Divergences and comparative convexity

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Outline

Kullback-Leibler divergence: relative entropy

- The Kullback-Leibler divergence (KLD) is a dissimilarity measure between probability distributions/measures P and Q :

$$D_{\mathrm{KL}}(P:Q) = \begin{cases} \int p \log \frac{p}{q}\,\mathrm{d}\mu, \quad p = \frac{\mathrm{dP}}{\mathrm{d}\mu}, Q = \frac{\mathrm{dQ}}{\mathrm{d}\mu}, & P \ll Q \\ +\infty & P \not\ll Q \end{cases}$$

- Fails symmetry and triangle inequality of metrics but is always non-negative as known as Gibbs' inequality:

$$D_{\mathrm{KL}}(P:Q) \geq 0, \quad D_{\mathrm{KL}}(P:Q) \neq D_{\mathrm{KL}}(Q:P), \quad D_{\mathrm{KL}}(P:Q) \not\leq D_{\mathrm{KL}}(P:Q) + D_{\mathrm{KL}}(Q:R)$$

- KLD also called relative entropy because it is the difference between the cross-entropy and Shannon entropy:

$$D_{\mathrm{KL}}(P:Q) = H^{\times}(P:Q) - H(P), H^{\times}(P:Q) = -\int p \log q\,\mathrm{d}\mu, H(P) = H^{\times}(P:P) = -\int p \log p\,\mathrm{d}\mu$$

- Interpretations in information theory: expected difference of the number of bits required for Huffman encoding of P using a code optimized for Q rather than the Huffman code optimized for P.

Exponential families: Discrete/continuous/measures

- A parametric family of distributions $\{P_\lambda\}$ all dominated by a measure μ is an **exponential family** iff the densities wrt μ can be expressed canonically as

$$
\begin{aligned}
p_\lambda(x) &= \exp\left(\langle\theta(\lambda), t(x)\rangle - F(\theta(\lambda)) + k(x)\right) \\
&= \frac{1}{Z(\theta)} \exp\left(\langle\theta(\lambda), t(x)\rangle\right) h(x)
\end{aligned}
$$

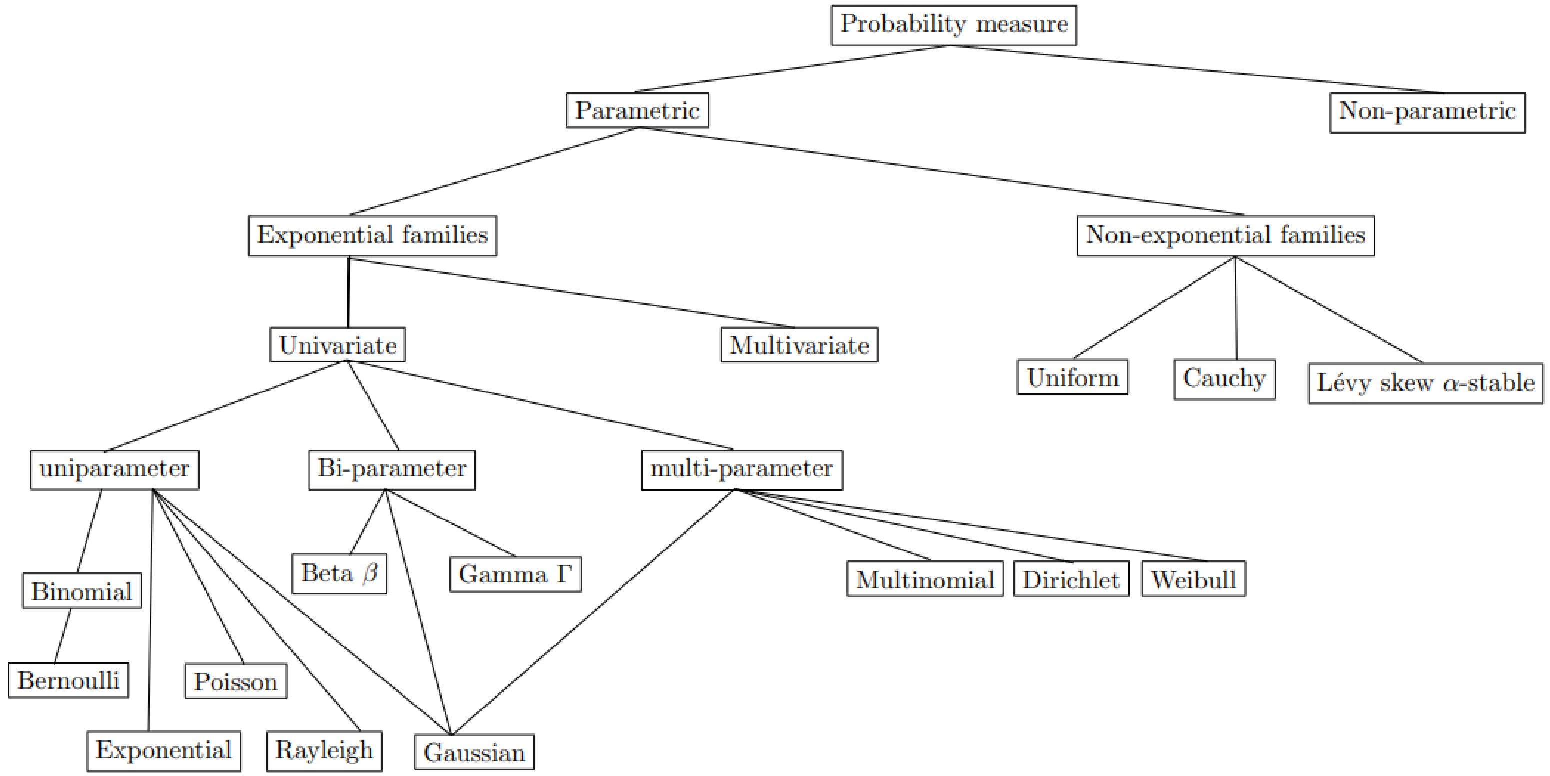
- θ is **natural parameter**
- t(x) is **sufficient statistics** and k(x) and h(x) are auxiliary carrier term
- Inner product (e.g., scalar product for vectors)

- Unnormalized density: $\tilde{p}_\lambda(x) = \exp\left(\langle\theta(\lambda), t(x)\rangle\right) h(x), \quad \tilde{p}_\theta(x) = \exp\left(\langle\theta, t(x)\rangle\right) h(x)$
- Subtractive normalization: $F(\theta) = \log Z(\theta) = \log \int_{\mathcal{X}} \tilde{p}_\theta(x)\, \mathrm{d}\mu(x)$
- Divisive normalization: $Z(\theta) = \exp(F(\theta)) = \int_{\mathcal{X}} \tilde{p}_\theta(x)\, \mathrm{d}\mu(x)$

- F called cumulant function in statistics
- F called free energy and Z called partition function in thermodynamics

Exponential families (EFs): Some examples

- Many common distributions in statistics are exponential families in disguise



- Many statistical models in machine learning are exponential families: undirected graphical models, energy-based models including Markov random fields and conditional random fields

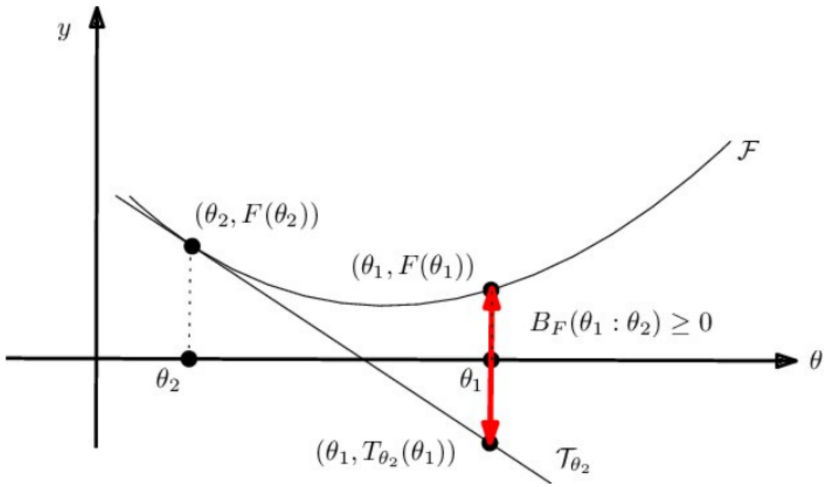
KLD between two densities of an EF

- Bypass integral calculations of KLDs and express it as a divergence between parameters: Bregman divergences

$$
\begin{aligned}
D_{\mathrm{KL}}(p_{\lambda_1} : p_{\lambda_2}) &= D_{\mathrm{KL}}(p_{\theta_1} : p_{\theta_2}) = \int p_{\theta_1} \log \frac{p_{\theta_1}}{p_{\theta_2}} \,\mathrm{d}\mu \\
&= B_F(\theta_2 : \theta_1) = B_F(\theta(\lambda_2) : \theta(\lambda_1)) \\
&= F(\theta_2) - F(\theta_1) - \langle \theta_2 - \theta_1, \nabla F(\theta_1) \rangle
\end{aligned}
$$

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

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



- Dual expectation/moment parameterization: $\eta = \nabla F(\theta) = E_{p_\theta}[t(X)]$
- Many equivalent parameterizations of EFs: $p_\lambda \leftrightarrow p_{\theta(\lambda)} \leftrightarrow p_{\eta(\theta)}$

Convex duality: convex conjugates (F,F*)

- **Legendre-Fenchel transformation** of a function:

  as known as slope transform: $$F^*(\eta) = \sup_{\theta \in \Theta} \langle \theta, \eta \rangle - F(\theta)$$

- Supremum reached for $\eta = \nabla F(\theta)$: defines the **gradient map**
- Moment parameter space: $H = \{\nabla F(\theta) \ : \ \theta \in \Theta\}$
- Restrict F to **Legendre-type function** $(F(\theta), \Theta)$ so that

convex conjugate is also of Legendre type: $(F^*(\eta), H)$

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

- And we have: $\theta = \nabla F^*(\eta)$ and $F^{**} = F$ reciprocal gradient: $\nabla F^* = (\nabla F)^{-1}$
- Legendre transformation:

  (need to invert ∇F) $$F^*(\eta) = \langle \eta, (\nabla F)^{-1}(\eta) \rangle - F((\nabla F)^{-1}(\eta))$$

Dual Bregman divergence/Fenchel-Young divergence

- Bregman divergence can be expressed equivalently as a **Fenchel-Young divergence**:

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

- **Dual Bregman divergence**: $B_F(\theta_1 : \theta_2) = B_{F^*}(\eta_2 : \eta_1)$

- Thus KLD between densities of an exponential family expressed as:

$$\begin{aligned} D_{\mathrm{KL}}(p_{\lambda_1} : p_{\lambda_2}) &= D_{\mathrm{KL}}(p_{\theta_1} : p_{\theta_2}) = \int p_{\theta_1} \log \frac{p_{\theta_1}}{p_{\theta_2}} \mathrm{d}\mu \\ &= B_F(\theta(\lambda_2) : \theta(\lambda_1)) = B_F(\theta_2 : \theta_1) = Y_{F,F^*}(\theta_2 : \eta_1) \\ &= B_{F^*}(\eta_1 : \eta_2) = Y_{F^*,F}(\eta_1 : \theta_2) \end{aligned}$$

Information geometry: Dually structures

- Riemannian metric g is smooth inner product on a manifold which allows to measure vector lengths and angles between vectors
- Affine connection ∇ defines how to connect vectors between infinitesimally close tangent spaces. Affine connection defines ∇-geodesic

- Information geometry considers dual structures: A manifold M equipped with a Riemannian metric tensor g and dual torsion-free affine connections ∇ and ∇^* coupled to the metric so that the Levi-Civita connection wrt g is $(\nabla+\nabla^*)/2$: Structure (M,g,∇,∇^*)

- Information geometry induced by statistical models $\{p_\theta\}$, information geometry induced by divergences, information geometry induced by convex functions, information geometry induced by regular cones, etc.

Information geometry of convex functions: Dually flat spaces

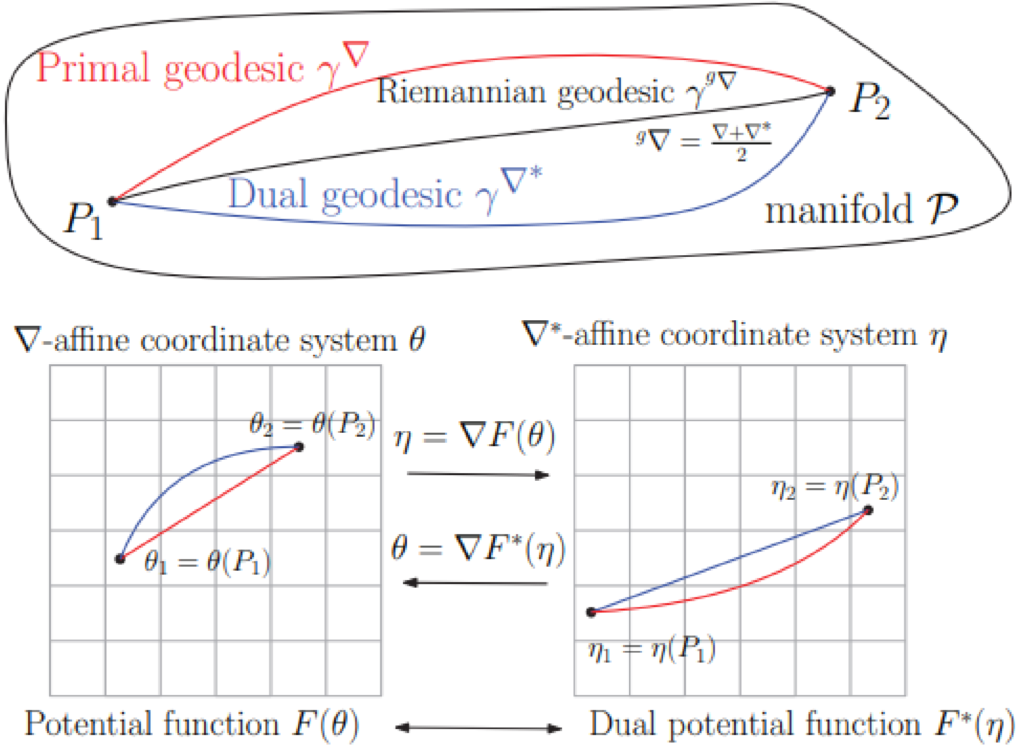
- An affine connection ∇ is flat if there exists a coordinate system θ called ∇-affine coordinate system such that the Christoffel symbols Γ vanish

- ∇-geodesics are straight lines in θ-chart

- Hessian metric tensor g expressed in θ-chart as $\nabla^2 F(\theta)$

- Legendre duality yields dual expression of Hessian metric $\nabla^2 F^*(\eta)$ and dual affine flat connection ∇^* with ∇^*-geodesics straight in η-chart

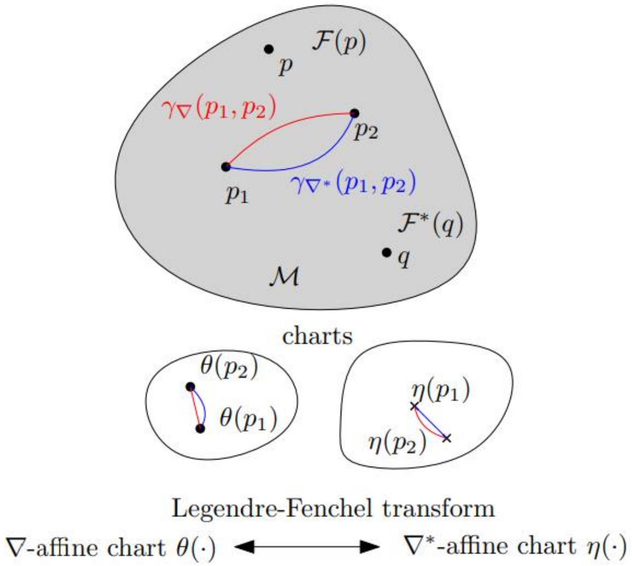
- Dually flat space DFS(F(θ), Θ)=(M,g, ∇, ∇^*)



Canonical divergences of dually flat spaces: Dually flat divergences

- Given a dually flat space (M, g, ∇, ∇^*), we can reconstruct locally two potential functions $F(\theta)$ and $F^*(\eta)$ related by Legendre-Fenchel transformation
- The dually flat divergence $D_{\nabla,\nabla^*}(P:Q)$ can be expressed using the mixed coordinate system θ and η as a Fenchel-Young divergence or equivalently using dual Bregman divergences either in the θ- or η-charts

$$\begin{aligned} D_{\nabla,\nabla^*}(P:Q) &= Y_{F,F^*}(\theta(P):\eta(Q)) \\ &= B_F(\theta(P):\theta(Q)) \\ &= B_{F^*}(\eta(Q):\eta(P)) \\ &= Y_{F^*,F}(\eta(Q):\theta(P)) \end{aligned}$$



$$\begin{aligned} \mathrm{DFS}(F(\theta),\Theta) &= \mathrm{DFS}(F^*(\eta),H) \\ \mathrm{DFS}(\bar F(\bar\theta),\bar\Theta) &= \mathrm{DFS}(F(\theta),\Theta), \quad \bar F(\bar\theta) = A\,F(\bar\theta)+a, \bar\theta = B\,\theta + b \end{aligned}$$

Canonical divergence of cumulant functions amount to statistical reverse KLD: $B_F(\theta_1:\theta_2)=D^*_{\mathrm{KL}}(p_{\theta_1}:p_{\theta_2})$

Usually, in Statistics/ML, we prove ⇒: $D_{\mathrm{KL}}(p_{\theta_1}:p_{\theta_2})={B_F}^*(\theta_1:\theta_2)=B_F(\theta_2:\theta_1)$

where D* is dual divergence: $D^*(p:q)=D(q:p)$

Let us prove ⇐ from information geometry of canonical divergence of DFS(F(θ), Θ)

① $F^*(\eta)=E_{p_\theta}[\log p_\theta]=-H(p_\theta)$:

$$
\begin{aligned}
H(p_\theta) &= -E_{p_\theta}[\log p_\theta],\\
&= -E_{p_\theta}[\langle\theta,x\rangle-F(\theta)],\\
&= F(\theta)-\langle\theta,E_{p_\theta}[x]\rangle,\\
&= F(\theta)-\langle\theta,\eta\rangle,\\
&= -F^*(\eta).
\end{aligned}
$$

②
$$
\begin{aligned}
\langle\theta_1,\eta_2\rangle &= \langle\theta_1,E_{p_{\theta_2}}[x]\rangle,\\
&= E_{p_{\theta_2}}[\langle\theta_1,x\rangle]=E_{p_{\theta_2}}[\log\tilde{p}_{\theta_1}(x)],\\
&= E_{p_{\theta_2}}[\log p_{\theta_1}(x)+F(\theta_1)],\\
&= E_{p_{\theta_2}}[\log p_{\theta_1}(x)]+F(\theta_1).
\end{aligned}
$$

③
$$
\begin{aligned}
D(p_{\theta_1}:p_{\theta_2})=Y_{F,F^*}(\theta_1:\eta_2) &= F(\theta_1)+F^*(\eta_2)-\langle\theta_1,\eta_2\rangle,\\
&= F(\theta_1)-H(p_{\theta_2})-E_{p_{\theta_2}}[\log p_{\theta_1}(x)]-F(\theta_1)\\
&= H^\times(p_{\theta_2}:p_{\theta_1})-H(p_{\theta_2}),\\
&= D_{\mathrm{KL}}(p_{\theta_2}:p_{\theta_1}),\\
&= D^*_{\mathrm{KL}}(p_{\theta_1}:p_{\theta_2}).
\end{aligned}
$$

Canonical divergence of cumulant functions amount to statistical reverse KLD:

$$D_{\mathrm{KL}}(p_{\theta_1} : p_{\theta_2}) = B_{F^*}(\theta_1 : \theta_2) = B_F(\theta_2 : \theta_1)$$

We reconstruct Kullback-Leibler divergence by relaxing to arbitrary densities

$B_F(\theta_1 : \theta_2) = D^*_{\mathrm{KL}}(p_{\theta_1} : p_{\theta_2})$ ⇒KLD

Interpretations:

- $F(\theta)$ is the cumulant function (also called free energy in thermodynamics),
- $\eta = \nabla F(\theta) = E_{p_\theta}[t(x)]$ is the moment of the sufficient statistic,
- $F^*(\eta) = -H(p_\theta)$ is the negentropy, and
- $\theta = \nabla F^*(\eta)$ are the Lagrangian multipliers in the maximum entropy problem

Natural parameter space Θ is convex

Proof. Let Θ denote the natural parameter space:

$$\Theta = \left\{\theta \;:\; Z(\theta) = \int \exp(\langle\theta, x\rangle)\mathrm{d}\mu < \infty\right\} = \left\{\theta \;:\; F(\theta) = \log \int \exp(\langle\theta, x\rangle)\mathrm{d}\mu < \infty\right\}.$$

Let $\theta_0, \theta_1 \in \Theta$ and consider $\theta_\alpha = \theta_0 + \alpha(\theta_1 - \theta_0)$ for $\alpha \in (0,1)$. In order to show that Θ is convex, we need to prove that $\theta_\alpha \in \Theta$, i.e., $Z(\theta_\alpha) < \infty$. We have

$$\begin{aligned} \int \exp(\langle\theta_\alpha, x\rangle)\,\mathrm{d}\mu(x) &= \int \exp(\langle\alpha\theta_0, x\rangle)\exp(\langle(1-\alpha)\theta_1, x\rangle)\mathrm{d}\mu(x), \\ &= \int (\exp(\langle\theta_0, x\rangle))^\alpha\,(\exp(\langle\theta_1, x\rangle))^{(1-\alpha)}\,\mathrm{d}\mu(x). \end{aligned} \tag{31}$$

Now, recall Hölder inequality for positive functions $f(x)$ and $g(x)$ with conjugate exponents p and q in $[1, \infty)$ such that $\frac{1}{p} + \frac{1}{q} = 1$:

$$\int f(x)g(x)\mathrm{d}\mu(x) \leq \left(\int f^p(x)\mathrm{d}\mu(x)\right)^{\frac{1}{p}} \left(\int g^q(x)\mathrm{d}\mu(x)\right)^{\frac{1}{q}}.$$

Consider $f(x) = (\exp(\langle\theta_0, x\rangle))^\alpha$ and $p = \frac{1}{\alpha} > 1$ and $g(x) = (\exp(\langle\theta_1, x\rangle))^{1-\alpha}$ with $q = \frac{1}{1-\alpha} > 1$ (we check that $\frac{1}{p} + \frac{1}{q} = \alpha + 1 - \alpha = 1$). Thus we upper bound Eq. 31 using Hölder inequality as follows:

$$\int \exp(\langle\theta_\alpha, x\rangle)\,\mathrm{d}\mu(x) \leq \left(\int \exp(\langle\theta_0, x\rangle)\mathrm{d}\mu(x)\right)^\alpha \left(\int \exp(\langle\theta_1, x\rangle)\mathrm{d}\mu(x)\right)^{1-\alpha} < \infty, \tag{32}$$

since both $\int \exp(\langle\theta_0, x\rangle)\mathrm{d}\mu(x) < \infty$ and $\int \exp(\langle\theta_1, x\rangle)\mathrm{d}\mu(x) < \infty$ because θ_0 and θ_1 both belong to Θ. Hence, we have shown that Θ is convex. □

Partition function Z(θ)=exp(F(θ)) is strictly log-convex
Cumulant function F(θ)=log Z(θ) is strictly convex

When we proved that natural parameter space is convex, we had

$$\int \exp(\langle\theta_\alpha, x\rangle)\,\mathrm{d}\mu(x) \leq \left(\int \exp(\langle\theta_0, x\rangle)\mathrm{d}\mu(x)\right)^{\alpha} \left(\int \exp(\langle\theta_1, x\rangle)\mathrm{d}\mu(x)\right)^{1-\alpha} < \infty$$

That is for short: $Z(\theta_\alpha) \leq Z(\theta_0)^{\alpha}\, Z(\theta_1)^{1-\alpha}.$

Take the logarithm on both sides:

$$\begin{aligned} \log Z(\theta_\alpha) &\leq \log\left(Z(\theta_0)^{\alpha}\, Z(\theta_1)^{1-\alpha}\right), \\ F(\alpha\theta_0 + (1-\alpha)\theta_1) &\leq \alpha F(\theta_0) + (1-\alpha)F(\theta_1) \end{aligned}$$

F is strictly convex since Eq. iff $\theta_1 = \theta_2$

Definition: A function Z is stricty log-convex is log Z is strictly convex

$\Rightarrow$ Z(θ)=exp(F(θ)) is strictly convex because F(θ) strictly convex:

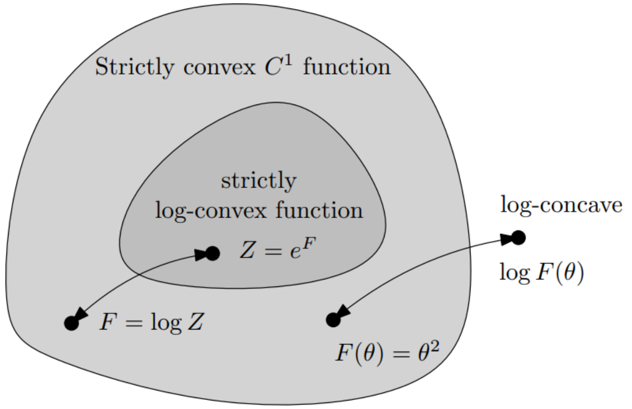
A log-convex function is also convex (but not necessarily the converse)

Proof. By definition, function $Z(\theta)$ is strictly log-convex if and only if:

$$\forall \theta_0 \neq \theta_1, \quad Z(\alpha\theta_0 + (1-\alpha\theta_1)) < Z(\theta_0)^\alpha \, Z(\theta_1)^{1-\alpha}, \tag{3}$$

i.e., by taking the logarithm on both sides of the inequality, $F = \log Z$ is strictly convex:

$$\begin{aligned} \forall \theta_0 \neq \theta_1, \quad \log Z(\alpha\theta_0 + (1-\alpha)\theta_1) &< \alpha \log Z(\theta_0) + (1-\alpha)\log Z(\theta_1), \\ \Leftrightarrow \quad F(\alpha\theta_0 + (1-\alpha)\theta_1) &< \alpha F(\theta_0) + (1-\alpha) F(\theta_1). \end{aligned}$$



Since $f(x) = \exp(x)$ is strictly convex (because $f''(x) = \exp(x) > 0$), we have for all $\alpha \in (0,1)$:

$$f(\alpha F(\theta_0) + (1-\alpha)F(\theta_1)) < \alpha f(F(\theta_0)) + (1-\alpha) f(F(\theta_1)).$$

Letting $F(\theta) = \log Z(\theta)$ in the above inequality, we get:

$$\exp(\alpha \log Z(\theta_0) + (1-\alpha)\log Z(\theta_1) < \alpha \exp(\log Z(\theta_0)) + (1-\alpha)\exp(\log Z(\theta_1)), \tag{4}$$

$$Z(\theta_0)^\alpha \, Z(\theta_1)^{1-\alpha} < \alpha Z(\theta_0) + (1-\alpha) Z(\theta_1), \tag{5}$$

and therefore we get from Eq. 3 and Eq. 5:

$$\forall \theta_0 \neq \theta_1, Z(\alpha\theta_0 + (1-\alpha\theta_1)) < Z(\theta_0)^\alpha \, Z(\theta_1)^{1-\alpha} < \alpha Z(\theta_0) + (1-\alpha) Z(\theta_1). \tag{6}$$

That is, Z is strictly convex.

Bregman divergences $B_{F=\log Z}$ and $B_{Z=\exp F}$

$$
\begin{aligned}
B_Z(\theta_1 : \theta_2) &= Z(\theta_1) - Z(\theta_2) - \langle \theta_1 - \theta_2, \nabla Z(\theta_2) \rangle \geq 0, \\
B_{\log Z}(\theta_1 : \theta_2) &= \log\left(\frac{Z(\theta_1)}{Z(\theta_2)}\right) - \left\langle \theta_1 - \theta_2, \frac{\nabla Z(\theta_2)}{Z(\theta_2)} \right\rangle \geq 0,
\end{aligned}
$$

And furthermore, we can define skewed Jensen divergences from the convex generators:

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

Including the symmetric Jensen divergence:

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

Bhattacharyya distances and Rényi divergences

- If KLD between EF densities = B_F^*, to what statistical divergences correspond J_F and $J_{\alpha,F}$?
- Define **scaled skewed Bhattacharyya distances**:

$$D^s_{B,\alpha}(p:q) = -\frac{1}{\alpha(1-\alpha)} \log \int p^\alpha q^{1-\alpha} \mathrm{d}\mu, \quad \alpha \in \mathbb{R}\backslash\{0,1\}$$

which are scaled **Rényi divergences**:

$$D^s_{B,\alpha}(p:q) = \frac{1}{\alpha} D_{R,\alpha}(p:q)$$

$$D_{R,\alpha}(p:q) = \frac{1}{\alpha-1} \log \int p^\alpha q^{1-\alpha} \mathrm{d}\mu$$

Scaling allows to unify KLD with Bhattacharyya distances:

$$D^s_{B,\alpha}(p:q) = \begin{cases} -\frac{1}{\alpha(1-\alpha)} \log \int p^\alpha q^{1-\alpha} \mathrm{d}\mu, & \alpha \in \mathbb{R}\backslash\{0,1\}, \\ D_{\mathrm{KL}}(p:q), & \alpha = 1, \\ 4\, D_B(p,q) & \alpha = \frac{1}{2}, \\ {D_{\mathrm{KL}}}^*(p:q) = D_{\mathrm{KL}}(q:p) & \alpha = 0. \end{cases}$$

Bhattacharyya distances and Rényi divergences between densities of an exponential family

Proposition 4 ([32]). *The scaled α-skewed Bhattacharyya distances between two probability densities p_{θ_1} and p_{θ_2} of an exponential family amounts to the scaled α-skewed Jensen divergence between their natural parameters:*

$$D_{B,\alpha}^{s}(p_{\theta_1} : p_{\theta_2}) = J_{F,\alpha}^{s}(\theta_1, \theta_2). \tag{13}$$

Proof: consider the α-skewed Bhattacharyya similarity coefficient:

$$\begin{aligned}\rho_\alpha(p_{\theta_1} : p_{\theta_2}) &= \int \exp\left(\langle \theta_1, x\rangle - F(\theta_1)\right)^{\alpha} \exp\left(\langle \theta_2, x\rangle - F(\theta_2)\right)^{1-\alpha} \mathrm{d}\mu, \\ &= \int \exp(\langle \alpha\theta_1 + (1-\alpha)\theta_2), x\rangle) \exp\left(-(\alpha F(\theta_1) + (1-\alpha)F(\theta_2))\right) \mathrm{d}\mu.\end{aligned}$$

$$\rho_\alpha(p_{\theta_1} : p_{\theta_2}) = \exp(-(\alpha F(\theta_1) + (1-\alpha)F(\theta_2)) \exp(F(\bar{\theta})) \int \exp(\langle \bar{\theta}, x\rangle - F(\bar{\theta}))\mathrm{d}\mu.$$

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

Overview of classical divergences

Normalized densities $p_\theta = \exp(x \cdot \theta - F(\theta)) = \frac{\exp(x\cdot\theta)}{Z(\theta)}$

Scaled Rényi α-divergence or α-skewed Bhattacharyya distance

$$\boxed{D^s_{B,\alpha}(p_{\theta_1} : p_{\theta_2}) = \frac{1}{\alpha} D_{R,\alpha}(p_{\theta_1} : p_{\theta_2}) = J^s_{F\alpha}(\theta_1 : \theta_2)}$$

$\alpha \to 0$	$\alpha = \frac{1}{2}$	$\alpha \to 1$
Reverse KLD	4 Bhattacharyya distance	KLD
$D_{\mathrm{KL}}{}^*(p_{\theta_1} : p_{\theta_2}) = B_F(\theta_1 : \theta_2)$	$4\, D_B(p_{\theta_1}, p_{\theta_2}) = 4\, J_F(\theta_1, \theta_2)$	$D_{\mathrm{KL}}(p_{\theta_1} : p_{\theta_2}) = B_F{}^*(\theta_1 : \theta_2)$
Bregman	4 Jensen	Reverse Bregman

Extended Kullback-Leibler divergences between unnormalized densities: Bregman divergence B_Z

Extend KLD to **unnormalized densities**: $D_{\mathrm{KL}}(\tilde{p}:\tilde{q}) = \int \left(\tilde{p}\log\frac{\tilde{p}}{\tilde{q}} + \tilde{q} - \tilde{p}\right)\mathrm{d}\mu$

$$D_{\mathrm{KL}}(\tilde{p}:\tilde{q}) \quad = \quad H^\times(\tilde{p}:\tilde{q}) - H(\tilde{p})$$

$$H^\times(\tilde{p}:\tilde{q}) = \int \left(\tilde{p}(x)\log\frac{1}{\tilde{q}(x)} + \tilde{q}(x)\right)\mathrm{d}\mu(x) - 1$$

Reverse extended KLD: $D^*_{\mathrm{KL}}(\tilde{p}:\tilde{q}) = D_{\mathrm{KL}}(\tilde{q}:\tilde{p})$

$$\begin{aligned}
D_{\mathrm{KL}}(\tilde{p}_{\theta_1}:\tilde{p}_{\theta_2}) &= \int \left(\tilde{p}_{\theta_1}(x)\log\frac{\tilde{p}_{\theta_1}(x)}{\tilde{p}_{\theta_2}(x)} + \tilde{p}_{\theta_2}(x) - \tilde{p}_{\theta_1}(x)\right)\mathrm{d}\mu(x),\\
&= \int \left(e^{\langle t(x),\theta_1\rangle}\langle\theta_1-\theta_2, t(x)\rangle + e^{\langle t(x),\theta_2\rangle} - e^{\langle t(x),\theta_1\rangle}\right)\mathrm{d}\mu(x),\\
&= \left\langle \int t(x)e^{\langle t(x),\theta_1\rangle}\mathrm{d}\mu(x), \theta_1-\theta_2\right\rangle + Z(\theta_2) - Z(\theta_1),\\
&= \langle\theta_1-\theta_2, \nabla Z(\theta_1)\rangle + Z(\theta_2) - Z(\theta_1) = B_Z(\theta_2:\theta_1),
\end{aligned}$$

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

KLD between arbitrary positive densities

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

$$p(x) = \frac{\tilde{p}(x)}{Z_p} \qquad q(x) = \frac{\tilde{q}(x)}{Z_q}$$

$$D_{\mathrm{KL}}(\tilde{p}:\tilde{q}) = Z_p \left(D_{\mathrm{KL}}(p:q) + \log \frac{Z_p}{Z_q} \right) + Z_q - Z_p.$$

$$
\begin{aligned}
H^{\times}(\tilde{p}:\tilde{q}) &= Z_p H^{\times}(p:q) - Z_p \log Z_q + Z_q - 1, \\
H(\tilde{p}) &= Z_p H(p) - Z_p \log Z_p + Z_p - 1,
\end{aligned}
$$

When specialized to densities of exponential family:

$$D_{\mathrm{KL}}(\tilde{p}_{\theta_1}:\tilde{p}_{\theta_2}) = \langle \theta_1 - \theta_2, \nabla Z(\theta_1) \rangle + Z(\theta_2) - Z(\theta_1) = B_Z(\theta_2:\theta_1)$$

α -divergences between unnormalized densities

- Statistical α -divergences between positive measures:

$$D_\alpha(\tilde{p} : \tilde{q}) = \begin{cases} \frac{1}{\alpha(1-\alpha)} \int \left(\alpha\tilde{p} + (1-\alpha)\tilde{q} - \tilde{p}^\alpha \tilde{q}^{1-\alpha}\right) \mathrm{d}\mu, & \alpha \notin \{0,1\} \\ D_{\mathrm{KL}}^*(\tilde{p} : \tilde{q}) = D_{\mathrm{KL}}(\tilde{q} : \tilde{p}) & \alpha = 0, \\ 4\, D_H^2(\tilde{p}, \tilde{q}) & \alpha = \frac{1}{2}, \\ D_{\mathrm{KL}}(\tilde{p} : \tilde{q}) & \alpha = 1. \end{cases}$$

- When considering unnormalized exponential family densities:

$$D_\alpha(\tilde{p}_{\theta_1} : \tilde{p}_{\theta_2}) = \begin{cases} \frac{1}{\alpha(1-\alpha)} J_{Z,\alpha}(\theta_1 : \theta_2), & \alpha \notin \{0,1\} \\ B_Z(\theta_1 : \theta_2) & \alpha = 0, \\ 4\, J_Z(\theta_1, \theta_2) & \alpha = \frac{1}{2}, \\ B_Z^*(\theta_1 : \theta_2) = B_Z(\theta_2 : \theta_1) & \alpha = 1 \end{cases}$$

Proposition 5. *The α-divergences between unnormalized densities of an exponential family amounts to scaled α-Jensen divergences between their natural parameters for the partition function:*

$$D_\alpha(\tilde{p}_{\theta_1} : \tilde{p}_{\theta_2}) = J^s_{Z,\alpha}(\theta_1 : \theta_2).$$

Overview of divergences between (un)normalized EF densities

Statistical divergences between densities of an exponential family $\mathcal{E}$

Normalized densities $p_\theta = \exp(x \cdot \theta - F(\theta)) = \frac{\exp(x\cdot\theta)}{Z(\theta)}$

Scaled Rényi α-divergence or α-skewed Bhattacharyya distance

$$\boxed{D^s_{B,\alpha}(p_{\theta_1} : p_{\theta_2}) = \frac{1}{\alpha} D_{R,\alpha}(p_{\theta_1} : p_{\theta_2}) = J^s_{F\alpha}(\theta_1 : \theta_2)}$$

$\alpha \to 0$ | $\alpha = \frac{1}{2}$ | $\alpha \to 1$

Reverse KLD

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

Bregman

4 Bhattacharyya distance

$4\, D_B(p_{\theta_1}, p_{\theta_2}) = 4\, J_F(\theta_1, \theta_2)$

4 Jensen

KLD

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

Reverse Bregman

F: cumulant function/free energy

Unnormalized densities $\tilde{p}_\theta = \exp(x \cdot \theta)$

α-divergences

$$\boxed{D_\alpha(\tilde{p}_{\theta_1} : \tilde{p}_{\theta_2}) = J^s_{Z,\alpha}(\theta_1 : \theta_2)}$$

$\alpha \to 0$ | $\alpha = \frac{1}{2}$ | $\alpha \to 1$

Reverse KLD

$D_{\mathrm{KL}}{}^*(p_{\theta_1} : p_{\theta_2}) = B_Z(\theta_1 : \theta_2)$

Bregman

4 squared Hellinger divergence

$4\, D^2_H(p_{\theta_1}, p_{\theta_2}) = 4\, J_Z(\theta_1, \theta_2)$

4 Jensen

KLD

$D_{\mathrm{KL}}(p_{\theta_1} : p_{\theta_2}) = B_Z{}^*(\theta_1 : \theta_2)$

Reverse Bregman

Z: partition function/Laplace transform

Comparative convexity: (M,N)-convexity

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

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

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

$$A(x,y;\alpha,1-\alpha)=\alpha x+(1-\alpha)y$$

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

$$G(x,y;\alpha,1-\alpha)=x^{\alpha}y^{1-\alpha}$$

Comparative convexity wrt quasi-arithmetic means

- Kolmogorov-Nagumo-De Finitti quasi-arithmetic mean for a strictly monotone generator h(u):

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

- Includes power means which are homogeneous means:

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

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

Include the geometric mean when p→0

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

Deforming convex functions with comparative convexity

Since log-convexity is $(A = M_{\mathrm{id}}, G = M_{\log})$-convexity, a function Z is strictly log-convex iff $\log \circ Z \circ \mathrm{id}^{-1} = \log \circ Z$ is strictly convex. We have

$$Z = \tau^{-1} \circ F \circ \rho \Leftrightarrow F = \tau \circ Z \circ \rho^{-1}.$$

We consider deformations with two strictly monotone functions which preserve convexity and thus induces family of Bregman and Jensen divergences, and families of dually flat spaces:

$$\underbrace{F = \tau \circ Z \circ \rho^{-1}}_{(M_{\rho^{-1}}, M_{\tau^{-1}})\text{-convex when } Z \text{ is convex}} \quad \underset{(\rho^{-1},\tau^{-1})\text{-deformation}}{\overset{(\rho,\tau)\text{-deformation}}{\rightleftarrows}} \quad \underbrace{Z = \tau^{-1} \circ F \circ \rho}_{(M_\rho, M_\tau)\text{-convex when } F \text{ is convex}}$$

We deform both the function F (by τ^{-1}) and the argument θ (by ρ) by considering functions Z

Generalizing Bregman divergences with (M,N)-convexity

- Skew Jensen comparative convexity divergence:

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

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

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

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

Generalizing Bregman divergences with quasi-arithmetic mean convexity

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

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

Amounts to a **conformal Bregman divergence**:

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

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

Remark: Conformal Bregman divergences may yield robustness in applications

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- Jensen divergence
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- Partition function is log-convex and hence convex
- Bregman divergence wrt Z: KLD between unnormalized EF densities
- Jensen divergence wrt Z: alpha divergences
- Overview of divergences between (un)normalized EF densities
- Comparative convexity
- Comparative convexity wrt quasi-arithmetic means
- Deforming convex functions wrt quasi-arithmetic generators
- (M,N)-Jensen divergence
- (M,N)-Bregman divergence
- Equivalence with a conformal Bregman divergence
- Power Bregman divergences
- Conclusion