# Jensen-Bregman Voronoi diagrams and centroidal tessellations

Frank Nielsen

www.informationgeometry.org

École Polytechnique, LIX, France

Sony Computer Science Laboratories, FRL, Japan

(joint work with Richard Nock)

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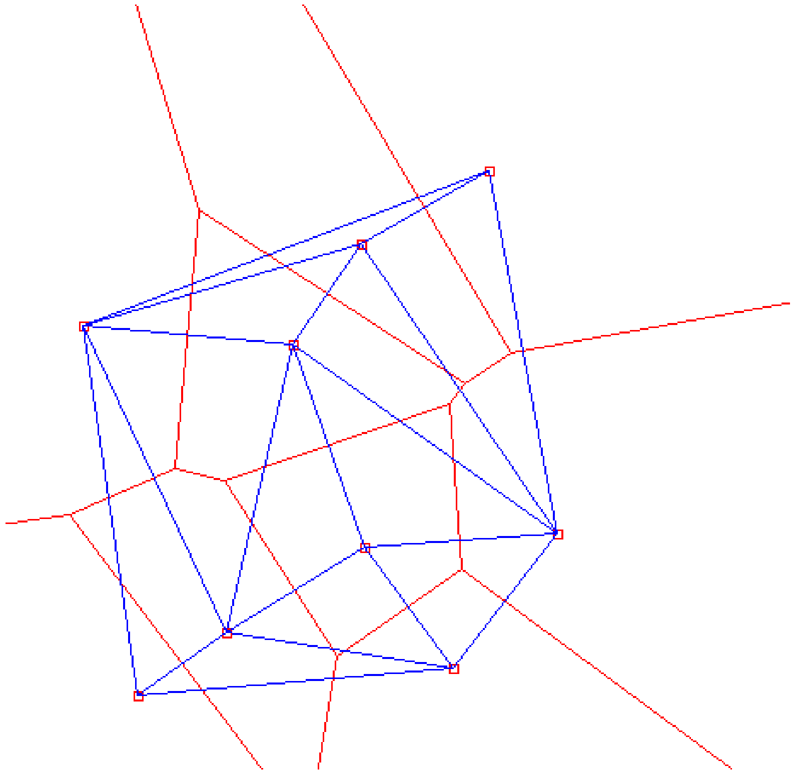
# Voronoi diagrams

Fundamental combinatorial structure for proximty locations:

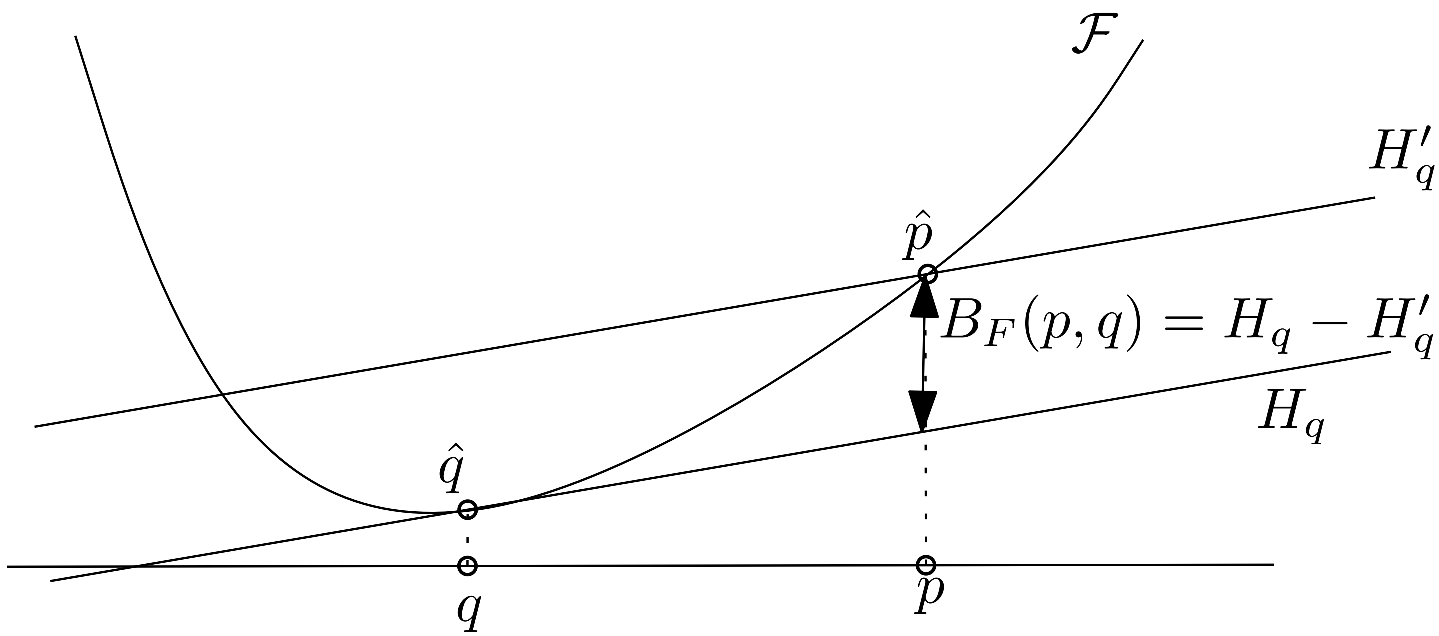


Dual Delaunay triangulation

$\rightarrow$ Extend Voronoi diagrams to Jensen-Bregman divergences.

# 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).**

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

# ensen-Bregman divergences: 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 $F(\cdot)$.

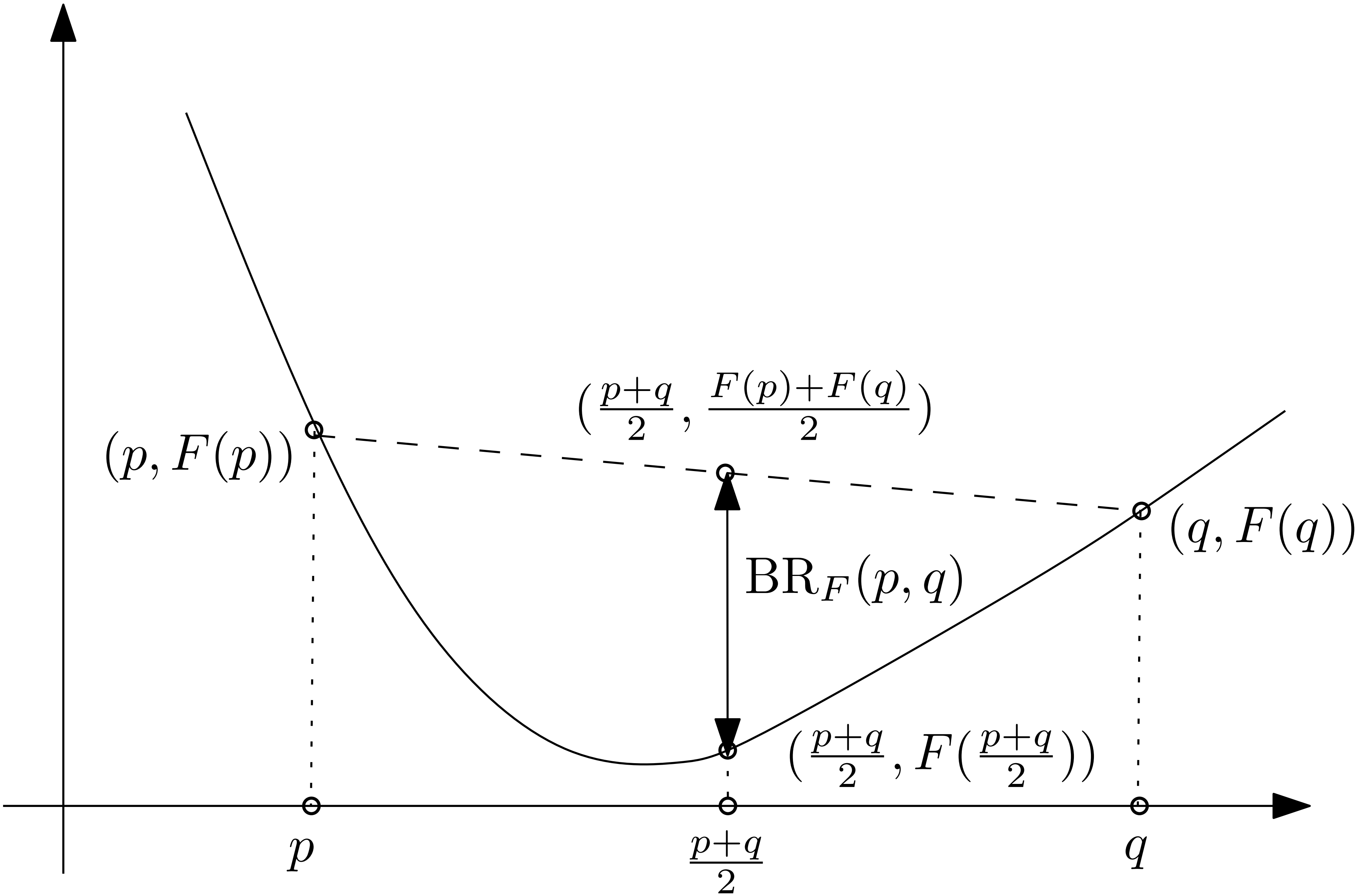
$$\mathrm{BR}_F(p,q) = \sum_{i=1}^{d} \mathrm{BR}_F(p^{(i)}, q^{(i)}),$$

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)

# Visualizing Burbea-Rao divergences



# 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.)
For $Q = I$, we get the squared Euclidean distance.

$\rightarrow$ Ordinary Voronoi diagrams are a special case of Jensen-Bregman Voronoi diagrams.

# Skew Burbea-Rao divergences

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

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

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 $\alpha\rightarrow 1-\alpha$:

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

$\rightarrow$ Extend to arbitrary $\alpha\in\mathbb{R}$ by dividing by $\alpha(1-\alpha)$:

$\mathrm{BR'}_F^{(\alpha)}(p,q) = \frac{1}{\alpha(1-\alpha)}\mathrm{BR}_F^{(\alpha)}(p,q)$ or $\mathrm{BR'}_F^{(\alpha')}(p,q) = \frac{4}{(1-\alpha'^2)}\mathrm{BR}_F^{(\frac{1-\alpha'}{2})}(p,q)$

(with $\alpha = \frac{1-\alpha'}{2}$)

$\rightarrow$ Bregman Voronoi diagrams are special cases of (scaled) skew Jensen-Bregman Voronoi diagrams.

Bregman Voronoi Diagrams, Discrete and Computational Geometry (Springer), 10.1007/s00454-010-9256-1, 2010.

# Non-homogeneous distances

Jensen-Bregman divergences are usually not homogeneous ($D(kp,kq)=k^\lambda D(p,q)$) except for

- Burg entropy ($\lambda=0$) $F(x)=-\log x$, $J_F(p,q)=\log\frac{p+q}{2\sqrt{pq}}$. (logarithm of the ratio of the arithmetic mean over the geometric mean),
- Shannon entropy ($\lambda=1$) $F(x)=x\log x$, $J_F(p,q)=\frac{1}{2}\left(p\log\frac{2p}{p+q}+q\log\frac{2q}{p+q}\right)$
- Squared entropy ($\lambda=2$) $F(x)=x^2$, $J_F(p,q)=\frac{1}{4}(p-q)^2$

For homogeneous distances,

$$D(p,q)=q^\lambda D\left(\frac{p}{q},1\right).$$

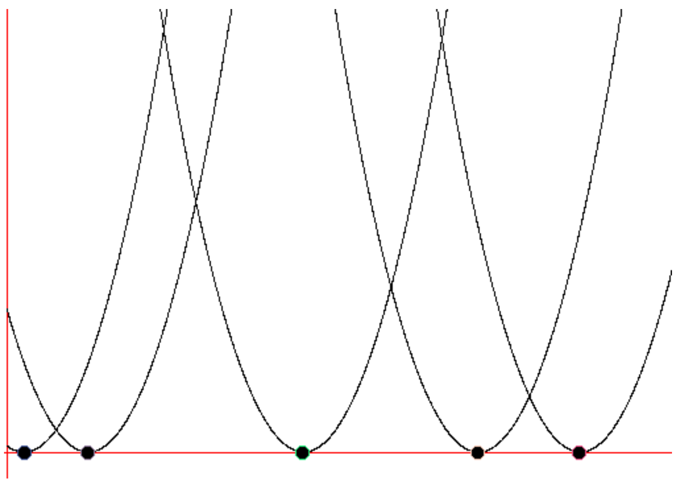
# Voronoi diagram as a minimization diagram

Sites (generators), cells.

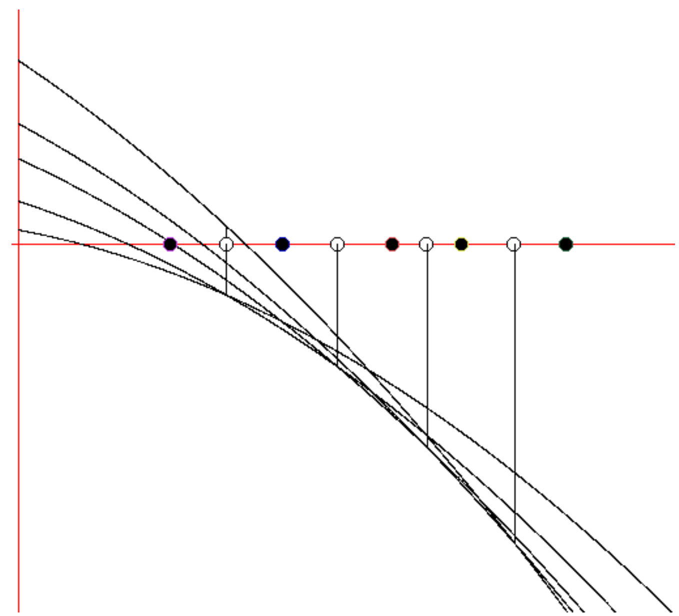
$$V(p_i) = \{p \mid J_F(p, p_i) < J_F(p, p_j)\ \forall j \neq i\}.$$

*Anchored* distance function

$$D_i(x) = J_F(x, p_i) = \frac{F(p_i)+F(x)}{2} - F\left(\frac{p_i+x}{2}\right)$$
$$\equiv D_i'(x) = \frac{1}{2}F(p_i) - F\left(\frac{p_i+x}{2}\right).$$

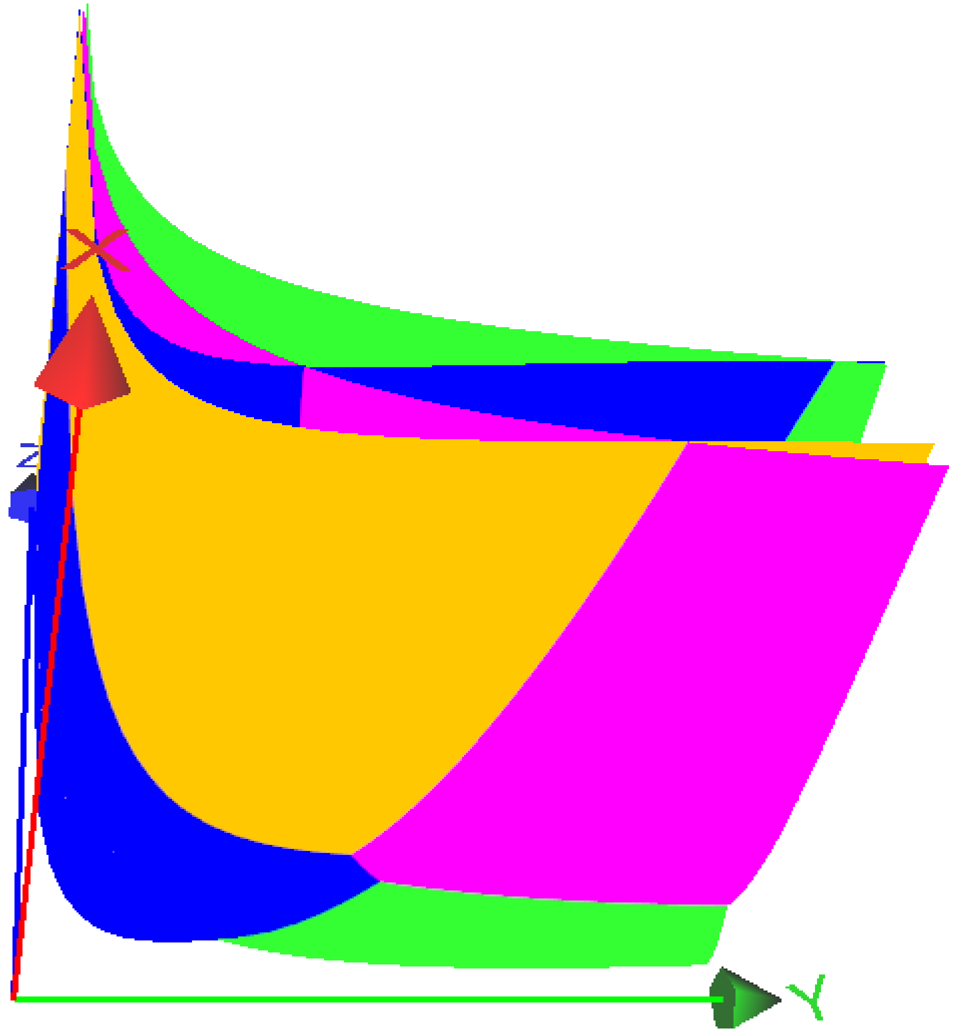


lower enveloppe Shannon $D_i(x)$



lower enveloppe Shannon $D_i'(x)$

# 3D Jensen-Burg envelope




$\rightarrow$ Vertical projection yields 2D Jensen-Burg Voronoi diagram.

# Jensen-Bregman Voronoi

Jensen-Bregman divergences are not necessarily convex.

For example, consider $F(x) = x^3$ on $\mathbb{R}^+$ (with $F''(x) = 6x$). We have $D_p''(x) = 3(x - \frac{p+x}{4})$; This is non-negative for $x \geq \frac{p}{3}$ only.

However, we have a special structure of the lower envelope.
Minimization diagram $\min_i D_i(x)$ is equivalent to the minimization diagram of the functions

$$D_i(x) \equiv D_i'(x) = \frac{1}{2}F(p_i) - F\left(\frac{p_i + x}{2}\right).$$

($D'$ does not mean derivative function but simply $D_i(x) = D_i'(x) + \frac{F(x)}{2}$ )

# Jensen-Bregman bisector

Bisector $(p, q)$ (after removing $\frac{F(x)}{2}$ terms):

$$\frac{F(p)}{2} - F\left(\frac{x+p}{2}\right) = \frac{F(q)}{2} - F\left(\frac{x+q}{2}\right).$$

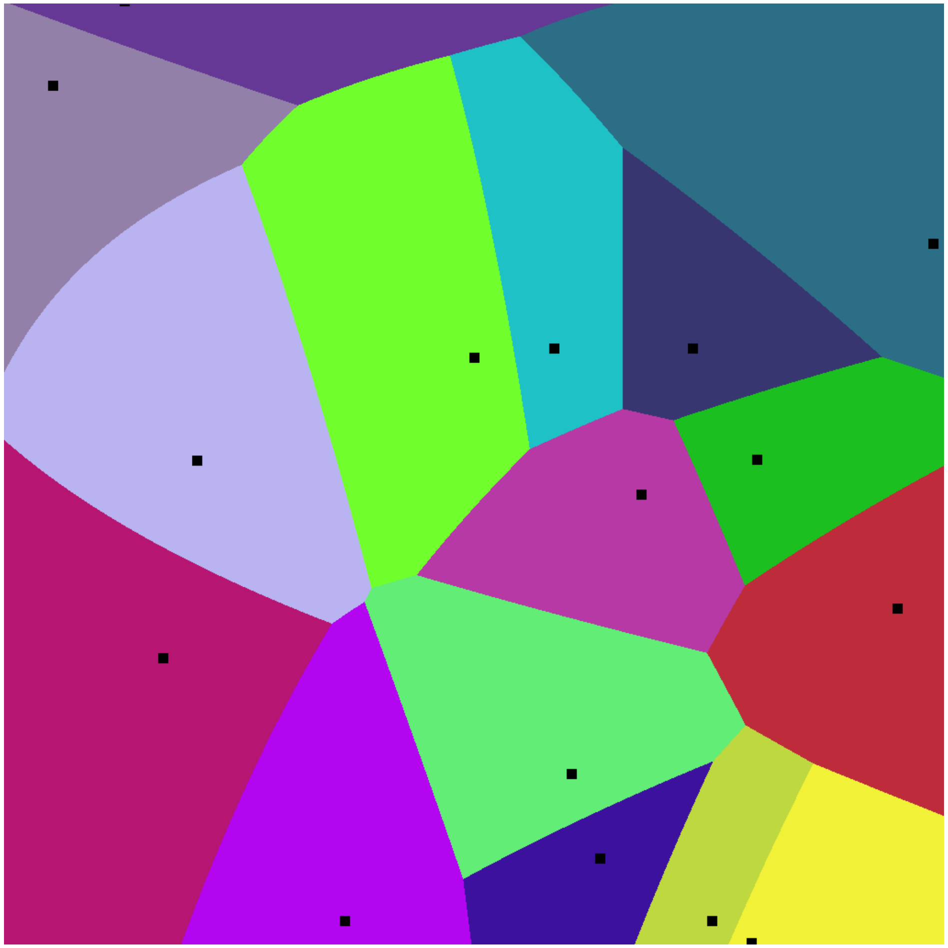
$$\underbrace{F\left(\frac{x+q}{2}\right)}_{\text{convex}} \underbrace{-F\left(\frac{x+p}{2}\right)}_{\text{Concave}} + \underbrace{\frac{F(p)}{2} - \frac{F(q)}{2}}_{\text{Constante}} = 0$$

Interpreted as the sum/intersection of a *convex* function $F\left(\frac{x+q}{2}\right) - \frac{F(p)}{2}$ with a *concave* function $-F\left(\frac{x+p}{2}\right) - \frac{F(q)}{2}$.

In 2D, the iso-distance curves intersect in at most two points.
(proof by contradiction, require strict convexity).

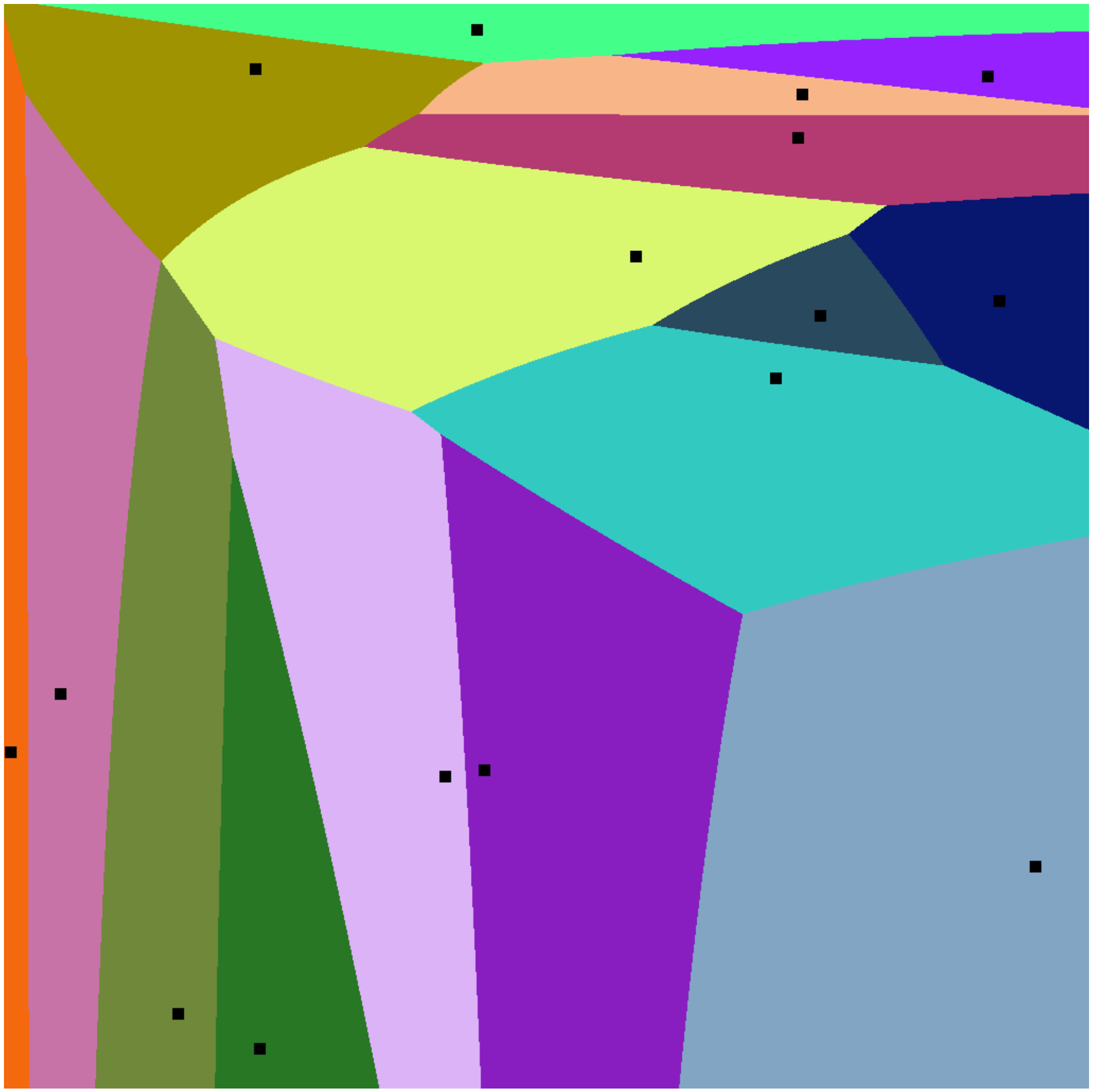
# Jensen-Bregman Voronoi

In 2D, bisectors are pseudo-lines (pseudo-circles iso-distance contours)
Complexity of the Jensen-Bregman Voronoi diagram is linear
(planar graph)



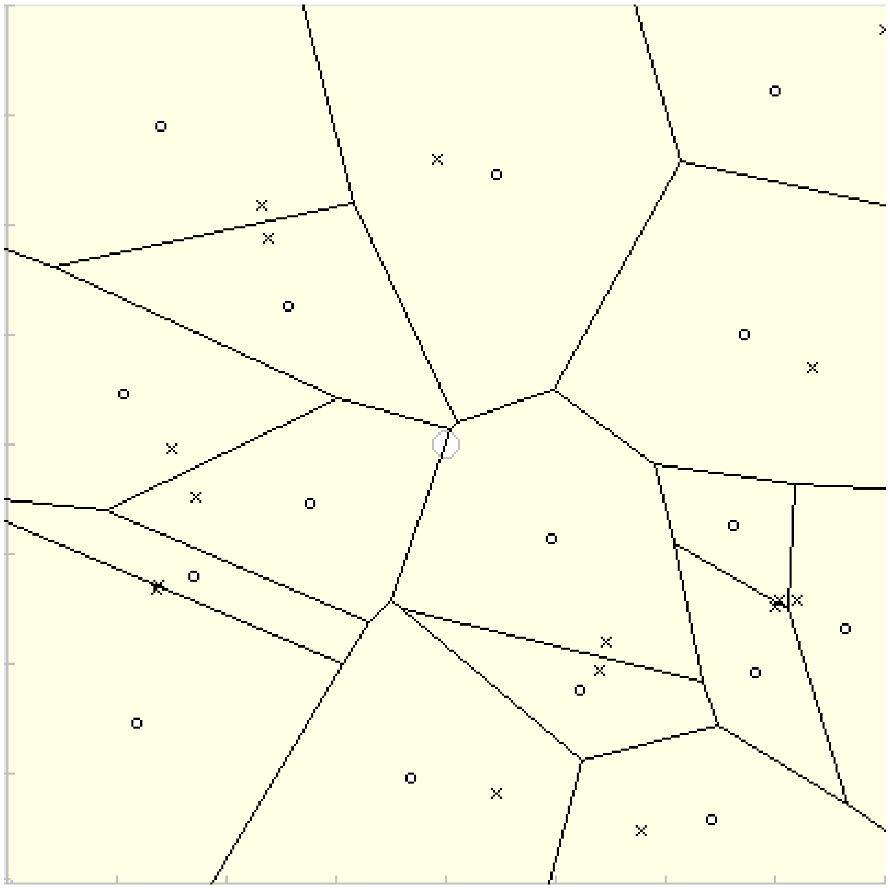
Jensen-Shannon Voronoi diagram

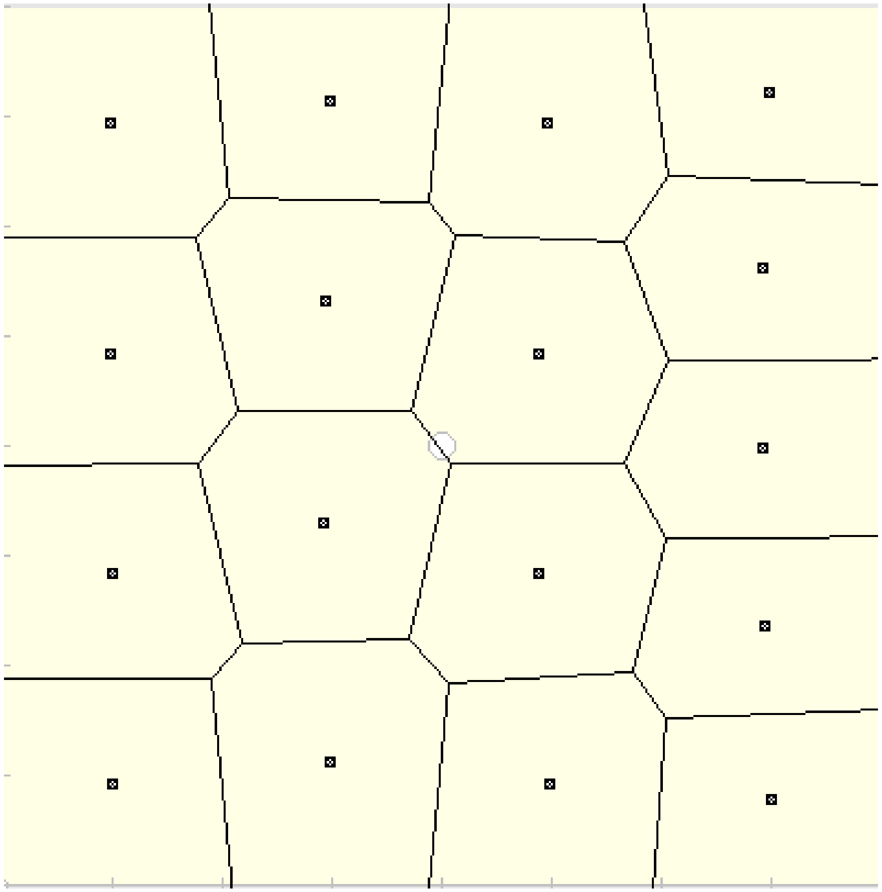
# 2D Jensen-Burg Voronoi



# Centroidal Voronoi Tesselations

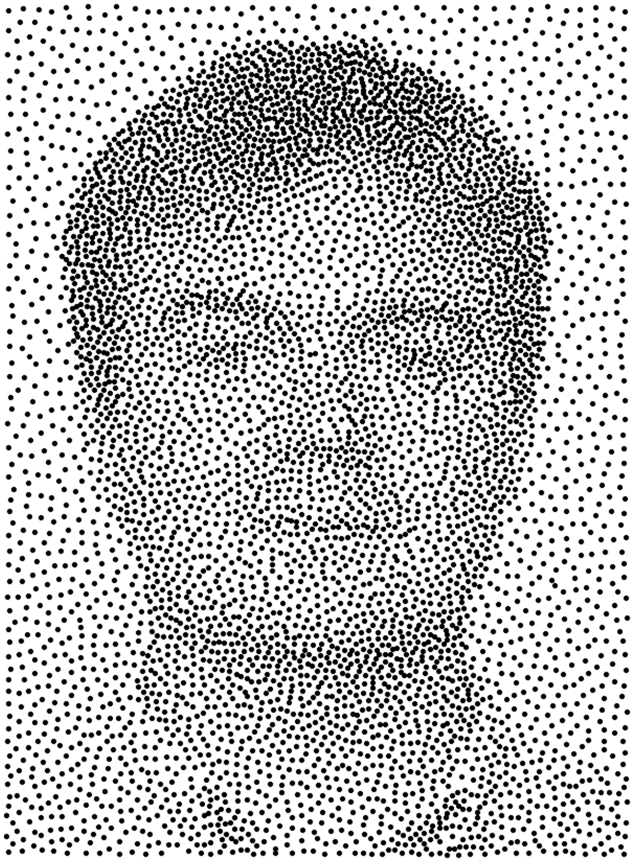
CVT using Lloyd or L-BFGS algorithms (Limited BroydenŰFletcherŰGoldfarbŰShanno).





# Applications of CVTs: Stippling

Also called pointillism in computer graphics.
(non-photorealistic renderings)



# Jensen-Bregman centroids

Consider a finite point set $\{p_1, ..., p_n\}$.

$$c^* = \arg\min_c \sum_{i=1}^n w_i J_F(p_i, c) = \arg\min_c L(c)$$

Minimization can be decomposed as

$$L(c) = L_{\mathrm{convex}}(c) + L_{\mathrm{concave}}(c).$$

(Under mild assumptions any function can be decomposed as a sum of a convex plus concave function)
For the Jensen-Bregman centroid, this decomposition is given *explicitly*:

$$\begin{aligned} L_{\mathrm{convex}}(c) &= \frac{F(c)}{2} \\ L_{\mathrm{concave}}(c) &= -\sum_{i=1}^n F\left(\frac{p_i + c}{2}\right), \end{aligned}$$

# Jensen-Bregman centroids (and barycenters)

Use framework of CCCP (ConCave Convex Procedure):

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

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

Start from arbitrary $c_0$ and iterate:

$$x_{t+1} = \nabla F^{-1}\left(\sum_{i=1}^{n} w_i \nabla F\left(\frac{x_t+p_i}{2}\right)\right).$$

Guaranteed convergence to a (local) minimum.
(gradient descent methods require to fix learning rates)

# Jensen-Bregman centroids

Consider a dense region $X$ with an underlying density function $\rho(\cdot)$.

$$\arg\min_{c \in X} \int_{p \in X} \rho(p) \mathrm{BR}_F(p, c) \mathrm{d}p$$

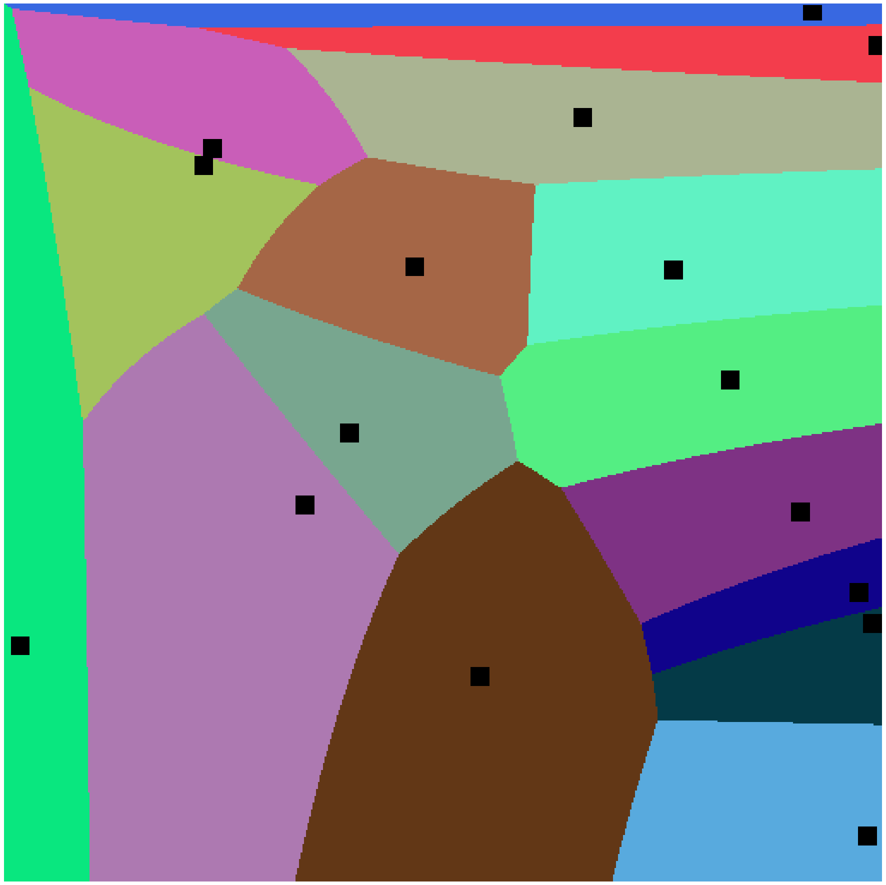
Integral CCCP using $c_0 = \int_{p \in X} \rho(p) \mathrm{d}p$, update as follows:

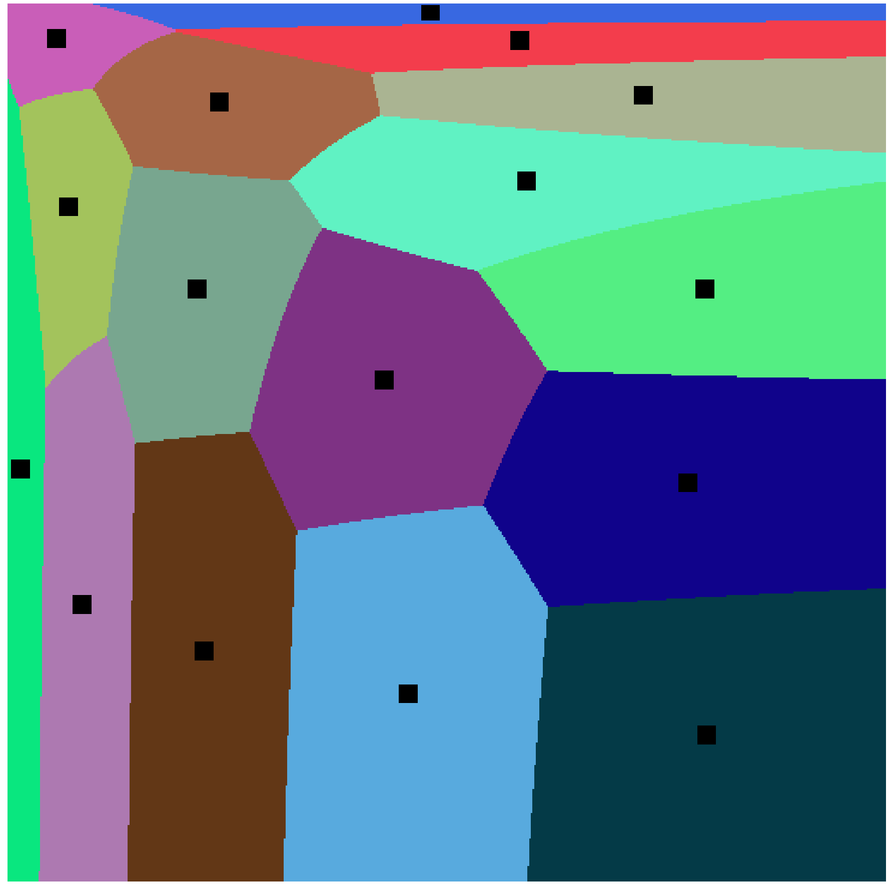
$$c_{t+1} = \nabla F^{-1} \left( \frac{\int_{p \in X} \rho(p) \nabla F \left( \frac{p + c_t}{2} \right) \mathrm{d}p}{\int_{p \in X} \rho(p) \mathrm{d}p} \right)$$

$\rightarrow$ In general, difficult to compute in closed-form (except for squared Mahalanobis). Approximate by discretizing.

# Jensen-Burg centroidal Voronoi tesselation

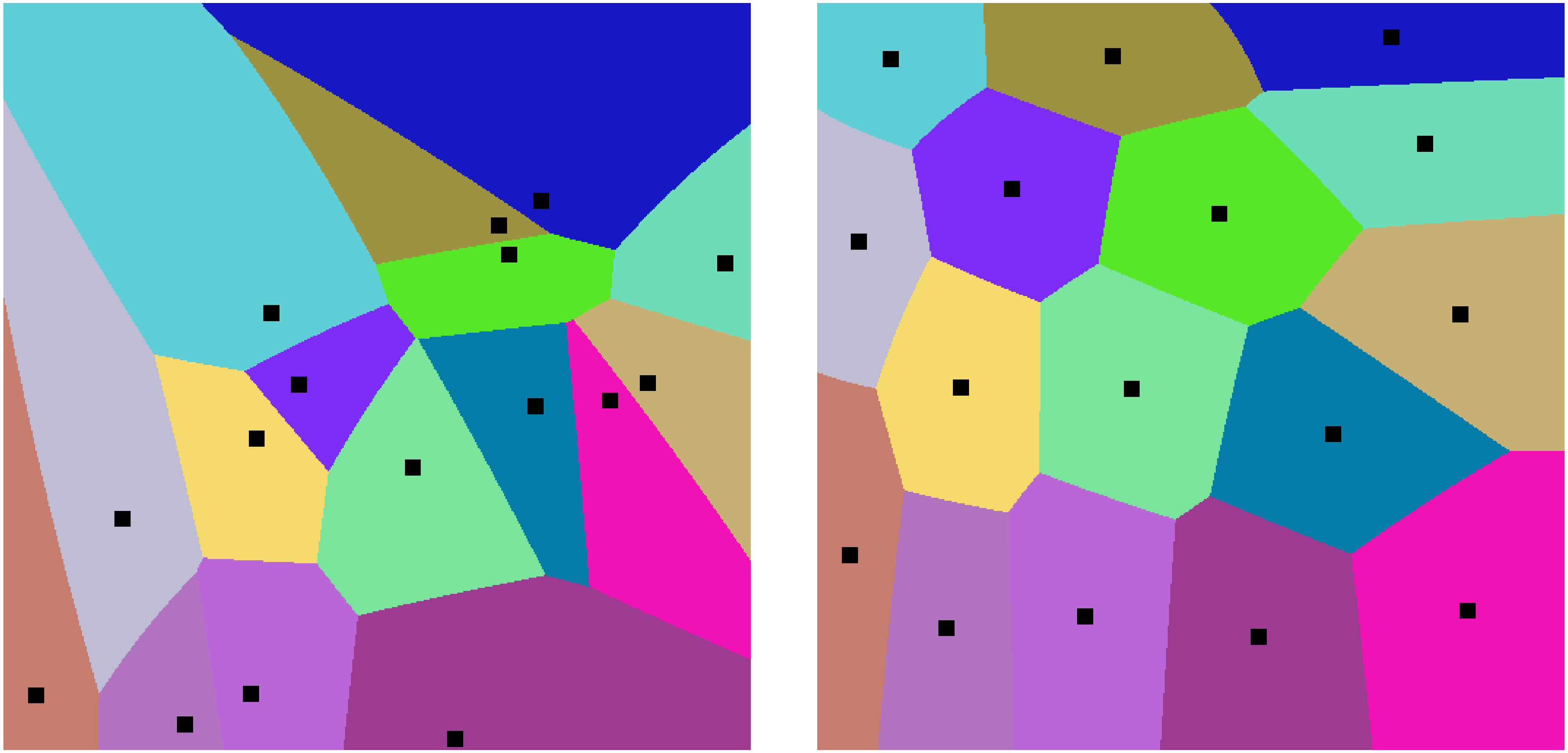
We discretize cells.





# Jensen-Shannon centroidal Voronoi tesselation

We discretize cells



# Application to statistical Voronoi diagrams

For probability densities, Bhattacharyya similarity coefficient (and non-metric symmetric distance):

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

(coefficient is always *strictly* positive)
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/$\alpha$-divergences

Skew Bhattacharrya divergences based on Chernoff $\alpha$-coefficients.

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

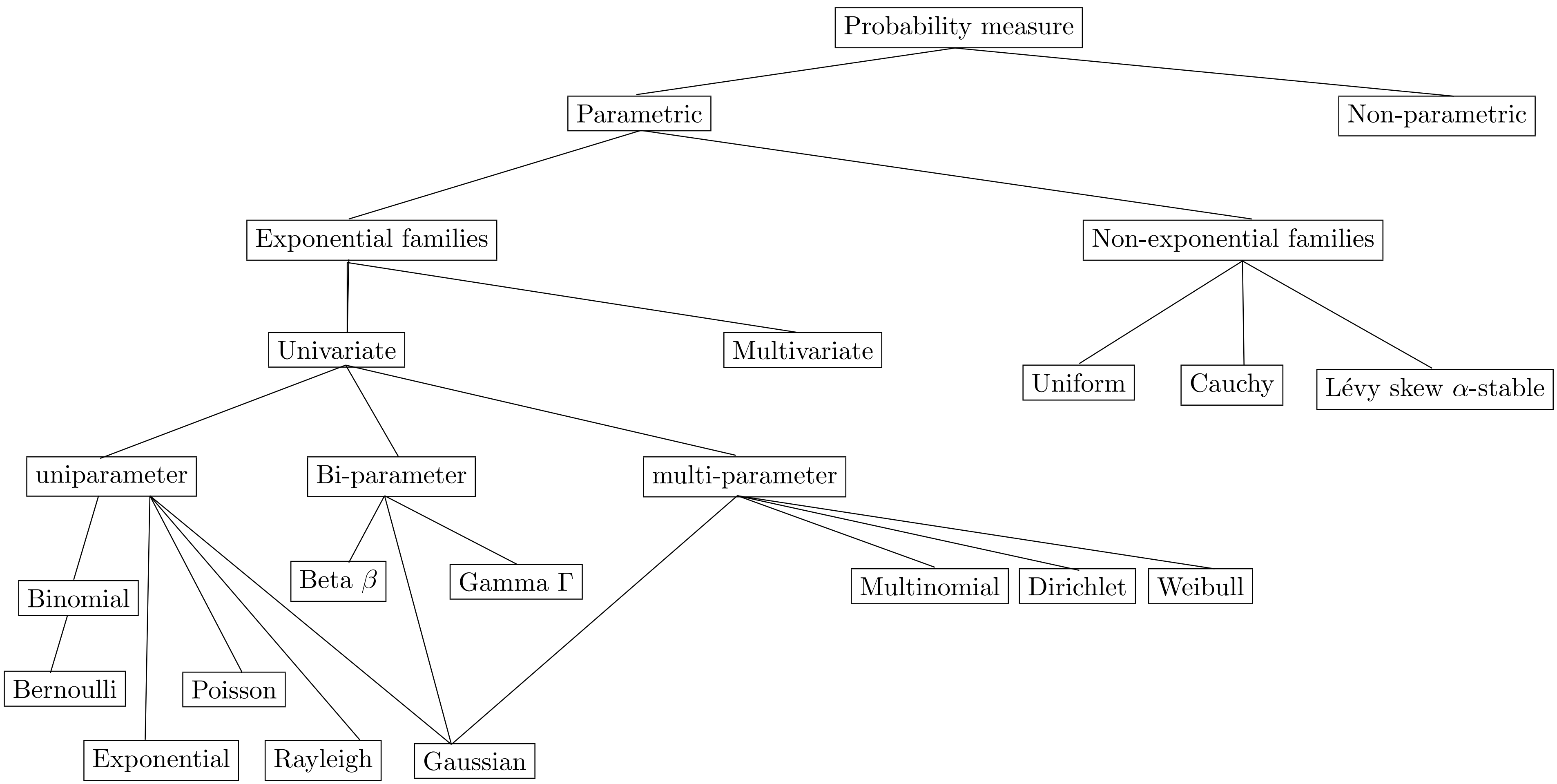
Amari $\alpha$-divergence:

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

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

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

# Exponential families in statistics




Finite moments of all orders.

# 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,
- $F(\theta) = \frac{1}{4}\mathrm{tr}(\theta_2^{-1}\theta_1\theta_1^T) - \frac{1}{2}\log\det\theta_2 + \frac{d}{2}\log\pi$,
- $t(x) = (x, -x^Tx)$,
- $k(x) = 0$.

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 $\mathcal{E}_F$:

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

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

$= \exp(-\mathrm{BR}_F^{(\alpha)}(\theta_p,\theta_q)) > 0.$ Coefficient is always strictly positive. For $\theta_p = \theta_q$, $C_\alpha(\theta_p,\theta_q) = \exp -0 = 1$ and $B_\alpha(\theta_p,\theta_q) = 0$.

# Summary of paper & results

- Extending Jensen-Shannon divergence to arbitrary convex (information) function (=negative entropy)
- Jensen-Bregman divergences (=Jensen or Burbea-Rao divergences)
- 2D Voronoi diagram is in *linear complexity* (bisector). Jensen-Bregman Voronoi diagrams extend Bregman Voronoi diagrams.
- Jensen-Bregman centroids (solved iteratively using CCCP)
- Jensen-Bregman centroidal Voronoi tesselations (CVTs, by discretization)
- Bhattacharyya distance of members of the same exponential family = Jensen-Bregman divergence on the natural parameters
- Statistical Voronoi diagrams, extending Bregman Voronoi diagrams (since asymptotically skewed Jensen-Bregman divergences yields Bregman divergences)

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