The Burbea-Rao and Bhattacharyya centroids

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(joint work with Sylvain Boltz)

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Means and centroids

In Euclidean geometry, centroid c of a point set $\mathcal{P} = \{p_1, ..., p_n\}$:
Center of mass (also known as center of gravity):

$$\frac{1}{n}\sum_{i=1}^{n} p_i$$

Unique minimizer of average *squared* Euclidean distances

$$c = \arg\min_p \sum_{i=1}^{n} \frac{1}{n}\|p - p_i\|^2.$$

Two major ways to define means:

- by axiomatization, or
- by optimization

Means by axiomatization

Axioms for mean function $M(x_1, x_2)$:

- Reflexivity. $M(x, x) = x$,
- Symmetry. $M(x_1, x_2) = M(x_2, x_1)$,
- Continuity and strict monotonicity. $M(\cdot, \cdot)$ continuous and $M(x_1, x_2) < M(x_1', x_2)$ for $x_1 < x_1'$, and
- Anonymity. $M(M(x_{11}, x_{12}), M(x_{21}, x_{22})) = M(M(x_{11}, x_{21}), M(x_{12}, x_{22}))$

x_{11}	x_{12}
x_{21}	x_{22}

Yields unique function f (up to an additive constant):

$$M(x_1, x_2) = f^{-1}\left(\frac{f(x_1) + f(x_2)}{2}\right) \stackrel{\text{equal}}{=} M_f(x_1, x_2)$$

f: continuous, strictly monotonous and increasing function.
(1930: Kolmogorov, Nagumo, + Aczél 1966)

Means by axiomatization: Quasi-arithmetic means

- arithmetic mean $\frac{x_1+x_2}{2} \longleftarrow f(x) = x$
- geometric mean $\sqrt{x_1 x_2} \longleftarrow f(x) = \log x$
- harmonic mean $\frac{2}{\frac{1}{x_1}+\frac{1}{x_2}} \longleftarrow f(x) = \frac{1}{x}$

Arithmetic barycenter on the f-representation ($y = f(x)$) :

$$M_f(x_1, ..., x_n; w_1, ..., w_n) = f^{-1}\left(\sum_{i=1}^n w_i f(x_i) = \bar{x}\right)$$

$$f(\bar{x}) = \sum_{i=1}^n w_i f(x_i)$$

$$\bar{y} = \sum_{i=1}^n w_i y_i$$

Dominance and interness of means

Dominance property:

$$M_f(x_1,...,x_n;w_1,...,w_n) < M_g(x_1,...,x_n;w_1,...,w_n),$$

if and only if g dominates f: $\forall x, g(x) > f(x)$.

Interness property:

$$\min(x_1,...,x_n) \leq M_f(x_1,...,x_n) \leq \max(x_1,...,x_n),$$

limit cases $p \to \pm\infty$ of *power means* for $f(x) = x^p, p \in \mathbb{R}_*$.

$$M_p(x_1,...,x_n) = \left(\sum_{i=1}^n w_i x_i^p\right)^{\frac{1}{p}}$$

name of power mean	value of p
maximum	$\to +\infty$
quadratic mean	2
arithmetic mean	1
geometric mean	$\to 0$
harmonic mean	$\to -1$
minimum	$\to -\infty$

also called Hölder means.

Means by optimization

$$\text{(OPT)} : \min_x \sum_{i=1}^n w_i d(x, p_i) = \min_x L(x; \mathcal{P}, d),$$

Entropic means (Ben-Tal et al., 1989)

$$I_f(x, p) = pf\left(\frac{x}{p}\right),$$

$f(\cdot)$: strictly convex differentiable function with $f(1) = 0$ and $f'(1) = 0$.
entropic means: linear scale-invariant (homogeneous degree 1):

$$M(\lambda p_1, ..., \lambda p_n; I_f) = \lambda M(p_1, ..., p_n; I_f)$$

Bregman means

$$B_F(x,p) = F(x) - F(p) - (x-p)F'(p),$$

$F(\cdot)$: strictly convex and differentiable function.
(OPT) is convex $\rightarrow$ admits a unique minimizer:

$$M(p_1, ..., p_n; B_F) = M_{F'}(p_1, ..., p_n) = F'^{-1}\left(\sum_{i=1}^n w_i F'(p_i)\right)$$

quasi-arithmetic mean for F', the derivative of F.

Since $d(x,p) \neq d(p,x)$, define a *right-sided* centroid M'

$$(\mathrm{OPT}') : \min_x \sum_{i=1}^n w_i d(p_i, x),$$

Information-theoretic sided means

Reference duality

- f-divergences

$$I_f(x,p) = I_{f*}(p,x),$$

for $f^*(x) = xf(1/x)$.
Any f-divergence can be symmetrized and stay in the class

- Bregman divergences

$$B_F(x,p) = B_{F^*}(F'(p), F'(x))$$

for $F^*(\cdot)$ the Legendre convex conjugate ($F^{*\prime} = (F')^{-1}$)
Only the squared Mahanalobis distances are symmetric Bregman divergences

Separable divergence and means as projections

Separable divergence:

$$d(x,p) = \sum_{i=1}^{d} d_i(x^{(i)}, p^{(i)}),$$

with $x^{(i)}$ denoting the i-th coordinate, and d_i's univariate divergences. Typical non separable divergence : squared Mahalanobis distance (or other matrix trace divergences)

$$d(x,p) = (x-p)^T Q (x-p)$$

View means of separable divergence as a projection

$$(\mathrm{PROJ}) : \inf_{u \in U} d(u,p)$$

with $u_1 = ... = u_{d \times n} > 0$, and p the $(n \times d)$-dimensional point obtained by stacking the d coordinates of each of the n points.

Burbea-Rao divergences

Based on Jensen's inequality for a convex function F:

$$d(x,p) = \frac{F(x)+F(p)}{2} - F\left(\frac{x+p}{2}\right) \stackrel{\text{equal}}{=} \mathrm{BR}_F(x,p) \geq 0.$$

strictly convex function $F(\cdot)$.

$$\mathrm{BR}_F(p,q) = \sum_{i=1}^{d} \mathrm{BR}_F(p^{(i)}, q^{(i)}),$$

Includes the special case of Jensen-Shannon divergence:

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

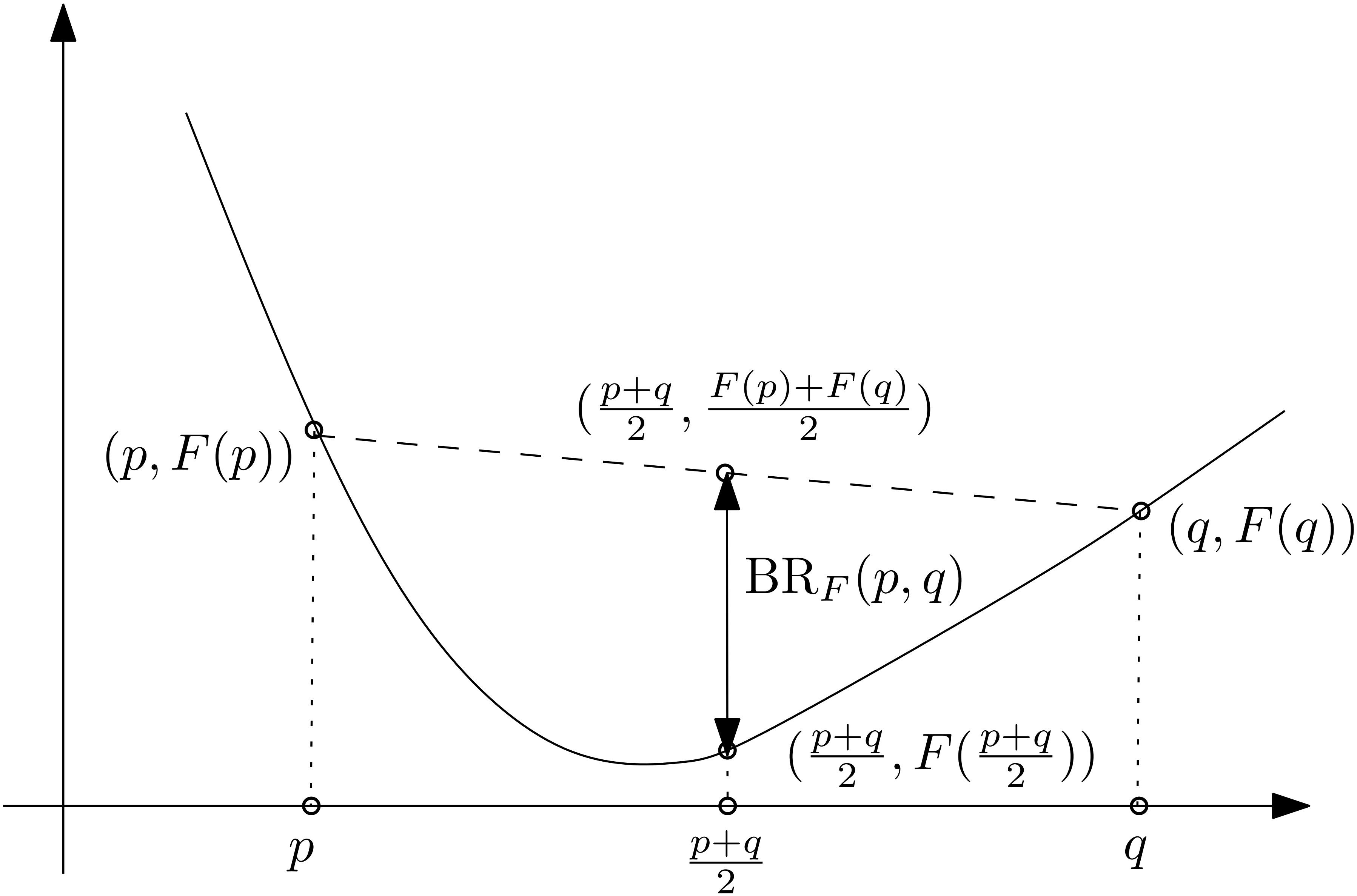
$F(x) = -H(x)$, the negative Shannon entropy $H(x) = -x \log x$.
$\rightarrow$ generators are convex and entropies are concave (negative generators)

Burbea-Rao divergences: Squared Mahalanobis

$$\begin{aligned}
\mathrm{BR}_F(p,q) &= \frac{F(p)+F(q)}{2} - F\left(\frac{p+q}{2}\right) \\
&= \frac{2\langle Qp,p\rangle + 2\langle Qq,q\rangle - \langle Q(p+q),p+q\rangle}{4} \\
&= \frac{1}{4}(\langle Qp,p\rangle + \langle Qq,q\rangle - 2\langle Qp,q\rangle) \\
&= \frac{1}{4}\langle Q(p-q),p-q\rangle = \frac{1}{4}\|p-q\|_Q^2.
\end{aligned}$$

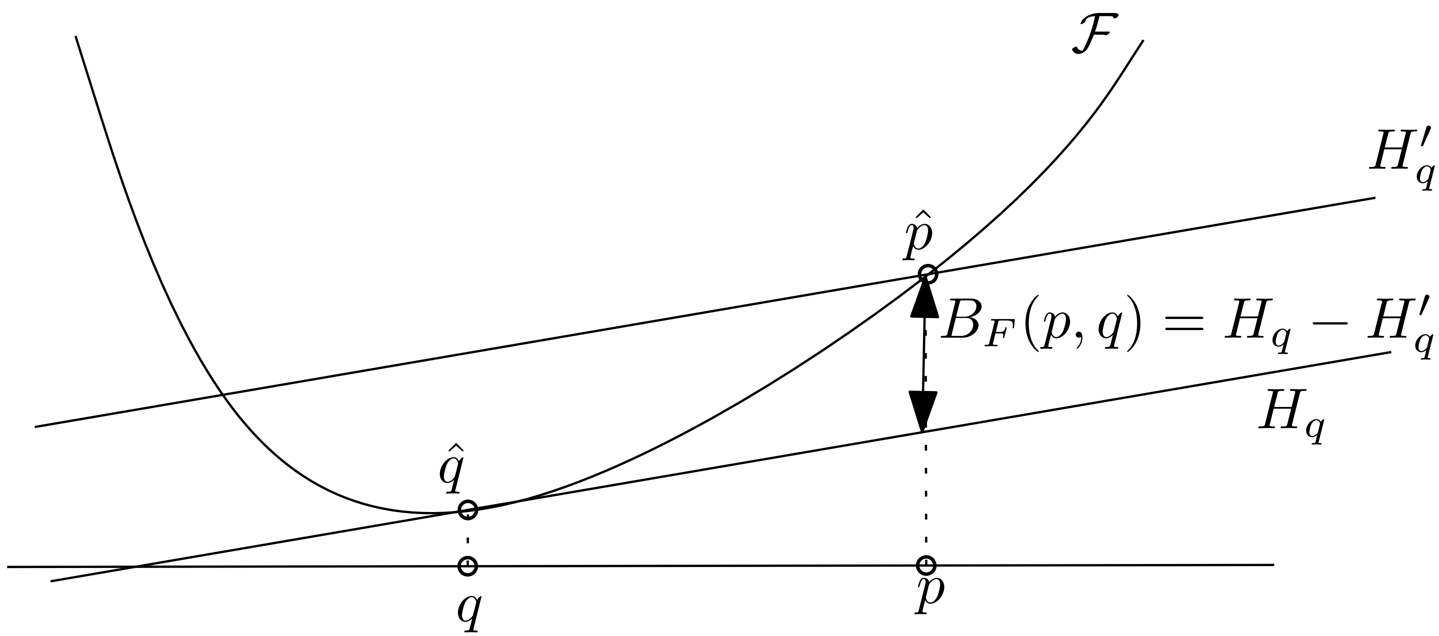
(Not a metric. square root of Jensen-Shannon is a metric but not the square roots of all Burbea-Rao divergences.)

Visualizing Burbea-Rao divergences



Visualizing Bregman divergences

$$B_F(p,q) = F(p) - F(q) - \langle p - q, \nabla F(q)\rangle,$$



- Kullback-Leibler ($F(x) = x \log x$): $\mathrm{KL}(p,q) = \sum_{i=1}^{d} p^{(i)} \log \frac{p^{(i)}}{q^{(i)}}$
- Squared Euclidean L_2^2 ($F(x) = x^2$): $L_2^2(p,q) = \sum_{i=1}^{d} (p^{(i)} - q^{(i)})^2 = \|p - q\|^2$

Symmetrizing Bregman divergences

- **Jeffreys-Bregman divergences.**

$$
\begin{aligned}
S_F(p;q) &= \frac{B_F(p,q)+B_F(q,p)}{2} \\
&= \frac{1}{2}\langle p-q, \nabla F(p) - \nabla F(q)\rangle,
\end{aligned}
$$

- **Jensen-Bregman divergences (diversity index).**

$$
\begin{aligned}
J_F(p;q) &= \frac{B_F(p,\frac{p+q}{2})+B_F(q,\frac{p+q}{2})}{2} \\
&= \frac{F(p)+F(q)}{2} - F(\frac{p+q}{2}) = \mathrm{BR}_F(p,q)
\end{aligned}
$$

Skew Burbea-Rao divergences

$$
\begin{aligned}
\mathrm{BR}_F^{(\alpha)} &: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+ \\
\mathrm{BR}_F^{(\alpha)}(p,q) &= \alpha F(p) + (1-\alpha) F(q) - F(\alpha p + (1-\alpha) q)
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{BR}_F^{(\alpha)}(p,q) &= \alpha F(p) + (1-\alpha) F(q) - F(\alpha p + (1-\alpha) q) \\
&= \mathrm{BR}_F^{(1-\alpha)}(q,p)
\end{aligned}
$$

Skew symmetrization of Bregman divergences:

$$
\alpha B_F(p, \alpha p + (1-\alpha) q) + (1-\alpha) B_F(q, \alpha p + (1-\alpha) q) \stackrel{\text{equal}}{=} \mathrm{BR}_F^{(\alpha)}(p,q)
$$

= skew Jensen-Bregman divergences.

Bregman as asymptotic skewed Burbea-Rao

$$B_F(p,q) = \lim_{\alpha\rightarrow 1} \frac{1}{1-\alpha} \mathrm{BR}_F^{(\alpha)}(p,q)$$
$$B_F(q,p) = \lim_{\alpha\rightarrow 0} \frac{1}{\alpha} \mathrm{BR}_F^{(\alpha)}(p,q)$$

Proof: $F(\alpha p + (1-\alpha)q) = F(p + (1-\alpha)(q-p)) \simeq_{\alpha\simeq 1} F(p) + (1-\alpha)(q-p)\nabla F(p)$

Taylor

$F(\alpha p+(1-\alpha)q)-\alpha F(p)-(1-\alpha)F(q) \simeq_{\alpha\rightarrow 1} (1-\alpha)F(p)+(1-\alpha)(q-p)\nabla F(p)-(1-\alpha)F(q)$

$\simeq_{\alpha\rightarrow 1} (1-\alpha)\left(F(p) - F(q) - (p-q)\nabla F(p)\right)$

$\lim_{\alpha\rightarrow 1} \mathrm{BR}_F^{(\alpha)}(p,q) = (1-\alpha)B_F(p,q)$

For $0<\alpha<1$, swap arguments by setting $\alpha\rightarrow 1-\alpha$:

$$\mathrm{BR}_F^{(\alpha)}(p,q) = \mathrm{BR}_F^{(1-\alpha)}(q,p)$$

Burbea-Rao centroids

$$\mathrm{OPT} : c = \arg\min_x \sum_{i=1}^n w_i \mathrm{BR}_F^{(\alpha_i)}(x, p_i) = \arg\min_x L(x)$$

Wlog., equivalent to minimize

$$E(c) = (\sum_{i=1}^n w_i \alpha_i) F(c) - \sum_{i=1}^n w_i F(\alpha_i c + (1 - \alpha_i) p_i)$$

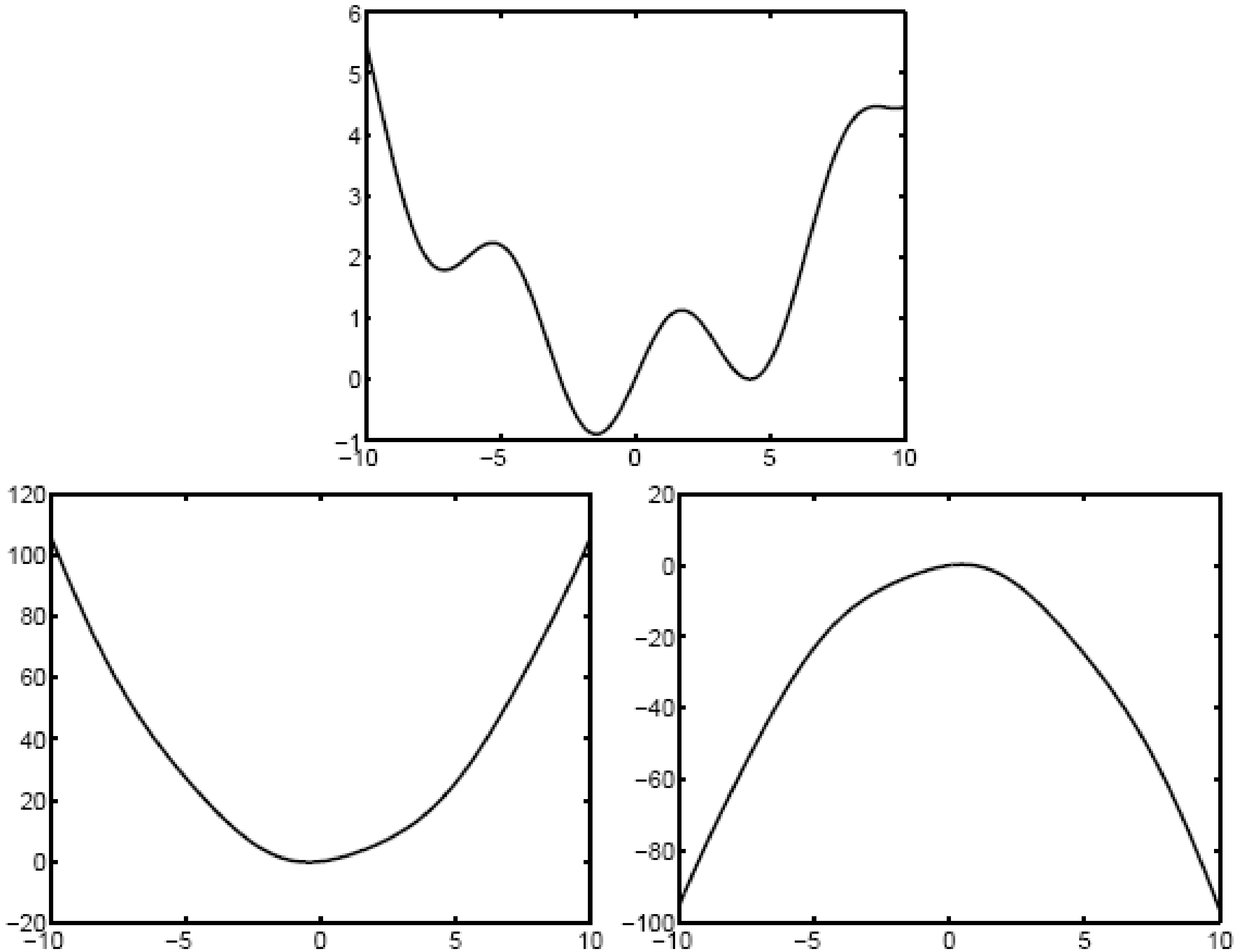
Sum $E = F + G$ of convex F + concave G function $\Rightarrow$ Convex-ConCave Procedure (CCCP, NIPS*01)
Start from arbitrary c_0, and iteratively update as:

$$\nabla F(c_{t+1}) = -\nabla G(c_t)$$

Guaranteed convergence to a local minimum.

ConCave Convex Procedure (CCCP)

$$\min_x E(x) = F(x) + G(x)$$
$$\nabla F(c_{t+1}) = -\nabla G(c_t)$$



Iterative algorithm for Burbea-Rao centroids

Apply CCCP scheme

$$\nabla F(c_{t+1}) = \frac{1}{\sum_{i=1}^n w_i \alpha_i} \sum_{i=1}^n w_i \alpha_i \nabla F\left(\alpha_i c_t + (1-\alpha_i) p_i\right)$$

$$c_{t+1} = \nabla F^{-1}\left(\frac{1}{\sum_{i=1}^n w_i \alpha_i} \sum_{i=1}^n w_i \alpha_i \nabla F\left(\alpha_i c_t + (1-\alpha_i) p_i\right)\right)$$

Get arbitrarily fine approximations of the (skew) Burbea-Rao centroids and barycenters.

Special cases: Closed-form Burbea-Rao centroids

Consider $F(x) = \langle x, x \rangle$.

$$\min E(x) = \frac{F(x)}{2} - \sum_{i=1}^{n} w_i F\left(\frac{p_i + x}{2}\right),$$

$$= \quad \min \frac{\langle x, x \rangle}{2} - \frac{1}{4} \sum_{i=1}^{n} w_i \left(\langle x, x \rangle + 2\langle x, p_i \rangle + \langle p_i, p_i \rangle\right)$$

The minimum obtained when $\nabla E(x) = 0$

$$x = \bar{p} = \sum_{i=1}^{n} w_i p_i$$

Extremal skew cases (for $\alpha \rightarrow 0$ or $\alpha \rightarrow 1$):
Bregman sided centroids in closed-forms: $\bar{x} = \sum_{i=1}^{n} w_i p_i$ (right-sided) or
$\bar{x} = (\nabla F)^{-1} \left(\sum_{i=1}^{n} w_i \nabla F(p_i)\right)$ (left-sided)
But usually only approximation using CCCP iterations.

Bhattacharyya coefficients/distances

Bhattacharyya coefficient and non-metric distance:

$$C_(p,q) = \int \sqrt{p(x)q(x)}\mathrm{d}x, \qquad 0 \leq C(p,q) \leq 1, \qquad B(p,q) = -\ln C(p,q).$$

Hellinger metric

$$H(p,q) = \sqrt{\frac{1}{2}\int (\sqrt{p(x)} - \sqrt{q(x)})^2 \mathrm{d}x},$$

such that $0 \leq H(p,q) \leq 1$.

$$\begin{aligned} H(p,q) &= \sqrt{\frac{1}{2}\left(\int p(x)\mathrm{d}x + \int q(x)\mathrm{d}x - 2\int \sqrt{p(x)}\sqrt{q(x)}\mathrm{d}x\right)} \\ &= \sqrt{1 - C(p,q)}. \end{aligned}$$

Chernoff coefficients/α-divergences

$$
\begin{aligned}
B_\alpha(p,q) &= -\ln \int_x p^\alpha(x) q^{1-\alpha}(x) \mathrm{d}x = -\ln C_\alpha(p,q) \\
&= -\ln \int_x q(x) \left(\frac{p(x)}{q(x)}\right)^\alpha \mathrm{d}x \\
&= -\ln E_q[L^\alpha(x)]
\end{aligned}
$$

Amari α-divergence:

$$
D_\alpha(p||q) = \begin{cases} \frac{4}{1-\alpha^2}\left(1 - \int p(x)^{\frac{1-\alpha}{2}} q(x)^{\frac{1+\alpha}{2}} \mathrm{d}x\right), & \alpha \neq \pm 1, \\ \int p(x) \log \frac{p(x)}{q(x)} \mathrm{d}x = \mathrm{KL}(p,q), & \alpha = -1, \\ \int q(x) \log \frac{q(x)}{p(x)} \mathrm{d}x = \mathrm{KL}(q,p), & \alpha = 1, \end{cases}
$$

$$
D_\alpha(p||q) = D_{-\alpha}(q||p)
$$

Remapping $\alpha' = \frac{1-\alpha}{2}$ ($\alpha = 1 - 2\alpha'$) to get Chernoff α'-divergences

Exponential families in statistics

Gaussian, Poisson, Bernoulli/multinomial, Gamma/Beta, etc.:

$$p(x;\lambda) = p_F(x;\theta) = \exp\left(\langle t(x), \theta\rangle - F(\theta) + k(x)\right).$$

Example: Poisson distribution

$$p(x;\lambda) = \frac{\lambda^x}{x!}\exp(-\lambda),$$

- the sufficient statistic $t(x) = x$,
- $\theta = \log\lambda$, the natural parameter,
- $F(\theta) = \exp\theta$, the log-normalizer,
- and $k(x) = -\log x!$ the carrier measure (with respect to the counting measure).

Gaussians as an exponential family

$$p(x;\lambda) = p(x;\mu,\Sigma) = \frac{1}{2\pi\sqrt{\det\Sigma}} \exp\left(-\frac{(x-\mu)^T\Sigma^{-1}(x-\mu))}{2}\right)$$

- $\theta = (\Sigma^{-1}\mu, \frac{1}{2}\Sigma^{-1}) \in \Theta = \mathbb{R}^d \times \mathbb{K}_{d\times d}$, with $\mathbb{K}_{d\times d}$ cone of positive definite matrices,
- $F(\theta) = \frac{1}{4}\mathrm{tr}(\theta_2^{-1}\theta_1\theta_1^T) - \frac{1}{2}\log\det\theta_2 + \frac{d}{2}\log\pi$,
- $t(x) = (x, -x^T x)$,
- $k(x) = 0$.

Inner product : composite, sum of a dot product and a matrix trace :

$$\langle\theta,\theta'\rangle = \theta_1^T\theta_1' + \mathrm{tr}(\theta_2^T\theta_2').$$

The coordinate transformation $\tau : \Lambda \to \Theta$ is given for $\lambda = (\mu,\Sigma)$ by

$$\tau(\lambda) = \left(\lambda_2^{-1}\lambda_1, \frac{1}{2}\lambda_2^{-1}\right), \qquad \tau^{-1}(\theta) = \left(\frac{1}{2}\theta_2^{-1}\theta_1, \frac{1}{2}\theta_2^{-1}\right)$$

Bhattacharyya/Chernoff of exponential families

Equivalence with skew Burbea-Rao distances:

$$B_\alpha(p_F(x;\theta_p), p_F(x;\theta_q)) = \mathrm{BR}_F^{(\alpha)}(\theta_p, \theta_q) = \alpha F(\theta_p) + (1-\alpha)F(\theta_q) - F(\alpha\theta_p + (1-\alpha)\theta_q)$$

Proof: Chernoff coefficients $C_\alpha(p,q)$ of members $p = p_F(x;\theta_p)$ and $q = p_F(x;\theta_q)$ of the *same* exponential family $\mathcal{E}_F$:

$C_\alpha(p,q) = \int p^\alpha(x) q^{1-\alpha}(x) \mathrm{d}x = \int p_F^\alpha(x;\theta_p) p_F^{1-\alpha}(x;\theta_q) \mathrm{d}x$
$= \int \exp(\alpha(\langle x, \theta_p\rangle - F(\theta_p))) \times \exp((1-\alpha)(\langle x, \theta_q\rangle - F(\theta_q)))\mathrm{d}x$
$= \int \exp\left(\langle x, \alpha\theta_p + (1-\alpha)\theta_q\rangle - (\alpha F(\theta_p) + (1-\alpha)F(\theta_q)\right)\mathrm{d}x$
$= \exp -(\alpha F(\theta_p) + (1-\alpha)F(\theta_q)) \times$
$\int \exp\left(\langle x, \alpha\theta_p + (1-\alpha)\theta_q\rangle - F(\alpha\theta_p + (1-\alpha)\theta_q) + F(\alpha\theta_p + (1-\alpha)\theta_q)\right)\mathrm{d}x$
$= \exp\left(F(\alpha\theta_p + (1-\alpha)\theta_q) - (\alpha F(\theta_p) + (1-\alpha)F(\theta_q)\right) \times \int \exp\langle x, \alpha\theta_p + (1-\alpha)\theta_q\rangle -$
$F(\alpha\theta_p + (1-\alpha)\theta_q)\mathrm{d}x$

$$= \exp\left(F(\alpha\theta_p + (1-\alpha)\theta_q) - (\alpha F(\theta_p) + (1-\alpha)F(\theta_q)\right) \times \underbrace{\int p_F(x;\alpha\theta_p + (1-\alpha)\theta_q)\mathrm{d}x}_{=1}$$

$= \exp(-\mathrm{BR}_F^{(\alpha)}(\theta_p, \theta_q)) \geq 0.$

α-div./Kullback-Leibler $\leftrightarrow$ Burbea-Rao/Bregman

Skew Bhattacharyya distances on members of the same exponential family is equivalent to skew Burbea-Rao divergences on the natural parameters (without swapping order).

$$B_\alpha(p_F(x;\theta_p), p_F(x;\theta_q)) = \mathrm{BR}_F^{(\alpha)}(\theta_p, \theta_q)$$

For $\alpha = \pm 1$, Kullback-Leibler of exp. fam. = *Bregman divergence* (limit as $\alpha \to 1$ or $\alpha \to 0$).

$$\begin{aligned}
\mathrm{KL}(p,q) &= \mathrm{KL}(p_F(x;\theta_p), p_F(x;\theta_q)) \\
&= \lim_{\alpha' \to 1} D_{\alpha'}(p_F(x;\theta_p), p_F(x;\theta_q)) \\
&= \lim_{\alpha' \to 1} \frac{1}{\alpha'(1-\alpha')}(1 - \underbrace{C_\alpha(p_F(x;\theta_p), p_F(x;\theta_q))}_{\text{since } \exp x \simeq_{x\simeq 0} 1+x}) \\
&= \lim_{\alpha' \to 1} \frac{1}{\alpha'(1-\alpha')} \underbrace{\mathrm{BR}_F^{\alpha'}(\theta_p, \theta_q)}_{(1-\alpha')B_F(\theta_q,\theta_p)} \\
&= \lim_{\alpha' \to 1} \frac{1}{\alpha'} B_F(\theta_q, \theta_p) = B_F(\theta_q, \theta_p)
\end{aligned}$$

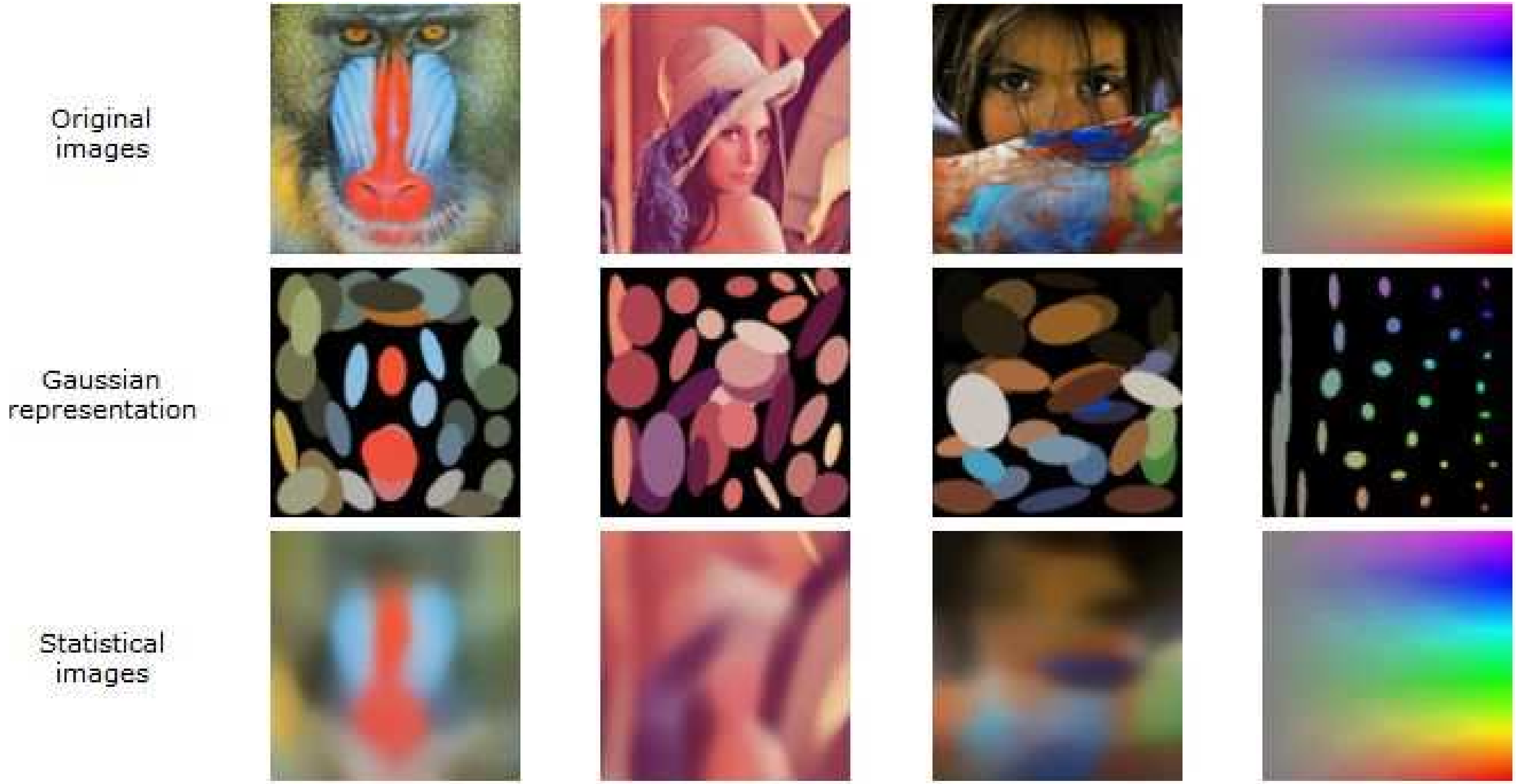
Closed-form Bhattacharyya distances for exp. fam.

Exp. fam.	$F(\theta)$ (up to a constant)	Bhattacharyya/Burbea-Rao $\mathrm{BR}_F(\lambda_p, \lambda_q) = \mathrm{BR}_F(\tau(\lambda_p)$
Multinomial	$\log(1 + \sum_{i=1}^{d-1} \exp\theta_i)$	$-\ln\sum_{i=1}^{d} \sqrt{p_i q_i}$
Poisson	$\exp\theta$	$\frac{1}{2}(\sqrt{\mu_p} - \sqrt{\mu_q})^2$
Gaussian	$-\frac{\theta_1^2}{4\theta_2} + \frac{1}{2}\log(-\frac{\pi}{\theta_2})$	$\frac{1}{4}\frac{(\mu_p-\mu_q)^2}{\sigma_p^2+\sigma_q^2} + \frac{1}{2}\ln\frac{\sigma_p^2+\sigma_q^2}{2\sigma_p\sigma_q}$
Gaussian	$\frac{1}{4}\mathrm{tr}(\Theta^{-1}\theta\theta^T) - \frac{1}{2}\log\det\Theta$	$\frac{1}{8}(\mu_p - \mu_q)^T\left(\frac{\Sigma_p+\Sigma_q}{2}\right)^{-1}(\mu_p - \mu_q) + \frac{1}{2}\ln\frac{\det\frac{\Sigma_p+\Sigma_q}{2}}{\det\Sigma_p\det\Sigma_q}$

Bhattacharyya, Burbea-Rao, Tsallis, Rényi, $\alpha-$, β-divergences are in closed forms for members of the same exponential family.

Application: Statistical images and Gaussians

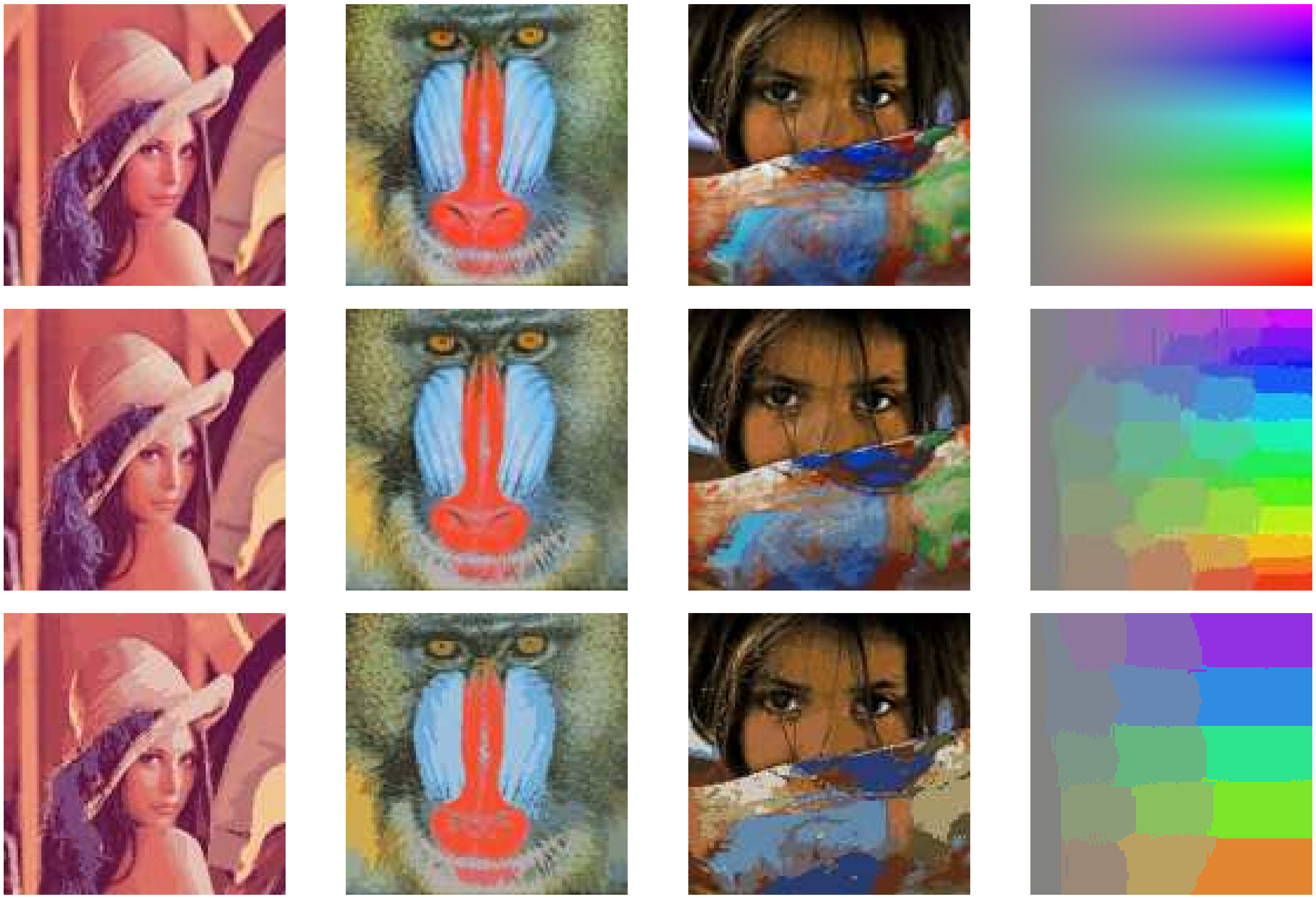
Consider 5D Gaussian Mixture Models (GMMs) of color images (image=RGBxy point set)



Get open source Java(TM) jMEF library:
`www.informationgeometry.org/MEF/`

Hierarchical clustering of GMMs

Hierarchical clustering of GMMs wrt. Bhattacharyya distance. Simplify the number of components of an initial GMM.



(a) source

(b) $k = 48$

(c) $k = 16$

Summary of results

- Skew Burbea-Rao divergences occur when
  - Symmetrizing skew Bregman divergences: Jensen-Bregman divergences
  - Bhattacharyya/Chernoff coefficients/distances of exponential families
- Apply ConCave-Convex procedure (CCCP) for computing Burbea-Rao centroids
- Skewed Burbea-Rao yields *in the limit* Bregman divergences
- Application: Hierarchical clustering of Gaussian mixtures
- (In arXiv:1004.5049, alternative tailored matrix method generalizing ICASSP 2000 but not so efficient as the general scheme)

`www.informationgeometry.org/BurbeaRao/`

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