)

## **Quasi-convex Jensen and Bregman divergences**

• Strictly quasiconvex function:  $Q((\theta\theta')_{\alpha}) < \max\{Q(\theta), Q(\theta')\}, \quad \theta \neq \theta' \in \Theta$ 

 $(\theta\theta')_{\alpha} := (1-\alpha)\theta + \alpha\theta'$ 

![](_page_53_Figure_3.jpeg)

• Quasiconvex Jensen divergence:

 $\begin{aligned} {}^{\mathrm{qcvx}}J_Q^{\alpha}(\theta:\theta') &:= \max\{Q(\theta),Q(\theta')\} - Q((\theta\theta')_{\alpha}) \ge 0, \\ &= \max\{Q(\theta),Q(\theta')\} - Q((1-\alpha)\theta + \alpha\theta')). \end{aligned}$ 

• Quasic-convex Jensen divergence is a (Max,A)-Jensen divergence!

N. and Hadjeres, Quasiconvex Jensen Divergences and Quasiconvex Bregman Divergences, Workshop on Joint Structures and Common Foundations of Statistical Physics, Information Geometry and Inference for Learning. Springer, 2020.

# Multivariate Bregman divergence as a family of univariate Bregman divergences

**Proposition** A multivariate Bregman divergence  $B_F(\theta_1 : \theta_2)$  can be written equivalently as a univariate Bregman divergence  $B_{F_{\theta_1,\theta_2}}(0:1)$ :

$$\forall \theta_1, \theta_2 \in \Theta, \quad B_F(\theta_1 : \theta_2) = B_{F_{\theta_1, \theta_2}}(0 : 1),$$

**1D Bregman generator** 

where

$$F_{\theta_1,\theta_2}(u) := F(\theta_1 + u(\theta_2 - \theta_1))$$

#### is a univariate Bregman divergence.

**Proof:** The univariate functions  $F_{\theta_1,\theta_2}$  are proper 1D Bregman generators: We have the directional derivative:

$$\nabla_{\theta_2-\theta_1} F_{\theta_1,\theta_2}(u) = \lim_{\epsilon \to 0} \frac{F(\theta_1 + (\epsilon + u)(\theta_2 - \theta_1)) - F(\theta_1 + u(\theta_2 - \theta_1))}{\epsilon},$$
  
=  $(\theta_2 - \theta_1)^\top \nabla F(\theta_1 + u(\theta_2 - \theta_1)),$ 

Since  $F_{\theta_1,\theta_2}(0) = F(\theta_1)$ ,  $F_{\theta_1,\theta_2}(1) = F(\theta_2)$ , and  $F'_{\theta_1,\theta_2}(u) = \nabla_{\theta_2-\theta_1}F_{\theta_1,\theta_2}(u)$ , it follows that

$$B_{F_{\theta_1,\theta_2}}(0:1) = F_{\theta_1,\theta_2}(0) - F_{\theta_1,\theta_2}(1) - (0-1)\nabla_{\theta_2-\theta_1}F_{\theta_1,\theta_2}(1), = F(\theta_1) - F(\theta_2) + (\theta_2 - \theta_1)^{\top}\nabla F(\theta_2) = B_F(\theta_1:\theta_2).$$

The Bregman chord divergence, GSI, Springer, 2019

# Designing divergences by measuring convexity gaps

![](_page_55_Figure_1.jpeg)

$$J_F^{\alpha,\beta,\gamma}(\theta:\theta') := (F(\theta)F(\theta'))_{\gamma} - (F((\theta\theta')_{\alpha})F((\theta\theta')_{\beta}))_{\frac{\gamma-\alpha}{\beta-\alpha}},$$

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

#### The Bregman chord divergence, GSI, Springer, 2019

![](_page_56_Picture_0.jpeg)

### "The only constant in life is change" -Heraclitus

My motto: "Invariance is the only constant in change!"

![](_page_56_Picture_3.jpeg)

https://franknielsen.github.io/

![](_page_57_Figure_0.jpeg)

- Fast stabbing of boxes in high dimensions, Theoretical Computer Science 246.1-2 (2000): 53-72.
- On point covers of c-oriented polygons, Theoretical computer science 263.1-2 (2001): 17-29.

# Adaptive computational geometry (PhD, 1996)

### **Computational geometry: Output-sensitive algorithms**

![](_page_57_Figure_6.jpeg)

**2D** lower envelopes

convex hull of objects

![](_page_58_Figure_0.jpeg)

(a) Squared Euclidean distance

(b) Itakura-Saito divergence

Figure 13.2. Voronoi diagram and convex polyhedron.

[Voronoi by mapping to the paraboloid]

[Bregman Voronoi by mapping to Bregman potential functions]

Bregman voronoi diagrams, Discrete & Computational Geometry 44.2 (2010): 281-307.

### The **fabric** of information geometry and the **untangling** of its **geometry**, **divergence**, **statistical** models

![](_page_59_Picture_1.jpeg)