

Fully-Connected Network on Noncompact Symmetric Space and Ridgelet Transform based on Helgason-Fourier Analysis

Sho Sonoda ¹ Isao Ishikawa ^{1,2} Masahiro Ikeda ¹

¹RIKEN Center for Advanced Intelligence Project (RIKEN AIP), Tokyo, Japan

²Ehime University, Ehime, Japan

The 39th International Conference on Machine Learning (ICML2022),
Baltimore, Maryland USA
July 17-23, 2022



Main Contributions

In this study, we have

- devised a *fully-connected network* $S[\gamma]$ on noncompact symmetric spaces $X = G/K$, which covers Hyperbolic NNs and SPD Nets as special cases;
- derived the *ridgelet transform* $R[f; \rho]$, a closed-form analysis operator satisfying the reconstruction formula $S[R[f; \rho]] = ((\sigma, \rho))f$, based on the *Helgason-Fourier transform on G/K* , and
- presented a constructive proof of the *cc-universality of finite networks on G/K* by discretizing the reconstruction formula in a *coordinate-free and unified manner*

A Noncompact Symmetric Space G/K

- is a homogeneous space G/K with *nonpositive sectional curvature* on which G acts transitively

Definition (Noncompact Symmetric Space G/K)

- Let G be a connected semisimple real Lie group, and
- let $G = KAN$ be the Iwasawa decomposition.
- The quotient (the set of all left cosets)

$$X := G/K = \{gK \mid g \in G\},$$

is called a noncompact symmetric space.

Example (Hyperbolic Space \mathbb{H}^m)

for embedding words, and tree-structured dataset

Example (SPD Manifold \mathbb{P}_m)

or a manifold of positive definite matrices, e.g., covariance matrices

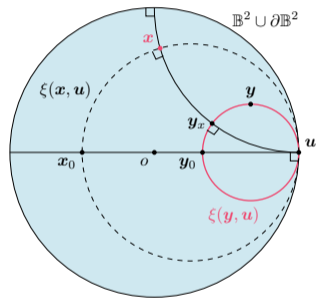


Figure: The Poincaré Disk \mathbb{B}^2 is a 2-dim. Hyperbolic space

Neural Networks on G/K

- are developing, but lack expressive power analysis
- Difficulty: There are no canonical ways to define an “affine map $\mathbf{a} \cdot \mathbf{x} - b$ on manifold”

(Reference) Euclidean NN

For any nonlinear function $\sigma : \mathbb{R} \rightarrow \mathbb{R}$, parameters $(\mathbf{a}_i, b_i, c_i) \in \mathbb{R}^m \times \mathbb{R} \times \mathbb{R}$, a Euclidean NN (a depth-2 fully-connected neural network on \mathbb{R}^m) is given by

$$f(\mathbf{x}) = \sum_{i=1}^p c_i \sigma(\mathbf{a}_i \cdot \mathbf{x} - b_i), \quad \mathbf{x} \in \mathbb{R}^m$$

Hyperbolic NNs (Ganea+18, Gulcehre+19, Shimizu+21)

- For each point $x \in \mathbb{H}^m$,
- the affine map is re-defined by Gyrovector calculus,
- the elementwise activation is defined on a tangent space: $\exp_0 \circ \sigma \circ \log_0(x)$

SPDNets (Huang-Gool17, Dong+17, Gao+19)

- For an SPD matrix $x \in \mathbb{P}_m$,
- BiMap layer: $w^\top x w$
- ReEig layer: $u^\top \max(0, \lambda - b) u$
where $x = u^\top \lambda u$

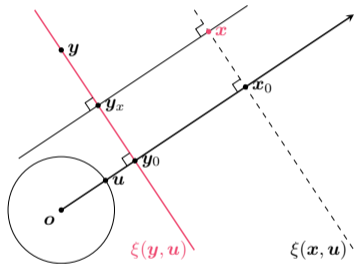
Geometric Reformulation of Euclidean Fully-Connected Neuron $\sigma(\mathbf{a} \cdot \mathbf{x} - b)$

As a “*wavelet function* on the *signed distance* between a *point* \mathbf{x} and a *hyperplane* ξ ”:

$$\sigma(\mathbf{a} \cdot \mathbf{x} - b) = \sigma(rd(\mathbf{x}, \xi)), \quad (\text{geometric, or coordinate-free})$$

where

- $\mathbf{a} = r\mathbf{u}$ (polar coordinates $(r, \mathbf{u}) \in \mathbb{R} \times \mathbb{S}^{m-1}$)
- $\xi := \{\mathbf{y} \in \mathbb{R}^m \mid r\mathbf{u} \cdot \mathbf{y} = b\}$ (a hyperplane passing through point $(b/r)\mathbf{u}$ with normal \mathbf{u})
- $d(\mathbf{x}, \xi)$ signed distance from point \mathbf{x} to hyperplane ξ
- $d \mapsto \sigma(rd)$ wavelet function



Main Results 1/3: A Continuous Neural Network on G/K

Definition (Continuous Horospherical X -NN)

$$S[\gamma](x) := \int_{\mathfrak{a}^* \times \partial X \times \mathbb{R}} \gamma(a, u, b) \sigma(a \cdot \langle x, u \rangle - b) e^{\rho \langle x, u \rangle} da du db, \quad x \in X$$

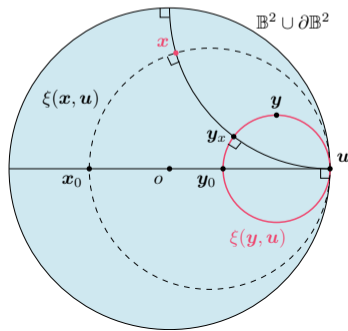
- i.e., a continuous frame defined by weighted fully-connected neurons $x \mapsto \sigma(\dots)$
- $\mathfrak{a} = \mathfrak{a}^* = \mathbb{R}^r$ for $r := \text{rank } X$ (Lie algebra and its dual of A of $G = KAN$)
- $\rho \in \mathfrak{a}^*$ constant vector

\mathfrak{a} -valued composite distance $\langle x, u \rangle$

is a vector distance from the origin o to a horosphere $\xi(x, u)$ (i.e., $|\langle x, u \rangle|$ becomes the Riemannian distance)

horosphere $\xi(x, u)$ passing through point $x \in X$ normal $u \in \partial X$

is a sphere in G/K with infinite radius (Recall that a Euclidean hyperplane is a *Euclidean sphere with infinite radius*)



Main Results 2/3: Ridgelet Transform

- is an analysis operator (or a pseudo-inverse operator) of integral representation operator S

Definition (Ridgelet Transform)

For any function $f : G/K \rightarrow \mathbb{C}$ and an auxiliary function $\rho : \mathbb{R} \rightarrow \mathbb{R}$,

$$R[f](a, u, b) := \int_X c[f](x) \overline{\rho(a \cdot \langle x, u \rangle - b)} e^{g\langle x, u \rangle} dx$$

where $c[f]$ is a Helgason-Fourier multiplier.

Theorem (Reconstruction Formula)

For any $f \in L^2(X)$ (or $f \in C_c^\infty(X)$), $\sigma \in \mathcal{S}'(\mathbb{R})$, $\rho \in \mathcal{S}(\mathbb{R})$,

$$S[R[f; \rho]] = ((\sigma, \rho))f.$$

where $((\sigma, \rho))$ is a scalar product.

- i.e., a *constructive* universal approximation theorem for *continuous* neural networks on G/K

Main Results 3/3: cc -Universality

- is a *constructive* universal approximation theorem for *finite* neural networks on G/K

Theorem (cc -Universality of X -NNs)

For any $\varepsilon > 0$, compact set $Z \subset X$, functions $f \in C(Z)$, $\sigma \in \mathcal{S}'(\mathbb{R})$, $\rho \in \mathcal{S}(\mathbb{R})$, there exists a finite neural network of the form

$$f(x) := \sum_{i=1}^n c_i \sigma(a_i \cdot \langle x, u_i \rangle - b_i) e^{\rho \langle x, u_i \rangle}, \quad x \in X = G/K$$

satisfying

$$\sup_{x \in Z} |f_n(x) - f(x)| < \varepsilon.$$

- i.e., the density of finite NNs in continuous functions w.r.t. the compact convergence

Examples: Horospherical HNN and SPD Net

Continuous Horospherical Hyperbolic NN

On the *Poincaré ball model* $\mathbb{B}^m := \{\mathbf{x} \in \mathbb{R}^m \mid |\mathbf{x}| < 1\}$ equipped with the Riemannian metric $\mathfrak{g} = 4(1 - |\mathbf{x}|)^{-2} \sum_{i=1}^m dx_i \otimes dx_i$,

$$S[\gamma](\mathbf{x}) := \int_{\mathbb{R} \times \partial\mathbb{B}^m \times \mathbb{R}} \gamma(\mathbf{a}, \mathbf{u}, b) \sigma(\mathbf{a} \langle \mathbf{x}, \mathbf{u} \rangle - b) e^{\varrho \langle \mathbf{x}, \mathbf{u} \rangle} d\mathbf{a} d\mathbf{u} db, \quad \mathbf{x} \in \mathbb{B}^m$$

$$\varrho = (m - 1)/2, \quad \langle \mathbf{x}, \mathbf{u} \rangle = \log \left(\frac{1 - |\mathbf{x}|_E^2}{|\mathbf{x} - \mathbf{u}|_E^2} \right), \quad (\mathbf{x}, \mathbf{u}) \in \mathbb{B}^m \times \partial\mathbb{B}^m$$

Continuous Horospherical SPD Net

$$S[\gamma](\mathbf{x}) := \int_{\mathbb{R}^m \times \partial\mathbb{P}_m \times \mathbb{R}} \gamma(\mathbf{a}, \mathbf{u}, b) \sigma(\mathbf{a} \cdot \langle \mathbf{x}, \mathbf{u} \rangle - b) e^{\varrho \cdot \langle \mathbf{x}, \mathbf{u} \rangle} d\mathbf{a} d\mathbf{u} db, \quad \mathbf{x} \in \mathbb{P}_m$$

$\varrho = (-\frac{1}{2}, \dots, -\frac{1}{2}, \frac{m-1}{4})$, $\langle \mathbf{x}, \mathbf{u} \rangle = \frac{1}{2} \log \lambda(\mathbf{u} \mathbf{x} \mathbf{u}^\top)$, $(\mathbf{x}, \mathbf{u}) \in \mathbb{P}_m \times \partial\mathbb{P}_m$ where λ is the diagonal in the *Cholesky decomposition*

Sketch Proof of Reconstruction Formula

- is based on *Helgason-Fourier analysis* on G/K
- Given a function $f : G/K \rightarrow \mathbb{C}$, solve an integral equation $S[\gamma] = f$ of unknown γ .
- **Step 1:** Turn $S[\gamma]$ to a *Helgason-Fourier expression*:

$$\begin{aligned} S[\gamma](x) &:= \int_{\mathfrak{a}^* \times \partial X \times \mathbb{R}} \gamma(a, u, b) \sigma(a \cdot \langle x, u \rangle - b) e^{\varrho \langle x, u \rangle} da du db \\ &= \frac{1}{2\pi} \int_{\mathbb{R}} \left[\int_{\mathfrak{a}^* \times \partial X} \gamma^\sharp(\lambda/\omega, u, \omega) |\mathbf{c}(\lambda)|^2 e^{(i\lambda + \varrho)\langle x, u \rangle} \frac{d\lambda du}{|\mathbf{c}(\lambda)|^2} \right] |\omega|^{-r} \sigma^\sharp(\omega) d\omega. \end{aligned}$$

- **Step 2:** Since inside $[\dots]$ is the *inverse Helgason-Fourier transform*, put a separation-of-variables form:

$$\gamma_{f,\rho}^\sharp(\lambda/\omega, \mathbf{u}, \omega) = \widehat{f}(\lambda, \mathbf{u}) \overline{\rho^\sharp(\omega)} |\mathbf{c}(\lambda)|^{-2}.$$

Then, by the construction, it is a particular solution:

$$S[\gamma_{f,\rho}] = ((\sigma, \rho)) f,$$

where $((\sigma, \rho)) := \frac{|W|}{2\pi} \int_{\mathbb{R}} \sigma^\sharp(\omega) \overline{\rho^\sharp(\omega)} |\omega|^{-m} d\omega$.

- In the end, we employ $\gamma_{f,\rho}$ as the definition of $R[f; \rho]$