Computational Information Geometry
for Machine Learning

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Computational Information Geometry (CIG) : Background

Computational Information Geometry (CIG) relies seamlessly on:

- statistics and probability (STAT & PR),
- information theory (IT),
- differential geometry (DG, including multilinear algebra of tensors),
- computation:
  Yes, we are computer scientists and programmers! How do we compute friendly? (make wide & wise use of dualities...)

Many application fields: computational statistics, machine learning (ML), information retrievals (IRs), computer vision (CV), medical imaging, radar signal processing, etc.

Motivations: Setting goals!
Computational Information Geometry: Main goals

1. understand “distances” and group them axiomatically into classes and build generic meta-algorithms (unifying former algorithms): Bregman divergences $B_F$, Csiszár $f$-divergences $l_f$, proper scoring rules, etc.

   → seek for “properties with exhaustivity”,

2. understand relationships between distances and geometries,

3. understand generalized entropies, cross-entropies, maximum entropy probability distributions, and their induced geometries (beyond Shannon/Boltzmann/Gibbs).

4. provide (coordinate-free) intrinsic computing using the language/affordances of geometry (for computational statistics, machine learning and predictive analytics)
Goal 1. Dissimilarities (distances) and meta-algorithms

- unify algorithms into **meta-algorithms** working on classes of distances (metrics, divergences):
  - parameter estimation (with goodness-of-fit),
  - center-based clustering (with Bregman distances),
  - learning (boosting with surrogate loss functions),
  - forecasting (with proper score functions),
  - etc.

- propose new **principled** classes of distances:
  - total Bregman divergences [17],
  - total Jensen divergences [41],
  - conformal divergences [45], etc.

- understand axiomatically properties and relationships between distances (or multi-entity diversity indexes) and search for their **exhaustive characterizations**.
Goal 2. Distances and geometries

Not 1-to-1 (because same geometry can be realized for different distances).
Geometry = meta-model
Embedding (isometrically) a geometry into another geometry : =model interpreted into another larger model.

- Underlying geometries of distances/divergences :
  - Riemannian geometry with metric distances (with the metric Levi-Civita connection),
  - Dually coupled affine differential geometry ($\pm \alpha$-geometry) and non-metric distances (aka. divergences),
  - monotone embeddings into $(\rho, \tau)$-structure (extending $l_\alpha$-embedding),
  - etc.

- geometries of probability distributions/positive measures and distances :
  How to define statistical manifolds?
Goal 3. Entropies, cross-entropies, relative entropies and MaxEnt distributions

- entropies $H(P)$ (Shannon-Boltzmann-Gibbs), cross-entropies $H^\times(P : Q)$ and relative entropies KL. $KL(P : Q) = H^\times(P : Q) - H(P)$ with $H(P) = H^\times(P : P)$.
- generalized entropies (so called deformed "logarithms"), the concept of escort distributions,
- maximum entropy principle and equilibrium distributions (Boltzmann-Gibbs, Tsallis’s heavy tailed distributions, etc.)
- entropies, information (=neg-entropy) and complexity (Kolmogorov, non-computability)
Goal 4. Geometric computing for intrinsic computing

Propose a paradigm for data science : from “datum” (biased) processing to geometric “pointum” (non-biased) coordinate-free computing

- get unbiased processing : coordinate-free!,
- use affordances of the geometric language for building/explaining algorithms:
  points, geodesics, balls, orthogonality, projection, Pythagoras, flat, submanifold, etc.

- analytic and synthetic geometries (closed-form or exact geometric characterization).
  Example : Two pseudo-segments always intersect in a common point... that may not be in closed-form.

- invariance (and statistical invariance) and geometry:
  group of invariance, invariance and sufficiency, statistical invariance, etc.

Geometrizing probability spaces yields statistical manifolds
Part I: Geometry of statistical manifolds
Outline of Part I

1. Fisher information (Cramér-Rao lower bound) & sufficiency (1922)
2. Structures from differential geometry of population spaces (Hotelling, 1930, Rao, 1945, Amari-Centsov 1980’s)
3. Maximum entropy principle (exponential families) (1957, Jaynes)
4. Information projections (and Pythagoras’ theorem)
I. Statistical Information
Fisher Information

$I(\theta)$
Old days - :) Discrete and Continuous random variables

- Discrete RV: probability mass function (pmf) $X \sim p$, discrete support $\mathcal{X}$.

$$\mathbb{E}[X] = \sum_{x \in \mathcal{X}} p(x)x = \langle X \rangle$$

Distributions: Bernoulli, binomial, multinomial, Poisson, etc.-$\infty$.

- Continuous RV: probability density function (pdf) $X \sim p$, continuous support $\mathcal{X}$.

$$\mathbb{E}[X] = \int_{x \in \mathcal{X}} p(x)x \, dx = \langle X \rangle$$

Distributions: exponential, normal, lognormal, gamma, beta, Dirichlet, Wishart, etc.-$\infty$.
From data sets to empirical (discrete) distributions

Given $X = \{x_1, \ldots, x_n\}$ observations...

...build the empirical distribution:

$$p_e(X) = \frac{1}{n} \sum_{i=1}^{n} \delta(X - X(i))$$

$$F_e(x) = \frac{1}{n} \sum_{i=1}^{n} 1_{[x_i \leq x]} \ (\text{cdf})$$

$$p_e^i = \frac{1}{n} \#\{x = i\} \ (\text{frequency})$$

Support $X$ is unknown a priori: not a multinomial distribution nor a finite mixture!

Sample mean $\bar{\mu} = \frac{1}{n} \sum_i x_i = \langle X \rangle_{pe} = \sum_{i \in \text{??}} p_e^i i$.

Estimation $X \sim D(\theta)$ by the method of moments:

$$\langle X \rangle_{pe} = \mathbb{E}[X] = \langle X \rangle$$
Old days : Discrete and continuous random variables

- **Discrete RV. Shannon entropy** :

\[
H(X) = \sum_{x \in \mathcal{X}} p(x) \log \frac{1}{p(x)} \geq 0
\]

always positive (notion of uncertainty! max uncertainty for uniform distribution : \(H(U) = \log n\))

- **Continuous RV. Differential entropy** :

\[
H(X) = \int_{x \in \mathcal{X}} p(x) \log \frac{1}{p(x)} \, dx
\]

can be negative (physical interpretation !) ... 

For example, for multivariate normals (MVNs) \(N(\mu, \Sigma)\) :

\[
H(X) = \frac{1}{2} \log(2\pi e)^d |\Sigma|
\]
Mixture sampling: Example of a Gaussian Mixture Model (GMM)

To sample a variate \( x \) from a GMM:

- Choose a component \( l \) according to the weight distribution \( w_1, \ldots, w_k \).
- Draw a variate \( x \) according to \( N(\mu_l, \Sigma_l) \).

→ Sampling is a **doubly stochastic process**:

- throw a biased dice with \( k \) faces to choose the component:
  \[
  l \sim \text{Multinomial}(w_1, \ldots, w_k)
  \]
  (Multinomial is normalized histogram without void bins)

- then draw at random a variate \( x \) from the \( l \)-th component
  \[
  x \sim N(\mu_l, \Sigma_l)
  \]
  \[
  x = \mu + Cz \text{ with Cholesky: } \Sigma = CC^T \text{ and } z = [z_1 \ldots z_d]^T \text{ standard normal random variate: } z_i = \sqrt{-2 \log U_1 \cos(2\pi U_2)}
  \]
Statistical mixtures: discrete, continuous or mixed!

Finite mixture models \((k \in \mathbb{N})\) have pmf/pdf:

\[
m(x) = \sum_{i=1}^{k} w_i p_i(x)
\]

(not sum of RVs, \(M \neq \sum_i w_i X_i\) that have convolutional densities)

- mixtures of Gaussians (universal representation for smooth densities)
- multinomial distribution is a mixture
  (and also an exponential family in information geometry…)

What about the mixture of a standard Gaussian with a binomial distribution? \(\rightarrow\) Neither discrete nor continuous!
Measure theory (axiom system of Kolmogorov, 1933)

- unify discrete and continuous RVs as probability measures (pm) $\mu, \nu$, etc.
- can handle RVs that are neither continuous nor discrete (e.g., a mixture of Poisson with a Gaussian)
- for probability measures, pmfs/pdfs are Radon-Nikodym derivatives
- expectation notation is unified as:

$$E[X] = \int_{x \in X} xp(x) \, d\nu(x)$$

- Two usual base measures:
  - counting measure: $\nu_C$ ($\int \to \Sigma$)
  - Lebesgue measure: $\nu_L$
Measure theory: Probability space (recalling terminology)

- $\mathcal{X}$ a set, the sample space
- $\sigma$-algebra $\mathcal{F}$ over $\mathcal{X}$: subsets of $\mathcal{X}$ closed under countable many intersections, unions, and complements.
- $(\mathcal{X}, \mathcal{F})$: measurable space
- measure $\mu : \mathcal{F} \to \mathbb{R} \cup \{\pm\infty\}$ with
  - $\mu(E) \geq 0, \forall E \in \mathcal{F}, \mu(\emptyset) = 0$
  - $\mu(\bigcup_{i \geq 1} E_i) = \sum_{i \geq 1} \mu(E_i)$ for pairwise disjoint sequence $\{E_i \in \mathcal{F}\}$
- $(\mathcal{X}, \mathcal{F}, \mu)$, a (positive) measure space
- $(\mathcal{X}, \mathcal{F}, \mu)$ with $\mu(\mathcal{X}) = 1$, a probability space, $F \in \mathcal{F}$ are events
Measurable functions and random variables

- **Measurable function** $f : \mathcal{X} \to \mathcal{Y}$ between two measurable spaces $(\mathcal{X}, \mathcal{F})$ and $(\mathcal{Y}, \mathcal{G})$:

  $$\forall G \in \mathcal{G}, \quad f^{-1}(G) \in \mathcal{F}$$

- **Random variable** $X = \text{measurable function } X : \mathcal{X} \to \mathbb{R}$. Therefore:

  $$\{x \in X \mid a < X(x) < b\} \in \mathcal{F}$$

  all sample states with $X$ taking values between $a$ and $b$ is an event (CDF)

- **continuous RV** = measures on Borel $\sigma$-algebra
Dominance and Radon-Nikodym derivatives

- measure $\mu$ is dominated by measure $\nu$ ($\mu \ll \nu$) iff.

\[ \nu(E) = 0 \Rightarrow \mu(E) = 0 \]

- $\mu \ll \nu$ $\sigma$-finite ($X$=countable union of measurable sets with finite measure) then $\mu$ admits a density $f$ wrt to $\nu$, the Radon-Nikodym derivative:

\[ f \equiv \frac{d\mu}{d\nu} \]

\[ \forall \ \nu \text{— measurable } E, \ \mu(E) \equiv \int_{e \in E} f \, d\nu(e) \]

- $P \ll \nu$, Shannon entropy: $H(P) = - \int p(x) \log p(x) \, d\nu(x)$. 
Statistical estimation : parametric estimation $\hat{\theta}$

- Given idd. $X = \{x_1, ..., x_n\} \sim p_{\theta_0}(x)$ (hidden by Nature), estimate $\theta$ in family $\{p_\theta(x)\}_\theta$?
  → from observation sets to random vectors

- **Maximum Likelihood Principle (MLE):**

\[
\hat{\theta}_n = \arg\max_\theta \prod_i p_\theta(x_i) = \arg\max_\theta l(X; \theta) = \sum_i \log p_\theta(x_i)
\]

- **Consistency:** $\lim_{n \to \infty} \hat{\theta}_n = \theta_0$

- **score function:** $s(\theta, x) = \nabla_\theta \log p_\theta(x)$ with $\nabla_\theta = (\partial_i = \frac{\partial}{\partial \theta_i})_i$. score indicates the sensitivity of the log-likelihood curve.

- For strictly concave log-likelihood, unique $\hat{\theta}$ such that $s(\hat{\theta}, x) = 0$ (MVNs, Beta, Poisson, Dirichlet, etc).
Fisher information $I(\theta) = \text{Variance of the score}$

Amount of information that an observable random variable $X$ carries about an unknown parameter $\theta$:
First moment of score: $0$, not discriminative!

$$\mathbb{E} \left[ \frac{\partial}{\partial \theta} \log p(X; \theta) \mid \theta \right] = \mathbb{E} \left[ \frac{\partial}{\partial \theta} \frac{p(X; \theta)}{p(X; \theta)} \mid \theta \right] = \int \frac{\partial}{\partial \theta} \frac{p(x; \theta)}{p(x; \theta)} p(x; \theta) \, dx$$

$$= \int \frac{\partial}{\partial \theta} p(x; \theta) \, dx = \frac{\partial}{\partial \theta} \int f(x; \theta) \, dx$$

$$= \frac{\partial}{\partial \theta} 1 = 0.$$

Second moment of score: (with $\partial_i l(x; \theta) = \frac{\partial}{\partial \theta_i} l(x; \theta)$)

$$\mathcal{I}(\theta) = \mathbb{E} \left[ \left( \frac{\partial}{\partial \theta} \log f(X; \theta) \right)^2 \right] = \int \left( \frac{\partial}{\partial \theta} \log f(x; \theta) \right)^2 f(x; \theta) \, dx > 0$$

Multi-parameter: $l_{i,j}(\theta) = \mathbb{E}_{\theta} [\partial_i l(x; \theta) \partial_j l(x; \theta)]$, $I(\theta) \succeq 0$, PS(S)D

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2. Fisher Information-2. FIM
Fisher information and Cramér-Rao lower bound

How good is an estimator? how to measure goodness?

- **Mean Square Error (MSE)**: \( \text{MSE}(\theta) \equiv \mathbb{E}[||\hat{\theta} - \theta_0||^2] \) (consistency: \( \text{MSE} \to 0 \))

- **Cramér-Rao lower bound**: for an unbiased estimator \( \hat{\theta} \):
  \[
  \nabla[\hat{\theta}] \succeq I^{-1}(\theta_0)
  \]

- **efficiency**: unbiased estimator matching the CR lower bound

- **asymptotic normality** of \( \hat{\theta} \) (on random vectors):
  \[
  \hat{\theta} \sim \mathcal{N}\left(\theta_0, \frac{1}{n}I^{-1}(\theta_0)\right)
  \]
Fisher Information Matrix (FIM)

\[ I(\theta) = [I_{i,j}(\theta)]_{i,j}, \quad I_{i,j}(\theta) = \mathbb{E}_\theta[\partial_i l(x; \theta) \partial_j l(x; \theta)] \]

- For **multinomials** \((p_1, \ldots, p_d)\):

\[
I(\theta) = \begin{bmatrix}
 p_1(1 - p_1) & -p_1 p_2 & \ldots & -p_1 p_k \\
 -p_1 p_2 & p_2(1 - p_2) & \ldots & -p_2 p_k \\
 \vdots & \vdots & \ddots & \vdots \\
 -p_1 p_k & -p_2 p_k & \ldots & p_k(1 - p_k)
\end{bmatrix}
\]

- For **multivariate normals** (MVNs) \(N(\mu, \Sigma)\):

\[
I_{i,j}(\theta) = \frac{\partial \mu^\top}{\partial \theta_i} \Sigma^{-1} \frac{\partial \mu}{\partial \theta_j} + \frac{1}{2} \text{tr} \left( \Sigma^{-1} \frac{\partial \Sigma}{\partial \theta_i} \Sigma^{-1} \frac{\partial \Sigma}{\partial \theta_j} \right)
\]

matrix trace : \(\text{tr}\).
Reparameterization of the Fisher information matrix

- Let $\theta = \theta(\eta)$ and $\eta$ be two 1-to-1 parameterizations
- $J = [J_{i,j}]_{i,j}$: Jacobian matrix $J_{i,j} = \frac{\partial \theta_i}{\partial \eta_j}$.

$$I_\eta(\eta) = J^\top \times I_\theta(\theta(\eta)) \times J$$

Fisher information matrix depends on the parameterization of the parameter space (covariant)
Statistics: Information and sufficiency

- **sufficiency**: $P(x|t, \theta) = P(x|t)$
  \[ \Rightarrow \text{all information about } \theta \text{ is contained inside } t \]

- $I_s(x)(\theta) \leq I_x(\theta)$ for a statistic $s$, with equality iff. $s$ is **sufficient**

- Fisher-Neyman’s factorization criterion: $t(x)$ is sufficient then we have the following canonical factorization:

  \[ p(x; \theta) = g(t(x); \theta) h(x) \]

- Ex.: $t(x) = (\sum_i x_i, \sum_i x_i^2)$ sufficient for univariate normals.
  - All information about $\theta$ in two quantities: data reduction without loss of statistical information
  - Sample mean $\bar{\mu} = \frac{1}{n} \sum_i x_i$, sample variance

  \[ \bar{\nu} = \frac{1}{n} \sum_i (x_i - \bar{\mu})^2 = \frac{1}{n} \sum_i x_i^2 - \bar{\mu}^2 = \frac{1}{n} \sum_i x_i^2 - (\frac{1}{n} \sum_i x_i)^2 \]

- Not all statistics carry information on $\theta$: **ancillary statistics**, statistics that does not depend on the parameter $\theta$.
We are interested in finite-dimensional sufficient statistics... (statistical lossless data reduction)
Exponential families and finite sufficiency

- Probability measure
  - Parametric
    - Exponential families
      - Univariate
        - uniparameter
          - Bernoulli
          - Binomial
          - Exponential
          - Poisson
          - Rayleigh
          - Gamma
      - Bi-parameter
          - Beta
          - Gamma
    - Multi-parameter
      - multi-parameter
      - multi-parameter
  - Non-parametric
    - Non-exponential families
      - Uniform
      - Cauchy
      - Lévy skew α-stable

Beware: Exponential distribution belongs to the exponential families too.
Exponential families: families of parametric distributions

- Canonical decomposition ($t(x)$ sufficient statistics, $k(x)$ auxiliary carrier term):

$$p(x; \theta) = \exp(\langle t(x), \theta \rangle - F(\theta) + k(x))$$

- log-Laplace transform:

$$F(\theta) = \log \int \exp(\langle t(x), \theta \rangle + k(x))dx$$

- many distributions $p(x; \lambda)$ (normal, gamma, beta, multinomial, Poisson) are exponential families with $\theta(\lambda)$

- $F$ is strictly convex on convex natural parameter space

$$\Theta = \{ \theta \in \mathbb{R}^D \mid F(\theta) < \infty \}$$

- Dual parameterizations: $\theta(\lambda)$ or $\eta(\lambda) = \nabla F(\theta(\lambda)) = \mathbb{E}[t(X)]$

- Fisher information matrix: $I(\theta) = \nabla^2 F(\theta) \succ 0$ (Hessian of strictly convex function)

- MLE: $\hat{\eta} = \frac{1}{n} \sum_i t(x_i) = \nabla F(\theta)$ (condition on existence)
Convex duality: Legendre-Fenchel transformation [21, 19]

- For a strictly convex and differentiable function $F : \mathcal{X} \to \mathbb{R}$, define the **convex conjugate**:

$$F^*(y) = \sup_{x \in \mathcal{X}} \left\{ \langle y, x \rangle - F(x) \right\}$$

- Maximum obtained for $y = \nabla F(x)$:

$$\nabla_x l_F(y; x) = y - \nabla F(x) = 0 \implies y = \nabla F(x)$$

- Maximum **unique** from convexity of $F$ ($\nabla^2 F \succ 0$):

$$\nabla^2_x l_F(y; x) = -\nabla^2 F(x) \prec 0$$

- **Convex conjugates with domains**:

$$(F, \mathcal{X}) \Leftrightarrow (F^*, \mathcal{Y}), \quad \mathcal{Y} = \{ \nabla F(x) \mid x \in \mathcal{X} \}$$
Legendre duality: Geometric interpretation

Consider the **epigraph** of \( F \) as a convex object:

- **convex hull** (vertex, \( V \)-representation), versus
- **half-space** (halfspace, \( H \)-representation).

\[
\begin{align*}
\mathcal{P} &= \{ x_P \} \\
\mathcal{H}_P : z = (x - x_P)F'(x_P) + F(x_P)
\end{align*}
\]

\[
\mathcal{H}_Q : z = (x - x_Q)F'(p) + F(x_Q)
\]

Legendre transform also called “slope” transform.
Legendre duality & Canonical divergence

- Convex conjugates have *functional inverse* gradients $\nabla F^{-1} = \nabla F^*$.
  $\nabla F^*$ may require numerical approximation
  (not always available in analytical closed-form)

- **Involution**: $(F^*)^* = F$ with $\nabla F^* = (\nabla F)^{-1}$.

- Convex conjugate $F^*$ expressed using $(\nabla F)^{-1}$:

\[
F^*(y) = \langle x, y \rangle - F(x), \quad x = \nabla_y F^*(y) \\
F^*(y) = \langle (\nabla F)^{-1}(y), y \rangle - F((\nabla F)^{-1}(y))
\]

- **Fenchel-Young inequality** at the heart of the canonical divergence:

\[
F(x) + F^*(y) \geq \langle x, y \rangle
\]

\[
A_F(x : y) = A_{F^*}(y : x) = F(x) + F^*(y) - \langle x, y \rangle \geq 0
\]
Parameters of exponential families

- $D$: order of the exponential family
- $d$: uni- ($d = 1$) or multi-variate family

Many parameterizations are possible but only two are canonical: natural parameters and expectation parameters.

Original parameters

\[ \lambda \in \Lambda \]

Exponential family
dual parameterization

\[ \theta \in \Theta \]

\[ \eta = \nabla_\theta F(\theta) \]

Natural parameters

\[ \theta = \nabla_\eta F^*(\eta) \]

Expectation parameters

Legendre transform

\[ (\Theta, F) \leftrightarrow (H, F^*) \]
Canonical decomposition of exponential families

\[ \langle \cdot, \cdot \rangle : \text{inner product on vectors (scalar product), matrices (ReTr}(AB^*)) \]

\( t(x) \) sufficient statistics, \( k(x) \) auxiliary carrier term:

\[
p(x; \theta) = \exp(\langle t(x), \theta \rangle - F(\theta) + k(x))
\]

Not unique decomposition because:

- natural parameter and sufficient statistic: \( t'(x) = At(x) \) and \( \theta' = A^{-1}\theta \) (for \( |A| \neq 0 \) affine transformation)
- constant in \( F'(\theta) = F(\theta) + c \) and \( k'(x) = k(x) - c \)

Let us give some decomposition examples…
Statistical mixtures: Rayleigh MMs [28]

IntraVascular UltraSound (IVUS) imaging:

Rayleigh distribution:

\[ p(x; \lambda) = \frac{x}{\lambda^2} e^{-\frac{x^2}{2\lambda^2}} \]

\( x \in \mathbb{R}^+ \)

\( d = 1 \) (univariate)

\( D = 1 \) (order 1)

\( \theta = -\frac{1}{2\lambda^2} \)

\( \Theta = (-\infty, 0) \)

\[ F(\theta) = -\log(-2\theta) \]

\[ t(x) = x^2 \]

\[ k(x) = \log x \]

(Weibull \( k = 2 \))

Coronary plaques: fibrotic tissues, calcified tissues, lipidic tissues

Rayleigh Mixture Models (RMMs):

for segmentation and classification tasks

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Statistical mixtures : Gaussian MMs [12, 28, 13]

Gaussian mixture models (GMMs) : model low frequency.
Color image interpreted as a 5D xyRGB point set.

Gaussian distribution $p(x; \mu, \Sigma)$:
\[
\frac{1}{(2\pi)^{d/2} \sqrt{\det \Sigma}} e^{-\frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu)}
\]

Squared Mahalanobis distance:
\[
D_Q(x, y) = (x - y)^T Q(x - y)
\]
\[x \in \mathbb{R}^d\]
d (multivariate)
\[
D = \frac{d(d+3)}{2} \text{ (order)}
\]
\[
\theta = (\Sigma^{-1}\mu, \frac{1}{2}\Sigma^{-1}) = (\theta_v, \theta_M)
\]
\[
\Theta = \mathbb{R} \times S^d_{++}
\]
\[
F(\theta) = \frac{1}{4} \theta_v^T \theta_M^{-1} \theta_v - \frac{1}{2} \log |\theta_M| + \frac{d}{2} \log \pi
\]
\[
t(x) = (x, -xx^T)
\]
\[
k(x) = 0
\]
MLE of exponential families: Two coordinate systems

\[ \eta = \mathbb{E}[t(x)] = \nabla F(\theta), \quad \theta = (\nabla F)^{-1}(\eta) = \nabla F^*(\eta) \]

**Closed-form in expectation parameter coordinate system** \( \eta \): 
\[ \hat{\eta} = \frac{1}{n} \sum_i t(x_i) \]

**Convex optimization in the natural parameter coordinate system** \( \theta \). 
\[ \max_{\theta} l(\theta; x_1, \ldots, x_n) = \frac{1}{n} \sum_i (\langle t(x_i), \theta \rangle - F(\theta)) \equiv \min_{\theta} F(\theta) - \langle \theta, \bar{t} \rangle \] (that is, \( \nabla F(\hat{\theta}) = \bar{t} \))
Exponential families: Universal families!

Universal representations of “smooth” densities:

- **mixtures** of exponential families approximate any smooth density (mixtures of Gaussians)
- a **single** exponential family (possibly multimodal) approximates also any smooth density: Similar to approximations of functions by polynomials. We can choose the sufficient statistics in \((1, x, x^2, x^3, \ldots)\) and \((\log x, \log^2 x, \log^3 x, \ldots)\). But then \(F(\theta)\) *not* in closed form:

\[
F(\theta) = \int_x \exp \left( \theta^\top t(x) + k(x) \right) \, d\nu(x)
\]

(common problem met in practice not to have closed-form expression of \(F\), Ising and Potts models, etc.)
Boltzmann-Gibbs distribution in statistical physics

Let $E(X; \theta)$ be an energy function.

$$p(X; \theta) = \frac{1}{Z(\theta)} \exp(-E(X; \theta))$$

$Z(\theta)$ normalization factor (aka. partition function) :

$$Z(\theta) = \int_x \exp(-E(X; \theta)) \, d\nu(x)$$

$$F(\theta) = \log Z(\theta)$$
The observed point \( \hat{P} \) in information geometry

- \( \{ P_\theta \}_\theta \) : a parametric (exponential family) model, \textbf{identifiable}  
- View \( P_\theta \) as a point on a manifold (dual coordinates \( \theta \) and \( \eta \))  
- Observed point \( \hat{P} \) with \( \eta \)-coordinate \( t(x) = \frac{1}{n} \sum_i t(x_i) \) (MLE)

\[
\hat{P}(\eta = \hat{\eta} = \frac{1}{n} \sum_i t(x_i))
\]

We shall see later that \( \hat{P} \) is \( m \)-projection of the empirical distribution on the e-flat...
MLE of exponential families [20]

- \( \hat{\eta} = \overline{t(x)} \) but we would like \( \hat{\theta} = (\nabla F^{-1})(\hat{\eta}) \)
- value of the maximum likelihood :
  \[
  l(\theta; x_1, \ldots, x_n) = F^*(\hat{\eta}) + \overline{k(x)}
  \]

\[
\overline{k(x)} = \frac{1}{n} \sum_{i=1}^{n} k(x_i)
\]
\( F^* \) is neg-entropy
- When \( F(\theta) \) not in closed-form : Contrastive Divergence (MCMC), score matching (Fisher divergence), etc.
II. Geometric structures of probability manifolds:

- $(M, g)$
- $(M, g, \nabla, \nabla^*) \iff (M, g, T)$
Population space & Parameter space


- $\mathcal{P} = \{p(x|\theta) \mid \theta \in \Theta\}$ a parametric family of distributions, the population space,
- $\Theta$, the parameter space of dimension $D$
- immersion $i(\theta) = p(x|\theta)$ from the parameter space to the population space:
  - $i$ : one-to-one (model identifiability)
  - $i$ of rank $\dim(\Theta) = D$:
    $$\frac{\partial p(x|\theta)}{\partial \theta_1}, \ldots, \frac{\partial p(x|\theta)}{\partial \theta_D}$$
    ... are linearly independent
- Geometric structures of SPD matrices when we consider the particular space $\{N(0, \Sigma) \mid \Sigma \succ 0\}$
Fisher information matrix (FIM)

- log-likelihood $l(\theta|x) = \log p(x|\theta)$, $\partial_i = \frac{\partial}{\partial \theta_i}$.
- Metric tensor, $D \times D$ matrix: $g = [g_{ij}] = \sum_{i,j} g_{ij} dx_i \otimes dx_j$ (tensor product)
  $$g_{ij} = \mathbb{E}_\theta[\partial_i l(\theta) \partial_j l(\theta)]$$
- FIM can be rewritten equivalently as:
  $$g_{ij} = 4 \int_x \partial_i \sqrt{p(x|\theta)} \partial_j \sqrt{p(x|\theta)} dx$$
- $g$ symmetric positive definite ( SPD), non-degenerate when $\{\partial_i p(x|\theta)\}_i$ are linear independent (problem with mixture models where $\exists \theta, l(\theta) = 0$)
Fisher information matrix & Hessian

Negative expectation of the Hessian of the log-likelihood function:

\[ g_{ij} = \mathbb{E}_\theta [\partial_i l(\theta) \partial_j l(\theta)] \]

\[ g_{ij} = 4 \int_x \partial_i \sqrt{p(x|\theta)} \partial_j \sqrt{p(x|\theta)} dx \]

\[ g_{ij} = \begin{cases} -\mathbb{E}_\theta [\partial_i \partial_j l(\theta)] \end{cases} \]

For natural exponential families \( p(x|\theta) = \exp(\langle \theta, x \rangle - F(\theta)) \),

\[ l(\theta) = \nabla^2 F(\theta) \succeq 0 \]
Fisher information: invariance and covariance

Invariant under reparameterization of the sample space: \( X \) RV. with \( p(x|\theta) \) and \( Y = f(X) \) for an invertible transformation \( f(\cdot) \) with density \( \bar{p}(y|\theta) \).

\[
g_{ij}(\theta) = \bar{g}_{ij}(\theta)
\]

Covariant under reparameterization of the parameter space: Let \( \eta = \eta(\theta) \) be an invertible transformation with \( \bar{p}_\eta(x) = p_{\eta(\theta)}(x) \)

\[
\bar{g}_{ij}(\eta) = g_{kr} \big|_{\eta=\eta(\theta)} \frac{\partial \theta_k}{\partial \eta_i} \frac{\partial \theta_r}{\partial \eta_j}
\]

sufficient statistics: \( p(x|t, \theta) = p(x|t) \), non-deterministic Markov morphism transformations (statistical invariance).
Basics of Riemannian geometry

- \((M, g)\) : Riemannian manifold
- \(\langle \cdot, \cdot \rangle\), Riemannian metric tensor \(g\) : definite positive bilinear form on each tangent space \(T_x M\) (depends smoothly on \(x\))
- \(\| \cdot \|_x : \|u\| = \langle u, u \rangle^{1/2} \) : Associated norm in \(T_x M\)
- \(\rho(x, y)\) : metric distance between two points on the manifold \(M\) (length space)

\[
\rho(x, y) = \inf \left\{ \int_0^1 \| \dot{\gamma}(t) \| \, dt, \quad \gamma \in C^1([0, 1], M), \quad \gamma(0) = x, \quad \gamma(1) = y \right\}
\]

- Shortest paths (length space)
- but technically parallel transport wrt. Levi-Civita metric connection \(\nabla_{LC}\).
Basics of Riemannian geometry: Exponential map

- Local map from the tangent space $T_x M$ to the manifold defined with geodesics (wrt $\nabla$).

\[ \forall x \in M, D(x) \subseteq T_x M : D(x) = \{ v \in T_x M : \gamma_v(1) \text{ is defined} \} \]

with $\gamma_v$ maximal (i.e., largest domain) geodesic with $\gamma_v(0) = x$ and $\gamma_v'(0) = v$.

- Exponential map:

\[
\exp_x(\cdot) : \quad D(x) \subseteq T_x M \rightarrow M \\
\exp_x(v) = \gamma_v(1)
\]

$D$ is star-shaped.
Riemannian geometry: Exponential and Logarithmic maps

\[ \exp : \, y \in M \rightarrow X_p \in T_p \]

\[ \log = \exp^{-1} : \, X_p \in T_p \rightarrow y \in M \]
Basics of Riemannian geometry: Geodesics

- **Geodesic**: smooth path which locally minimizes the distance between two points.

- Given a vector \( v \in T_x M \) with base point \( x \), there is a unique geodesic started at \( x \) with speed \( v \) at time 0: \( t \mapsto \exp_x(tv) \) or \( t \mapsto \gamma_t(v) \).

- Geodesic on \([a, b]\) is *minimal* if its length is less or equal to others. For complete \( M \) (i.e., \( \exp_x(v) \)), taking \( x, y \in M \), there exists a *minimal* geodesic from \( x \) to \( y \) in time 1.

\[ \gamma(x, y): [0, 1] \rightarrow M, \ t \mapsto \gamma_t(x, y) \] with the conditions \( \gamma_0(x, y) = x \) and \( \gamma_1(x, y) = y \).

- \( U \subseteq M \) is *convex* if for any \( x, y \in U \), there exists a unique minimal geodesic \( \gamma(x, y) \) in \( M \) from \( x \) to \( y \). Geodesic *fully lies* in \( U \) and depends smoothly on \( x, y, t \).
Basics of Riemannian geometry: Geodesics

- Geodesic $\gamma(x, y)$: locally minimizing curves linking $x$ to $y$
- Speed vector $\gamma'(t)$ parallel along $\gamma$:
  \[
  \frac{D\gamma'(t)}{dt} = \nabla_{\gamma'(t)}\gamma'(t) = 0
  \]

- When manifold $M$ embedded in $\mathbb{R}^d$, acceleration is normal to tangent plane:
  \[
  \gamma''(t) \perp T_{\gamma(t)}M
  \]

- $\|\gamma'(t)\| = c$, a constant (say, unit).

$\Rightarrow$ Parameterization of curves with constant speed (otherwise, you get the trace of the geodesic only...)
Basics of Riemannian geometry: Geodesics and means

Constant speed geodesic $\gamma(t)$ so that $\gamma(0) = x$ and $\gamma(\rho(x, y)) = y$ (constant speed 1, the unit of length).

\[ x \#_t y = m = \gamma(t) : \rho(x, m) = t \times \rho(x, y) \]

For example, in the Euclidean space:

\[ x \#_t y = (1 - t)x + ty = x + t(y - x) = m \]

\[ \rho_E(x, m) = \| t(y - x) \| = t \| y - x \| = t \times \rho(x, y), t \in [0, 1] \]

$\Rightarrow m$ interpreted as a mean (barycenter) between $x$ and $y$
Diffeomorphism from the tangent space to the manifold

- **Injectivity radius** $\text{inj}(M)$: largest $r > 0$ such that for all $x \in M$, the map $\exp_x(\cdot)$ restricted to the open ball in $T_x M$ with radius $r$ is an embedding.
- **Global injectivity radius**: infimum of the injectivity radius over all points of the manifold.

Important for navigating back and forth from $T_x M$ to $M$ (extrinsic/intrinsic computing)...

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Riemannian geometry of population spaces

- Consider \((M, g)\) with \(g = I(\theta)\), Hotelling (1930), Rao (1945). Fisher information matrix is unique up to a constant (for statistical invariance).
- Geometry of multinomials is **spherical** (on the orthant)
- For univariate location-scale families, **hyperbolic geometry** or **Euclidean geometry** (location only)

\[
p(x|\mu, \sigma) = \frac{1}{\sigma} p_0 \left( \frac{x - \mu}{\sigma} \right), \quad X = \mu + \sigma X_0
\]

(Normal, Cauchy, Laplace, Student \(t\)-, etc.)
Tangent planes, tangent bundles, vector fields

- $T_p$ : tangent plane at $p$
- $TM$, tangent bundle
- vector field = global section of the tangent bundle
- Mahalanobis metric distance on tangent planes $T_x$ :

\[
M_Q(p, q) = \sqrt{(p - q)^\top Q(x)(p - q)}
\]

axioms of the metric for $Q(x) = g(x) \succ 0$ (SPD).

- Rao’s distance between close points amounts to $\rho \simeq \sqrt{2KL} = \sqrt{SKL}$.
For exponential families, $\rho \simeq \text{Mahalanobis} = \sqrt{\Delta \theta^\top I(\theta) \Delta \theta}$. 
Tangent plane: basis vectors

- \((\partial_i)_x = \left(\frac{\partial}{\partial \theta^i}\right)_x\)
- \(X_x = \sum_{i=1}^{D} X^i(\partial_i)_x\)
- Define proper metric tensor: \(g_{ij}(x) = g_x(\partial_i, \partial_j) > 0\)
\( \alpha \)-representations and parameterizations of the tangent planes

\[
f_\alpha(u) = \begin{cases} \frac{2}{1-\alpha} u^{1-\alpha} / 2, & \alpha \neq 1 \\ \log u, & \alpha = 1. \end{cases}
\]

- \( \alpha = -1 \) : \( p(x|\theta) \rightarrow f_{-1}(p(x|\theta)) = p(x|\theta) \) : usual parameterization of the tangent plane \( T^{(-1)}_x M \) with basis \( \partial_i^{(-1)} = \partial_i \).

- \( \alpha = 0 \) : square root representation : \( p(x|\theta) \rightarrow f_0(p(x|\theta)) = 2\sqrt{p(x|\theta)} \).

- \( \alpha = 1 \) : logarithmic representation : \( p(x|\theta) \rightarrow f_1(p(x|\theta)) = \log p(x|\theta) \).

\[
\partial^{(1)} = \partial_i f_1(p(x|\theta)) = \frac{1}{p(x|\theta)} \partial_i p(x|\theta)
\]

Tangent planes are invariant objects : do not depend on the \( \alpha \)-representation.
Extrinsic Computational Geometry on tangent planes

- Tensor \( g = Q(x) \succ 0 \) defines smooth inner product
  \[
  \langle p, q \rangle_x = (p - q)^\top Q(x)(p - q)
  \]
  that induces a normed distance:
  \[
  d_x(p, q) = \|p - q\|_x = \sqrt{(p - q)^\top Q(x)(p - q)}
  \]

- Mahalanobis metric distance on tangent planes :
  \[
  \Delta_{\Sigma}(X_1, X_2) = \sqrt{(\mu_1 - \mu_2)^\top \Sigma^{-1}(\mu_1 - \mu_2)} = \sqrt{\Delta \mu^\top \Sigma^{-1} \Delta \mu}
  \]

- Cholesky decomposition \( \Sigma = LL^\top \), lower triangular matrix \( L \):
  \[
  \Delta(X_1, X_2) = D_E(L^{-1} \mu_1, L^{-1} \mu_2)
  \]

- Computing on tangent planes = Euclidean computing on transformed points \( x' \leftarrow L^{-1}x \).

\textit{Extrinsic vs intrinsic} computations.
Riemannian Mahalanobis metric tensor ($\Sigma^{-1}$, PSD)

\[
\rho(p_1, p_2) = \sqrt{(p_1 - p_2)^\top \Sigma^{-1} (p_1 - p_2)}, \quad g(p) = \Sigma^{-1} = \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix}
\]

non-conformal geometry : $g(p) \neq f(p)/l$
(Visualization with Tissot indicatrix)
Normal/Gaussian family and 2D location-scale families

- Fisher Information Matrix (FIM):

\[
I(\theta) = \begin{bmatrix}
I_{i,j}(\theta) = \mathbb{E}_{\theta} \left[ \frac{\partial}{\partial \theta_i} \log p(x|\theta) \frac{\partial}{\partial \theta_j} \log p(x|\theta) \right] \end{bmatrix} = \mathbb{E}_{\theta}[\partial_i I \partial_j I]
\]

- FIM for univariate normal/multivariate spherical distributions:

\[
I(\mu, \sigma) = \begin{bmatrix}
\frac{1}{\sigma^2} & 0 \\
0 & \frac{2}{\sigma^2}
\end{bmatrix} = \frac{1}{\sigma^2} \begin{bmatrix}
1 & 0 \\
0 & 2
\end{bmatrix}
\]

\[
I(\mu, \sigma) = \text{diag} \left( \frac{1}{\sigma^2}, \ldots, \frac{1}{\sigma^2}, \frac{2}{\sigma^2} \right)
\]

- Amount to Poincaré metric \( \frac{dx^2 + dy^2}{y^2} \), hyperbolic geometry in upper half plane/space.
Riemannian Poincaré upper plane metric tensor (conformal)

\[
\cosh \rho(p_1, p_2) = 1 + \frac{\|p_1 - p_2\|^2}{2y_1 y_2}, \quad g(p) = \begin{bmatrix}
\frac{1}{y^2} & 0 \\
0 & \frac{1}{y^2}
\end{bmatrix} = \frac{1}{y^2} I
\]

\[
\text{conformal : } g(p) = \frac{1}{y^2} I
\]
Matrix SPD spaces and hyperbolic geometry

Symmetric Positive Definite matrices $M : \forall x \neq 0, x^\top M x > 0.$

- 2D SPD(2) matrix space has dimension $d = 3$ : A positive cone.

$$\text{SPD}(2) \{ (a, b, c) \in \mathbb{R}^3 : a > 0, \quad ab - c^2 > 0 \}$$

- Can be peeled into sheets of dimension 2, each sheet corresponding to a constant value of the determinant of the elements

$$\text{SPD}(2) = \text{SSPD}(2) \times \mathbb{R}^+$$

where SSPD(2) = \{a, b, c = \sqrt{1 - ab}) : a > 0, ab - c^2 = 1\}

- Mapping $M(a, b, c) \to \mathbb{H}^2$ :
  - $(x_0 = \frac{a+b}{2} \geq 1, x_1 = \frac{a-b}{2}, x_2 = c)$ in hyperboloid model [39]
  - $z = \frac{a-b+2i c}{2+a+b}$ in Poincaré disk [39].
Riemannian Poincaré disk metric tensor (conformal)

→ often used in Human Computer Interfaces, network routing (embedding trees), etc.
Riemannian Klein disk metric tensor (non-conformal)

- recommended for “computing space” since geodesics are straight line segments
- Klein is also conformal at the origin (so we can perform translation from and back to the origin via Möbius transform.)
- Geodesics passing through $O$ in the Poincaré disk are straight (so we can perform translation from and back to the origin)
Riemannian geometry: Optimization on the manifold with the **natural gradient** [1]

Numerical optimization on manifolds:

- defined on a manifold, generalize Euclidean gradient
  \[ \nabla_x f(x) = (\frac{\partial}{\partial x_1} f(x), ..., \frac{\partial}{\partial x_D} f(x)) \] .
- natural gradient respects intrinsic geometry of the manifold:
  \[ \tilde{\nabla}_{\theta} f(\theta) = (I(\theta))^{-1} \times \nabla_{\theta} f(\theta) \]

(Euclidean geometry: \( I(\theta) = I \))

- invariant under changes of the parameterization (natural gradient = contravariant form of the gradient)
- Information-geometric optimization (IGO), black-box optimization
Jeffrey’s prior from volume element

- **Volume of the manifold:**

  $$v(M) = \int \sqrt{|g(\theta)|} d\theta < \infty$$

- **Consider the prior distribution:**

  $$q(\theta) = \frac{1}{v(M)} \sqrt{|g(\theta)|}$$

- Invariant under reparameterization

- Bayesian statistics (and other $\pm \alpha$-volume element in $|G : |g(\theta)|^{\frac{1+\alpha}{2}}$)
Affine differential geometry: dual connections $\nabla$ and $\nabla^*$ coupled with a metric $g$
Connections $\prod$ and covariant derivatives $\nabla$

- Connections $\prod$ set correspondences between vectors in tangent spaces $T_p$ and $T_q$. When manifold $M$ is embedded in $\mathbb{R}^d$, there exists a natural correspondence. Otherwise, connections $\prod$ need to be formally defined.

- Covariant derivatives $\nabla$: differentiation of a vector field $Y$ in the direction of another vector field $X$, yielding a vector field $Z = \nabla_X Y$.

- Connections and covariant derivatives induce the same geometric structure. Yield notions of geodesics, flatness/curvature, parallelness, torsion.

- Riemannian structure $(M, g)$ has an induced metric connection $\nabla_g = \nabla_{\text{LC}} = \nabla^{(0)}$, called the Levi-Civita connection.
Connections and parallel transport

- $\prod_{p,q}$ a connection from $T_p$ to $T_q$

$$\prod_{p,q} : T_p \to T_q$$

so that $v \in T_p$ yields $w = \prod_{p,q}(v) \in T_q$

- from linear isomorphism between tangent spaces of neighboring points to tangent points between arbitrary points by integrating along a curve $\gamma_{p,q}$ connecting $p$ with $q$. 

- $d^3$ coefficients $\Gamma_{ijk}(p)$ required for defining $\prod$.

- Vector field $X$ along $\gamma$ with $X(t + dt) = \prod_{\gamma(t),\gamma(t+dt)} X(t)$. We say vector fields $\{X(t) \mid t\}$ along $\gamma$ are \underline{parallel} with respect to the connection $\prod$. Parallel transport.
Covariant derivatives $\nabla$

$\nabla$ : differentiation of a vector field $Y$ in the direction of another vector field $X$, yielding a vector field $Z = \nabla_X Y$.

$$\nabla : V(M) \times V(M) \rightarrow V(M)$$

Properties $\nabla$ should have:

$$\nabla_{f_1 X_1 + f_2 X_2} Y = f_1 \nabla_{X_1} Y + f_2 \nabla_{X_2} Y$$
$$\nabla_X (Y_1 + Y_2) = \nabla_X Y_1 + \nabla_X Y_2$$
$$\nabla_X (fY) = f \nabla_X Y + (Xf) Y$$

Linear combinations of covariant derivatives is a covariant derivative
Vector field parallel to a curve

Vector field $Y \in V(M)$ is $\nabla$-parallel to a curve $\gamma(t)$:

$$\forall t, \forall X \in V(M), \quad \nabla_{\dot{\gamma}(t)} Y = 0$$
Curves $\gamma$ on $(M, \nabla)$ such that

$$\forall t, \quad \nabla_{\dot{\gamma}(t)} \dot{\gamma}(t) = 0$$
Affine coordinate system and flat connection

In general, specify a connection/covariant $\nabla$ by $D^3$ coefficients:

$$\nabla \partial_i \partial_j = \Gamma^k_{ij} \partial_k, \quad \forall i, j, k \in \{1, \ldots, D\}$$

$(M, \nabla)$, $\theta$ a coordinate system.

$\theta$ is an affine coordinate system iff:

- Vector fields $\{\partial_i = \frac{\partial}{\partial \theta_i}\}$ are parallel in $M$
- Equivalent to $\forall i, j, \quad \nabla \partial_i \partial_j = 0$
- Equivalent to $\forall i, j, k, \quad \Gamma^k_{ij} = 0$ (Christoffel symbols)

When there exists an affine coordinate system for $(M, \nabla)$, we say that $M$ is flat.
Metric connection : Special case of Levi-Civita connection
\( \nabla_{LC} = \nabla^{(0)} \)

Given \((M, g)\), there exists a unique metric connection, the Levi-Civita connection:

- \( \Gamma_{ij}^k = \frac{\partial_i g_{jk} + \partial_j g_{ki} - \partial_k g_{ij}}{2} \)
- and we have \( g(\nabla_{\partial_i}^{(0)} \partial_j, \partial_k) = \Gamma_{ij}^k \).
- Parallel transport of tangent vectors preserves the inner product.
- Therefore angles are kept, henceforth “parallel transport”
Autoparallel submanifold

$N \subset M$ of $(M, N)$ is autoparallel:

- Property on the tangent bundle $TN$

\[
\forall X, Y \in TN, \quad \nabla_X Y \in TN
\]

- Parallel ($\nabla$)-transport of tangent vectors for $N$ are tangent vectors of $N$.

- Notion of “hyperplanes” in differential geometry

- For an affine connection with coordinate system $\theta$, equivalent to an affine subspace of $\theta \in \mathbb{R}^D$. 

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Differential-geometric structures: Summary

- **Manifold** $M$
  - **Riemannian manifold**
    - metric tensor $g$ (inner product)
      - (angle, orthogonality)
      - $(M, g)$
  - **connection** $\Pi$, $\nabla$
    - *covariant derivatives* $\nabla$
      - $\Pi \Leftrightarrow \nabla$
      - parallel transport
        - (flatness, autoparallel)
        - $(M, \nabla)$

**Differential structure** $(M, g, \nabla)$

- **Levi-Civita connection**
  - $\nabla_{\text{LC}} = \nabla(g)$ (coefficients $\Gamma^k_{ij}$)
  - geodesics preserves $\langle \cdot, \cdot \rangle$
  - $\rho(P, Q)$ metric distance
    - (shortest paths)

- **Dual connections** $(M, g, \nabla, \nabla^*)$
Dually affine connections

- Two affine connections $\Pi$ and $\Pi^*$ (and covariant derivatives $\nabla$ and $\nabla^*$)
- Property of inner product:

\[
\langle X, Y \rangle_g = \langle \Pi X, \Pi^* Y \rangle_g
\]

- Riemannian geometry: $\Pi = \Pi^*$
Dually affine connections: $e$-connection and $m$-connection

Exponential $e$-geodesics and mixture $m$-geodesics for probability densities:

\[
\gamma_m(p, q, \alpha) : \ r(x, \alpha) = \alpha p(x) + (1 - \alpha) q(x)
\]
\[
\gamma_e(p, q, \alpha) : \ \log r(x, \alpha) = \alpha p(x) + (1 - \alpha) q(x) - F(t)
\]

\[
\nabla^{(e)} \gamma_e(t) = 0, \quad \nabla^{(m)} \gamma_m(t) = 0
\]

Flat but not Riemannian flat: $e$-flat and $m$-flat.
Dually $\alpha$-affine connections

$\alpha \in \mathbb{R}$,

$$\nabla^{(\alpha)} = \frac{1 + \alpha}{2} \nabla + \frac{1 - \alpha}{2} \nabla^*$$

- $\nabla = \nabla^e$ or $\nabla^m$
- Dually-coupled affine connections: $\nabla^{(\alpha)}$ and $\nabla^{(-\alpha)}$
- $\alpha = 0 : \nabla^{(0)} = \frac{\nabla + \nabla^*}{2} = \nabla_{\text{LC}}$, Levi-Civita metric connection (self-dual $\nabla^{(0)} = \nabla^{(0)*}$)
- 0-geometry is Riemannian geometry (often curved but not for isotropic Gaussians)
Dually flat orthogonal coordinate systems

- \( \theta \)- and \( \eta \)-coordinate systems
- partial derivatives: \( \partial_i = \frac{\partial}{\partial \theta_i}, \partial^i = \frac{\partial}{\partial \eta^i} \)
- \( \langle \partial_i, \partial^j \rangle = \delta_{ij} \) (biorthogonal coordinate systems)
- metric-coupled connection:

\[
X\langle Y, Z \rangle = \langle \nabla_X Y, Z \rangle + \langle Y, \nabla^*_X Z \rangle
\]

- \( \Gamma_{ijk}(\theta) = \Gamma^*_{ijk}(\eta) = 0 \)

This is key advantage over the Riemannian \( (\nabla_{LC}) \) structure: Geodesics are known in closed form with the affine coordinate systems. Line segments in either the \( \theta \)- or \( \eta \)-coordinate systems.
Dually flat manifolds from a convex function $F$

Canonical geometry induced by strictly convex and differentiable convex function $F$.

- **Potential functions**: $F$ and Legendre convex conjugate $G = F^*$
- **Dual coordinate systems**: $\theta = \nabla F^*(\eta)$ and $\eta = \nabla F(\theta)$.
- **Metric tensor $g$**: written equivalently using the two coordinate systems:

\[
g_{ij}(\theta) = \frac{\partial^2}{\partial \theta_i \partial \theta_j} F(\theta), \quad g^{ij}(\eta) = \frac{\partial^2}{\partial \eta_i \partial \eta_j} G(\eta)
\]

- **Divergence from Young’s inequality of convex conjugates**:

\[
D(P : Q) = F(\theta(P)) + F^*(\eta(Q)) - \langle \theta(P), \eta(Q) \rangle
\]

This is a Bregman divergence in disguise - :) ...

- **exponential family**: $p(x|\theta) = \exp(\langle \theta, x \rangle - F(\theta))$
- **Terminology**: $F = \text{cumulant function}$, $G = \text{negative entropy}$
Geometry induced from a potential function

$F$ a strictly convex potential function

$$
g_{ij} = \frac{\partial^2 F}{\partial i \partial j}
$$

$$
\Gamma_{ijk}^{(\alpha)} = \frac{1 - \alpha}{2} \frac{\partial^3 F}{\partial i \partial j \partial k}
$$

Dually coupled $\pm \alpha$-connections (affine torsion-free, Kurose [16], 1994):

$$
\forall X, Y, Z \in V(M), \quad Xg(Y, Z) = g(\nabla_X^{(\alpha)} Y, Z) + g(Y, \nabla_X^{(\alpha)} Z)
$$

Curvature : $\kappa = \frac{1 - \alpha^2}{4}$ (and hence $\alpha = \pm 1 \Leftrightarrow \kappa = 0$, flat)
Bregman divergences: An old friend from the optimization community
Bregman divergences

\[ D_F(p : q) = F(p) - F(q) - \langle p - q, \nabla F(q) \rangle \]

includes...

- squared Euclidean distance: \( F(x) = \langle x, x \rangle \), and squared Mahalanobis \( F(x) = x^\top Qx \) (only symmetric divergences)
- (extended) Kullback-Leibler divergence: \( F(x) = \sum_i x_i \log x_i - x_i \) (Shannon information),

\[ eKL(p : q) = \sum_i \left( p_i \log \frac{p_i}{q_i} + q_i - p_i \right) \]

- \( F(x) = - \sum_i \log x_i \) (Burg information), Itakura-Saito divergence:

\[ IS(p : q) = \sum_i \left( \frac{p_i}{q_i} - \log \frac{p_i}{q_i} - 1 \right) \]

- and many others!
Bregman divergence: Geometric interpretation (I)

Potential function $F$, graph plot $\mathcal{F} : (x, F(x))$.

$$D_F(p : q) = F(p) - F(q) - \langle p - q, \nabla F(q) \rangle$$
Bregman divergence: Geometric interpretation (II)

Potential function $f$, graph plot $\mathcal{F} : (x, f(x))$.

$$B_f(p\|q) = f(p) - f(q) - (p - q)f'(q)$$

$B_f(.\|q)$: vertical distance between the hyperplane $H_q$ tangent to $\mathcal{F}$ at lifted point $\hat{q}$, and the translated hyperplane at $\hat{p}$. 
Bregman divergence: Geometric interpretation (III)

Bregman divergence and path integrals

\[ B(\theta_1 : \theta_2) = F(\theta_1) - F(\theta_2) - \langle \theta_1 - \theta_2, \nabla F(\theta_2) \rangle, \]  

\[ = \int_{\theta_2}^{\theta_1} \langle \nabla F(t) - \nabla F(\theta_2), dt \rangle, \]  

\[ = \int_{\eta_1}^{\eta_2} \langle \nabla F^*(t) - \nabla F^*(\eta_1), dt \rangle, \]  

\[ = B^*(\eta_2 : \eta_1) \]
Dual Bregman divergences & canonical divergence [34]

For $P$ and $Q$ belonging to the same exponential families

$$\text{KL}(P : Q) = E_P \left[ \log \frac{p(x)}{q(x)} \right] \geq 0$$

$$= B_F(\theta_Q : \theta_P) = B_{F^*}(\eta_P : \eta_Q)$$

$$= F(\theta_Q) + F^*(\eta_P) - \langle \theta_Q, \eta_P \rangle$$

$$= A_F(\theta_Q : \eta_P) = A_{F^*}(\eta_P : \theta_Q)$$

with $\theta_Q$ (natural parameterization) and $\eta_P = E_P[t(X)] = \nabla F(\theta_P)$ (moment parameterization).

$$\text{KL}(P : Q) = \int p(x) \log \frac{1}{q(x)} \, dx - \int p(x) \log \frac{1}{p(x)} \, dx$$

$$H^\times(P : Q) = H^\times(P : P)$$

Shannon cross-entropy and entropy of EF [34] :

$$H^\times(P : Q) = F(\theta_Q) - \langle \theta_Q, \nabla F(\theta_P) \rangle - E_P[k(x)]$$

$$H(P) = F(\theta_P) - \langle \theta_P, \nabla F(\theta_P) \rangle - E_P[k(x)]$$

$$H(P) = -F^*(\eta_P) - E_P[k(x)]$$
III. Principle of Maximum Entropy (MaxEnt)
Maximum entropy (MaxEnt)

Underconstrained optimization problem (Jaynes’s principle for maximum ignorance):

\[
\max_p H(p) = \sum_x p(x) \log \frac{1}{p(x)}
\]

\[
\sum_x p(x) t_i(x) = m_i, \quad \forall i \in \{1, \ldots, D\}
\]

\[
p(x) \geq 0, \quad \forall x \in \{1, \ldots, n\}
\]

\[
\sum_x p(x) = 1
\]

- Maximizing a concave function \((H)\) subject to linear constraints
- Convex optimization problem.
A more general setting for MaxEnt

Given a prior \( q \), find the closest distribution which satisfies the linear constraints:

\[
\min_p \text{KL}(p : q) = \sum_x p(x) \log \frac{p(x)}{q(x)}
\]

\[
\sum_x p(x) t_i(x) = m_i, \quad \forall i \in \{1, ..., D\}
\]

\[
p(x) \geq 0, \quad \forall x \in \{1, ..., n\}
\]

\[
\sum_x p(x) = 1
\]

→ Maximum entropy when \( q = \frac{1}{n} \), the uniform prior
An illustration...

$\text{prior } q$

$e$-projection

affine subspace induced by constraints

\[ p^* = \min_p \text{KL}(p : q) \quad \text{m-flat} \]
Analytic solution: exponential families!

Using Lagrange multipliers $\theta$ with $t(x) = (t_1(x), \ldots, t_D(x))$:

$$p(x) = \frac{1}{Z(\theta)} \exp(\langle \theta, t(x) \rangle) q(x)$$

... but Lagrange multipliers usually not in explicit form.

- Canonical exponential families: $\exp(\langle \theta, t(x) \rangle - F(\theta) + k(x))$
- Prior $q$ gives the carrier measure $q(x) = e^{k(x)}$
- $Z(\theta)$ is the normalizer
- called Gibbs distribution, Maxwell-Boltzmann distribution in statistical mechanics
A toy example for MaxEnt

- A distribution $p$ with support $\mathbb{R}$ has $\mathbb{E}[X] = 3$ and $\mathbb{E}[X^2] = 25$. Which distribution should we choose for $p$?
- $t(x) = (x, x^2)$ defines the univariate Gaussian family of distributions.
- So we choose $p \sim N(\mu = 3, \sigma = 5)$

in general not so easy if we are given $E[X^k]$ for $k \geq 2$... uniqueness but no closed form...
Another insightful proof

Any other distribution \( p \neq p^* \) satisfying the constraints is such that 
\( \text{KL}(p : q) > \text{KL}(p^* : q) \).
Consider the difference \( \text{KL}(p : q) - \text{KL}(p^* : q) : \)

\[
\begin{align*}
= & \sum_x p(x) \log \frac{p(x)}{q(x)} - \sum_x p^*(x) \log \frac{p^*(x)}{q(x)} \\
= & \sum_x p(x) \log \frac{p(x)}{q(x)} - \sum_x p(x) \log \frac{p^*(x)}{q(x)} \\
= & \sum_x p(x) \log \frac{p(x)}{p^*(x)} = \text{KL}(p : p^*) > 0
\end{align*}
\]

Pythagorean relation: \( \text{KL}(p : q) = \text{KL}(p : p^*) + \text{KL}(p^* : q) \)
An illustration of MaxEnt with prior \( q(x) \)...

\[
KL(p : q) = KL(p : p^*) + KL(p^* : q)
\]

\( p^* = \min_p KL(p : q) \)

affine subspace induced by constraints

e-projection

\[ KL(p^* : q) \]

prior \( q \)

\[ KL(p : q) \]

\[ KL(p : p^*) \]

\( m \)-geodesic

\( p \)

\( m \)-flat
Computing information projections easily

- Project the prior $q$ onto $A = \{ p \mid \mathbb{E}_p[t_i(x)] = m_i, \forall i \in \{1, ..., D\} \}$. Let $A_i = \{ p \mid \mathbb{E}_p[t_i(x)] = m_i \}$
- Let $t = 0$ and $p_0 = q$
- Repeat until convergence (within a threshold):
  $$p_{t+1} = \text{l-projection of } p_t \text{ onto } L_t \mod D$$
- 1D projection easy: Find $\theta_i$ such that $F_{\neq i}(\theta_i) = m_i$ (for example, using line search)
Cyclic (line search) 1D information projections
IV. Information projection
Projections: $e$-projection and $m$-projection

\[
\nabla^{(e)} = \nabla^{(1)}, \quad \nabla^{(m)} = \nabla^{(-1)}
\]

- **$e$-projection** $q$ is **unique** if $M \subseteq S$ is $m$-flat and minimizes the $m$-divergence $\text{KL}(q : p)$.

- **$m$-projection** $q$ is **unique** if $M \subseteq S$ is $e$-flat and minimizes the $e$-divergence $\text{KL}(p : q)$.

$\text{KL}$ and reverse $\text{KL}$ are $\alpha$-divergences for $\alpha = \pm 1$...
MLE as min KL : Information projection

- Empirical distribution: \( p_e(x) = \frac{1}{n} \sum_i \delta(x - x_i) \).
- \( p_e \) is absolutely continuous with respect to \( p_\theta(x) \)

\[
\min\text{KL}(p_e(x) : p_\theta(x)) = \int p_e(x) \log p_e(x) \, dx - \int p_e(x) \log p_\theta(x) \, dx
\]

\[
= \min -H(p_e) - E_{p_e}[\log p_\theta(x)]
\]

\[
\equiv \max \frac{1}{n} \sum \delta(x - x_i) \log p_\theta(x)
\]

\[
= \max \frac{1}{n} \sum_i \log p_\theta(x_i) = \boxed{\text{MLE}}
\]
Log-likelihood function

\[ l(\theta; X) = \frac{1}{n} \sum_{i=1}^{n} \log p(x_i|\theta) = \langle \log p(x|\theta) \rangle_{p_e} \]

Empirical distribution: \( p_e(X) = \frac{1}{n} \sum_{i=1}^{n} \delta(X - X(i)) \)

MLE = \textit{m-projection from} \( p_e \) \textit{to the model submanifold}
Nested and curved exponential families

\( \mathcal{P}(\theta) \) an exponential family

- **nested EFs**: Fix some parameters \( \theta = (\theta_{\text{fixed}}, \theta_{\text{variable}}) \). Then \( \mathcal{P}_{\theta_{\text{fixed}}} (\theta_{\text{variable}}) \) is a nested exponential family. Get stratified EFs with uni-order EF easy to handle algorithmically (Legendre)

- **curved EFs**: \( C(\gamma) \subseteq \mathcal{P}(\theta) \) embedded in \( \mathcal{P}(\theta) \). Example: \( \{N(\mu, \mu^2) \mid \mu \in \mathbb{R}\} \) is embedded into \( \{N(\mu, \sigma^2)\} \).
MLE for curved exponential families

Entropy $H(\theta) = -E_\theta[\log p(x|\theta)] = F(\theta) - \langle \theta, \nabla F(\theta) \rangle = -F^*(\eta)$ (when $k(x) = 0$, otherwise add $-E[k(x)]$).

$$D(p(\hat{\eta}) : p(\gamma)) = -H(\hat{\eta}) - \frac{1}{n} \log L(\gamma)$$

$$\max_{\gamma} L(\gamma) \equiv \min_{\gamma} D(p(\hat{\eta}) : p(\gamma))$$

$\hat{\gamma}$ is the $m$-projection of the observation point (with $\eta$-coordinate $\hat{\eta}$)
Illustration: MLE for curved exponential families

MLE observed point
$(\hat{\eta} = \frac{1}{n} \sum_{i=1}^{n} t(x_i))$ m-projection
$
\hat{\gamma} = \min_{\gamma} KL(p(\hat{\eta}) : p(\gamma))$

curved exponential family
information loss, statistical curvature.
Simplifying a mixture model into a single component \cite{48}

$m$-projection of the mixture model $m$ onto the e-flat (exponential family manifold) : Best single distribution that approximates an exponential family mixture is found by taking the center of mass of the moment parameters : $$\bar{\eta} = \sum_i w_i \eta_i.$$
Kullback-Leibler divergence and Fisher information

$$\text{KL}(\theta + \Delta \theta : \theta) \approx \frac{1}{2} \theta^\top I(\theta) \theta$$

... square Mahalanobis induced locally by half squared Mahalanobis distance for the Fisher information matrix.

$$g_{ij}(\theta_0) = \left. \frac{\partial^2}{\partial \theta_i \partial \theta_j} \right|_{\theta = \theta_0} \text{KL}(P(\theta) \| P(\theta_0))$$

This holds for $f$-divergences $\int p(x) f\left(\frac{q(x)}{p(x)}\right) d\nu(x)$ (that includes Kullback-Leibler divergence) : divergence inducing a metric proportional to Fisher information (Part II).
Additive Shannon/Rényi versus non-additive Tsallis entropies

- additive (Shannon-Rényi)

\[ H(P \times Q) = H(P) + H(Q) \]

- non-additive (Tsallis) \( T_q(X) = \frac{1}{q-1}(1 - \sum_i p_i^q) \)

\[ T_q(X \times Y) = T_q(X) + T_q(Y) + (1 - q) T_q(X) T_q(Y) \]

- Both can be unified with Sharma-Mittal [37] 2-parameter family of entropies

- Sharma-Mittal entropies, cross-entropies and relative entropies are known in closed-form for exponential families.
Part I : Summary

- Fisher information (Cramér-Rao lower bound) & sufficiency (1922)
- Differential geometry of population spaces:
  - Fisher-Rao geometry (Hotelling, 1930): $g(\theta) = I(\theta)$
  - Dually-coupled connection geometry (1970’s-1980’s, Cencov, Amari, Kurose): $(M, g, \nabla^{(\alpha)}, \nabla^{(-\alpha)})$, or $(M, g, T)$
  - Dually-flat manifold from a potential function $F$ and canonical divergence (=Bregman divergence).
- Exhaustivity: Bregman divergences=canonical divergences in dually flat spaces
- Maximum entropy principle (Shannon entropy & exponential families)
- Information-geometric projections: MLE from empirical distribution, MLE in curved exponential families, and in mixture simplification.
Part II: Algorithms & Space of spheres
Brief historical review of Computational Geometry (CG)

- **Three research periods**:
  1. **Geometric algorithms**:
     Voronoi/Delaunay, minimum spanning trees, data-structures for proximity queries
  2. **Geometric computing**:
     robustness, algebraic degree of predicates, programs that work/scale!
  3. **Computational topology** (global geometry):
     simplicial complexes, filtrations, input=distance matrix
     → paradigm of Topological Data Analysis (TDA)

- **Showcasing libraries for CG software**:
  - CGAL [http://www.cgal.org/]
  - Geometry Factory [http://geometryfactory.com/]
  - Gudhi [https://project.inria.fr/gudhi/]
  - Ayasdi [http://www.ayasdi.com/]

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Basics of Euclidean Computational Geometry: Voronoi diagrams and dual Delaunay complexes
Euclidean (ordinary) Voronoi diagrams

\[ \mathcal{P} = \{ P_1, \ldots, P_n \} : n \text{ distinct point generators in Euclidean space } \mathbb{E}^d \]

\[ V(P_i) = \{ X : D_E(P_i, X) \leq D_E(P_j, X), \forall j \neq i \} \]

Voronoi diagram = cell complex \( V(P_i)'s \) with their faces
Voronoi diagrams from bisectors and \( \cap \) halfspaces

**Bisectors**

\[
\text{Bi}(P, Q) = \{ X : D_E(P, X) = D_E(Q, X) \}
\]

→ are **hyperplanes** in Euclidean geometry

Voronoi cells as halfspace intersections:

\[
V(P_i) = \{ X : D_E(P_i, X) \leq D_E(P_j, X), \; \forall j \neq i \} = \cap_{i=1}^{n} \text{Bi}^{+}(P_i, P_j)
\]

\[
D_E(P, Q) = \|\theta(P) - \theta(Q)\|_2 = \sqrt{\sum_{i=1}^{d}(\theta_i(P) - \theta_i(Q))^2}
\]

\( \theta(P) = p \): **Cartesian coordinate system** with \( \theta_j(P_i) = p_i^{(j)} \).

⇒ Many applications of Voronoï diagrams: crystal growth, codebook/quantization, molecule interfaces/docking, motion planning, etc.
Voronoi diagrams and **dual** Delaunay simplicial complex

- **Empty sphere** property, **max min angle** triangulation, etc
- Voronoi & dual **Delaunay** triangulation
  - → non-degenerate point set = no \((d + 2)\) points co-spherical
- Duality: **Voronoi** \(k\)-face \(\Leftrightarrow\) **Delaunay** \((d - k)\)-simplex
- Bisector \(\text{Bi}(P, Q)\) **perpendicular** \(\perp\) to segment \([PQ]\)
Voronoi & Delaunay: Complexity and algorithms

- Combinatorial complexity: $\Theta(n^{\lceil d/2 \rceil})$ (→ quadratic in 3D) matched for points on the moment curve: $t \mapsto (t, t^2, \ldots, t^d)$
- Construction: $\Theta(n \log n + n^{\lceil d/2 \rceil})$, optimal
- Some output-sensitive algorithms but...
- $\Omega(n \log n + f)$, not yet optimal output-sensitive algorithms.
Birth of differential-geometric methods in statistics.

- Fisher information matrix (non-degenerate positive definite) can be used as a (smooth) Riemannian metric tensor $g$.
- Distance between two populations indexed by $\theta_1$ and $\theta_2$ : Riemannian distance (metric length)

First applications in statistics :

- Fisher-Hotelling-Rao (FHR) geodesic distance used in classification :
  Find the closest population to a given set of populations
- Used in tests of significance (null versus alternative hypothesis), power of a test : $\mathbb{P}(\text{reject } H_0 | H_0 \text{ is false})$
  $\rightarrow$ define surfaces in population spaces
Rao’s distance (1945, introduced by Hotelling 1930 [15])

- Infinitesimal squared length element:

\[
\begin{align*}
\text{ds}^2 &= \sum_{i,j} g_{ij}(\theta) \text{d}\theta_i \text{d}\theta_j = \text{d}\theta^T I(\theta) \text{d}\theta \\
\end{align*}
\]

- Geodesic and distance are hard to explicitly calculate:

\[
\begin{align*}
\rho(p(x; \theta_1), p(x; \theta_2)) &= \min_{\theta(s)} \int_0^1 \sqrt{\left(\frac{\text{d}\theta}{\text{d}s}\right)^T I(\theta) \frac{\text{d}\theta}{\text{d}s}} \text{d}s \\
\theta(0) &= \theta_1 \\
\theta(1) &= \theta_2
\end{align*}
\]

Rao’s distance not known in closed-form for multivariate normals

- Advantages: Metric property of \(\rho\) + many tools of differential geometry [3]: Riemannian Log/Exp tangent/manifold mapping
Extrinsic Computational Geometry on tangent planes

- Tensor $g = Q(x) > 0$ defines smooth inner product
  \[ \langle p, q \rangle_x = (p - q)^\top Q(x)(p - q) \] that induces a normed distance:
  \[ d_x(p, q) = \|p - q\|_x = \sqrt{(p - q)^\top Q(x)(p - q)} \]

- Mahalanobis metric distance on tangent planes:
  \[
  \Delta_{\Sigma}(X_1, X_2) = \sqrt{(\mu_1 - \mu_2)^\top \Sigma^{-1}(\mu_1 - \mu_2)} = \sqrt{\Delta\mu^\top \Sigma^{-1} \Delta\mu}
  \]

- Cholesky decomposition $\Sigma = LL^\top$
  \[
  \Delta(X_1, X_2) = D_E(L^{-1}\mu_1, L^{-1}\mu_2)
  \]

- CG on tangent planes = ordinary CG on transformed points $x' \leftarrow L^{-1}x$. Extrinsic vs intrinsic means [11]
Mahalanobis Voronoi diagrams on tangent planes (extrinsic)

In statistics, covariance matrix $\Sigma$ account for both correlation and dimension (feature) scaling

Dual structure $\equiv$ anisotropic Delaunay triangulation
$\Rightarrow$ ”empty circumellipse” property (Cholesky decomposition)
Riemannian manifolds: Choice of equivalent models?

Many equivalent models of hyperbolic geometry:

- **Conformal** (good for visualization since we can measure angles) versus non-conformal (computationally-friendly for geodesics) models.
- Convert *equivalently* to other models of hyperbolic geometry: Poincaré disk, upper half space, hyperboloid, Beltrami hemisphere, etc.
Riemannian Poincaré disk metric tensor (conformal)

→ often used in Human Computer Interfaces, network routing (embedding trees), etc.
Riemannian Klein disk metric tensor (non-conformal)

- recommended for “computing space” since geodesics are straight line segments
- Klein is also **conformal at the origin** (so we can perform translation from and back to the origin)
- Geodesics passing through $O$ in the Poincaré disk are straight (so we can perform translation from and back to the origin)
Hyperbolic Voronoi diagrams [35, 40]

In arbitrary dimension, $\mathbb{H}^d$

- In Klein disk, the hyperbolic Voronoi diagram amounts to a clipped affine Voronoi diagram, or a clipped power diagram with efficient clipping algorithm [6].
- then convert to other models of hyperbolic geometry: Poincaré disk, upper half space, hyperboloid, Beltrami hemisphere, etc.
- **Conformal** (good for visualization) versus **non-conformal** (good for computing) models.
Hyperbolic Voronoi diagrams [35, 40]

Hyperbolic Voronoi diagram in Klein disk = clipped power diagram.
Power distance:

\[ \|x - p\|^2 - w_p \]

→ additively weighted ordinary Voronoi = ordinary CG
Hyperbolic Voronoi diagrams [35, 40]

5 common models of the abstract hyperbolic geometry

https://www.youtube.com/watch?v=i9IUzNxeH4o (5 min. video)
ACM Symposium on Computational Geometry (SoCG’14)
Voronoï diagrams in dually affine information geometry
Dually flat space construction from convex functions $F$

- Convex and strictly differentiable function $F(\theta)$ admits a Legendre-Fenchel convex conjugate $F^*(\eta)$:

$$F^*(\eta) = \sup_{\theta}(\theta^\top \eta - F(\theta)), \quad \nabla F(\theta) = \eta = (\nabla F^*)^{-1}(\theta)$$

- Young’s inequality gives rise to canonical divergence [19]:

$$F(\theta) + F^*(\eta') \geq \theta^\top \eta' \Rightarrow A_{F,F^*}(\theta,\eta') = F(\theta) + F^*(\eta') - \theta^\top \eta'$$

- Writing using single coordinate system, get dual Bregman divergences:

$$B_F(\theta_p : \theta_q) = F(\theta_p) - F(\theta_q) - (\theta_p - \theta_q)^\top \nabla F(\theta_q) = B_{F^*}(\eta_q : \eta_p) = A_{F,F^*}(\theta_p,\eta_q) = A_{F^*,F}(\eta_q : \theta_p)$$

- Dual affine coordinate systems with geodesics “straight”:

$$\eta = \nabla F(\theta) \iff \theta = \nabla F^*(\eta). \quad \text{Tensor} \quad g(\theta) = g^*(\eta)$$
Dual divergence/Bregman dual bisectors \([7, 32, 36]\)

Bregman sided (reference) bisectors related by convex duality:

\[
\begin{align*}
\text{Bi}_F(\theta_1, \theta_2) &= \{ \theta \in \Theta \mid B_F(\theta : \theta_1) = B_F(\theta : \theta_1) \} \\
\text{Bi}_{F^*}(\eta_1, \eta_2) &= \{ \eta \in H \mid B_{F^*}(\eta : \eta_1) = B_{F^*}(\eta : \eta_1) \}
\end{align*}
\]

**Right-sided bisector**: \(\rightarrow \theta\)-hyperplane, \(\eta\)-hypersurface

\[
H_F(p, q) = \{ x \in X \mid B_F(x : [p]) = B_F(x : [q]) \}.
\]

\[
H_F : \langle \nabla F(p) - \nabla F(q), x \rangle + (F(p) - F(q) + \langle q, \nabla F(q) \rangle - \langle p, \nabla F(p) \rangle) = 0
\]

**Left-sided bisector**: \(\rightarrow \theta\)-hypersurface, \(\eta\)-hyperplane

\[
H_F'(p, q) = \{ x \in X \mid B_F([p] : x) = B_F([q] : x) \}
\]

\[
H_F' : \langle \nabla F(x), q - p \rangle + F(p) - F(q) = 0
\]

**hyperplane = autoparallel submanifold of dimension** \(d - 1\)
Visualizing Bregman bisectors in $\theta$- and $\eta$-coordinate systems

Primal coordinates $\theta$
natural parameters

Dual coordinates $\eta$
expectation parameters

$\text{Bi}(P, Q)$ and $\text{Bi}^*(P, Q)$ can be expressed in either $\theta/\eta$ coordinate systems
Spaces of spheres: 1-to-1 mapping between $d$-spheres and $(d+1)$-hyperplanes using potential functions
Space of Bregman spheres and Bregman balls [7]

Dual sided Bregman balls (bounding Bregman spheres):

\[
\begin{align*}
\text{Ball}_F^r(c, r) &= \{ x \in \mathcal{X} \mid B_F(x : c) \leq r \} \\
\text{Ball}_F^l(c, r) &= \{ x \in \mathcal{X} \mid B_F(c : x) \leq r \}
\end{align*}
\]

Legendre duality:

\[
\text{Ball}_F^l(c, r) = (\nabla F)^{-1}(\text{Ball}_{F^*}^r(\nabla F(c), r))
\]

Illustration for Itakura-Saito divergence, \( F(x) = -\log x \)
Generalized law of cosines and generalized Pythagoras’ theorem

- Generalized law of cosines: \( \theta = \text{angle made at } Q \text{ by the } \nabla\text{-geodesic } \gamma_{PQ} \text{ with the } \nabla^*\text{-geodesic } \gamma_{QR}^* \)

\[
D(P : R) = D(P : Q) + D(Q : R) - \left( \|\gamma_{PQ}\|\|\gamma_{QR}^*\| \cos(\theta) \right) \\
\langle \theta_P - \theta_Q, \eta_R - \eta_Q \rangle
\]

- Euclidean law of cosines when \( D = B_F \) for \( F = \frac{1}{2}x^\top x \):

\[
\|\overrightarrow{PR}\|^2 = \|\overrightarrow{PQ}\|^2 + \|\overrightarrow{QR}\|^2 - 2\|\overrightarrow{PQ}\|\|\overrightarrow{QR}\| \cos \theta
\]

- Generalized Pythagoras’ theorem when \( \theta = \frac{\pi}{2} \):

\[
D(P : R) = D(P : Q) + D(Q : R)
\]

amount to check that \( \cos \theta = 0 \), that is \( \langle \theta_P - \theta_Q, \eta_R - \eta_Q \rangle = 0 \)
Space of Bregman spheres: Lifting map [7]

\( \mathcal{F} : x \mapsto \hat{x} = (x, F(x)) \), hypersurface in \( \mathbb{R}^{d+1} \), potential function

\( H_p : \) Tangent hyperplane at \( \hat{p} \), \( z = H_p(x) = \langle x - p, \nabla F(p) \rangle + F(p) \)

- Bregman sphere \( \sigma \longrightarrow \hat{\sigma} \) with supporting hyperplane
  \( H_\sigma : z = \langle x - c, \nabla F(c) \rangle + F(c) + r. \)
  (// to \( H_c \) and shifted vertically by \( r \))
  \( \hat{\sigma} = \mathcal{F} \cap H_\sigma. \)

- Intersection of any hyperplane \( H \) with \( \mathcal{F} \) projects onto \( \mathcal{X} \) as a Bregman sphere:

\[
H : z = \langle x, a \rangle + b \rightarrow \sigma : \text{Ball}_F(c = (\nabla F)^{-1}(a), r = \langle a, c \rangle - F(c) + b)
\]
Lifting/Polarity : Potential function graph $\mathcal{F}$
Space of Bregman spheres: Algorithmic applications [7]

- Vapnik-Chervonenkis dimension (VC-dim) is \(d + 1\) for the class of Bregman balls.
- Union/intersection of Bregman \(d\)-spheres from representational \((d + 1)\)-polytope [7]
- **Radical axis** of two Bregman balls is an **hyperplane**: Applications to Nearest Neighbor search trees like Bregman ball trees or Bregman vantage point trees [43].
Bregman proximity data structures [43]

Vantage point trees: partition space according to Bregman balls

Partitionning space with intersection of Kullback-Leibler balls
→ efficient nearest neighbour queries in information spaces
Application: Minimum Enclosing Ball [30, 44]

To a hyperplane \( H_\sigma = H(a, b) : z = \langle a, x \rangle + b \) in \( \mathbb{R}^{d+1} \), corresponds a ball \( \sigma = \text{Ball}(c, r) \) in \( \mathbb{R}^d \) with center \( c = \nabla F^*(a) \) and radius:

\[
\begin{align*}
    r &= \langle a, c \rangle - F(c) + b = \langle a, \nabla F^*(a) \rangle - F(\nabla F^*(a)) + b = F^*(a) + b
\end{align*}
\]

since \( F(\nabla F^*(a)) = \langle \nabla F^*(a), a \rangle - F^*(a) \) (Young equality)

**SEB**: Find halfspace \( H(a, b)^- : z \leq \langle a, x \rangle + b \) that contains all lifted points:

\[
\min_{a, b} r = F^*(a) + b,
\]

\[
\forall i \in \{1, \ldots, n\}, \quad \langle a, x_i \rangle + b - F(x_i) \geq 0
\]

→ Convex Program (CP) with linear inequality constraints

\[
F(\theta) = F^*(\eta) = \frac{1}{2} x^\top x : \text{CP} \rightarrow \text{Quadratic Programming (QP)} \ [14]
\]

used in SVM. Smallest enclosing ball used as a primitive in SVM [49]
Smallest Bregman enclosing balls [44, 29]

Algorithm 1: BCCA(\(\mathcal{P}, l\)).

\(c_1 \leftarrow \) choose randomly a point in \(\mathcal{P}\);

for \(i = 2\) to \(l - 1\) do

\(/ /\) farthest point from \(c_i\) wrt. \(B_F\)

\(s_i \leftarrow \operatorname{argmax}_{j=1}^{n} B_F(c_i : p_j);\)

\(/ /\) update the center: walk on the \(\eta\)-segment \([c_i, p_{s_i}]_\eta\)

\(c_{i+1} \leftarrow \nabla F^{-1}(\nabla F(c_i)\# \frac{1}{i+1} \nabla F(p_{s_i}));\)

end

\(/ /\) Return the SEBB approximation

\textbf{return} \(\text{Ball}(c_I, r_I = B_F(c_I : X));\)

\(\theta\)-, \(\eta\)-geodesic segments in dually flat geometry.
Smallest enclosing balls : Core-sets [44]

Core-set $\mathcal{C} \subseteq \mathcal{S}$ : 

$$\text{SOL}(\mathcal{S}) \leq \text{SOL}(\mathcal{C}) \leq (1 + \epsilon)\text{SOL}(\mathcal{S})$$

extended Kullback-Leibler

Itakura-Saito
InSphere predicates wrt Bregman divergences [7]

Implicit representation of Bregman spheres/balls: consider $d + 1$ support points on the boundary

- Is $x$ inside the Bregman ball defined by $d + 1$ support points?

\[
\text{InSphere}(x; p_0, ..., p_d) = \begin{vmatrix}
1 & \ldots & 1 & 1 \\
\vdots & \ddots & \vdots & \vdots \\
p_0 & \ldots & p_d & x \\
F(p_0) & \ldots & F(p_d) & F(x)
\end{vmatrix}
\]

- Sign of a $(d + 2) \times (d + 2)$ matrix determinant
- InSphere($x; p_0, ..., p_d$) is negative, null or positive depending on whether $x$ lies inside, on, or outside $\sigma$. 
Smallest enclosing ball in Riemannian manifolds [3]

c = a#^M_t b : point γ(t) on the geodesic line segment [ab] wrt M such that
ρ_M(a, c) = t × ρ_M(a, b) (with ρ_M the metric distance on manifold M)

Algorithm 2: GeoA

c_1 ← choose randomly a point in 𝒫;
for i = 2 to l do
  // farthest point from c_i
  s_i ← argmax_j^n ρ(c_i, p_j);
  // update the center: walk on the geodesic line segment
  \[ c_i, p_{s_i} \]
  c_{i+1} ← c_i#^M_{i+1} p_{s_i};
end

// Return the SEB approximation
return Ball(c_l, r_l = ρ(c_l, 𝒫));
Approximating the smallest enclosing ball in hyperbolic space

Initialization

First iteration

Second iteration

Third iteration

Fourth iteration after 104 iterations

http://www.sonycs1.co.jp/person/nielsen/infogeo/RiemannMinimax/

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Bregman dual regular/Delaunay triangulations

Embedded geodesic Delaunay triangulations + empty Bregman balls

- Delaunay
- Exponential Del.
- Hellinger-like Del.

- empty Bregman sphere property,
- geodesic triangles: embedded Delaunay.
Dually orthogonal Bregman Voronoi & Triangulations

Ordinary Voronoi diagram is perpendicular to Delaunay triangulation:
Voronoi $k$-face $\perp$ Delaunay $d - k$-face

\[
\begin{align*}
\text{Bi}(P, Q) & \perp \gamma^*(P, Q) \\
\gamma(P, Q) & \perp \text{Bi}^*(P, Q)
\end{align*}
\]
Synthetic geometry : Exact characterization of the Bayesian error exponent but no closed-form known
Bayesian hypothesis testing, MAP rule and probability of error $P_e$

- Mixture $p(x) = \sum_i w_i p_i(x)$. **Task = Classify** $x$ Which component?
- Prior probabilities: $w_i = \mathbb{P}(X \sim P_i) > 0$ (with $\sum_{i=1}^n w_i = 1$)
- Conditional probabilities: $\mathbb{P}(X = x|X \sim P_i)$.

\[
\mathbb{P}(X = x) = \sum_{i=1}^n \mathbb{P}(X \sim P_i)\mathbb{P}(X = x|X \sim P_i) = \sum_{i=1}^n w_i \mathbb{P}(X|P_i)
\]

- Best rule = **Maximum A Posteriori** probability (MAP) rule:

\[
\text{map}(x) = \arg\max_{i\in\{1,...,n\}} w_i p_i(x)
\]

where $p_i(x) = \mathbb{P}(X = x|X \sim P_i)$ are the conditional probabilities.

- For $w_1 = w_2 = \frac{1}{2}$, probability of error

\[
P_e = \frac{1}{2} \int \min(p_1(x), p_2(x)) dx \leq \frac{1}{2} \int p_1(x)^\alpha p_2(x)^{1-\alpha} dx, \text{ for } \alpha \in (0, 1). 
\]

Best exponent $\alpha^*$
Error exponent for exponential families: duality $\text{EF} \leftrightarrow \text{BD}$

- **Exponential families** have finite dimensional sufficient statistics: $\rightarrow$
  Reduce $n$ data to $D$ statistics.

\[
\forall x \in \mathcal{X}, \quad p(x|\theta) = \exp(\theta^\top t(x) - F(\theta) + k(x))
\]

$F(\cdot)$: log-normalizer/cumulant/partition function, $k(x)$: auxiliary term for carrier measure.

- Maximum likelihood estimator (MLE): $\nabla F(\hat{\theta}) = \frac{1}{n} \sum_i t(X_i) = \hat{\eta}$

- **Injection between exponential families and Bregman divergences**:

\[
\log p(x|\theta) = -B_{F^*}(t(x) : \eta) + F^*(t(x)) + k(x)
\]

Exponential families are log-concave
Geometry of the best error exponent

On the exponential family manifold, **Chernoff $\alpha$-coefficient** [8]:

$$c_{\alpha}(P_{\theta_1} : P_{\theta_2}) = \int p_{\theta_1}^\alpha(x)p_{\theta_2}^{1-\alpha}(x)d\mu(x) = \exp(-J_F^{(\alpha)}(\theta_1 : \theta_2))$$

**Skew Jensen divergence** [26] on the natural parameters:

$$J_F^{(\alpha)}(\theta_1 : \theta_2) = \alpha F(\theta_1) + (1 - \alpha)F(\theta_2) - F(\theta_{12}^{(\alpha)})$$

**Chernoff information** = **Bregman divergence for exponential families**:

$$C(P_{\theta_1} : P_{\theta_2}) = B(\theta_1 : \theta_{12}^{(\alpha*)}) = B(\theta_2 : \theta_{12}^{(\alpha*)})$$

Finding best error exponent $\alpha^*$?
Geometry of the best error exponent: binary hypothesis [23]

Chernoff distribution $P^*$:

$$P^* = P_{\theta_{12}^*} = G_e(P_1, P_2) \cap \text{Bi}_m(P_1, P_2)$$

e-geodesic:

$$G_e(P_1, P_2) = \left\{ E_{12}^{(\lambda)} \mid \theta(E_{12}^{(\lambda)}) = (1 - \lambda)\theta_1 + \lambda\theta_2, \lambda \in [0, 1] \right\},$$

$m$-bisector:

$$\text{Bi}_m(P_1, P_2) : \left\{ P \mid F(\theta_1) - F(\theta_2) + \eta(P)^\top \Delta\theta = 0 \right\},$$

Optimal natural parameter of $P^*$:

$$\theta^* = \theta_{12}^{(\alpha^*)} = \arg\min_{\theta \in \Theta} B(\theta_1 : \theta) = \arg\min_{\theta \in \Theta} B(\theta_2 : \theta).$$

$\rightarrow$ closed-form for order-1 family, or efficient bisection search.
Geometry of the best error exponent: binary hypothesis

\[ P^* = P_{\theta^*_{12}} = G_e(P_1, P_2) \cap B_{im}(P_1, P_2) \]

\( m \)-bisector

\( B_{im}(P_{\theta_1}, P_{\theta_2}) \)

\( \eta \)-coordinate system

\( e \)-geodesic \( G_e(P_{\theta_1}, P_{\theta_2}) \)

\( C(\theta_1 : \theta_2) = B(\theta_1 : \theta^*_{12}) \)

Binary Hypothesis Testing: \( P_e \) bounded using Bregman divergence between Chernoff distribution and class-conditional distributions.
Clustering and Learning finite statistical mixtures
The distortion class of $\alpha$-divergences

For $\alpha \in \mathbb{R} \neq \pm 1$, $\alpha$-divergences [9] on positive arrays [51]:

\[
D_\alpha(p : q) \overset{\text{eq}}{=} \sum_{i=1}^{d} \frac{4}{1 - \alpha^2} \left( \frac{1 - \alpha}{2} p^i + \frac{1 + \alpha}{2} q^i - (p^i)^{\frac{1-\alpha}{2}} (q^i)^{\frac{1+\alpha}{2}} \right)
\]

with

\[
D_\alpha(p : q) = D_{-\alpha}(q : p)
\]

and in the limit cases $D_{-1}(p : q) = KL(p : q)$ and $D_1(p : q) = KL(q : p)$, where $KL$ is the extended Kullback–Leibler divergence

\[
KL(p : q) \overset{\text{eq}}{=} \sum_{i=1}^{d} p^i \log \frac{p^i}{q^i} + q^i - p^i
\]

$\alpha$-divergences belong to the class of Csiszár $f$-divergences

\[
l_f(p : q) \overset{\text{eq}}{=} \sum_{i=1}^{d} q^i f \left( \frac{p^i}{q^i} \right)
\]

with the following generator:

\[
f(t) = \begin{cases} 
\frac{4}{1 - \alpha^2} (1 - t^{(1+\alpha)/2}), & \text{if } \alpha \neq \pm 1, \\
t \ln t, & \text{if } \alpha = 1, \\
- \ln t, & \text{if } \alpha = -1 
\end{cases}
\]

Information monotonicity

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9. Bayesian error exponent
Pythagoras’ theorem for $\alpha$-divergences [16]

Use $\nabla^{(\alpha)}$ and $\nabla^{(-\alpha)}$ dually coupled connections with respect to $g$.

\[
Xg(Y, Z) = g(\nabla^{(\alpha)}_X, Z) + g(Y, \nabla^{(-\alpha)}_X Z)
\]

\[
\gamma^{(\alpha)}_{PQ} \perp \gamma^{(-\alpha)}_{QR}
\]

\[
D_\alpha(P : Q) = D_\alpha(P : Q) + D_\alpha(Q : R) - \kappa D_\alpha(P : Q)D_\alpha(Q : R)
\]

Curvature $\kappa = \frac{\alpha^2 - 1}{4}$. 
Mixed divergences [42]

Defined on three parameters $p$, $q$ and $r$:

$$M_{\lambda}(p : q : r) \overset{eq}{=} \lambda D(p : q) + (1 - \lambda) D(q : r)$$

for $\lambda \in [0, 1]$.

Mixed divergences include:

- the **sided divergences** for $\lambda \in \{0, 1\}$,
- the **symmetrized** (arithmetic mean) divergence for $\lambda = \frac{1}{2}$, or skew symmetrized for $\lambda \neq \frac{1}{2}$.
Symmetrizing $\alpha$-divergences

\[ S_{\alpha}(p, q) = \frac{1}{2} (D_{\alpha}(p : q) + D_{\alpha}(q : p)) = S_{-\alpha}(p, q), \]
\[ = M_{\frac{1}{2}}(p : q : p), \]

For $\alpha = \pm 1$, we get half of Jeffreys divergence:

\[ S_{\pm 1}(p, q) = \frac{1}{2} \sum_{i=1}^{d} (p^{i} - q^{i}) \log \frac{p^{i}}{q^{i}} \]

- Centroids for symmetrized $\alpha$-divergence usually not in closed form.
- How to perform center-based clustering without closed form centroids?
Jeffreys positive centroid [22]

- Jeffreys divergence is symmetrized $\alpha = \pm 1$ divergences.
- The Jeffreys positive centroid $c = (c^1, ..., c^d)$ of a set $\{h_1, ..., h_n\}$ of $n$ weighted positive histograms with $d$ bins can be calculated component-wise exactly using the Lambert $W$ analytic function:

$$c^i = \frac{a^i}{W \left( \frac{a^i}{g^i} e \right)}$$

where $a^i = \sum_{j=1}^{n} \pi_j h_j^i$ denotes the coordinate-wise arithmetic weighted means and $g^i = \prod_{j=1}^{n} (h_j^i)^{\pi_j}$ the coordinate-wise geometric weighted means.

- The Lambert analytic function $W$ [5] (positive branch) is defined by $W(x)e^{W(x)} = x$ for $x \geq 0$.
- $\rightarrow$ Jeffreys $k$-means clustering. But for $\alpha \neq 1$, how to cluster?
Mixed $\alpha$-divergences/$\alpha$-Jeffreys symmetrized divergence

- Mixed $\alpha$-divergence between a histogram $x$ to **two** histograms $p$ and $q$:

\[
M_{\lambda,\alpha}(p : x : q) = \lambda D_{\alpha}(p : x) + (1 - \lambda) D_{\alpha}(x : q),
\]

\[
= \lambda D_{-\alpha}(x : p) + (1 - \lambda) D_{-\alpha}(q : x),
\]

\[
= M_{1-\lambda, -\alpha}(q : x : p),
\]

- $\alpha$-Jeffreys symmetrized divergence is obtained for $\lambda = \frac{1}{2}$:

\[
S_{\alpha}(p, q) = M_{\frac{1}{2}, \alpha}(q : p : q) = M_{\frac{1}{2}, \alpha}(p : q : p)
\]

- Skew symmetrized $\alpha$-divergence is defined by:

\[
S_{\lambda, \alpha}(p : q) = \lambda D_{\alpha}(p : q) + (1 - \lambda) D_{\alpha}(q : p)
\]
Mixed divergence-based $k$-means clustering

$k$ distinct seeds from the dataset with $l_i = r_i$.

**Input:** Weighted histogram set $\mathcal{H}$, divergence $D(\cdot, \cdot)$, integer $k > 0$, real $\lambda \in [0, 1]$;

Initialize left-sided/right-sided seeds $C = \{(l_i, r_i)\}_{i=1}^k$;

**repeat**

// Assignment

for $i = 1, 2, \ldots, k$ do

\[ C_i \leftarrow \{ h \in \mathcal{H} : i = \arg\min_j M_\lambda(l_j : h : r_i) \}; \]

end

// Dual-sided centroid relocation

for $i = 1, 2, \ldots, k$ do

\[ r_i \leftarrow \arg\min_x D(C_i : x) = \sum_{h \in C_i} w_j D(h : x); \]

\[ l_i \leftarrow \arg\min_x D(x : C_i) = \sum_{h \in C_i} w_j D(x : h); \]

end

**until** convergence;
Mixed $\alpha$-hard clustering : $\text{MAhC}(\mathcal{H}, k, \lambda, \alpha)$

**Input**: Weighted histogram set $\mathcal{H}$, integer $k > 0$, real $\lambda \in [0, 1]$, real $\alpha \in \mathbb{R}$;

Let $C = \{ (l_i, r_i) \}_{i=1}^k \leftarrow \text{MAS}(\mathcal{H}, k, \lambda, \alpha)$;

repeat
  // Assignment
  for $i = 1, 2, ..., k$ do
    $A_i \leftarrow \{ h \in \mathcal{H} : i = \arg \min_j M_{\lambda, \alpha}(l_j : h : r_j) \}$;
  end

  // Centroid relocation
  for $i = 1, 2, ..., k$ do
    $r_i \leftarrow \left( \sum_{h \in A_i} w_i h^{\frac{1-\alpha}{2}} \right)^{\frac{2}{1-\alpha}}$;
    $l_i \leftarrow \left( \sum_{h \in A_i} w_i h^{\frac{1+\alpha}{2}} \right)^{\frac{2}{1+\alpha}}$;
  end

until convergence;
Coupled $k$-Means++ $\alpha$-Seeding

**Algorithm 3:** Mixed $\alpha$-seeding; $\text{MAS}(\mathcal{H}, k, \lambda, \alpha)$

**Input:** Weighted histogram set $\mathcal{H}$, integer $k \geq 1$, real $\lambda \in [0, 1]$, real $\alpha \in \mathbb{R}$; Let $C \leftarrow h_j$ with uniform probability;

**for** $i = 2, 3, \ldots, k$ **do**

Pick at random histogram $h \in \mathcal{H}$ with probability:

$$\pi_{\mathcal{H}}(h) \overset{\text{eq}}{=} \frac{w_h M_{\lambda, \alpha}(c_h : h : c_h)}{\sum_{y \in \mathcal{H}} w_y M_{\lambda, \alpha}(c_y : y : c_y)} ,$$

//where $(c_h, c_h) \overset{\text{eq}}{=} \text{arg min}_{(z, z) \in \mathcal{C}} M_{\lambda, \alpha}(z : h : z)$;

$C \leftarrow C \cup \{(h, h)\};$

**end**

**Output:** Set of initial cluster centers $C$;

→ Guaranteed probabilistic bound. Just need to initialize! No centroid computations
Learning MMs: A geometric hard clustering viewpoint

Learn the parameters of a mixture \( m(x) = \sum_{i=1}^{k} w_i p(x|\theta_i) \)

Maximize the complete data likelihood = clustering objective function

\[
\max_{W,\Lambda} l_c(W, \Lambda) = \sum_{i=1}^{n} \sum_{j=1}^{k} z_{i,j} \log(w_j p(x_i|\theta_j)) \\
= \max_{\Lambda} \sum_{i=1}^{n} \max_{j=1}^{k} \log(w_j p(x_i|\theta_j)) \\
\equiv \min_{W,\Lambda} \sum_{i=1}^{n} \min_{j=1}^{k} D_j(x_i),
\]

where \( c_j = (w_j, \theta_j) \) (cluster prototype) and \( D_j(x_i) = -\log p(x_i|\theta_j) - \log w_j \) are potential distance-like functions.

further attach to each cluster a different family of probability distributions.
Generalized $k$-MLE for learning statistical mixtures

Model-based clustering : Assignment of points to clusters :

$$D_{w_j, \theta_j, F_j}(x) = - \log p_{F_j}(x; \theta_j) - \log w_j$$

$k$-GMLE :

1. Initialize weight $W \in \Delta_k$ and family type $(F_1, \ldots, F_k)$ for each cluster
2. Solve $\min \sum \min_j D_j(x_i)$ (center-based clustering for $W$ fixed) with potential functions : $D_j(x_i) = - \log p_{F_j}(x_i|\theta_j) - \log w_j$
3. Solve family types maximizing the MLE in each cluster $C_j$ by choosing the parametric family of distributions $F_j = F(\gamma_j)$ that yields the best likelihood : $\min_{F_1=F(\gamma_1), \ldots, F_k=F(\gamma_k)\in F(\gamma)} \sum_i \min_j D_{w_j, \theta_j, F_j}(x_i)$. 
   $\forall l, \gamma_l = \max_j F^*_j(\hat{\eta}_l = \frac{1}{n_l} \sum_{x \in C_l} t_j(x)) + \frac{1}{n_l} \sum_{x \in C_l} k(x)$.
4. Update weight $W$ as the cluster point proportion
5. Test for convergence and go to step 2) otherwise.

Drawback = biased, non-consistent estimator due to Voronoi support truncation.
Computing $f$-divergences for generic $f$ : Beyond stochastic Monte-Carlo numerical integration
Ali-Silvey-Csiszár $f$-divergences

\[ l_f(X_1 : X_2) = \int x_1(x) f \left( \frac{x_2(x)}{x_1(x)} \right) \, d\nu(x) \geq 0 \]

<table>
<thead>
<tr>
<th>Name of the $f$-divergence</th>
<th>Formula $l_f(P : Q)$</th>
<th>Generator $f(u)$ with $f(1) = 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total variation (metric)</td>
<td>$\frac{1}{2} \int</td>
<td>p(x) - q(x)</td>
</tr>
<tr>
<td>Squared Hellinger</td>
<td>$\int (\sqrt{p(x)} - \sqrt{q(x)})^2 , d\nu(x)$</td>
<td>$(\sqrt{u} - 1)^2$</td>
</tr>
<tr>
<td>Pearson $\chi_P^2$</td>
<td>$\int \frac{(q(x) - p(x))^2}{p(x)} , d\nu(x)$</td>
<td>$(u - 1)^2$</td>
</tr>
<tr>
<td>Neyman $\chi_N^2$</td>
<td>$\int \frac{(p(x) - q(x))^2}{q(x)} , d\nu(x)$</td>
<td>$\frac{(1-u)^2}{u}$</td>
</tr>
<tr>
<td>Pearson-Vajda $\chi_P^k$</td>
<td>$\int \frac{(q(x) - \lambda p(x))^k}{p^{k-1}(x)} , d\nu(x)$</td>
<td>$(u - 1)^k$</td>
</tr>
<tr>
<td>Pearson-Vajda $</td>
<td>\chi</td>
<td>^k_P$</td>
</tr>
<tr>
<td>Kullback-Leibler</td>
<td>$\int p(x) \log \frac{p(x)}{q(x)} , d\nu(x)$</td>
<td>$- \log u$</td>
</tr>
<tr>
<td>reverse Kullback-Leibler</td>
<td>$\int q(x) \log \frac{q(x)}{p(x)} , d\nu(x)$</td>
<td>$u \log u$</td>
</tr>
<tr>
<td>$\alpha$-divergence</td>
<td>$\frac{4}{1 - \alpha^2} \left( 1 - \int p \frac{1 - \alpha}{2} (x) q^{1 + \alpha}(x) , d\nu(x) \right)$</td>
<td>$\frac{4}{1 - \alpha^2} \left( 1 - u \frac{1 + \alpha}{2} \right)$</td>
</tr>
<tr>
<td>Jensen-Shannon</td>
<td>$\frac{1}{2} \int (p(x) \log \frac{2p(x)}{p(x) + q(x)} + q(x) \log \frac{2q(x)}{p(x) + q(x)}) , d\nu(x)$</td>
<td>$-(u + 1) \log \frac{1 + u}{2} + u \log u$</td>
</tr>
</tbody>
</table>
Information monotonicity of $f$-divergences

Do coarse binning: from $d$ bins to $k < d$ bins:

$$\mathcal{X} = \biguplus_{i=1}^{k} A_i$$

Let $p^A = (p_i)_A$ with $p_i = \sum_{j \in A_i} p_j$.

**Information monotonicity**:

$$D(p : q) \geq D(p^A : q^A)$$

$\Rightarrow$ $f$-divergences are the *only* divergences preserving the information monotonicity.
$f$-divergences and higher-order Vajda $\chi^k$ divergences

\[
I_f(X_1 : X_2) = \sum_{k=0}^{\infty} \frac{f^{(k)}(1)}{k!} \chi^k_P(X_1 : X_2)
\]

\[
\chi^k_P(X_1 : X_2) = \int \frac{(x_2(x) - x_1(x))^k}{x_1(x)^{k-1}} d\nu(x),
\]

\[
|\chi|^k_P(X_1 : X_2) = \int \frac{|x_2(x) - x_1(x)|^k}{x_1(x)^{k-1}} d\nu(x),
\]

are $f$-divergences for the generators $(u - 1)^k$ and $|u - 1|^k$.

- When $k = 1$, $\chi^1_P(X_1 : X_2) = \int (x_1(x) - x_2(x)) d\nu(x) = 0$ (never discriminative), and $|\chi^1_P|(X_1, X_2)$ is twice the total variation distance.
- $\chi^k_P$ is a signed distance
Affine exponential families

Canonical decomposition of the probability measure:

\[ p_\theta(x) = \exp(\langle t(x), \theta \rangle - F(\theta) + k(x)), \]

consider natural parameter space \( \Theta \) affine (like multinomials).

\[ \text{Poi}(\lambda) : \quad p(x|\lambda) = \frac{\lambda^x e^{-\lambda}}{x!}, \lambda > 0, x \in \{0, 1, \ldots\} \]

\[ \text{Nor}_I(\mu) : \quad p(x|\mu) = (2\pi)^{-\frac{d}{2}} e^{-\frac{1}{2}(x-\mu)^\top(x-\mu)}, \mu \in \mathbb{R}^d, x \in \mathbb{R}^d \]

<table>
<thead>
<tr>
<th>Family</th>
<th>( \theta )</th>
<th>( \Theta )</th>
<th>( F(\theta) )</th>
<th>( k(x) )</th>
<th>( t(x) )</th>
<th>( \nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson</td>
<td>( \log \lambda )</td>
<td>( \mathbb{R} )</td>
<td>( e^\theta )</td>
<td>( - \log x! )</td>
<td>( x )</td>
<td>( \nu_c )</td>
</tr>
<tr>
<td>Iso. Gaussian</td>
<td>( \mu )</td>
<td>( \mathbb{R}^d )</td>
<td>( \frac{1}{2} \theta^\top \theta )</td>
<td>( \frac{d}{2} \log 2\pi - \frac{1}{2} x^\top x )</td>
<td>( x )</td>
<td>( \nu_L )</td>
</tr>
</tbody>
</table>
Higher-order Vajda $\chi^k$ divergences

The (signed) $\chi_P^k$ distance between members $X_1 \sim \mathcal{E}_F(\theta_1)$ and $X_2 \sim \mathcal{E}_F(\theta_2)$ of the same affine exponential family is ($k \in \mathbb{N}$) always bounded and equal to:

$$\chi_P^k(X_1 : X_2) = \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} \frac{e^{F((1-j)\theta_1 + j\theta_2)}}{e^{(1-j)F(\theta_1) + jF(\theta_2)}}$$

For Poisson/Normal distributions, we get closed-form formula:

$$\chi_P^k(\lambda_1 : \lambda_2) = \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} e^{\lambda_1^{1-j}\lambda_2^j - ((1-j)\lambda_1 + j\lambda_2)},$$

$$\chi_P^k(\mu_1 : \mu_2) = \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} e^{\frac{1}{2}j(j-1)(\mu_1 - \mu_2)^	op (\mu_1 - \mu_2)}.$$
\( f \)-divergences: Analytic formula \([18]\)

\[ \lambda = 1 \in \text{int}(\text{dom}(f^{(i)})), \text{ } f\text{-divergence (Theorem 1 of [4])}: \]

\[
\left| l_f(X_1 : X_2) - \sum_{k=0}^{s} \frac{f^{(k)}(1)}{k!} \chi_P(X_1 : X_2) \right| \\
\leq \frac{1}{(s + 1)!} \| f^{(s+1)} \|_\infty (M - m)^s,
\]

where \( \| f^{(s+1)} \|_\infty = \sup_{t \in [m, M]} |f^{(s+1)}(t)| \) and \( m \leq \frac{p}{q} \leq M \).

\( \lambda = 0 \) (whenever \( 0 \in \text{int}(\text{dom}(f^{(i)})) \)) and affine exponential families, simpler expression:

\[
l_f(X_1 : X_2) = \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!} l_{1-i,i}(\theta_1 : \theta_2),
\]

\[
l_{1-i,i}(\theta_1 : \theta_2) = \frac{e^{F(i \theta_2 + (1-i) \theta_1)}}{e^{iF(\theta_2) + (1-i)F(\theta_1)}}.
\]
Designing conformal divergences: Finding graphical gaps!
Geometrically designed divergences

Plot of the convex generator $F$. 

$F : (x, F(x))$

$(q, F(q))$

$(p, F(p))$

$J(p, q)$

$tB(p : q)$

$p + \frac{q}{2}$

$q$

$p$

$B(p : q)$
Divergences: skew Jensen & Bregman divergences

\( F \) a smooth convex function, the generator.

- **Skew Jensen divergences:**

\[
J'_\alpha(p : q) = \alpha F(p) + (1 - \alpha)F(q) - F(\alpha p + (1 - \alpha)q),
\]

\[
= (F(p)F(q))_\alpha - F((pq)_\alpha),
\]

where \((pq)_\gamma = \gamma p + (1 - \gamma)q = q + \gamma(p - q)\) and \((F(p)F(q))_\gamma = \gamma F(p) + (1 - \gamma)F(q) = F(q) + \gamma(F(p) - F(q))\).

- **Bregman divergences:**

\[
B(p : q) = F(p) - F(q) - \langle p - q, \nabla F(q) \rangle,
\]

\[
\lim_{\alpha \to 0} J_\alpha(p : q) = B(p : q), \quad \lim_{\alpha \to 1} J_\alpha(p : q) = B(q : p)
\]

- **Statistical skewed Bhattacharrya divergence:**

\[
\text{Bhat}(p_1 : p_2) = -\log \int p_1(x)^\alpha p_2(x)^{1-\alpha} d\nu(x) = J'_\alpha(\theta_1 : \theta_2)
\]

for exponential families [27].
Divergences and centroids [33, 27]

Population minimizers: \( \arg \min_c \sum_{i=1}^n w_i D(p_i : c) \)

- useful for center-based clustering algorithms (\( k \)-means)
- For Bregman divergences: \( c^R = \sum_i w_i p_i \) (invariant, center of mass).
  \( c^L = (\nabla F)^{-1}(\sum_i w_i \nabla F(p_i)) \) a f-mean also called
  quasi-arithmetic mean: \( f^{-1}(\sum_i w_i f(x_i)) \) that generalizes arithmetic
  \( f(x) = x \), harmonic \( f(x) = \frac{1}{x} \) and geometric means \( f(x) = \log x \).
- Bregman information \( \sum_{i=1}^n w_i D(p_i : c^R) = F(\sum_i w_i p_i) - \sum_i w_i F(p_i) \), a
  Jensen diversity index.
- For Jensen divergences, use Concave-Convex Procedure from
  \( c_0 = \sum_i w_i p_i \) to solve \( \sum_i w_i J'_{\alpha}(c : p_i) : \)

\[
c_{t+1} = (\nabla F)^{-1} \left( \sum_i w_i \nabla F(\alpha c_t + (1 - \alpha)p_i) \right)
\]
Quasi-arithmetic mean:
\[ M_f(x_1, \ldots, x_n) = f^{-1}(\frac{1}{n} f(x_i)) \]

Bregman divergence:
\[ B_F(p : q) = F(p) - F(q) - \langle p - q, \nabla F(q) \rangle \]

Probability:
\[ p_F(x|\theta) = e^{\langle t(x), \theta \rangle - F(\theta) + k(x)} \]
\[ p_F(x|\theta) = e^{-B^*(t(x) : \nabla F(\theta)) + F^*(t(x)) + k(x)} \]

Convexity
\[ f = \nabla F \text{ Monotone increasing} \]

Legendre transform

Distances

Aggregators

Probabilities
Total Bregman divergences [17]

Conformal divergence, conformal factor $\rho$:

$$D'(p : q) = \rho(p, q)D(p : q)$$

plays the rôle of “regularizer” [50]

Invariance by rotation of the axes of the design space

$$tB(p : q) = \frac{B(p : q)}{\sqrt{1 + \langle \nabla F(q), \nabla F(q) \rangle}} = \rho_B(q)B(p : q),$$

$$\rho_B(q) = \frac{1}{\sqrt{1 + \langle \nabla F(q), \nabla F(q) \rangle}}.$$ 

For example, total squared Euclidean divergence:

$$tE(p, q) = \frac{1}{2} \frac{\langle p - q, p - q \rangle}{\sqrt{1 + \langle q, q \rangle}}.$$
Total skew Jensen divergences [38]

\[
\begin{align*}
\text{tB}(p : q) &= \rho_B(q)B(p : q), \quad \rho_B(q) = \sqrt{\frac{1}{1 + \langle \nabla F(q), \nabla F(q) \rangle}} \\
\text{tJ}_\alpha(p : q) &= \rho_J(p, q)J_\alpha(p : q), \quad \rho_J(p, q) = \sqrt{\frac{1}{1 + \langle F(p) - F(q) \rangle^2 \langle p - q, p - q \rangle}}
\end{align*}
\]

Jensen-Shannon divergence, square root is a metric:

\[
J\text{S}(p, q) = \frac{1}{2} \sum_{i=1}^{d} p_i \log \frac{2p_i}{p_i + q_i} + \frac{1}{2} \sum_{i=1}^{d} q_i \log \frac{2q_i}{p_i + q_i}
\]

But the square root of the total Jensen-Shannon divergence is not a metric.
If $(P : Q) = \int p(x) f\left(\frac{q(x)}{p(x)}\right) d\nu(x)$

$D^v(P : Q) = D(v(P) : v(Q))$

$I_f(P : Q) = \int p(x) f\left(\frac{q(x)}{p(x)}\right) d\nu(x)$

$B_F(P : Q) = F(P) - F(Q) - \langle P - Q, \nabla F(Q) \rangle$

$tB_F(P : Q) = \frac{B_F(P; Q)}{\sqrt{1 + \|\nabla F(Q)\|^2}}$

$C_{D,g}(P : Q) = g(Q)D(P : Q)$

$B_{F,g}(P : Q; W) = WB_F\left(\frac{P}{Q} : \frac{Q}{W}\right)$
Summary : Part II. Geometric Computing in Information Spaces

- Location-scale families, spherical normal, symmetric positive definite matrices $\rightarrow$ hyperbolic geometry.
- Hyperbolic geometry : CG affine constructions in Klein disk
- Space of spheres in dually affine connection geometry
- Synthetic geometry for characterizing the best error exponent in Bayes error
- Conformal divergences : total Bregman/total Jensen divergences
- Clustering using pair of centroids for clusters using mixed divergences for symmetrized alpha divergences
- Learning statistical mixtures maximizing the complete likelihood as a sequence of geometric clustering problems : $k$-GLME
- In search of closed-form solutions : Jeffreys centroid using Lambert $W$ function, $f$-divergence approximation for affine exponential families.
Geometric Sciences of Information (GSI) 2015


http://www.gsi2015.org/
Summary: Computational Information Geometry

- Originally, IG studied the space of (parametric) probability distributions, but now geometry of "parameter spaces" in general (matrices, dynamic systems, etc.)
- Fisher-Rao Riemannian geometry has often geodesics not in closed form
- Dual connections coupled with metric has dual geodesics straight in biorthogonal affine coordinate systems
- Bregman divergences are canonical divergences in dually flat spaces
- Csiszár $f$-divergences preserve information monotonicity and induce locally Fisher tensor metric geometry.
- Algorithm designs are often based on information projections.
Closing philosophical view...

Super-model $M^+$

Model $M$

Structure

Parameter $\theta$

Configuration space $\Theta$

coordinate-based (biased)

Geometry embedding $G^+$

Geometry $G$

Structure

Point $P_\theta$

Space $\{P_\theta | \theta \in \Theta\}$

coordinate-free!
The next big wave...
Quantum Information Geometry (and QIT)

- Quantum states: density matrices = Hermitian positive semi-definite matrices of unit trace (John von Neumann, 1927)
- A generalization of probability theory (classical probability=diagonal matrices=commutative matrices)
- Several Quantum Fisher Information metrics [46]
- Quantum random walks to define distance between graphs (simulated on classical computers [10])
- Quantum Voronoi diagrams [31]
- etc.
Thank you!

Next time, why not consider ClG for your ML problems - :)?
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