

# Non-Euclidean Computational Geometry and Its Applications in Machine Learning

Frank Nielsen  
Sony Computer Science Laboratories, Inc  
Tokyo, Japan

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## Abstract

This note provides a concise overview of my work in computational geometry and geometric computing on non-Euclidean and information-geometric spaces. It also highlights applications to machine learning, including unsupervised clustering and supervised classification, across a range of domains such as computational statistics, computer vision, medical imaging, and finance.

Since its inception, Artificial Intelligence (AI) builds upon concepts from computational geometry [1] (CG), e.g., the celebrated book “Perceptrons: An Introduction to Computational Geometry” [2] by Marvin Minsky and Seymour Papert (1969). Key supervised learning methods like  $k$ -Nearest Neighbor ( $k$ -NN rule) classifications [3][4] and support vector machines [5] (SVMs) rely on geometric  $k$ -order Voronoi partitions [6] and smallest enclosing ball procedures [7][8], respectively. Computational geometry in Euclidean spaces and more generally in normed  $\ell_p$ -spaces have been thoroughly investigated<sup>1</sup> [9] but geometric computing in other spaces has received comparatively little consideration.

A main focus of my research is to consider computational geometry and geometric computing primitives in non-Euclidean spaces, specially in “information spaces” where points denote *typed objects* (e.g., model parameters like vectors or matrices, probability measures, functions, etc) and consider applications ranging from computational statistics [11] to computer vision [12] or medical imaging [13], just to name a few. In particular, information geometry [14][15] (IG) originally started by studying families of statistical models (parametric or not) with main applications in statistics and mathematical neuroscience [16]. Information geometry highlights a fundamental *dual geometric structure*<sup>2</sup> which can be studied purely from the mathematical point of view. In fact, the mechanism of the information-geometric dual structures was independently found in the specific cases of Hessian manifolds [17] and in affine differential geometry [18] by pure geometers (e.g., Professor Koszul and Professor Nomizu). There is a rich interplay between smooth dissimilarities (called divergences, yokes, or contrast functions) and underlying information-geometric structures [19]. Some information-geometric structures yield canonical divergences: For example, Bregman divergences are canonical divergences of dually flat spaces and logarithmic divergences [20] yield dualistic structures with constant section curvatures, and vice-versa. Thus in our work, we have also proposed new dissimilarity measures (e.g., total Bregman divergence [12], geometric Jensen-Shannon

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<sup>1</sup>The lead author of the textbook [9] is Professor Jean-Daniel Boissonnat who advised my PhD [10] (defended in 1996).

<sup>2</sup>Namely, a pair of torsion-free affine connections coupled to a Riemannian metric.

divergence [21, 22], Hölder projective divergence [23], duo Bregman pseudo-divergence [24], statistical Minkowski distances [25], etc), studied their properties, and considered applications in machine learning (ML). Some statistical problems like simplifying statistical mixtures can be tackled as clustering problems [26] (unsupervised learning) of corresponding weighted parameter point sets sitting in information spaces. Also interestingly, some methods to approximate the calculations of dissimilarities rely on tasks of computational geometry: For example, we show how computing upper and lower envelopes [27] of parametric-density function graphs is useful to bound the Kullback-Leibler divergence,  $\alpha$ -divergences [28, 29], and more generally Ali-Silvey-Csiszár  $f$ -divergences in [30, 31].

I shall report concisely my main contributions to non-Euclidean computational geometry. The contributions are categorized by types of geometry as follows:

**Hyperbolic geometry.** Hyperbolic geometry is frequently encountered in many scientific areas like (a) in machine learning since it can embed discrete hierarchical structures into continuous hyperbolic spaces with low distortions [32], (b) in information geometry as the Fisher-Rao geometry of location-scale families [14, 33] for example, (c) in computer vision/medical imaging as the geometry of symmetric positive-definite (SPD) matrices equipped with the Riemannian trace metric [34]. We described a practical robust method to calculate the hyperbolic Voronoi diagram of a finite point set as a clipped power diagram in Klein non-conformal ball model [35] which can then be converted and visualized in other conformal models [36] like the Poincaré ball or upper half-space, or the hyperboloid models. The method extends to  $k$ -order hyperbolic Voronoi diagrams and we reported the closed-form formula for the constant speed velocity parametrizations of geodesics in Klein model<sup>3</sup> [37]. The hyperbolic Delaunay complex as the dual of the hyperbolic Voronoi diagram was studied in [38]. There is no known closed-form formula for calculating the center of mass in hyperbolic geometry, so we considered alternatively the closed-form formula of Galperin model centroid in [39] and used this primitive to simplify kernel density estimators (KDEs) by clustering methods. Next, we designed a fast iterative geodesic-walk algorithm extending [40] for computing the smallest enclosing ball of finite point sets and theoretically guaranteed its performance [41]. We investigated a novel class of so-called Poincaré probability distributions in the Poincaré disk, study their invariance properties, and provided various formula for measuring their dissimilarities [42]. Computational hyperbolic geometry is very useful in machine learning because hierarchical graph structures can be embedded with low distortions as Delaunay trees [43] but embedding techniques face robustness and numerical problems in practice. We considered the novel problem of hyperbolic embeddings of supervised models in [44] and studied a robust tempered calculus for hyperbolic embeddings [45].

**Hilbert/Birkhoff geometry.** The Klein model of hyperbolic geometry can be interpreted as a Riemannian manifold equipped with the Klein Riemannian metric [46] or as a Hilbert geometry induced by an open bounded convex domain<sup>4</sup> [47]. When the considered domain is an open ellipsoid, the corresponding Hilbert geometry yields the Cayley-Klein geometry [48, 49]. Hilbert geometry is very-well suited to computational geometry because straight lines are pregeodesics (i.e., unparameterized geodesics) but geodesics may not be unique depending on the domain. Geodesics are unique when the Hilbert domain boundary is smooth. We extended Klein Hilbert geometry to the Siegel matrix ball model [50] and termed this space

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<sup>3</sup>Pregeodesics in Klein model of hyperbolic geometry are straight lines in the Cartesian coordinate system.

<sup>4</sup>Thus Hilbert geometry are never Hilbert spaces because vector spaces cannot be Hilbert geometry domains!

the Siegel-Klein model<sup>5</sup> [51]. Many statistical models encountered in machine learning have open convex parameter domains. For example, let us mention (i) the probability simplex of categorical distributions [52] whose Hilbert simplex balls have hexagonal shapes [53], (ii) the ellipsope of correlation matrices [52], (iii) the double cone model [54] of symmetric-positive definite matrices [55]. We considered the Hilbert geometry for those open bounded convex domains with various applications in machine learning. The case of simplicial domains (like the probability simplex) is very particular (and unique) in as sense that the Hilbert geometry is isomorphic to a vector space equipped with a polyhedral norm [52]. We compare several geometric structures of the probability simplex for dimension reduction tasks [56] including the Aitchison geometry [57] which is used in compositional data analysis (CoDA, e.g., often used in hyperspectral imaging [58]). Birkhoff geometry is related to Hilbert geometry [59] and the contraction theorem of the Birkhoff distance is often used in machine learning to prove convergence of Sinkhorn-type algorithms in optimal transport [60][61]. Recently, Hilbert geometry gained attention from the computational geometry community: For example, refer to the recent works on Hilbert Voronoi/Delaunay studies [62] and classifiers in Hilbert geometry [63, 64].

**Riemannian and Finslerian geometry.** Riemannian geometry [65] generalizes Euclidean geometry by introducing a metric tensor field smoothly varying on tangent planes. The metric tensor provides the notion of lengths of vectors and angles between vectors (e.g., thus allowing one to check for orthogonality between vectors). To move a vector from one tangent plane to another tangent plane, one needs to specify explicitly the parallel transport along curves connecting tangents planes. Local notions of curvature and torsions are derived from the connection in general, and geodesic lengths with respect to metric connections provide a metric distance called the Riemannian distance. In Riemannian geometry, the default connection is built from the metric tensor and is called the Levi-Civita (LC) connection. The LC connection is unique and torsion-free: This is the fundamental theorem of Riemannian geometry [65]. In information geometry [14], regular statistical models (i.e., with symmetric positive-definite Fisher information matrix) induce Fisher metrics [66, 67, 68][69] and the domains of statistical models are then interpreted as Fisher-Rao manifolds with the geodesic distances called Fisher-Rao distances (or Rao distances [70]). We designed and analyzed an interactive approximation algorithm for calculating the circumcenter of the smallest enclosing ball on arbitrary Riemannian manifolds [71] with sectional curvature constraints. Although very attractive in statistical applications, the Fisher-Rao distances can be difficult to calculate for some statistical models. For example, there is no known closed-form formula for the Fisher-Rao distance between any two multivariate normal distributions [72] (MVNs) although we can approximate arbitrarily finely this distance [73, 74]. Hilbert geometry with smooth ellipsoid boundaries can be analyzed using Riemannian metrics. In general, Hilbert geometry can be studied from the viewpoint of differential geometry using a Finsler metric [47][75]. We studied the uniqueness of  $p$ -means (e.g., medians when  $p = 1$ , centroids when  $p = 2$ , and circumcenters when  $p \rightarrow \infty$ ) on Finsler manifolds in [76].

**Neuromanifold geometry.** Stochastic (deep) neural networks (NNs) can be analyzed from the viewpoint of information geometry [77]. Stochasticity can be obtained by adding some Gaus-

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<sup>5</sup>The Siegel upper space [50] is a matrix extension of Poincaré upper plane which consists of symmetric complex matrices with SPD imaginary parts.

sian noise in the output or inside the activation functions of NN layers themselves [78]. Training neural networks can be visualized as trajectories on the (usually huge) parameter spaces of NNs which exhibit symmetries and Fisher metric degeneracies. Indeed, the Fisher information matrix (FIM) is only guaranteed to be symmetric semi-positive definite (as a covariance matrix) and its rank may vary locally. Intrinsic learning is often performed using natural gradient descents [79] (NGDs) or some of its variants but are often not practical because of their time complexity or numerical instability. We proposed several improved methods of NGDs like using local reparameterizations or adding momentum, and carried out experiments in [80, 81]. Natural gradient is related to mirror descent [82][83]. We also introduced a modular view of NN architectures where geometry is defined relatively (and dynamically) using the concept of relative Fisher information matrix [84]. One striking property of deep learning is that despite the huge numbers of parameters of NNs, the stochastic gradient descent (SGD) learning algorithm generalizes well with several phenomena observed during the training stage (e.g., double descent [85]). We studied why overparameterization in NNs work for learning from the viewpoint of minimum description length principle [86] (MDL) and reported an Occam’s razor based on a geometric modeling of the parameter spaces as lightlike manifolds [87]. In another work, we considered geodesic latent space regularization for variational autoencoder architectures (VAEs) in [88].

**Information geometry/Hessian geometry.** At the core of information geometry [14] is the dualistic differential-geometric structure which consists of two torsion-free affine connections coupled to the metric tensor which ensures that the metric is preserved under dual parallel transports [33, 15]. When considering parametric statistical models as manifolds, we can equip those manifolds with Amari dual  $\pm\alpha$ -connections [14] which are coupled to the Fisher-Rao metric. The dual structures can also be built from smooth divergences [19] (divergence-based information geometry) or convex functions [17] (Bregman manifolds<sup>6</sup> [89] which are Hessian manifolds with global charts, commonly called dually flat spaces in information geometry). Since convex functions remain convex after affine reparameterizations and additional affine terms, there is a gauge freedom [90] on Bregman manifolds which manifests itself by affine invariance of the (geometric) Legendre transform.

From a dualistic information-geometric structure, we can recover the Amari-Chentsov cubic tensor from which we can then build a family of dual geometries called the  $\alpha$ -geometries [33]. I considered algorithmic geometry on Bregman manifolds because they admit dual canonical affine coordinate systems where geodesics are straight in the proper coordinate systems and thus well-suited for computational geometry. Moreover, dual parallel transports on Bregman manifolds is path independent because the dual connections have zero curvature. A fundamental property on Bregman manifolds is the dual Pythagoras’ theorem [91] which allows one to prove the uniqueness of Bregman information projections [92] met in applications as minimization problems of Bregman divergences.

Let us describe the computational toolbox we developed for Bregman manifolds: First, we considered computing exactly [93] or approximating [94] the smallest enclosing Bregman balls [95]. The Bregman Voronoi diagrams [96] and its dual Bregman Delaunay complexes where studied in [97] where we generalize the paraboloid lifting technique [98, 99] of computational geometry (related to the polarity duality [100] with respect to the paraboloid). See [101]

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<sup>6</sup>See the software library named `pyBregMan`, <https://franknielsen.github.io/pyBregMan/index.html>

for a pedagogical video which illustrates the space of Bregman balls and its boolean algebra of union and intersection operations manipulated as intersections of halfspaces. In particular, we proved that the Vapnik-Chervonenkis dimensions<sup>7</sup> of  $d$ -variate Bregman balls [102] is  $d + 1$ . The reduction technique of Bregman Voronoi diagrams to power diagrams can further incorporate representational functions to compute representational Voronoi diagrams [103] which allows one to further consider  $\alpha$ -divergences and  $\beta$ -divergences as particular examples. Voronoi diagrams with respect to skew Jensen-Voronoi diagrams (including Bregman Voronoi diagrams in limit skewing cases) were studied in [104]. We described Bregman proximity query data-structures (useful for supervised classification with respect to Bregman divergences): Bregman vantage point trees [105] and Bregman ball trees [106].

Soft/hard clustering with Bregman divergences [107] allows one to unify  $k$ -means (vector quantization) and expectation-maximization (EM) algorithms for learning locally statistical mixtures. In particular, Bregman  $k$ -means can also be interpreted as a classification EM for mixtures of densities of a given exponential family<sup>8</sup>, termed  $k$ -MLE [111]. We may extend  $k$ -MLE to learning mixtures with different exponential families for components (e.g., generalized Gaussians [112]) and reported our implementation for Wishart mixtures in [113]. We studied Bregman sided and Bregman symmetrized centroids in [114]: Symmetrized Bregman centroids are geometrically characterized as the intersection of a mixed bisector with a geodesic yielding a fast numerical approximation scheme. The centroids with respect to conformal divergences is addressed in [115]. We further considered  $k$ -means clustering with respect to  $\alpha$ -divergences [116] and total Bregman/Jensen divergences [117]. We can also reinterpret symmetrized Bregman divergences as curved Bregman divergences [118]. The particular case of Jeffreys centroid (i.e., symmetrized Kullback-Leibler centroid interpreted as a symmetrized Bregman centroid) is expressed using Lambert  $W$  function [119] and the Jeffreys' centroids can be approximated fast [120] using proxy centroids (e.g., Gauss-Bregman inductive mean [121]). Jeffreys divergence between Gaussian mixture models (GMMs) are not known in closed-form but can be approximated efficiently [122]. Information-theoretic weighted clustering unifying various clustering techniques was reported in [123]. More generally, we studied the centroids with respect to skew Jensen divergences [124] (including Bregman sided centroids in limit skewing cases). In general,  $k$ -means type algorithms are NP-hard as soon as the dimension is greater or equal than 2. In 1D, we can use dynamic programming (DP) to solve for the optimal interval clustering [125].

Chernoff information [126] (CI) between two densities of an exponential family (CI is commonly used for example when bounding the exponent error in Bayesian hypothesis testing [127] or in information fusion [128]) can be explained from the information-geometric viewpoint as the intersection of a bisector with a dual geodesic [129]. For arbitrary two probability measures, their geometric mixture arc forms an exponential family called a Likelihood ratio exponential family (LREF) [130] and the CI analysis of [129] is generalized in [131]. As a byproduct, this CI study proves that the intersection of a primal bisector with a dual

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<sup>7</sup>VC-dimension is used to characterize performance of algorithms in machine learning.

<sup>8</sup>Exponential families [108] are families which maximize entropies given moments constraints. For example, the Gaussian family maximizes the differential entropy under the first and second moments constraints (i.e., a continuous exponential family). Similarly, lattice Gaussian families are discrete exponential families under the first two moment constraints for samples spaces being lattices [109]. Thus exponential families are also called maximal entropy distributions [110].

geodesic is unique: This is a pure information geometric result. More general paths between probability/unnormalized distributions than the arithmetic and geometric mixtures can be considered: For example, the  $q$ -power paths was shown to yield useful results in simulated annealing and thermodynamic integration methods [132, 133] often used in statistics and ML.

The cumulant functions of exponential families [134] are Legendre-type convex analytic functions. Their corresponding partition functions are log-convex and thus also convex (because the geometric mean is dominated by the arithmetic mean). The statistical divergences corresponding to the Bregman divergences induced by the cumulants and partition functions of exponential families are the reverse Kullback-Leibler divergence (KLD) and reverse extended KLD between normalized and unnormalized densities [135], respectively.

Another class of statistical models admitting dually flat connections are mixture families [136], i.e., linear combinations of linearly independent (probability) densities. It can be shown that the neg-entropy of such statistical mixtures with prescribed components (called  $w$ -mixtures in [137]) are Legendre-type generators which yields Hessian/Bregman manifolds. In general, the neg-entropy of continuous mixtures is not available in closed form: But let us note in passing that there is an interesting case of mixtures of two Cauchy distributions (i.e., mixture family of order 1 parameterized by a scalar weight  $w \in (0, 1)$ ) for which the differential entropy and the Jensen-Shannon divergence admit closed-form formula [138]. Cauchy distributions enjoy the property that their Kullback-Leibler divergence and any other  $f$ -divergences [139] is symmetric and can be expressed as scalar functions of their closed-form chi-square distances [140]. The Jensen-Shannon centroid [141] of a set of categorical distributions amount to a Jensen divergence on the mixture parameters (because mixtures are closed by linear combinations) and can be calculated using the convex-concave procedure [142] (i.e., difference of convex function algorithm, DCA [143] for short).

On a Bregman manifold, the Hessian metric can be expressed equivalently as the matrix Hessians of the dual convex potential functions in the respective primal/dual parameterizations. Remarkably, the squared Hessian matrices of the convex function encodes the Euclidean metric in the dual coordinate systems [144], and thus the Riemannian geodesic distances for the squared Hessian matrices are the Euclidean distance expressed in the dual coordinate systems (see [145] for the case of separable potential functions).

A novel dualistic structure on the James' SPD double cone model equipped with a mix of logdet and identity-complementary logdet barrier functions was studied in [75].

In practice, the generator  $F$  and/or its inverse gradient  $(\nabla F)^{-1}$  may not be available in closed form or is computationally intractable when handling log-normalizers of exponential families (e.g., discrete exponential families of some learning machines like Boltzmann machines). We proposed Monte Carlo information geometry which samples the log-normalizer integrals and yields with high probability a proper Bregman tractable generator [146] (random information geometry). We also consider using NNs to estimate Legendre transforms [147] using the affine gauge freedom [90] of Legendre transform. We currently work on the framework of neural information geometry (NIG) which uses NNs as function approximators to implement information-geometric structures in practice.

Information geometry of  $f$ -divergences are studied in [148]. When not available in closed-form,  $f$ -divergences can be estimated using Monte Carlo techniques [149]. Invariance and

spectral structures of  $f$ -divergences between multivariate location-scale families are reported in [150].

**Optimal transport geometry.** Optimal transport [60] (OT) is a mathematical field that gained a lot of attention in machine learning and computer vision because it allows to flexibly measure dissimilarities between discrete (empirical) distributions, or between continuous and discrete distributions. We proposed the earth mover distance [151] (i.e., with respect to ground distance  $\ell_1$ ) between superpixels obtained by oversegmentation for computer vision tasks [152]. Sinkhorn algorithm [153] is one of the most important computational methods for solving OTs through entropic regularization. We considered Tsallis regularized OT (instead of Shannon entropy [154]) with applications to ecological inference tasks [155]. We compared several distances for clustering multivariate time series [156, 157] based on Sklar’s theorem, and proposed optimal copula transport in [158]. We gave an approximation method based on the chain rule and marginalization of probabilities in [159]. We proposed a Sinkhorn autoencoder architecture [61]. Kantorovich unregularized OT yields a sparse plan but is time consuming while Sinkhorn entropic-regularized OT is fast but yields dense transport plans. We built a middle ground technique for fast OT approximation algorithm which allows one to control the degree of sparsity based on tempered exponential measures [160] (TEMs) in [161]. Otto proposed a Riemannian geometry by means of a regular Riemannian metric [162] (Otto metric), and information-geometric dualistic structures [163] are studied in the Wasserstein information geometry.

**Cone geometry.** A domain  $K$  of a vector space is a cone if for any  $\lambda > 0$ , we have  $\lambda K \subseteq K$ . Cones need not necessarily to be convex and may potentially contain lines. We consider regular cones defined as open convex pointed cones. The most studied cone is the cone of symmetric positive-definite (SPD) matrices. The geometry of cones was studied by Vinberg [164] where he defined a characteristic function  $\chi_K$  associated to each regular cone  $K$ . Since the characteristic function is Legendre-type, we recover a dual Hessian structure [17]. We considered the diffeomorphic embeddings of  $d$ -variate normal distributions into  $(d + 1)$ -SPD cone in [165] to define a fast distance between normal distributions. We considered also an equivariant mean on irreducible symmetric cones [166] with an application to  $k$ -mean clustering of SPD matrices in [167].

**Infinite-dimensional (RKHS) Hilbert space.** Bregman already considered (potentially infinite-dimensional) Hilbert metrics in his celebrated paper [168] that gave rise to the so-called (finite-dimensional vector) Bregman divergences. Matrix Bregman divergences with respect to inner products were investigated in [169] and in [170] with an application to portfolio theory. Gaussian measures in infinite-dimensional Hilbert spaces behave very differently from the finite-dimensional cases (e.g., there is no infinite-dimensional Lebesgue measure and the usual notion of covariance matrices is replaced by trace-class operators, etc.). We extend the geometric Jensen-Shannon divergence [21] which admits a closed-form<sup>9</sup> between finite-dimensional Gaussians to the Gaussian measures in a general Hilbert space in [172]. We generalize the maximum mean discrepancy (MMD) in [173] and proposed kernelised functional Bregman divergences using reproducible kernel Hilbert spaces [174] (RKHSs). Functional Bregman divergences have proven useful in Bayesian statistics [175]

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<sup>9</sup>The ordinary Jensen-Shannon divergence between Gaussians is not even analytic [171].

and pointwise Bregman divergences [176] are commonly considered, e.g., in rate-distortion view of uncertainty quantification [177].

**Euclidean geometry.** At infinitesimal scale, manifolds can be locally considered as Euclidean spaces (i.e., extrinsic geometry on tangent planes). Euclidean geometry can also be handled as a particular Riemannian manifold equipped with the Euclidean (Riemannian) metric. My PhD work focused on adaptive computational geometry [10] which generalizes the notion of output-sensitive algorithms: For example, I considered output-sensitive algorithms for computing a given number of maximal layers (Pareto fronts [178]) or convex layers [179] (onion peelings) which finds useful applications in database applications for computing skylines [180]. I designed a paradigm called grouping-and-querying [181] to get output-sensitive algorithms and used this paradigm to calculate the convex hulls of arbitrary objects (i.e., ellipses) on the plane [27]. The concept of adaptive algorithms vs output-sensitive algorithms is well illustrated when calculating the union of  $n$  intervals on a line [182]: We report a  $O(n \log p)$ -time algorithm for calculating the union of intervals where  $p \geq c$  is the minimum number of piercing points and  $c$  is the number of connected components (in worst-case scenario,  $c = 1$  but  $p = n - 1$ ). Thus given a problem, it is open to find new measures varying with instances and design algorithms taking into account those adaptive parameters. For example, we considered data structures for point location using the notion of fatness of objects in [183], etc. Combinatorial piercing/covering problems are such kinds of NP-hard problems with applications in telecommunications where adaptive heuristics can be designed (e.g., finding locations of base transceiver stations [184]).

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