

On the f -divergences between hyperboloid and Poincaré distributions

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Abstract. Hyperbolic geometry has become popular in machine learning due to its capacity to embed hierarchical graph structures with low distortions for further downstream processing. It has thus become important to consider statistical models and inference methods for data sets grounded in hyperbolic spaces. In this note, we study f -divergences between the Poincaré distributions and the related hyperboloid distributions.

Keywords: exponential family · group action · maximal invariant · Csiszár's f -divergence.

1 Introduction

Hyperbolic geometry³ [2] is very well suited for embedded tree graphs with low distortions [20] as hyperbolic Delaunay subgraphs of embedded tree nodes. So a recent trend in machine learning and data science is to embed discrete hierarchical graphs into continuous spaces with low distortions for further downstream tasks. There exists many models of hyperbolic geometry [2] like the Poincaré disk or upper-half plane conformal models, the Klein non-conformal disk model, the Beltrami hemisphere model, the Minkowski or Lorentz hyperboloid model, etc. We can transform one model of hyperbolic geometry to another model by a bijective mapping yielding a corresponding isometric embedding [11]. As a byproduct of the low-distortion hyperbolic embeddings of hierarchical graphs, many embedded data sets are available in hyperbolic model spaces, and those data sets need to be further processed. Thus it is important to build *statistical models* and *inference methods* for these hyperbolic data sets using probability distributions with support hyperbolic model spaces, and to consider statistical mixtures in those spaces.

Let us quickly review some of the various families of probability distributions defined in hyperbolic models as follows: One of the very first proposed family

³ Hyperbolic geometry has constant negative curvature and the volume of hyperbolic balls increases exponentially with respect to their radii rather than polynomially as in Euclidean space.

of such “hyperbolic distributions” was proposed in 1981 [16] and are nowadays commonly called the *hyperboloid distributions*. The hyperboloid distributions are defined on the Minkowski upper sheet hyperboloid by analogy to the von-Mises Fisher distributions [3] which are defined on the sphere. Barbaresco [4] defined the so-called Souriau-Gibbs distributions (2019) in the Poincaré disk (Eq. 57 of [4], a natural exponential family) with its Fisher information metric coinciding with the Poincaré hyperbolic Riemannian metric (the Poincaré unit disk is a homogeneous space where $SU(1, 1)$ Lie group acts transitively).

In this note, we focus on Ali-Silvey-Csiszár’s f -divergences for these distributions [14, 1]. In section 2, we prove using Eaton’s method of group action maximal invariants [15, 19] that all f -divergences (including the Kullback-Leibler divergence) between Poincaré distributions can be expressed canonically as functions of three terms (Proposition 1 and Theorem 1). Then, we deal with the hyperboloid distributions in dimension 2 in §3. We also consider q -deformed family of these distributions. We exhibit a correspondence in §4 between the upper-half plane and the Minkowski hyperboloid 2D sheet. The f -divergences between the hyperboloid distributions are very geometric because it exhibits a beautiful and clear maximal invariant which has connections with the side-angle-side congruence criteria for triangles in hyperbolic geometry. This note is a summarized version of the preprint [18] with some proofs omitted: we refer the reader to it for more details and other topics than f -divergences.

2 The Poincaré distributions

Tojo and Yoshino [22, 21, 23] described a versatile method to build exponential families of distributions on homogeneous spaces which are invariant under the action of a Lie group G generalizing the construction in [13]. They exemplify their “ G/H -method” on the upper-half plane $\mathbb{H} := \{(x, y) \in \mathbb{R}^2 : y > 0\}$ by constructing an exponential family with probability density functions invariant under the action of Lie group $G = SL(2, \mathbb{R})$, the set of invertible matrices with unit determinant. We shall call these distributions the Poincaré distributions, since their sample space $\mathcal{X} = G/H \simeq \mathbb{H}$, and we study this set of distributions as an exponential family [8]: The probability density function (pdf) of a Poincaré distribution [21] expressed using a 3D vector parameter $\theta = (a, b, c) \in \mathbb{R}^3$ is given by

$$p_\theta(x, y) := \frac{\sqrt{ac - b^2} \exp(2\sqrt{ac - b^2})}{\pi} \exp\left(-\frac{a(x^2 + y^2) + 2bx + c}{y}\right) \frac{1}{y^2}, \quad (1)$$

where θ belongs to the parameter space $\Theta := \{(a, b, c) \in \mathbb{R}^3 : a > 0, c > 0, ac - b^2 > 0\}$. The set Θ forms an open 3D convex cone. Thus the Poincaré distribution family has a 3D parameter cone space and the sample space is the hyperbolic upper plane. We also have a matrix form. Indeed, we can naturally identify Θ with the set of real symmetric positive-definite matrices $\text{Sym}^+(2, \mathbb{R})$

by the mapping $(a, b, c) \mapsto \begin{bmatrix} a & b \\ b & c \end{bmatrix}$. Hereafter, we denote the determinant of θ by $|\theta| := \sqrt{ac - b^2} > 0$ and the trace of θ by $\text{tr}(\theta) = a + c$ for $\theta = (a, b, c) \simeq \begin{bmatrix} a & b \\ b & c \end{bmatrix}$.

The f -divergence [14, 1] induced by a convex generator $f : (0, \infty) \rightarrow \mathbb{R}$ between two pdfs $p(x, y)$ and $q(x, y)$ defined on the support \mathbb{H} is defined by

$$D_f(p : q) := \int_{\mathbb{H}} p(x, y) f\left(\frac{q(x, y)}{p(x, y)}\right) dx dy.$$

Since $D_f(p : q) \geq f(1)$, we consider convex generators $f(u)$ such that $f(1) = 0$. The class of f -divergences includes the total variation distance ($f(u) = |u - 1|$), the Kullback-Leibler divergence ($f(u) = -\log(u)$, and its two common symmetrizations, namely, the Jeffreys divergence and the Jensen-Shannon divergence), the squared Hellinger divergence, the Pearson and Neyman sided χ^2 -divergences, etc.

We state the notion of maximal invariant by following [15]: Let G be a group acting on a set X . We denote it by $(g, x) \mapsto gx$.

Definition 1. We say that a map φ from X to a set Y is maximal invariant if it is invariant, specifically, $\varphi(gx) = \varphi(x)$ for every $g \in G$ and $x \in X$, and furthermore, whenever $\varphi(x_1) = \varphi(x_2)$ there exists $g \in G$ such that $x_2 = gx_1$. Every invariant map is a function of a maximal invariant. Specifically, if a map ψ from X to a set Z is invariant, then, there exists a map Φ from $\varphi(X)$ to Z such that $\Phi \circ \varphi = \psi$.

For each $x \in X$, we may consider its orbit $O_x := \{gx : g \in G\}$. A map is invariant when it is constant on orbits and maximal invariant when orbits have distinct map values.

Proposition 1. Define a group action of $\text{SL}(2, \mathbb{R})$ to $\text{Sym}(2, \mathbb{R})^2$ by

$$(g, (\theta, \theta')) \mapsto (g^{-\top} \theta g^{-1}, g^{-\top} \theta' g^{-1}).$$

Then, $S(\theta, \theta') := (|\theta|, |\theta'|, \text{tr}(\theta' \theta^{-1}))$ is maximal invariant of the action.

Proof. Observe that S is invariant with respect to the group action: $S(\theta, \theta') = S(g.\theta, g.\theta')$. Assume that $S(\theta^{(1)}, \theta^{(2)}) = S(\widetilde{\theta^{(1)}}, \widetilde{\theta^{(2)}})$. We see that there exists $g_{\theta^{(1)}} \in \text{SL}(2, \mathbb{R})$ such that $g_{\theta^{(1)}}.\theta^{(1)} = g_{\theta^{(1)}}^{-\top} \theta^{(1)} g_{\theta^{(1)}}^{-1} = \sqrt{|\theta^{(1)}|} I_2$, where I_2 denotes the 2×2 identity matrix. Then, $\theta^{(1)} = \sqrt{|\theta^{(1)}|} g_{\theta^{(1)}}^{\top} g_{\theta^{(1)}}$. Let $\theta^{(3)} := g_{\theta^{(1)}}.\theta^{(2)} = g_{\theta^{(1)}}^{-\top} \theta^{(2)} g_{\theta^{(1)}}^{-1}$. Then $\text{tr}(\theta^{(3)}) = \text{tr}(\theta^{(2)} g_{\theta^{(1)}}^{-1} g_{\theta^{(1)}}^{-\top}) = \sqrt{|\theta^{(1)}|} \text{tr}(\theta^{(2)} (\theta^{(1)})^{-1})$. We define $g_{\widetilde{\theta^{(1)}}}$ and $\widetilde{\theta^{(3)}}$ in the same manner. Then, $\text{tr}(\theta^{(3)}) = \text{tr}(\widetilde{\theta^{(3)}})$ and $|\theta^{(3)}| = |\widetilde{\theta^{(3)}}|$. Hence the set of eigenvalues of $\theta^{(3)}$ and $\widetilde{\theta^{(3)}}$ are identical with each other. By this and $\theta^{(3)}, \widetilde{\theta^{(3)}} \in \text{Sym}(2, \mathbb{R})$, there exists $h \in \text{SO}(2, \mathbb{R})$ such that $h.\theta^{(3)} = \widetilde{\theta^{(3)}}$. Hence $(hg_{\theta^{(1)}}).\theta^{(2)} = g_{\widetilde{\theta^{(1)}}}.\theta^{(2)}$. We also see that

$$(hg_{\theta^{(1)}}).\theta^{(1)} = g_{\theta^{(1)}}.\theta^{(1)} = \sqrt{|\theta^{(1)}|} I_2 = \sqrt{|\widetilde{\theta^{(1)}}|} I_2 = g_{\widetilde{\theta^{(1)}}}.\widetilde{\theta^{(1)}}.$$

Thus we have $(\widetilde{\theta^{(1)}}, \widetilde{\theta^{(2)}}) = (g_{\theta^{(1)}}^{-1} h g_{\theta^{(1)}}) \cdot (\theta^{(1)}, \theta^{(2)})$.

By direct calculations, we have that

Proposition 2. $D_f [p_\theta : p_{\theta'}] = D_f [p_{g^{-\top} \theta g^{-1}} : p_{g^{-\top} \theta' g^{-1}}]$

By Propositions 1 and 2, we get

Theorem 1. *Every f -divergence between two Poincaré distributions p_θ and $p_{\theta'}$ is a function of $(|\theta|, |\theta'|, \text{tr}(\theta' \theta^{-1}))$.*

We have exact formulae for the Kullback-Leibler divergence, the squared Hellinger divergence, and the Neyman chi-squared divergence.

Proposition 3. *We have the following results for two Poincaré distributions p_θ and $p_{\theta'}$.*

(i) (*Kullback-Leibler divergence*) Let $f(u) = -\log u$. Then,

$$D_f [p_\theta : p_{\theta'}] = \frac{1}{2} \log \frac{|\theta|}{|\theta'|} + 2 \left(\sqrt{|\theta|} - \sqrt{|\theta'|} \right) + \left(\frac{1}{2} + \sqrt{|\theta|} \right) (\text{tr}(\theta' \theta^{-1}) - 2).$$

(ii) (*squared Hellinger divergence*) Let $f(u) = (\sqrt{u} - 1)^2/2$. Then,

$$D_f [p_\theta : p_{\theta'}] = 1 - \frac{2|\theta|^{1/4} |\theta'|^{1/4} \exp((|\theta|^{1/2} + |\theta'|^{1/2})/2)}{|\theta + \theta'|^{1/2} \exp(|\theta + \theta'|^{1/2}/2)}.$$

(iii) (*Neyman chi-squared divergence*) Let $f(u) := (u-1)^2$. Assume that $2\theta' - \theta \in \Theta$. Then,

$$D_f [p_\theta : p_{\theta'}] = \frac{|\theta'| \exp(4|\theta'|^{1/2})}{|\theta|^{1/2} |2\theta' - \theta|^{1/2} \exp(2(|\theta|^{1/2} + |2\theta' - \theta|^{1/2}))} - 1.$$

Thus the KLD between two Poincaré distributions is asymmetric: $D_{\text{KL}}[p_\theta : p_{\theta'}] \neq D_{\text{KL}}[p_{\theta'} : p_\theta]$.

Recently, Tojo and Yoshino [23] introduced a notion of deformed exponential family associated with their G/H method in representation theory. As an example of it, they considered a family of *deformed Poincaré distributions* with index $q > 1$. For $x \in I_q := \{x \in \mathbb{R} : (1-q)x + 1 > 0\}$, let $\exp_q(x) := ((1-q)x + 1)^{1/(1-q)}$. For $q \in [1, 2)$, let a q -deformed Poincaré distribution be the distribution

$$p_\theta(x, y) := c_q(D) \exp_q \left(-\frac{a(x^2 + y^2) + 2bx + c}{y} \right) \frac{1}{y^2},$$

where $c_q(x) := \frac{(2-q)x}{\pi (\exp_q(-2x))^{2-q}}$. In this case, we also obtain that

Theorem 2. *Let $q \in [1, 2)$. Every f -divergence between two q -deformed Poincaré distributions p_θ and $p_{\theta'}$ is a function of $(|\theta|, |\theta'|, \text{tr}(\theta' \theta^{-1}))$.*

We proved this by Theorem 4 below and the correspondence principle in §4.

3 The two-dimensional hyperboloid distribution

We first give the definition of the Lobachevskii space (in reference to Minkowski hyperboloid model of hyperbolic geometry also called the Lorentz model) and the parameter space of the hyperboloid distribution. We focus on the case that $d = 2$. Let $\mathbb{L}^2 := \{(x_0, x_1, x_2) \in \mathbb{R}^3 : x_0 = \sqrt{1 + x_1^2 + x_2^2}\}$ and $\Theta_{\mathbb{L}^2} := \{(\theta_0, \theta_1, \theta_2) \in \mathbb{R}^3 : \theta_0 > \sqrt{\theta_1^2 + \theta_2^2}\}$. Let the Minkowski inner product [12] be $[(x_0, x_1, x_2), (y_0, y_1, y_2)] := x_0y_0 - x_1y_1 - x_2y_2$. We have $\mathbb{L}^2 = \{x \in \mathbb{R}^3 : [x, x] = 1\}$.

Now we define the *hyperboloid distribution* by following [5, 7, 9]. Hereafter, for ease of notation, we let $|\theta| := [\theta, \theta]^{1/2}$, $\theta \in \Theta_{\mathbb{L}^2}$. For $\theta \in \Theta_{\mathbb{L}^2}$, we define a probability measure P_θ on $\mathbb{L}^d \simeq \mathbb{R}^d$ by

$$P_\theta(dx_1dx_2) := c_2(|\theta|) \exp(-[\theta, \tilde{x}]) \mu(dx_1dx_2), \quad (2)$$

where we let $c_2(t) := \frac{t \exp(t)}{2(2\pi)^{1/2}}$, $t > 0$, $\tilde{x} := (\sqrt{1 + x_1^2 + x_2^2}, x_1, x_2)$, and $\mu(dx_1dx_2) := \frac{1}{\sqrt{1 + x_1^2 + x_2^2}} dx_1dx_2$. The 1d hyperboloid distribution was first introduced in statistics in 1977 [6] to model the log-size distributions of particles from aeolian sand deposits, but the 3D hyperboloid distribution was later found already studied in statistical physics in 1911 [17]. The 2d hyperboloid distribution was investigated in 1981 [10].

Now we consider group actions to the space of parameters $\Theta_{\mathbb{L}^2}$. Let the indefinite special orthogonal group be

$$\text{SO}(1, 2) := \{A \in \text{SL}(3, \mathbb{R}) : [Ax, Ay] = [x, y] \ \forall x, y \in \mathbb{R}^3\},$$

and $\text{SO}_0(1, 2) := \{A \in \text{SO}(1, 2) : A(\mathbb{L}^2) = \mathbb{L}^2\}$.

An action of $\text{SO}_0(1, 2)$ to $(\Theta_{\mathbb{L}^2})^2$ is defined by

$$\text{SO}_0(1, 2) \times (\Theta_{\mathbb{L}^2})^2 \ni (A, (\theta, \theta')) \mapsto (A\theta, A\theta') \in (\Theta_{\mathbb{L}^2})^2.$$

Proposition 4. $(\theta, \theta') \mapsto ([\theta, \theta], [\theta', \theta'], [\theta, \theta'])$ is maximal invariant for the action of $\text{SO}_0(1, 2)$ to $(\Theta_{\mathbb{L}^2})^2$.

In the following proof, all vectors are column vectors.

Proof. It is clear that the map is invariant with respect to the group action. Assume that

$$\left([\theta^{(1)}, \theta^{(1)}], [\theta^{(2)}, \theta^{(2)}], [\theta^{(1)}, \theta^{(2)}]\right) = \left([\widetilde{\theta}^{(1)}, \widetilde{\theta}^{(1)}], [\widetilde{\theta}^{(2)}, \widetilde{\theta}^{(2)}], [\widetilde{\theta}^{(1)}, \widetilde{\theta}^{(2)}]\right).$$

Let $\psi_i := \frac{\theta^{(i)}}{|\theta^{(i)}|}$, $\widetilde{\psi}_i := \frac{\widetilde{\theta}^{(i)}}{|\widetilde{\theta}^{(i)}|}$, $i = 1, 2$. Then, $[\psi_1, \psi_2] = [\widetilde{\psi}_1, \widetilde{\psi}_2]$.

We first consider the case that $\psi_1 = \widetilde{\psi}_1 = (1, 0, 0)^\top$. Let $\psi_i = (x_{i0}, x_{i1}, x_{i2})^\top$, $\widetilde{\psi}_i = (\widetilde{x}_{i0}, \widetilde{x}_{i1}, \widetilde{x}_{i2})^\top$, $i = 1, 2$. Then, $x_{20} = \widetilde{x}_{20} > 0$, $x_{21}^2 + x_{22}^2 = \widetilde{x}_{21}^2 + \widetilde{x}_{22}^2$ and hence

there exists an orthogonal matrix P such that $P(x_{21}, x_{22})^\top = (\widetilde{x}_{21}, \widetilde{x}_{22})^\top$. Let $A := \begin{pmatrix} 1 & 0 \\ 0 & P \end{pmatrix}$. Then, $A \in \text{SO}_0(1, 2)$, $A\psi_1 = (1, 0, 0)^\top = \widetilde{\psi}_1$ and $A\psi_2 = \widetilde{\psi}_2$.

We second consider the general case. Since the action of $\text{SO}_0(1, 2)$ to \mathbb{L}^2 defined by $(A, \psi) \mapsto A\psi$ is transitive, there exist $A, B \in \text{SO}_0(1, 2)$ such that $A\psi_1 = B\widetilde{\psi}_1 = (1, 0, 0)^\top$. Thus this case is attributed to the first case.

We regard μ as a probability measure on \mathbb{L}^2 . We recall that $[A\theta, A\widetilde{x}] = [\theta, \widetilde{x}]$ for $A \in \text{SO}_0(1, 2)$. We remark that μ is an $\text{SO}(1, 2)$ -invariant Borel measure [16] on \mathbb{L}^2 . Now we have that

Theorem 3. *Every f -divergence between p_θ and $p_{\theta'}$ is invariant with respect to the action of $\text{SO}_0(1, 2)$, and is a function of the triplet $([\theta, \theta], [\theta', \theta'], [\theta, \theta'])$.*

There is a clear geometric interpretation of this: The side-angle-side theorem for triangles in Euclidean geometry states that if two sides and the included angle of one triangle are equal to two sides and the included angle of another triangle, the triangles are congruent. This is also true for the hyperbolic geometry and it corresponds to Proposition 4 above. Every f -divergence is determined by the triangle formed by a pair of the parameters (θ, θ') when f is fixed.

Proposition 5. *We have the following results for two hyperboloid distributions p_θ and $p_{\theta'}$.*

(i) *(Kullback-Leibler divergence) Let $f(u) = -\log u$. Then,*

$$D_f[p_\theta : p_{\theta'}] = \log \left(\frac{|\theta|}{|\theta'|} \right) - |\theta'| + \frac{[\theta, \theta']}{[\theta, \theta]} + \frac{[\theta, \theta']}{|\theta|} - 1.$$

(ii) *(squared Hellinger divergence) Let $f(u) = (\sqrt{u} - 1)^2/2$. Then,*

$$D_f[p_\theta : p_{\theta'}] = 1 - \frac{2|\theta|^{1/2}|\theta'|^{1/2} \exp(|\theta|/2 + |\theta'|/2)}{|\theta + \theta'| \exp(|\theta + \theta'|/2)}.$$

(iii) *(Neyman chi-squared divergence) Let $f(u) := (u-1)^2$. Assume that $2\theta' - \theta \in \Theta_{\mathbb{L}^2}$. Then,*

$$D_f[p_\theta : p_{\theta'}] = \frac{|\theta'|^2 \exp(4|\theta'|)}{|\theta||2\theta' - \theta| \exp(2|\theta| + 2|2\theta' - \theta|)} - 1.$$

Now we consider deformations of the hyperboloid distribution. For $q \in [1, 2)$, we let a q -deformed hyperboloid distribution be the distribution

$$p_\theta(x_1, x_2) := c_q(|\theta|) \exp_q(-[\theta, \widetilde{x}]) \frac{1}{\sqrt{1 + x_1^2 + x_2^2}},$$

where $c_q(z) := \frac{(2-q)z}{2\pi(\exp_q(-z))^{2-q}}$.

In the same manner as in the derivation of Theorem 3, we obtain that

Theorem 4 (Canonical terms of the f -divergences between deformed hyperboloid distributions). *Let $q \in [1, 2)$. Then, every f -divergence between q -deformed hyperboloid distributions p_θ and $p_{\theta'}$ is invariant with respect to the action of $\text{SO}_0(1, 2)$, and is a function of the triplet $([\theta, \theta], [\theta', \theta'], [\theta, \theta'])$.*

4 Correspondence principle

It is well-known that there is a correspondence between the 2d Lobachevskii space $\mathbb{L} = \mathbb{L}^2$ and the Poincaré upper-half plane \mathbb{H} .

Proposition 6 (Correspondence between the parameter spaces). *For $\theta = (a, b, c) \in \Theta_{\mathbb{H}} := \{(a, b, c) : a > 0, c > 0, ac > b^2\}$, let $\theta_{\mathbb{L}} := (a+c, a-c, 2b) \in \Theta_{\mathbb{L}}$. We denote the f -divergence between $\{p_{\theta}\}_{\theta \in \Theta_{\mathbb{L}}}$ and $\{p_{\theta}\}_{\theta \in \Theta_{\mathbb{H}}}$ by $D_f^{\mathbb{L}}(\cdot : \cdot)$ and $D_f^{\mathbb{H}}(\cdot : \cdot)$ respectively. Then,*

(i) For $\theta, \theta' \in \Theta_{\mathbb{H}}$,

$$|\theta_{\mathbb{L}}|^2 = [\theta_{\mathbb{L}}, \theta_{\mathbb{L}}] = 4|\theta|, \quad |\theta'_{\mathbb{L}}|^2 = [\theta'_{\mathbb{L}}, \theta'_{\mathbb{L}}] = 4|\theta'|, \quad [\theta_{\mathbb{L}}, \theta'_{\mathbb{L}}] = 2|\theta| \operatorname{tr}(\theta' \theta^{-1}). \quad (3)$$

(ii) For every f and $\theta, \theta' \in \mathbb{H}$,

$$D_f^{\mathbb{L}}[p_{\theta_{\mathbb{L}}} : p_{\theta'_{\mathbb{L}}}] = D_f^{\mathbb{H}}[p_{\theta} : p_{\theta'}]. \quad (4)$$

For (i), at its first glance, there is an inconsistency in notation. However, $|\theta|$ is the Minkowski norm for $\theta \in \theta_{\mathbb{L}}$, and, $|\theta|$ is the determinant for $\theta \in \Theta_v$, so the notation is consistent in each setting. By this assertion, it suffices to compute the f -divergences between the hyperboloid distributions on \mathbb{L} .

Let $\mu_{\mathbb{H}}(dxdy) := \frac{dxdy}{y^2}$ and $\mu_{\mathbb{L}}(dxdy) := \frac{dxdy}{\sqrt{1+x^2+y^2}}$. By the change of variable $\mathbb{H} \ni (x, y) \mapsto (X, Y) = \left(\frac{1-x^2-y^2}{2y}, \frac{x}{y}\right) \in \mathbb{R}^2$, by recalling the correspondence between the parameters in Eq. (3), it holds that $y^2 p_{\theta}(x, y) = \sqrt{1+X^2+Y^2} p_{\theta_{\mathbb{L}}}(X, Y)$, and $\mu_{\mathbb{H}}(dxdy) = \mu_{\mathbb{L}}(dXdY)$.

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