

# AI Pictures at a Mathematical Exhibition: How Applied Harmonic Analysis meets Machine Learning

**Radu Balan**

Department of Mathematics and Norbert Wiener Center for Harmonic  
Analysis and Applications  
University of Maryland, College Park, MD

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University of Torino, Turin, Italy



Norbert Wiener Center  
for Harmonic Analysis and Applications

# Acknowledgments



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**Papers available online at:**

<https://www.math.umd.edu/~rvbalan/>

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# High-Level Overview

In this series of lectures, we discuss a few harmonic analysis techniques and problems applied to machine learning.

1. NN: Neural networks (NN) and their universal approximation property.
2. Lipschitz analysis: we provide rationals for studying Lipschitz properties of NNs, and then we perform a Lipschitz analysis of these networks. We focus on two aspects of this analysis: stochastic modeling of local vs. global analysis, and a scattering network inspired Lipschitz analysis of convolutive networks.
3. **Invariance and Equivariance**: We highlight the duality between invariance and covariance/equivariance, with focus on G-invariant representations.
4. Applications to data analysis and modeling: We present applications on a variety of problems: classification and regression on graphs; generative models for data sets; neural network based modeling of time-evolution of dynamical systems; discrete optimizatons.





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### Joint works with:

Naveed Haghani (UMD,APL-JHU) Daniel Levy (UMD)  
 Maneesh Singh (Verisk, Comcast) Efstratos Tsoukanis (UMD)

R. Balan, N. Haghani, M. Singh, “Permutation Invariant Representations with Applications to Graph Deep Learning”, arXiv preprint: 2203.07546 [math.FA], [cs.LG]

R. Balan, E. Tsoukanis, “Relationships between the Phase Retrieval Problem and Permutation Invariant Embeddings”, arXiv preprint: 2306.13111 [math.FA]

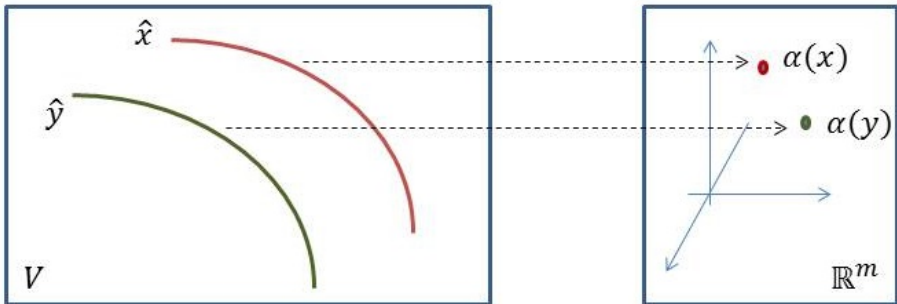


# High-Level View

Two related problems with many variations:

Given a (discrete) group  $G$  acting on a normed space  $V$ :

- 1 Construct a (bi)Lipschitz Euclidean embedding of the quotient space  $V/G$ ,  $\alpha : \hat{V} \rightarrow \mathbb{R}^m$ . **Classification of cosets.**
- 2 Construct the projection onto cosets,  $\pi : V \rightarrow [y] = \hat{y} = \{g \cdot y, g \in G\}$ .

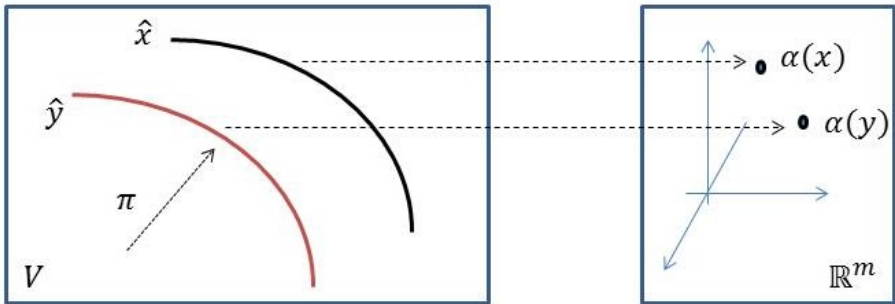


# Overview

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Optimizations within cosets.



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1. Motivation

# A. Similarity of Matrices

Consider two symmetric matrices  $A, B \in \text{Sym}(n)$ . When are they equivalent modulo an orthonormal change of coordinates?

Specifically, is there an orthogonal matrix  $U \in O(n)$  so that  $B = UAU^T$  ?

An elementary derivation in linear algebra shows that  $A \stackrel{O(n)}{\sim} B$  if and only if  $A$  and  $B$  have the same set of eigenvalues with exactly same multiplicities.

But what about other groups  $G$ ? For instance what about the group of permutation matrices  $\mathcal{S}_n$ ?

Find necessary and sufficient conditions so that  $A \stackrel{\mathcal{S}_n}{\sim} B$ .

Recall:

$$\mathcal{S}_n = \{P \in O(n) : P_{i,j} \in \{0, 1\}\} = O(n) \cap \{W \in [0, 1]^{n \times n} : W\mathbf{1} = \mathbf{1}, W^T\mathbf{1} = \mathbf{1}\}$$

1. Motivation

# A. The Graph Isomorphism Problem

Consider two graphs  $G = (\mathcal{V}, \mathcal{E})$  and  $\tilde{G} = (\tilde{\mathcal{V}}, \tilde{\mathcal{E}})$  with  $n$  nodes. The graph isomorphism problem is the computational problem of determining whether these graphs are identical after a relabeling of nodes.

If  $A$  and  $\tilde{A}$  denote their adjacency matrices, **these graphs are isomorphic if and only if  $\tilde{A} = \Pi A \Pi^T$  for some permutation matrix  $\Pi \in \mathcal{S}_n$ .**

Current state-of-the-art (Wikipedia): Babai (2015,2017) presented a quasi-polynomial algorithm with running time  $2^{O((\log n)^c)}$ , for some fixed  $c > 0$ . Helfgott (2017) claims that one can take  $c = 3$ .

Similar problem can be stated for weighted graphs:  $A, \tilde{A} \in \text{Sym}(n)$  with nonnegative entries, isomorphic if and only if  $\tilde{A} = \Pi A \Pi^T$  for some  $\Pi \in \mathcal{S}_n$ .





1. Motivation

# C. Graph Learning Problems

**Given** a data graph (e.g., social network, transportation network, citation network, chemical network, protein network, biological networks):

- Graph adjacency or weight matrix,  $A \in \mathbb{R}^{n \times n}$ ;
- Data matrix,  $X \in \mathbb{R}^{n \times r}$ , where each row corresponds to a feature vector per node.

**Construct** a map  $f : (A, X) \rightarrow f(A, X)$  that performs:

- 1 classification:  $f(A, X) \in \{1, 2, \dots, c\}$
- 2 regression/prediction:  $f(A, X) \in \mathbb{R}$ .

**Key observation:** The outcome should be invariant to vertex permutation:  
 $f(PAP^T, PX) = f(A, X)$ , for every  $P \in \mathcal{S}_n$ .



# Invariance vs. Equivariance

Graph learning problems are prime examples of the difference between *invariant* vs. *equivariant* representations.  
If the machine learning task is **node** classification or regression:

$$f : (A, X) \mapsto f(A, X) \in \{1, 2, \dots, c\}^n \text{ or } \mathbb{R}^n$$

where  $f(A, X)$  is a graph signal, i.e.,  $f(A, X)_i$  is signal at node  $i$ , then the nonlinear map  $f$  is *equivariant* and must satisfy  $f(PAP^T, PX) = Pf(A, X)$ , for all  $P \in \mathcal{S}_n$ .

## 1. Motivation

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On the other hand, if the machine learning task is **graph** classification or regression,

$$f : (A, X) \mapsto f(A, X) \in \{1, 2, \dots, c\} \text{ or } \mathbb{R}$$

where  $f(A, X)$  is assigned for the entire graph, then the nonlinear map  $f$  is *invariant* and must satisfy  $f(PAP^T, PX) = f(A, X)$ , for all  $P \in \mathcal{S}_n$ .

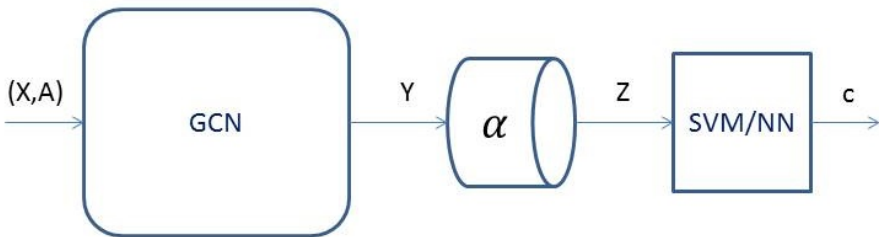




1. Motivation

# C. Deep Learning with GCN/GNN

The approach for the two learning tasks (classification or regression) is based on the following scheme (see also Maron et.al. ('19)):



where  $\alpha$  is a permutation invariant map (embedding), and SVM/NN is a single-layer or a deep neural network (Support Vector Machine or a Fully Connected Neural Network) trained on invariant representations.

The purpose of this talk is to analyze the  $\alpha$  component.









2. Permutation Invariant Representations for  $V = \mathbb{R}^{n \times d}$

# A Universal Embedding

Consider the map

$$\mu : \widehat{\mathbb{R}^{n \times d}} \rightarrow \mathcal{P}(\mathbb{R}^d) \quad , \quad \mu(X)(x) = \frac{1}{n} \sum_{k=1}^n \delta(x - x_k)$$

where  $\mathcal{P}(\mathbb{R}^d)$  denotes the convex set of probability measures over  $\mathbb{R}^d$ , and  $\delta$  denotes the Dirac measure.  $x_k$  is the  $k^{th}$  row of  $X$ .

Clearly  $\mu(X') = \mu(X)$  iff  $X' = PX$  for some  $P \in S_n$ .

The Wasserstein-2 distance is isometrically equivalent to  $\mathbf{d}$ :

$$W_2(\mu(X), \mu(Y))^2 := \inf_{q \in J(\mu(X), \mu(Y))} \mathbb{E}_q[\|x - y\|_2^2] = \min_{P \in S_n} \|Y - PX\|^2$$

By Kantorovich-Rubinstein theorem, the Wasserstein-1 distance (the Earth moving distance) extends to a norm on the space of signed Borel measures.

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By Kantorovich-Rubinstein theorem, the Wasserstein-1 distance (the Earth moving distance) extends to a norm on the space of signed Borel measures.

Main drawback:  $\mathcal{P}(\mathbb{R}^d)$  is infinite dimensional!

2. Permutation Invariant Representations for  $V = \mathbb{R}^{n \times d}$ 

## Finite Dimensional Embeddings

Idea: “Project” the measure onto a finite dimensional space. This is accomplished by *kernel methods*:

Fix a family of functions  $f_1, \dots, f_m$  and consider:

$$\mu(X) \mapsto \int_{\mathbb{R}^d} f_j(x) d\mu(X) = \frac{1}{n} \sum_{k=1}^n f_j(x_k) \quad , \quad j \in [m]$$

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Possible choices:

- ❶ Polynomial embeddings:  $\mathbb{R}[X]^{\mathcal{S}_n}$ , ring of invariant polynomials; [Lipman&al.],[Peyré&al.],[Sanay&al.],[Kemper book] ...
- ❷ Gaussian kernels:  $f_j(x) = \exp(-\|x - a_j\|^2 / \sigma_j^2)$  ; [Gilmer&al.],[Zaheer&al.], [Vinyals&al.],...
- ❸ Fourier kernels (cmplx embd):  $f_j(x) = \exp(2\pi i \langle x, \omega_j \rangle)$ ; related to Prony method; [Li&Liao] for bi-Lipschitz estimates.

Main drawback: No global bi-Lipschitz embeddings [Cahill&al.'19]. Ok on (some) compacts.

### 3. Polynomial Embeddings

# Polynomial Expansions - Quadratics

In the case  $d = 1$  recall Vieta's formulas, Newton-Girard identities

$$P(X) = \prod_{k=1}^N (X - x_k) \leftrightarrow \left( \sum_k x_k, \sum_k x_k^2, \dots, \sum_k x_k^n \right)$$

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For  $d > 1$ , consider the quadratic  $d$ -variate polynomial:

$$\begin{aligned} P(Z_1, \dots, Z_d) &= \prod_{k=1}^n \left( (Z_1 - x_{k,1})^2 + \dots + (Z_d - x_{k,d})^2 \right) \\ &= \sum_{p_1, \dots, p_d=0}^{2n} a_{p_1, \dots, p_d} Z_1^{p_1} \dots Z_d^{p_d} \end{aligned}$$

Encoding complexity:

$$m = \binom{2n+d}{d} \sim (2n)^d.$$

## 3. Polynomial Embeddings

## Polynomial Expansions - Quadratics (2)

A more careful analysis of  $P(Z_1, \dots, Z_d)$  reveals a form:

$$P(Z_1, \dots, Z_d) = t^n + Q_1(Z_1, \dots, Z_d)t^{n-1} + \dots + Q_{n-1}(Z_1, \dots, Z_d)t + Q_n(Z_1, \dots, Z_d)$$

where  $t = Z_1^2 + \dots + Z_d^2$  and each  $Q_k(Z_1, \dots, Z_d) \in \mathbb{R}_k[Z_1, \dots, Z_d]$  is a (non-homogeneous) polynomial of degree  $k$ . Hence one needs to encode:

$$m = \binom{d+1}{1} + \binom{d+2}{2} + \dots + \binom{d+n}{n} = \binom{d+n+1}{n} - 1$$

number of coefficients.

**A significant drawback:** Inversion is numerically unstable and embedding is not Lipschitz.

## 3. Polynomial Embeddings

## Readout Mapping Approach

## Polynomial Expansion - Linear Forms

A stable (Lipschitz, not bi-Lipschitz!) embedding can be constructed as follows (see also Gobels' algorithm (1996) or [Derksen, Kemper '02]).

Consider the  $n$  linear forms  $\lambda_k(Z_1, \dots, Z_d) = x_{k,1}Z_1 + \dots + x_{k,d}Z_d$ . Construct the polynomial in variable  $t$  with coefficients in  $\mathbb{R}[Z_1, \dots, Z_d]$ :

$$\begin{aligned}
 P(t) &= \prod_{k=1}^n (t - \lambda_k(Z_1, \dots, Z_d)) = t^n - e_1(Z_1, \dots, Z_d)t^{n-1} + \dots + (-1)^n e_n(Z_1, \dots, Z_d) \\
 &= t^n + \sum_{\substack{p_0, p_1, \dots, p_d \geq 0 \\ p_0 + p_1 + \dots + p_d = n, \quad p_0 < n}} c_{p_0, p_1, \dots, p_d} t^{p_0} Z_1^{p_1} \dots Z_d^{p_d}
 \end{aligned}$$

The elementary symmetric polynomials  $(e_1, \dots, e_n)$  are in 1-1 correspondence (Newton-Girard theorem) with the moments:

$$\mu_p = \sum_{k=1}^n \lambda_k^p(Z_1, \dots, Z_d), \quad 1 \leq p \leq n.$$



### 3. Polynomial Embeddings

# Polynomial Expansions - Linear Forms (2)

Each  $\mu_p$  is a homogeneous polynomial of degree  $p$  in  $d$  variables. Hence to encode each of them one needs  $\binom{d+p-1}{p}$  coefficients. Hence the embedding dimension is

$$m_0 = \binom{d}{1} + \binom{d+1}{2} + \dots + \binom{d+n-1}{n} = \binom{d+n}{n} - 1$$

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The map  $\alpha_0 : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^{m_0}$ ,  $X \mapsto (c_{p_0, p_1, \dots, p_d})_{p_0, p_1, \dots, p_d}$  is injective modulo  $S_n$  but it is not Lipschitz. However a simple modification as suggested by [Cahill et.al.'19] makes it Lipschitz.

## 3. Polynomial Embeddings

## Polynomial Lipschitz embedding

Denote by  $L_0$  the Lipschitz constant of  $\alpha_0$  when restricted to the closed unit ball  $B_1(\mathbb{R}^{n \times d}) : \{X \in \mathbb{R}^{n \times d}, \|X\| \leq 1\}$  of  $\mathbb{R}^{n \times d}$ , i.e.

$\|\alpha_0(X) - \alpha_0(Y)\| \leq L_0 \|X - Y\|$  for any  $X, Y \in \mathbb{R}^{n \times d}$  with  $\|X\|, \|Y\| \leq 1$ .

Let  $\varphi_0 : \mathbb{R} \rightarrow [0, 1]$ ,  $\varphi_0(x) = \min(1, \frac{1}{x})$  be a Lipschitz monotone decreasing function with Lipschitz constant 1.

## Theorem

*The map:*

$$\alpha_1 : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^m, \quad \alpha_1(X) = \begin{pmatrix} \alpha_0(\varphi_0(\|X\|)X) \\ \|X\| \end{pmatrix},$$

with  $m = \binom{n+d}{d} = m_0 + 1$  lifts to an injective and globally Lipschitz

map  $\hat{\alpha}_1 : \widehat{\mathbb{R}^{n \times d}} \rightarrow \mathbb{R}^m$  with Lipschitz constant  $\text{Lip}(\hat{\alpha}_1) \leq \sqrt{1 + L_0^2}$ .



## 3. Polynomial Embeddings

## Minimality

For  $d = 1$ ,  $m = n$  which is minimal.

For  $d = 2$ ,  $m = \frac{n^2+3n}{2}$ . Is this minimal?

## 3. Polynomial Embeddings

## Algebraic Embedding

## Encoding using Complex Roots

**Idea:** Consider the case  $d = 2$ . Then each  $x_1, \dots, x_n \in \mathbb{R}^2$  can be replaced by  $n$  complex numbers  $z_1, \dots, z_n \in \mathbb{C}$ ,  $z_k = x_{k,1} + ix_{k,2}$ .

Consider the complex polynomial:

$$Q(z) = \prod_{k=1}^n (z - z_k) = z^n + \sum_{k=1}^n \sigma_k z^{n-k}$$

which requires  $n$  complex numbers, or  $2n$  real numbers.

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**Open problem:** Can this construction be extended to  $d \geq 3$ ?

**Remark:** A drawback of polynomial (algebraic) embeddings: [Cahill'19] showed that polynomial embeddings of translation invariant spaces cannot be bi-Lipschitz.

## 4. Sorting based Embeddings

## The Max Pool approach

The idea is provided by the following observation.

Let  $\downarrow: \mathbb{R}^n \rightarrow \mathbb{R}^n$  denote the *sorting map*  $x \mapsto \downarrow x = \Pi x$ ,  $\Pi \in \mathcal{S}_n$ , so that

$$(\Pi x)_1 \geq (\Pi x)_2 \geq \dots \geq (\Pi x)_n.$$

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## Lemma

$\downarrow: \widehat{\mathbb{R}^n} \rightarrow \mathbb{R}^n$  is an isometry (hence bi-Lipschitz):

$$\|\downarrow(x) - \downarrow(y)\| = \min_{P \in \mathcal{S}_n} \|x - Py\|, \quad \text{for all } x, y \in \mathbb{R}^n.$$

Proof is based on the rearrangement inequality (see Wikipedia, or Hardy-Littlewood-Pólya “Inequalities” §10.2).

Our main goal is to extend this construction from  $\mathbb{R}^n$  to  $\mathbb{R}^{n \times d}$



## 4. Sorting based Embeddings

The Encoder  $\beta_A$ 

## Notations

Recall the equivalence relation, for  $X, Y \in \mathbb{R}^{n \times d}$ ,

$$X \sim Y \Leftrightarrow \exists \Pi \in \mathcal{S}_n, Y = \Pi X$$

that induces a quotient space  $\widehat{\mathbb{R}^{n \times d}} = \mathbb{R}^{n \times d} / \sim$  and the natural distance

$$\mathbf{d} : \widehat{\mathbb{R}^{n \times d}} \times \widehat{\mathbb{R}^{n \times d}} \rightarrow \mathbb{R}, \quad \mathbf{d}([X], [Y]) = \min_{\Pi \in \mathcal{S}_n} \|X - \Pi Y\|_F$$

In the following we construct an Euclidean embedding of the form

$$\beta_A : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^{n \times D}, \quad \beta_A(X) = \downarrow (XA)$$

where  $\downarrow (\cdot)$  sorts decreasingly each column of  $\cdot$ , independently.

The matrix  $A \in \mathbb{R}^{d \times D}$  is called the *key* of encoder  $\beta_A$ .

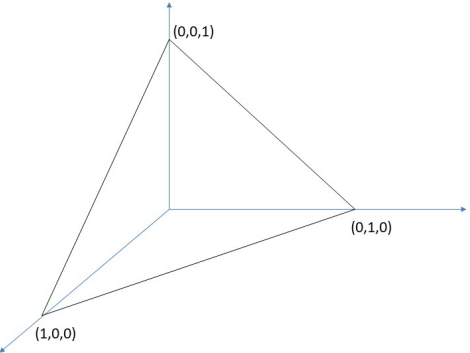
The key is called *universal* if  $\widehat{\beta}_A : \widehat{\mathbb{R}^{n \times d}} \rightarrow \mathbb{R}^{n \times D}$  is injective.

4. Sorting based Embeddings

# Intuition behind universality of keys

Consider the case  
 $n = 2, d = 3$

$$X = \begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \end{bmatrix}$$



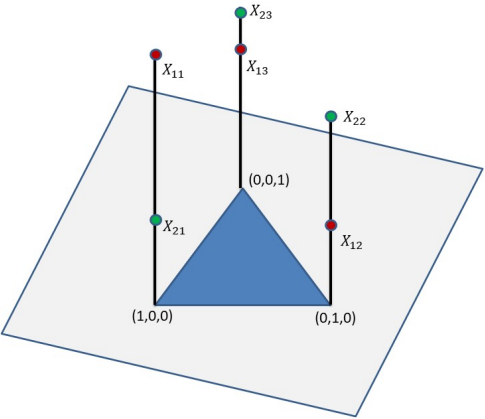
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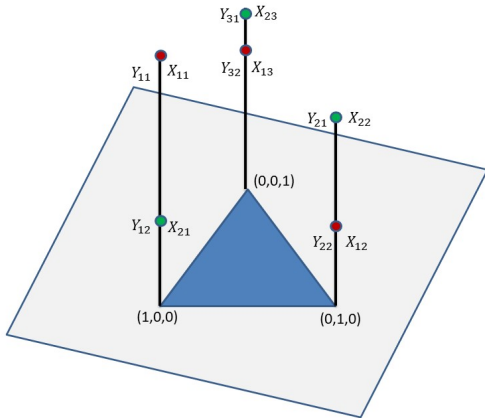
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Information lost!



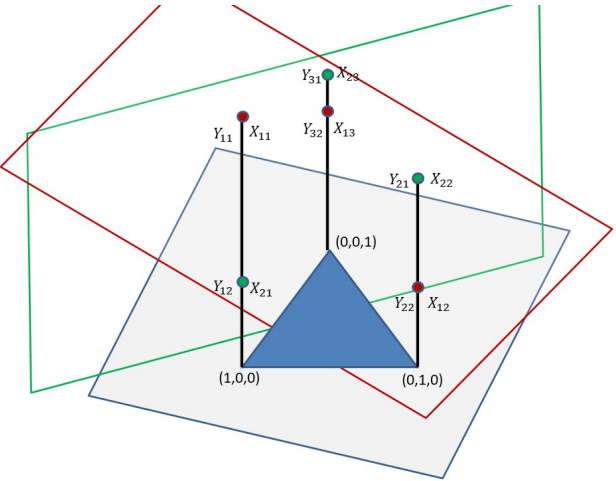
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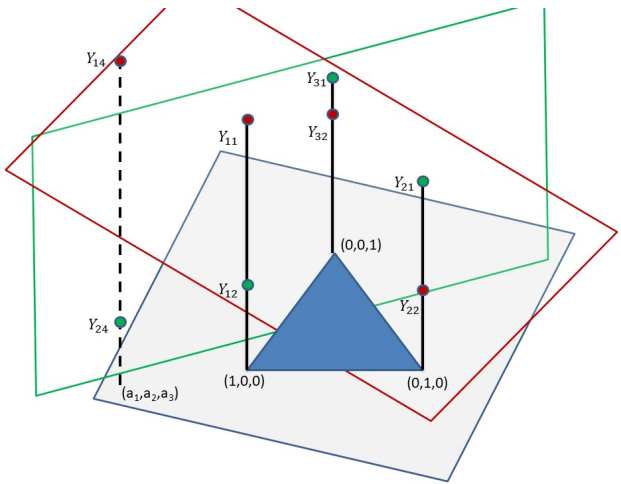
## 4. Sorting based Embeddings

## Intuition for this encoder

$$X = \begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \end{bmatrix}$$

$$Y \Rightarrow \downarrow \begin{bmatrix} X & Xa \end{bmatrix}$$

$$Y = \begin{bmatrix} Y_{11} & Y_{12} & Y_{13} & Y_{14} \\ Y_{21} & Y_{22} & Y_{23} & Y_{24} \end{bmatrix}$$



## 4. Sorting based Embeddings

## Three results (1)

## Existence of Universal Keys

## Theorem

Consider the metric space  $(\widehat{\mathbb{R}^{n \times d}}, \mathbf{d})$ . Set  $D = 1 + (d - 1)n!$  and let  $A \in \mathbb{R}^{d \times D}$  be a matrix whose columns form a full spark frame. Then the key  $A$  is universal and the induced map  $\hat{\beta}_A : \widehat{\mathbb{R}^{n \times d}} \rightarrow \mathbb{R}^{n \times D}$ ,  $\hat{\beta}_A([X]) = \downarrow(XA)$  is injective. Furthermore,  $\hat{\beta}_A$  is bi-Lipschitz with constants  $a_0 = \min_{J \subset [D], |J|=d} s_d(A[J])$  and  $b_0 = s_1(A)$ , where  $s_1(A)$  denotes the largest singular value of  $A$ ,  $A[J]$  denotes the submatrix of  $A$  formed by columns indexed by  $J$ , and  $s_d(A[J])$  denotes the  $d^{\text{th}}$  singular value (in this case, the smallest) of  $A[J]$ . Specifically, for any  $X, Y \in \mathbb{R}^{n \times d}$ ,

$$a_0 \mathbf{d}([X], [Y]) \leq \|\beta_A(X) - \beta_A(Y)\| \leq b_0 \mathbf{d}([X], [Y]) \quad (3.1)$$

where all norms are Frobenius norms.

4. Sorting based Embeddings

# Three results (2)

## Bi-Lipschitz Property of Universal Keys

### Theorem

Assume the key  $A \in \mathbb{R}^{d \times D}$  is universal, i.e., the induced map  $\hat{\beta}_A : \widehat{\mathbb{R}^{n \times d}} \rightarrow \mathbb{R}^{n \times D}$ ,  $[X] \mapsto \beta_A(X) = \downarrow(XA)$  is injective. Then  $\hat{\beta}_A$  is bi-Lipschitz, that is, there are constants  $a_0 > 0$  and  $b_0 > 0$  so that for all  $X, Y \in \mathbb{R}^{n \times d}$ ,

$$a_0 \mathbf{d}([X], [Y]) \leq \|\beta_A(X) - \beta_A(Y)\| \leq b_0 \mathbf{d}([X], [Y]) \quad (3.2)$$

where all are Frobenius norms. Furthermore, an estimate for  $b_0$  is provided by the largest singular value of  $A$ ,  $b_0 = s_1(A)$ .



4. Sorting based Embeddings

# Three results (3)

## Dimension Reduction

### Theorem

Assume  $A \in \mathbb{R}^{d \times D}$  is a universal key for  $\widehat{\mathbb{R}^{n \times d}}$  with  $D \geq 2d$ . Then, for  $m \geq 2nd$ , a generic linear operator  $B : \mathbb{R}^{n \times D} \rightarrow \mathbb{R}^m$  with respect to Zariski topology on  $\mathbb{R}^{n \times D \times m}$ , the map

$$\hat{\beta}_{A,B} : \widehat{\mathbb{R}^{n \times d}} \rightarrow \mathbb{R}^{2nd}, \quad \hat{\beta}_{A,B}(\hat{X}) = B(\hat{\beta}_A(\hat{X})) \tag{3.3}$$

is bi-Lipschitz. In particular, almost every full-rank linear operator  $B : \mathbb{R}^{n \times D} \rightarrow \mathbb{R}^{2nd}$  produces such a bi-Lipschitz map.

This result is compatible with a Whitney embedding theorem with the important caveat that the Whitney embedding result applies to smooth manifolds, whereas  $\widehat{\mathbb{R}^{n \times d}}$  is not a manifold.

## 4. Sorting based Embeddings

## Highlights of proofs

First result: Universal keys

The upper bound is immediate. For lower bound, fix  $X, Y \in \mathbb{R}^{n \times d}$ :

$$\|\beta_A(X) - \beta_A(Y)\|_2^2 = \sum_{k=1}^D \|\downarrow(Xa_k) - \downarrow(Ya_k)\|_2^2 = \sum_{k=1}^D \|P_k X a_k - Q_k Y a_k\|_2^2$$

$$\stackrel{\Pi_k := Q_k^T P_k}{=} \sum_{k=1}^D \|(\Pi_k X - Y) a_k\|_2^2$$

## 4. Sorting based Embeddings

## Highlights of proofs

First result: Universal keys

The upper bound is immediate. For lower bound, fix  $X, Y \in \mathbb{R}^{n \times d}$ :

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$$\stackrel{\Pi_k := Q_k^T P_k}{=} \sum_{k=1}^D \|(\Pi_k X - Y) a_k\|_2^2 \geq \sum_{j=1}^d \|(\Pi_{k_j} X - Y) a_{k_j}\|_2^2$$

so that  $\Pi_{k_1} = \dots = \Pi_{k_d} = \Pi_0$  (pigeonhole principle: needs  $D > (d-1)n!$ ).

4. Sorting based Embeddings

# Highlights of proofs

First result: Universal keys

The upper bound is immediate. For lower bound, fix  $X, Y \in \mathbb{R}^{n \times d}$ :

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so that  $\Pi_{k_1} = \dots = \Pi_{k_d} = \Pi_0$  (pigeonhole principle: needs  $D > (d-1)n!$ ). Then:

$$\begin{aligned} \|\beta_A(X) - \beta_A(Y)\|_2^2 &\geq \sum_{j=1}^d \|(\Pi_0 X - Y)a_{k_j}\|_2^2 \stackrel{\text{full spark}}{\geq} s_d(A[J])^2 \|\Pi_0 X - Y\|_2^2 \\ &\geq s_d(A[J])^2 \min_{\Pi \in \mathcal{S}_n} \|\Pi X - Y\|_2^2 = s_d(A[J])^2 \mathbf{d}([X], [Y])^2 \end{aligned}$$

4. Sorting based Embeddings

# Highlights of proofs

Second result: Bi-Lipschitz Property

The proof resembles the treatment of phase retrieval problem:

- 1 Homogeneity and compactness reduce the problem to local analysis.
- 2 The encoder is “locally” linearized. The failure of local lower Lipschitz bound implies a certain behavior for a Quadratically Constrained Ratio of Quadratics (QCRQ).
- 3 QCRQ has a minimizer:  $\inf \Rightarrow \min$ . [Teboulle&al.]  
This step took most of time and lots of (self)convincing !
- 4 Contradiction to injectivity assumption.

## 4. Sorting based Embeddings

# More detailed proof of the bi-Lipschitz result (1)

## 1. Reduction to local lower Lipschitz bound.

Assume  $\inf_{X \neq Y} \|\beta_A(X) - \beta_A(Y)\|_2 / \mathbf{d}([X], [Y]) = 0$ . By *homogeneity* and *compactness*, extract/construct sequences  $(X_j)_j$  and  $(Y_j)_j$  so that: (i)

$X_j \rightarrow Z$ ; (ii)  $Y_j \rightarrow Z$ ; (iii)  $\|Y_j\| \leq \|X_j\| = \|Z\| = 1$ ; (iv)

$\mathbf{d}([X_j], [Z]) = \|X_j - Z\|$ ; (v)  $\mathbf{d}([X_j], [Y_j]) = \|X_j - Y_j\|$ ; (vi)

$\mathbf{d}([Y_j], [Z]) = \|Y_j - Z\|$ .

## 2. Local linearization.

Let  $H = \{P \in \mathcal{S}_n ; PZ = Z\}$  denote the stabilizer of  $Z$ . Let  $U_j = X_j - Z$  and  $V_j = Y_j - Z$ . Then:

$$\lim_{j \rightarrow \infty} \frac{\sum_{k=1}^D \min_{Q \in H} \|QU_j a_k - V_j a_k\|^2}{\|U_j - V_j\|^2} = 0, \quad \|U_j - V_j\| \leq \|U_j - PV_j\|, \quad \forall P \in H.$$

## 4. Sorting based Embeddings

## More detailed proof of the bi-Lipschitz result (2)

## 3. QCQP

Last limit implies:

$$\inf_{\substack{(u, v) \in \mathbb{R}^{n \times d} : \\ U \neq QV, \forall V \in H}} \max_{P \in H} \frac{\sum_{k=1}^D \|(U - \Pi_k V) a_k\|_2^2}{\|U - PV\|^2} = 0$$

where  $\Pi_k$  achieves alignment between  $U_j a_k$  and  $V_j a_k$ .

Since these groups are finite, we obtain that the infimum is achieved!

Hence:

## 4. Injectivity no-go

There are  $U, V \in \mathbb{R}^{n \times d}$  so that  $Z + U \not\sim Z + V$  and yet

$(Z + U) a_k = \Pi_k (Z + V) a_k$  for all  $k \in [D]$ . This shows

$\beta_A(Z + U) = \beta_A(Z + V)$  which contradicts injectivity!

Q.E.D.

# Highlights of proofs

## Third result: Dimension Reduction

The proof follows the approach in [Cahill&al.], [Dufresne]:

$$0 = B(\beta_A(X)) - B(\beta_A(Y)) \Rightarrow \beta_A(X) - \beta_A(Y) \in \ker(B)$$

Need to show:  $\beta_A(X) - \beta_A(Y) = 0$ , or,  $Ran(\Delta) \cap \ker(B) = \{0\}$ , where

$$\Delta : \mathbb{R}^{n \times d} \times \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^{n \times D}, \quad \Delta(X, Y) = \beta_A(X) - \beta_A(Y).$$

In the polynomial case, [Cahill&al.] exploit arguments from algebraic geometry. Here the problem is simpler since  $Ran(\Delta)$  is included in a finite union of linear subspaces of dimension at most  $2nd$ .

By a dimension argument it follows that the target space for  $B$  must be of dimension at least  $2nd$  to obtain an injective embedding. In this case, generically,  $Ran(\Delta)$  and  $\ker(B)$  intersect transversally.



4. Sorting based Embeddings

# Towards universal keys

The arXiv preprint provides necessary and sufficient conditions for a key to be universal.

**Open Problem:** Given  $(n, d)$  find the smallest dimension  $D$  so that there exists a universal key  $A \in \mathbb{R}^{d \times D}$  for  $\mathbb{R}^{n \times d}$ .

So far we obtained (joint with **Daniel Levy** (UMD) ):

n	d	D-d
2	2	1
3	2	2
4	2	2
5	2	3
6	2	$\geq 4$

**Open Problem:** If a universal key exists for a triple  $(n, d, D)$  then is it true that universal keys are generic in  $\mathbb{R}^{d \times D}$  ?

4. Sorting based Embeddings

# Related results

A sequence of preprints came out almost simultaneously:

- ❶ R. Balan, N. Haghani, M. Singh, Permutation Invariant Representations with Applications to Graph Deep Learning, arXiv:2203.07546 (2022)
- ❷ N. Dym, S. J. Gortler, Low Dimensional Invariant Embeddings for Universal Geometric Learning, arXiv:2205.02956 (2022)
- ❸ J. Cahill, J. W. Iverson, D. G. Mixon, D. Packer, Group-invariant max filtering, arXiv:2205.14039 (2022)

all of them based on sorting in one way or another. [Dym and Gortler] shows that the key size should be significantly smaller than  $n!$ . [Cahill et.al.'22] introduced the concept of *max filter* which is a special case of a more general G-invariant representation discussed next.

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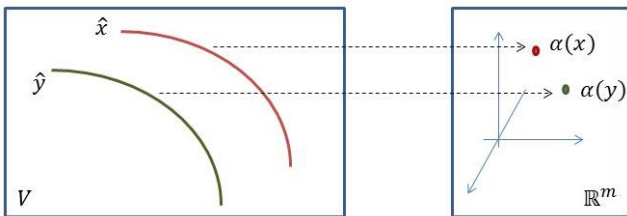
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- 2 Day 1: Neural Networks and Lipschitz Analysis
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  - 1. Motivation
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  - 1. Invariant Coorbit Representations
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  - 3. Bi-Lipschitz Property
- 5 Day 3: Applications

# High-Level View

Recall the framework for Euclidean embeddings of metric spaces induced by orthogonal representations of (finite) groups  $G$  acting on a linear space  $V$ .

Metric space  $(\hat{V}, \mathbf{d})$  where:  $\hat{V} = V/G$  is the set of orbits,

$[\hat{x}] = \{U_g x, g \in G\}$ , for  $x \in V$ ; and  $\mathbf{d}(\hat{x}, \hat{y}) = \min_{u \in \hat{x}, v \in \hat{y}} \|u - v\|_V$ .





# The Program

Given a discrete group  $G$  acting unitarily on a normed space  $V$ , we formulate four general problems

- ① Construct injective embeddings of the quotient space  $V/G$ ,  $\alpha : \hat{V} \rightarrow \mathbb{R}^m$ . **The injectivity problem.**
- ② Construct/Obtain bi-Lipschitz properties for the Euclidean embedding  $\alpha : \hat{V} \rightarrow \mathbb{R}^m$ . **The stability problem.**
- ③ Develop algorithms for inversion  $\alpha^{-1} : \mathbb{R}^m \rightarrow \hat{V}$ . **The recovery problem.**
- ④ Analyze specific cases. **Applications.**



# Invariant Representations

Let  $V$  be a  $d$ -dimensional Hilbert space and  $G$  a finite group of size  $N = |G|$  acting unitarily on  $V$ ,  $\{U_g, g \in G\}$ .

The quotient space  $\hat{V} = V/G$  is the set of orbits  $[x] = \{U_g x, g \in G\}$  induced by the group action, where for  $x, y \in V$ ,  $x \sim y$  iff  $y = U_g x$  for some  $g \in G$ .  $(\hat{V}, \mathbf{d})$  becomes a **metric space** with the natural distance

$$\mathbf{d}([x], [y]) = \min_{g \in G} \|x - U_g y\|$$

How to construct an invariant representation?

The standard method in the computational invariant theory: Find generators of the **ring of invariant polynomials** in  $d$  variables. This method goes back to Cayley, Hilbert, Noether .... However this approach has a drawback: it cannot produce bi-Lipschitz embeddings <sup>1</sup>, unless special cases.

<sup>1</sup>J. Cahill, A. Contreras, A.C. Hip, Complete Set of translation Invariant Measurements with Lipschitz Bounds, ACHA 2020





1. Invariant Coorbit Representations

# Representations based on sorting (2)

$$\phi_w : V \rightarrow \mathbb{R}^N, \quad \phi_w(x) = \downarrow ((\langle x, U_g w \rangle))_{g \in G}.$$

Remarks:

- 1  $\phi_w(U_g x) = \phi_w(x)$  for every  $g \in G$  and  $x \in V$ . Thus  $\phi_w$  lifts to the quotient space  $\widehat{V}$ .
- 2 Invariant polynomials, and more generally, invariant functions obtained by the averaging operator (the Reynolds operator), can be obtained as:

$$K \mapsto F_K(x) = \frac{1}{|G|} \sum_{g \in G} K(\langle U_g x, w \rangle) = \frac{1}{|G|} \sum_{g \in G} K(\phi_w(x))$$



1. Invariant Coorbit Representations

# Invariant Coorbit Representations

Special cases:

1. If  $G = S_n$  and  $V = \mathbb{R}^{n \times d}$  with action  $(P, X) \mapsto PX$ , then <sup>5</sup> introduced the embedding  $\beta_A(X) = \downarrow (XA)$ , for key  $A \in \mathbb{R}^{d \times D}$  and sorting operator acting independently in each column.

Equivalent recasting: Let  $w_1 = \delta_1 \cdot a_1^T, \dots, w_D = \delta_1 \cdot a_D^T$ , where  $\delta_1 = (1, 0, \dots, 0)^T$  and  $A = [a_1 | \dots | a_D]$ . Then note

$\phi_{w_1}(X) = \downarrow (Xa_1) \otimes 1_{(n-1)!}$ . Thus  $\Phi_w(X) = \beta_A(X) \otimes 1_{(n-1)!}$ . Thus  $\beta_A(X) = \Phi_{w,S}(X)$  for an appropriate subset  $S \subset [n!] \times [D]$  of size  $nD$ .

2. The *max filter* introduced in <sup>6</sup> for some template  $w \in V$  is defined by  $\langle \langle \cdot, w \rangle \rangle : V \rightarrow \mathbb{R}$ ,  $\langle \langle x, w \rangle \rangle = \max_{g \in G} \langle x, U_g w \rangle$ . Equivalent recasting:  $\langle \langle x, w \rangle \rangle = \Phi_{w,S}(X)$ , for  $S = \{1\}$ .

<sup>5</sup>R. Balan, N. Haghani, M. Singh, Permutation Invariant Representations with Applications to Graph Deep Learning, arXiv:2203.07546 (2022)

<sup>6</sup>J. Cahill, J. W. Iverson, D. G. Mixon, D. Packer, Group-invariant max filtering, arXiv:2205.14039 (2022)

2. Injective Invariant Representations

# Sufficient conditions for an injective embedding

## Theorem

Consider  $G$  finite group of size  $N$  acting unitarily on the  $d$ -dimensional  $V$ . Let  $\mathbf{w} \in V^p$ ,  $S \subset [N] \times [p]$ ,  $S_k$  the  $k^{\text{th}}$  slice, and linear map  $\mathcal{L} : l^2(S) \rightarrow \mathbb{R}^m$ . Denote  $\gamma_2 = \min_{g \in G, g \neq 1} \min_{\lambda \in \mathbb{R}} \text{rank}(\lambda I_d - U_g)$ ,  $\gamma_3 = \max_{g \in G, g \neq 1} \min_{\lambda \in \mathbb{R}} \text{rank}(\lambda I_d - U_g)$ . Then for almost every  $\mathbf{w}$  and  $\mathcal{L}$  the maps  $\Phi_{\mathbf{w}, S}$  or  $\Psi_{\mathbf{w}, S, \mathcal{L}}$  are injective on  $\widehat{V}$  in any of the following cases:

- 1 (Max filter, Cahill et.al. 2022) If  $p \geq 2d$  and  $S_{\max} = \{(1, 1), \dots, (1, p)\}$  then the max filterbank  $\Phi_{\mathbf{w}, S_{\max}}$  is injective for a.e.  $\mathbf{w} \in V^p$ .
- 2 (variation of previous result) If  $p \geq 2d$  and  $|S_k| \geq 1$  for all  $k \in [p]$  then  $\Phi_{\mathbf{w}, S}$  is injective for a.e.  $\mathbf{w} \in V^p$ .
- 3<sup>a</sup> If  $G$  is a reflection group and  $p \geq d$  then the max filterbank  $\Phi_{\mathbf{w}, S_{\max}}$  is injective for a.e.  $\mathbf{w} \in V^p$ .

<sup>a</sup>D. Mixon, Y. Qaddura, Injectivity, stability, and positive definiteness of max filtering, arXiv:2212.11156

2. Injective Invariant Representations

# Sufficient conditions for injective embedding (cont)

## Theorem

- ④ If  $p \geq 2d - \gamma_2$ ,  $|S| \geq 2d$ , and for each  $k$ ,  $|S_k| \in \{1, 2\}$  then  $\Phi_{\mathbf{w},S}$  is injective for a.e.  $\mathbf{w} \in V^p$ .
- ⑤ If  $2d - \gamma_3 \leq p \leq 2d$ ,  $|S_1| = \dots = |S_{2d-p}| = N$ , and  $|S_{2d-p+1}| = \dots = |S_p| = 1$  then  $\Phi_{\mathbf{w},S}$  is injective for a.e.  $\mathbf{w} \in V^p$ .
- ⑥ If  $\Phi_{\mathbf{w},S}$  is injective and  $m \geq 2d$  then the map  $\Psi_{\mathbf{w},S,\mathcal{L}}$  is injective for a.e. linear map  $\mathcal{L} : l^2(S) \rightarrow \mathbb{R}^m$ .

Remark:

This result can be extended to the case when  $S$  has an irregular structure. However this requires some involved spectral conditions.



## 2. Injective Invariant Representations

## Injectivity – sketch of proof

The proof provides a semi-algebraic characterization of the set of “bad” windows, i.e., windows  $\mathbf{w}$  that fail to separate, say  $\mathcal{F}$ .

$$\mathcal{F} \subset \bigcup_{\mathbf{g}, \mathbf{h} \in G^{p^*}} \mathcal{F}_{\mathbf{g}, \mathbf{h}} \quad , \quad G^{p^*} = \{(g_i^k)_{(i,k) \in S} \quad , \quad \forall k, (g_i^k)_{i \in S_k} \in G^{|S_k|} \text{ are distinct}\}$$

$$\mathcal{F}_{\mathbf{g}, \mathbf{h}} = \bigcup_{(x,y) \in \Gamma} \otimes_{k=1}^p \{U_{g_1^k} x - U_{h_1^k} y, \dots, U_{g_{m_k}^k} x - U_{h_{m_k}^k} y\}^\perp$$

where  $\Gamma = \{(x, y) \in V^2 : x \not\sim y, \|x\|^2 + \|y\|^2 = 1\}$ ,  $m_k = |S_k|$ . Using the “lift-and-project” technique, we realize each  $\mathcal{F}_{\mathbf{g}, \mathbf{h}}$  as finite unions of projection onto second term of total manifolds of certain real-analytic vector bundles. The vector bundles have as base manifolds subsets of  $\Gamma$  where dimension of the orthogonal complement of constant. In turn those subsets are controlled by spectral properties of  $U_g$ 's.

2. Injective Invariant Representations

# Injectivity – sketch of proof

The base manifolds of these vector bundles are themselves total spaces of a different vector bundles living over Grassmanian manifolds. For instance, for  $|S_k| = m_k = 2$ , First construct the bundle  $(Gr(1, \mathbb{R}^2), \pi, E)$  over  $Gr(1, \mathbb{R}^2) = \mathbb{RP}^1 \sim [0, \pi)$  with total space

$$E = \{(\theta, x, y) \in [0, \pi) \times V^2 ; \cos(\theta)(U_{g_1}x - U_{h_1}y) + \sin(\theta)(U_{g_2}x - U_{h_2}y) = 0\}$$

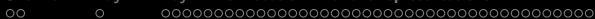
Most of fibers are  $d$ -dimensional except what  $\tan(\theta)$  is an eigenvalue of some unitary  $U_g$ . Those two cases induce a disjoint partition

$$\Gamma = (\Gamma \setminus \Pi_2(E)) \cup (\Gamma \cap \Pi_2(E)) \text{ so that}$$

$$\begin{aligned} (x, y) \in \Gamma_1 := \Gamma \setminus \Pi_2(E) &\rightarrow \dim\{U_{g_1}x - U_{h_1}y, (U_{g_2}x - U_{h_2}y)^\perp\} = d - 2 \\ (x, y) \in \Gamma_2 := \Gamma \cap \Pi_2(E) &\rightarrow \dim\{U_{g_1}x - U_{h_1}y, (U_{g_2}x - U_{h_2}y)^\perp\} = d - 1 \end{aligned}$$

from where the dimension estimates arise.





## 3. Bi-Lipschitz Property

## Main Result

## Theorem

Consider  $G$  finite group of size  $N$  acting unitarily on the  $d$ -dimensional  $V$ . Let  $\mathbf{w} \in V^p$ ,  $S \subset [N] \times [p]$  and  $\mathcal{L} : l^2(S) \rightarrow \mathbb{R}^m$ . Let

$$B = \max_{\substack{\sigma_1, \dots, \sigma_p \subset G, \\ |\sigma_k| = |S_k|, \forall k}} \lambda_{\max} \left( \sum_{k=1}^p \sum_{g \in \sigma_k} U_g w_k w_k^T U_g^T \right)$$

where  $S_k = \{i \in [N], (i, k) \in S\}$  for each  $k \in [p]$ .

- $\Phi_{\mathbf{w}, S} : (\widehat{V}, \mathbf{d}) \rightarrow l^2(S)$  is Lipschitz with constant upper bounded by  $\sqrt{B}$ .
- If  $S = [N] \times [p]$  and  $\Phi_{\mathbf{w}, S} : (\widehat{V}, \mathbf{d}) \rightarrow (\mathbb{R}^m, \|\cdot\|_2)$  is injective then it is also bi-Lipschitz;
- If  $S = [N] \times [p]$  and  $\Phi_{\mathbf{w}, S} : (\widehat{V}, \mathbf{d}) \rightarrow (\mathbb{R}^m, \|\cdot\|_2)$  is injective then for a generic  $\mathcal{L}$  with  $m \geq 2d$ , the map  $\Psi_{\mathbf{w}, S, \mathcal{L}} : (\widehat{V}, \mathbf{d}) \rightarrow (\mathbb{R}^m, \|\cdot\|_2)$  is injective and bi-Lipschitz.

3. Bi-Lipschitz Property

# Sketch of Proof

1. The upper Lipschitz bound is not too hard. A quick way to obtain it is by the Fundamental Theorem of Calculus: Fix  $x, y \in V$  and choose them so that  $\mathbf{d}([x], [y]) = \|x - y\|$ . The function  $f : [0, 1] \rightarrow I^2(S)$ ,  $f(t) = \Phi_{\mathbf{w}, S}((1 - t)x + ty)$  is Lipschitz because the sorting operator  $\downarrow$  is Lipschitz. The upper Lipschitz constant is computable from FTC and Lebesgue's differentiation theorem:

$$\|f(1) - f(0)\|_2 = \left\| \int_0^1 (Jf)|_{(1-t)x+ty} (y-x) dt \right\| \leq \sup_z \|J\Phi_{\mathbf{w}, S}(z)\|_\infty \mathbf{d}([x], [y])$$

But wherever  $\Phi$  is differentiable,  $J\Phi_{\mathbf{w}, S}(z) = \left[ (U_{g(\pi_k(i))} w_k)^T \right]_{(i,k) \in S}$  where  $\pi_k$  is the permutation that sorts  $\phi_{w_k}(z)$ . From here one obtains the upper bound.

The same goes for  $\Psi_{\mathbf{w}, S, \mathcal{L}}$ .



3. Bi-Lipschitz Property

# Sketch of Proof (2)

Step 4. By finiteness of  $G$ , we extract subsequences so that  $(\Phi_{\mathbf{w},S}(x_n))_{i,k} = \langle x_n, U_{g(1,i,k)} w_k \rangle$  and  $(\Phi_{\mathbf{w},S}(y_n))_{i,k} = \langle y_n, U_{g(2,i,k)} w_k \rangle$  (note the group elements are independent on  $n$ !). It follows:

$$\lim_{n \rightarrow \infty} \frac{1}{\|u_n - v_n\|^2} \sum_{(i,k) \in S} |\langle w_k, U_{g(1,i,k)}^T u_n - U_{g(2,i,k)}^T v_n \rangle|^2 = 0$$

Step 5. Using an argument about ratios of quadratics, it follows that one is able to produce  $u, v$  so that  $u \not\sim v$  and  $\langle w_k, U_{g(1,i,k)}^T u - U_{g(2,i,k)}^T v \rangle = 0$  for all  $(i, k) \in S$ . Then for  $s > 0$  small enough,  $x = z + su$  and  $y = z + sv$  we have  $\mathbf{d}([x], [y]) > 0$  and yet  $\Phi_{\mathbf{w},S}(x) = \Phi_{\mathbf{w},S}(y)$ . Contradiction!

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