

# Bi-Lipschitz Euclidean Embeddings of Metric Spaces induced by Finite Group Representations

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**AMSC** | APPLIED MATHEMATICS AND STATISTICS,  
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# Preprints

## Preprints:

1. R.B., Naveed Haghani, Maneesh Singh, “Permutation-Invariant Representations with Applications to Graph Deep Learning”, ACHA, vol. 9 (2025)
2. R.B., Efstratios Tsoukanis, “Relationships between the Phase Retrieval Problem and Permutation Invariant Embeddings”, arXiv:2306.13111 [math.FA] , [cs.IT] , [math.IT]
3. R.B., Efstratios Tsoukanis, “G-Invariant Representations using Coorbits: Bi-Lipschitz Properties”, arXiv:2308.11784 [math.RT]
4. R.B., Efstratios Tsoukanis, “G-Invariant Representations using Coorbits: Injectivity Properties”, arXiv:2310.16365 [math.RT]
5. R.B., Efstratios Tsoukanis, Matthias Wellershoff, “Stability of sorting based embeddings”, arXiv:2410.05446 [math.FA]
6. N. Dym, M. Wellershoff, E. Tsoukanis, D. Levy, R. Balan, “Quantitative Bounds for Sorting-based Permutation-Invariant Embeddings”, arXiv:2510.22186[cs.LG, cs.IT, math.FA, math.MG]

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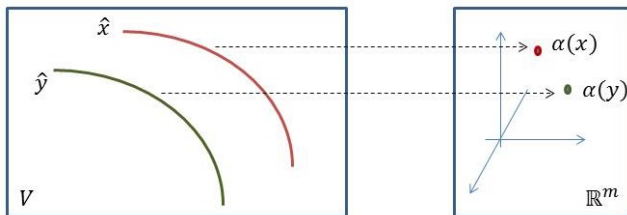
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# High-Level View

In this talk, we discuss Euclidean embeddings of metric spaces induced by orthogonal representations of finite groups  $G$  acting on a linear space  $V$  with inner product.

**Problem:** Construct bi-Lipschitz embeddings of the metric space  $\hat{V} = V / \sim$  of orbits,  $\alpha : \hat{V} \rightarrow \mathbb{R}^m$ , where  $\mathbf{d}([x], [y]) = \inf_{u \in [x], v \in [y]} \|u - v\|$

$$a_0 \mathbf{d}([x], [y]) \leq \|\alpha([x]) - \alpha([y])\|_2 \leq b_0 \mathbf{d}([x], [y]).$$



# The Program

Given a discrete group  $G$  acting unitarily on a normed real 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.](#)

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- ④ Analyze specific cases. **Applications.**

Today we discuss results about the first two problems: **injectivity**, **bi-Lipschitz stability**.

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# I. Phase Retrieval Problems

Since 2006 ACHA paper<sup>1</sup> lots of research on this theme.

The group:  $G = O(1) = \{+1, -1\}$  or  $G = U(1) \sim \mathbb{T}^1$  acting on  $\mathbb{K}^n$ .

Embedding:  $x \mapsto \{|\langle x, f_k \rangle|\}_{k \in [m]}$  for a fixed frame  $\{f_1, \dots, f_m\} \subset \mathbb{K}^n$ ,  
 $\mathbb{K} = \mathbb{R}$  or  $\mathbb{K} = \mathbb{C}$ .

Two type of results of particular interest:

- **Minimal embeddings:** For  $\mathbb{K} = \mathbb{R}$ ,  $m_{\min} \geq 2n - 1$ <sup>1</sup>; For  $\mathbb{K} = \mathbb{C}$ :  
 $m_{\min} \leq 4n - 4$ ;  $m_{\min} = 4n - 4$  when  $n = 2^p + 1$  [Conca, Edidin, Hering, Vinzant'15]; [Vinzant'15]:  $n = 4$ ,  $m_{\min} = 11 = 4n - 5$
- **Bi-Lipschitz:**  
 [EldarMend'14, BandCahlMixnNels'14, BWang'15, BZou'15'16] Any finite-dimensional injective embedding is bi-Lipschitz. Global inverse Lipschitz.

<sup>1</sup>R.B, Pete Casazza, Dan Edidin, On Signal Reconstruction without Noisy Phase, Appl. Comp. Harm. Anal., 20 (2006)

## II. 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.

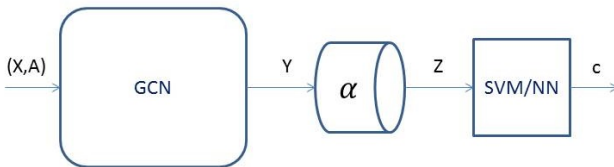
**Construct** a map  $f : (A, X) \rightarrow f(A, X)$  that performs:

- 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  $P \in \mathcal{S}_n$ .

# Graph Deep Learning with GCN/GNN

Our approach for these learning tasks (classification or regression) is based on the following scheme (see GCN<sup>2</sup> and equivariance<sup>3</sup>):



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.

[Our focus is on the  \$\alpha\$  component.](#)

<sup>2</sup>Kipf, T. N. and Welling, M., Semi-Supervised Classification with Graph Convolutional Networks, arXiv e-prints , arXiv:1609.02907 (Sep 2016).

<sup>3</sup>H. Maron, E. Fetaya, N. Segol, Y. Lipman, On the Universality of Invariant Networks, arXiv:1901.09342 [cs.LG] (May 2019).

# III. Assignment Problems

## 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  $\Pi \in \mathcal{S}_n$ .

# Graph Alignment Problems

Consider two  $n \times n$  symmetric matrices  $A, B$ . The “vanilla” alignment problem for quadratic forms asks for the orthogonal matrix  $U \in O(n)$  that minimizes

$$\|UAU^T - B\|_F^2 := \text{trace}((UAU^T - B)^2) = \|A\|_F^2 + \|B\|_F^2 - 2\text{trace}(UAU^T B).$$

The solution is well-known and depends on the eigendecomposition of matrices  $A, B$ : if  $A = U_1 D_1 U_1^T$ ,  $B = U_2 D_2 U_2^T$  then

$$U_{opt} = U_2 U_1^T, \quad \|U_{opt} A U_{opt}^T - B\|_F^2 = \sum_{k=1}^n |\lambda_k - \mu_k|^2,$$

where  $D_1 = \text{diag}(\lambda_k)$  and  $D_2 = \text{diag}(\mu_k)$  are diagonal matrices with eigenvalues ordered monotonically.

# Quadratic Assignment Problem (QAP)

The challenging case is when  $U$  is constrained to the permutation group as is the case in the *graph matching problem*. In this case, the optimization problem becomes

$$\min_{U \in \mathcal{S}_n} \|UAU^T - B\|_F$$

which turns into a QAP:  $\max_{U \in \mathcal{S}_n} \text{trace}(UAU^T B)$ .

This is equivalent to computing the natural distance

$d(\hat{A}, \hat{B}) = \min_{P, Q \in \mathcal{S}_n} \|PAP^T - QBQ^T\|_F$  between the equivalence classes  $\hat{A}, \hat{B} \in \widehat{\text{Sym}(n)}$  induced by action  $(\Pi, A) \mapsto \Pi A \Pi^T$ .

How is this connected to the embedding problem? If one can design an *efficient* nearly isometric map  $\Phi : \text{Sym}(n) \rightarrow \mathbb{R}^m$  so that

(1)  $\Phi(PAP^T) = \Phi(A)$  for all  $P \in \mathcal{S}_n$  and  $A \in \text{Sym}(n)$ , and

(2)  $(1-\delta) \min_{P \in \mathcal{S}_n} \|PAP^T - B\| \leq \|\Phi(A) - \Phi(B)\| \leq (1+\delta) \min_{P \in \mathcal{S}_n} \|PAP^T - B\|$ ,

then the QAP solved efficiently up to a multiplicative factor.



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# Problem Setup

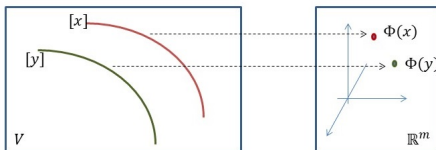
Consider a group  $G \subset O(d)$  acting on the Euclidean space  $V = \mathbb{R}^d$ .

## General problem

Construct an embedding map  $\Phi : V \rightarrow \mathbb{R}^m$

- ① Invariance:  $\Phi(U_g x) = \phi(x) \quad \forall g \in G, x \in V$
- ② Injectivity: if  $\Phi(x) = \Phi(y)$  then there exists  $g \in G$  so that  $y = U_g x$ .
- ③  $\Phi$  is bi-Lipschitz on  $(\hat{V} = V/G, \mathbf{d})$ :

$$a_0 \inf_{u \in [x], v \in [y]} \|u - v\| \leq \|\Phi(x) - \Phi(y)\| \leq b_0 \inf_{u \in [x], v \in [y]} \|u - v\|.$$



# Approaches

Over the past many years, several constructions have been proposed:

- ① Invariant Polynomials: Hilbert, Noether, ..., Cahill<sup>4</sup>, Bandeira<sup>5</sup>
- ② Kernels: replace monomials by other kernels, e.g.  $e^{i\omega x}$ ,  $e^{-x^2}$ ,  $\sigma(\langle x, a \rangle)$ <sup>6</sup>
- ③ Sorting: extends the 1-D sorting,  $x \mapsto \downarrow x$ <sup>7,8</sup>

~~1+2: *sum pooling* layer; 3: *max pooling* layer deep nets<sup>9, 10</sup>.~~

<sup>4</sup>J. Cahill, A. Contreras, A.C. Hip, Complete Set of translation Invariant Measurements with Lipschitz Bounds, Appl. Comput. Harm. Anal. 49 (2020), 521–539.

<sup>5</sup>A. Bandeira, B. Blum-Smith, J. Kileel, J. Niles-Weed, A. Perry, A.S. Wein, Estimation under group actions: Recovering orbits from invariants, ACHA 66 (2023)

<sup>6</sup>D. Yarotsky, Universal approximations of invariant maps by neural networks, Constructive Approximation (2021)

<sup>7</sup>R. Balan, N. Haghani, M. Singh, Permutation-Invariant Representations with Applications to Graph Deep Learning, arXiv:2203.07546

<sup>8</sup>J. Cahill, J.W. Iverson, D.G. Mixon, D. Packer, Group-invariant max filtering, arXiv:2205.14039.

<sup>9</sup>O. Vinyals, S. Bengio, M. Kudlur, Order Matters: Sequence to sequence for sets, ICLR 2016

<sup>10</sup>H. Maron, H. Ben-Hamu, N. Shamir, Y. Lipman, Invariant and equivariant graph networks, ICLR 2019

# Idea

Consider the special case  $G = S_n$  is the symmetric group acting by permutation matrices on  $V = \mathbb{R}^n$ .

The ring of invariant polynomials is generated by the elementary symmetric polynomials  $e_1, \dots, e_n$ ,  $\mathbb{R}[X_1, \dots, X_n]^{S_n} \simeq \mathbb{R}[e_1, \dots, e_n]$ . There is a natural embedding  $\mathbb{R}^n / S_n \hookrightarrow \mathbb{R}^n$ ,  $x \mapsto (e_1(x), \dots, e_n(x))$ .

Drawback: it is not bi-Lipschitz.

# Idea

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Drawback: it is not bi-Lipschitz.

Alternatively: Consider the embedding  $\downarrow: \mathbb{R}^n/S_n \hookrightarrow \mathbb{R}^n$ ,  $x \mapsto \downarrow(x)$ , that sorts monotone decreasing the vector  $x$ .

Key observation:  $\min_{P \in S_n} \|x - Py\|_2 = \|\downarrow x - \downarrow y\|_2$ .

Hence:  $\downarrow$  is an *isometric* embedding of  $\mathbb{R}^n/S_n$  into  $\mathbb{R}^n$ ,

# Sorting based Representations and G-invariance

Assume  $V$  is a real  $d$ -dimensional Hilbert space and  $G$  a finite orthogonal group of size  $N = |G|$ , acting on  $V$ ,  $\{U_g, g \in G\}$ .

Fix a generator  $w \in V$  (call it, *window*, or *template*, or *wavelet*) and consider the nonlinear map induced by sorting its coorbit:

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

where  $\downarrow(y) = (y_{\pi(i)})_{i \in [N]}$  is the non-increasing sorting operator:

$$y_{\pi(1)} \geq \cdots \geq y_{\pi(N)}.$$

Key observations:

- ①  $\phi_w(U_g x) = \phi_w(x)$ ,  $\phi$  is  $G$ -invariant.
- ②  $\phi_w$  is piecewise linear (in fact,  $\phi_w(x) = \phi_x(w)$ , and  $(w, x) \mapsto \phi_w(x)$  is piecewise bilinear).

# G-Invariant Coorbit Representations

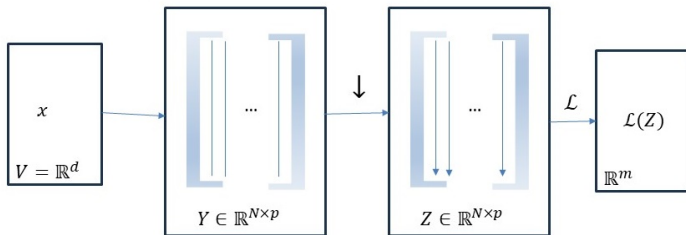
For a collection  $\mathbf{w} = (w_1, \dots, w_p) \in V^p$  the sorted coorbit representation:

$$\Phi_{\mathbf{w}} : V \rightarrow \mathbb{R}^{N \times p}, \quad \Phi_{\mathbf{w}}(x) = [\phi_{w_1}(x) | \dots | \phi_{w_p}(x)].$$

Apply a dimension-reduction linear map  $\mathcal{L} : \mathbb{R}^{N \times p} \rightarrow \mathbb{R}^m$ , the G-invariant coorbit representation:

$$\Psi_{\mathbf{w}, \mathcal{L}} : V \rightarrow \mathbb{R}^m, \quad \Psi_{\mathbf{w}, \mathcal{L}}(x) = \mathcal{L}(\Phi_{\mathbf{w}}(x))$$

$$x \mapsto Y := (\langle x, U_g w \rangle)_{g \in G} \times p \quad Y \mapsto Z := \downarrow (\langle x, U_g w \rangle)_{g \in G} \times p \quad Z \mapsto \mathcal{L}(Z)$$



In particular, if  $S \subset [N] \times [p]$ ,  $\Phi_{\mathbf{w}, S} := \Psi_{\mathbf{w}, 1_S} = \Phi_{\mathbf{w}}|_S$ .

# G-Invariant Coorbit Representations

Special cases:

1. For  $G = S_n$  and  $V = \mathbb{R}^{n \times d}$  with action  $(P, X) \mapsto PX$  <sup>11</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. This is of the type  $\Psi_{w, \mathcal{L}}$  for  $w_1 = \delta_1 \cdot a_1^T, \dots, w_D = \delta_1 \cdot a_D^T$ , where  $\delta_1 = (1, 0, \dots, 0)^T$  and  $A = [a_1 | \dots | a_D]$ , and  $\mathcal{L}$  a restriction operator to an appropriate subset  $S \subset [n!] \times [D]$  of size  $nD$ .

2. The *max filter* introduced in <sup>12</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:  $\langle \langle x, w \rangle \rangle = \mathcal{L}(\Phi_w(X))$ , for a restriction operator  $\mathcal{L}$  to the subset  $S = \{1\}$ .

3. The operator  $\Psi_{w, \mathcal{L}}$ ,  $\Psi_{w, \mathcal{L}}(X) = \mathcal{L}(\Phi_w(X))$  has been introduced in <sup>13</sup>

<sup>11</sup>R. Balan, N. Haghani, M. Singh, Permutation Invariant Representations with Applications to Graph Deep Learning, arXiv:2203.07546 (2022)

<sup>12</sup>J. Cahill, J. W. Iverson, D. G. Mixon, D. Packer, Group-invariant max filtering, arXiv:2205.14039 (2022)

<sup>13</sup>R.B, Efstratios Tsoukanis, Matthias Wellershoff, "Stability of sorting based embeddings", arXiv:2410.05446 (2024)



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# Main Results

## Injectivity

Let  $V_G = \{x \in V : U_g x = x, \forall g \in G\}$ ,  $d_G = \dim(V_G)$ ,  $q \geq 0$  and for  $g = (g_1, \dots, g_n)$ ,  $h = (h_1, \dots, h_n) \in H_n \subset G^n$  distinct,  $\rho_n(q) = \max_{g,h} \gamma_{g,h}^q$  where  $\gamma_{g,h}^q = \text{semi.alg.dim.} \{(x, y) \in V \times V : \dim(\text{span}\{U_{g_k} x - U_{h_k} y, k \in [n]\}) = q\}$

## Theorem (R.B., E. Tsoukanis '23-'25)

In any of the following cases

- ➊ Assume  $p \geq 2 \dim(V) - d_G$  and set  $\mathbf{n} = (k_1, \dots, k_p) \in [N]^p$ .
- ➋ Fix  $n \in [N]$  and choose  $p > \max_{q \in [n]} \frac{1}{q}(\rho_n(q) - d_G - 1)$ . Set  $\mathbf{n} = (n, \dots, n) \in [N]^p$ .
- ➌ Choose  $p \geq 1$  and  $\mathbf{n} = (n_1, \dots, n_p) \in [N]^p$  so that  $\max_{q_1 \in [n_1], \dots, q_p \in [n_p]} (\min_{i \in [p]} \rho_{n_i}(q_i) - (q_1 + \dots + q_p)) \leq d_G$ .

For a generic (w.r.t. Zariski topology)  $\mathbf{w}$  and for any  $S \subset [N] \times [p]$  with  $|\{k : (k, i) \in S\}| \geq n_i$ , the map  $\Phi_{\mathbf{w}, S} : (\widehat{V}, \mathbf{d}) \rightarrow (\mathbb{R}^{|S|}, \|\cdot\|_2)$  is injective.

# Main Results (2)

## Theorem (R.B, E.T., M. Wellershoff '24)

Consider the same setup as before. Assume  $\mathbf{w} \in V^p$  and  $\mathcal{L} : \mathbb{R}^{N \times p} \rightarrow \mathbb{R}^m$  so that  $\Psi_{\mathbf{w}, \mathcal{L}} : (\hat{V}, \mathbf{d}) \rightarrow (\mathbb{R}^m, \|\cdot\|_2)$  is **injective**.

- 1 *Themap  $\Psi_{\mathbf{w}, \mathcal{L}} : (\hat{V}, \mathbf{d}) \rightarrow (\mathbb{R}^m, \|\cdot\|_2)$  is bi-Lipschitz. Let  $a_0, b_0$  denote its bi-Lipschitz constants.*
- 2 *If  $f : V \rightarrow H$  is a Lipschitz continuous function so that  $f(U_g x) = f(x)$  for all  $g, x$ , where  $H$  is a Hilbert space, then there exists a Lipschitz continuous function  $g : \mathbb{R}^m \rightarrow H$  so that  $f = g \circ \Psi_{\mathbf{w}, \mathcal{L}}$ , i.e.  $f(x) = g(\Psi_{\mathbf{w}, \mathcal{L}}(x))$ . Furthermore,  $\text{Lip}(g) \leq \text{Lip}(f)/a_0$ .*
- 3 *Assume  $g : \mathbb{R}^m \rightarrow H$  is a Lipschitz function with Lipschitz constant  $\text{Lip}(g)$ . Then  $f = g \circ \Psi_{\mathbf{w}, \mathcal{L}} : V \rightarrow H$  is  $G$ -invariant and Lipschitz, with Lipschitz constant  $\text{Lip}(f) \leq b_0 \text{Lip}(g)$ .*

Its proof is based on Kirszbraun's extension theorem.

# Existing Results

## Injectivity problem

Over the past 15 years or so, there have been works that recognized the difference between *generating polynomials* and *separating invariants*<sup>14</sup>. A seminal paper that resurfaces results on semi-algebraic sets is <sup>15</sup>. The method goes back to earlier works in phase retrieval<sup>16</sup>.

More recently, in the context of G-invariance, <sup>17, 18</sup>, or permutation invariance<sup>19</sup>

<sup>14</sup>Emilie Dufresne, Separating invariants and finite reflection groups, Advances in Mathematics 221 (2009), no. 6, 1979–1989.

<sup>15</sup>Dym Nadav, Steven J. Gortler. "Low dimensional invariant embeddings for universal geometric learning." arXiv preprint arXiv:2205.02956.

<sup>16</sup>R. Balan, P. Casazza, D. Edidin, On signal reconstruction without phase, ACHA 20(2006)

<sup>17</sup>D. G. Mixon, D. Packer, Max filtering with reflection groups, arXiv:2212.05104

<sup>18</sup>R. Balan, E. Tsoukanis, G-invariant representations using coorbits: Injectivity properties, arXiv:2310.16365

<sup>19</sup>On the equivalence between graph isomorphism testing and function approximation with GNNs, Z. Chen, S. Villar, L. Chen, I. Bruna, NeurIPS 2019

## Existing Results (2)

### Lipschitz and Bi-Lipschitz properties

Earlier results obtain Lipschitz/bi-Lipschitz properties on compacts, or certain classes of functions.

Global L/bi-L are harder to establish and typically rule out polynomial based embeddings.

So far only sorting based embeddings showed such global properties <sup>20, 21, 22</sup>

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<sup>20</sup>R. Balan, E. Tsoukanis, G-invariant representations using coorbits: Bi-lipschitz properties, arXiv:2308.11784

<sup>21</sup>J. Cahill, J. W. Iverson, D. G. Mixon, Bilipschitz group invariants, arXiv:2305.17241

<sup>22</sup>D. G. Mixon, Y. Qaddura, Injectivity, stability, and positive definiteness of max filtering, arXiv:2212.11156

# Sketch of Proof: Injectivity Result

Define the “*bad*” set of  $\mathbf{w}$ 's that fail to separate all distinct classes:

$$\mathcal{F} = \{ \mathbf{w} \in V^p, \exists x \not\sim y \Phi_{\mathbf{w}}(x) = \Phi_{\mathbf{w}}(y) \}.$$

The work is to embed  $\mathcal{F}$  into a semi-algebraic set of semi-algebraic dimension strictly less than  $pd = p \dim(V)$ .

This technique is called “lift-and-project”<sup>23</sup>: we construct a semi-algebraic vector bundle embedded into a certain Grassmanian vector bundle  $\gamma_{n,k}^\perp$ . The bad set  $\mathcal{F}$  is then indentified with a subset of the projection of this vector bundle into its second component.

The full result for  $\Psi_{\mathbf{w},\mathcal{L}}$  follows from analyzing the semi-algebraic dimension of the difference-set  $\{ \Phi_{\mathbf{w}}(x) - \Phi_{\mathbf{w}}(y) \}$ .

---

<sup>23</sup>R. Balan, P. Casazza, D. Edidin, On signal reconstruction without phase, ACHA 20(2006)

## Sketch of Proof: Lower Lipschitz bound

The proof is by contradiction. Consider the simpler case when  $\mathcal{L}$  is given by restriction to a subset  $S \subset [N] \times [p]$ .

1. If lower Lipschitz constant vanishes, then it must vanish locally: there are  $(x_n)_n, (y_n)_n$  such that

$$\lim_{n \rightarrow \infty} \frac{\|\Phi_{\mathbf{w}, S}(x_n) - \Phi_{\mathbf{w}, S}(y_n)\|^2}{\mathbf{d}([x_n], [y_n])^2} = 0$$

and

$$\lim_{n \rightarrow \infty} x_n = \lim_{n \rightarrow \infty} y_n = z_1, \quad \|x_n\| = 1, \quad \|y_n\| \leq 1, \quad \|z_1\| = 1$$

and they are aligned with one another:

$$\|x_n - y_n\| = \min_{g \in G} \|x_n - U_g y_n\| \tag{4.1}$$

$$\|x_n - z_1\| = \min_{g \in G} \|x_n - U_g z_1\| \tag{4.2}$$

$$\|y_n - z_1\| = \min_{g \in G} \|y_n - U_g z_1\| \tag{4.3}$$

## Lower Lipschitz bound

2. We construct inductively  $z_2, z_3, \dots, z_d$  such that for all  $1 \leq k \leq d - 1$ :

$$\|z_{k+1}\| \ll \|z_k\|, \quad \dim(\text{span}(z_1, \dots, z_k)) = k$$

and the local lower Lipschitz constant vanishes in a convex set

$$\{\sum_{r=1}^k a_r z_r, \quad |a_r - 1| < \epsilon\}.$$

3. For  $k = d$  this construction defines a non-empty open set  $\{\sum_{r=1}^k a_r z_r, \quad |a_r - 1| < \epsilon\}$  where the local lower Lipschitz constant vanishes.

4. Finally, we can construct  $u, v \neq 0$ , so that  $x = u + \sum_{r=1}^d z_r$  and  $y = v + \sum_{r=1}^d z_r$  satisfy  $x \neq y$  and yet

$$\Phi_{w,S}(x) = \Phi_{w,S}(y).$$

This contradicts the injectivity hypothesis.



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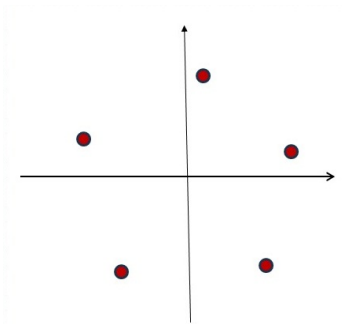
- 1 Problem Formulation
- 2 Motivation
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- 4 Main Results
- 5 Planar Rotations**
- 6 Numerical Examples in Graph Deep Learning
- 7 Extra

# Planar Rotations

Consider the group  $G = \langle U_{2\pi/N} \rangle \simeq \mathbb{Z}_N$  acting on  $V = \mathbb{R}^2$  by planar rotations

$$U_{2\pi/N}^k = U_{2\pi k/N} = \begin{bmatrix} \cos(\frac{2\pi k}{N}) & -\sin(\frac{2\pi k}{N}) \\ \sin(\frac{2\pi k}{N}) & \cos(\frac{2\pi k}{N}) \end{bmatrix}$$

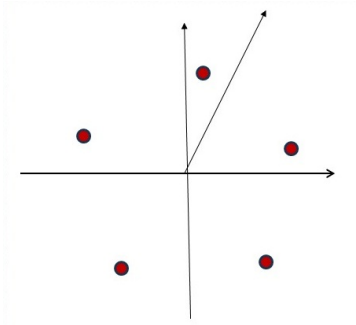
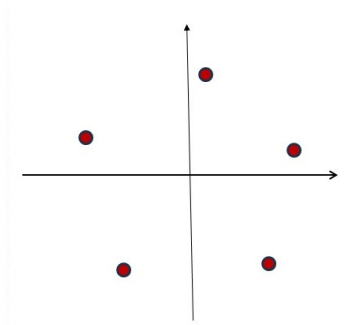
$N = 5$ . A generic orbit for rotations by  $\frac{2\pi}{5}$ .



# Planar Rotations: Metric Space

Consider the group  $G = \langle U_{2\pi/N} \rangle \simeq \mathbb{Z}_N$  acting on  $V = \mathbb{R}^2$  by planar rotations

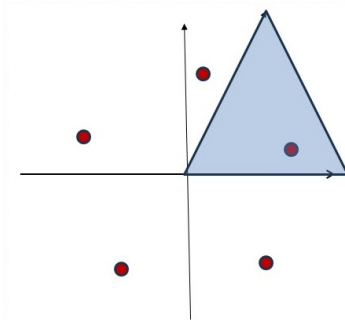
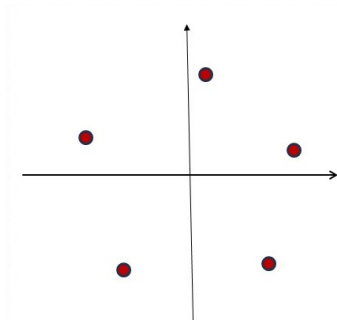
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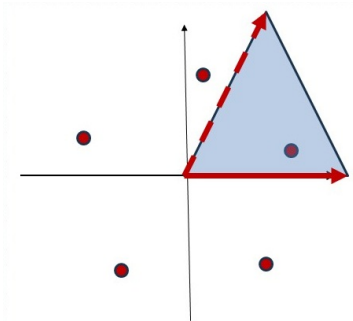
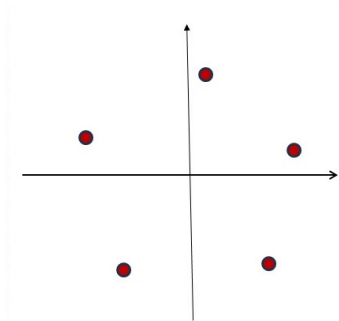
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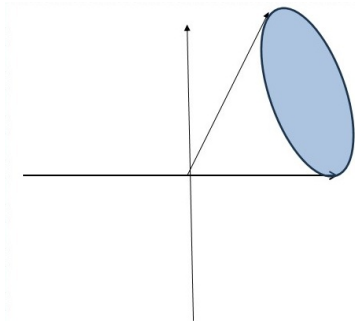
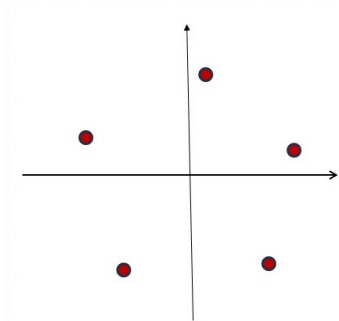
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# Planar Rotations: Metric Space

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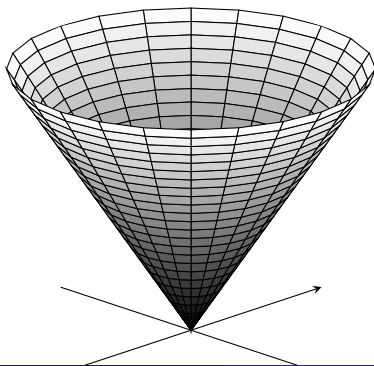


# Planar Rotations: Geometric Embedding

Explicit embedding with  $r = |x + iy| = \sqrt{x^2 + y^2}$  and  $\theta = \text{Arg}(x + iy)$ :

$$\Psi : \mathbb{R}^2 \rightarrow \mathbb{R}^3, (x, y) \mapsto \Psi(x, y) = \left( \frac{r}{N} \cos(N\theta), \frac{r}{N} \sin(N\theta), r \sqrt{1 - \frac{1}{N^2}} \right).$$

$$\frac{1}{N \sin(\frac{\pi}{2N})} \mathbf{d}((x_1, y_1), (x_2, y_2)) \leq \|\Psi(x_1, y_1) - \Psi(x_2, y_2)\|_2 \leq \mathbf{d}((x_1, y_1), (x_2, y_2))$$



3D embedding has distortion:

$$\frac{b_0}{a_0} = N \sin\left(\frac{\pi}{2N}\right) \xrightarrow{N \rightarrow \infty} \frac{\pi}{2} \approx 1.57.$$

The 2D projection:

$$(x, y) \mapsto \Psi_0(x, y) = \left( \frac{r}{N} \cos(N\theta), \frac{r}{N} \sin(N\theta) \right)$$

is bi-Lipschitz with distortion  $N$ .

# Planar Rotations: Sorted Coorbit Embedding (1)

The following result is proved by a careful analysis of this specific case ( $G = \langle U_a \rangle \simeq \mathbb{Z}_N$ ,  $a = \frac{2\pi}{N}$ ,  $V = \mathbb{R}^2$ ).

## Theorem (R.B, E.Tsoukanis'25)

- ① For any  $w \in \mathbb{R}^2$ , the map  $\Phi_w : \widehat{\mathbb{R}^2} \rightarrow \mathbb{R}^N$  is never injective.
- ② For any  $w_1, w_2 \in \mathbb{R}^2$  and  $S = \{(q_1, 1), (q_2, 2)\}$  the map  $\Phi_{w,S} : \widehat{\mathbb{R}^2} \rightarrow \mathbb{R}^2$  is never injective.
- ③ Assume either one of the following holds:
  - ①  $\mathbf{w} = (w_1, w_2, w_3) \in (\mathbb{R}^2)^3$  so that  $\{U_a^{k_1} w_1, U_a^{k_2} w_2, U_a^{k_3} w_3\}$  is a full spark frame for all integers  $k_1, k_2, k_3$ , and  $S = \{(1, 1), (1, 2), (1, 3)\}$  (the max filter);
  - ②  $\mathbf{w} = (w_1, w_2) \in (\mathbb{R}^2)^2$  so that  $\{U_{a/2}^{k_1} w_1, U_{a/2}^{k_2} w_2\}$  is linearly independent for all  $k_1, k_2$  integers, and  $S = \{(i, 1), (j, 1), (k, 2)\}$  ( $a \mathbf{n} = (2, 1)$  configuration) with  $i \neq j$  and, if  $N$  is even then  $i + j \neq N + 1$ .

Then generically, the map  $\Phi_{w,S} : \widehat{\mathbb{R}^2} \rightarrow \mathbb{R}^3$  is injective and hence



# Planar Rotations: Semi-algebraic indices

Cyclic group  $\langle U_a \rangle \simeq \mathbb{Z}_N$  generated by the planar rotation by  $a = \frac{2\pi}{N}$ .

Recall for  $g, h \in G^n$ ,

$$\gamma_{g,h}^q = \text{semi.alg.dim.} \{ (x, y) \in V \times V : \dim(\text{span}\{U_{g_k}x - U_{h_k}y, k \in [n]\}) = q \}$$

$$\rho_n(q) = \max_{g,h \in H_n} \gamma_{g,h}^q$$

where  $H_n = \{(g_1, \dots, g_n) \in G^n, g_i \neq g_j, \forall i \neq j\}$ .

Explicit computations:

$$\rho_1(q) = \begin{cases} 2, & q = 0, \\ 4, & q = 1, \\ -1, & q \geq 2. \end{cases} \quad \rho_2(q) = \begin{cases} 2, & q = 0, \\ 3, & q = 1 \text{ \& } N \text{ odd}, \\ 4, & q = 1 \text{ \& } N \text{ even}, \\ 4, & q = 2 \\ -1, & q \geq 3. \end{cases}$$

## Planar Rotations: Sorted Coorbit Embedding (2)

The expressions of semi-algebraic indices imply the following result:

### Theorem (R.B, E.Tsoukanis'25)

*Assume  $N$  is odd. For generic  $w_1, w_2, w_3 \in \mathbb{R}^2$  and every  $S = \{(k_1, 1), (k_2, 1), (k_3, 2), (k_4, 3)\}$  with  $k_1 \neq k_2$ , the map  $\Phi_{w,S} : \widehat{\mathbb{R}^2} \rightarrow \mathbb{R}^4$  is injective and hence bi-Lipschitz.*

With additional work (replacing  $H_n = \{(g_1, \dots, g_n) \in G^n, g_i \neq g_j, \forall i \neq j\}$  with  $\tilde{H}_n = \{h = (h_1, \dots, h_n) \in H_n, \exists x \in V, \downarrow (\langle x, U_g w \rangle)_{g \in G} = (\langle x, U_{h_i} w \rangle)_{i \in [n]}\}$ ), it is possible to show the following result:

### Theorem (R.B, E.Tsoukanis'25)

*Assume  $N$  is even. For generic  $w_1, w_2, w_3 \in \mathbb{R}^2$  and every  $S = \{(k_1, 1), (k_2, 1), (k_3, 2), (k_4, 3)\}$  with  $k_1 \neq k_2$  and  $k_1 + 1 + k_2 \neq N + 1$ , the map  $\Phi_{w,S} : \widehat{\mathbb{R}^2} \rightarrow \mathbb{R}^4$  is injective and hence bi-Lipschitz.*

Thank you!

Questions?

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- 1 Problem Formulation
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# The Protein Dataset

**Protein Dataset:** PROTEINS\_FULLL<sup>24</sup> consists of 1113 proteins: 663 non-enzymes and 450 enzymes. Each graph associated to one protein: nodes represent amino acids and edges represent the bonds between them. Number of nodes (aminoacids): varying between 20 and 620 with average of 39. Input feature vectors of size  $r = 29$ .

**Task:** the task is classification of each protein into *enzyme* or *non-enzyme*.

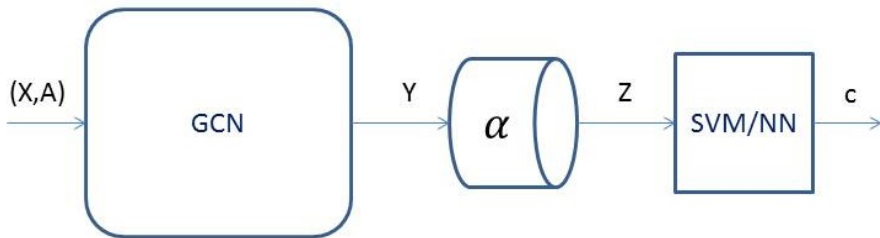
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<sup>24</sup>P.D. Dobson, A.J. Doig, "Distinguishing Enzyme Structures from Non-enzymes without Alignments", J. Mol. Biol. 330, 771-783, 2003.

# The Deep Network Architecture

**Architecture:** ReLU activation and

- GCN with  $L = 3$  layers and 29 input feature vectors, and 50 hidden nodes in each layer; no dropouts, no batch normalization. output of GCN:  $d = 1, 10, 50, 100$ .
- Mid-layer component:  $\alpha$
- Fully connected NN with dense 3-layers and 150 internal units; no dropouts, with batch normalization.



# The Network

Training has been done over 300 epochs with a batch size of 128. Loss function: binary cross-entropy.

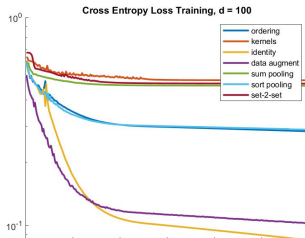
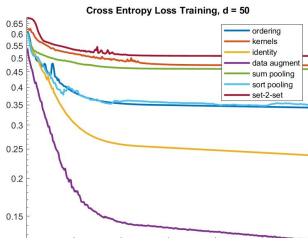
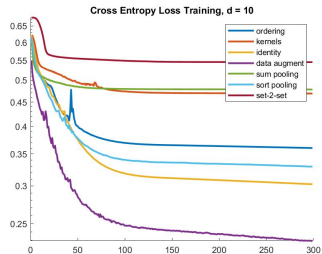
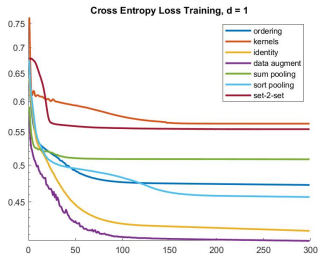
The following 7  $\alpha$  modules have been tested:

- ① identity:  $\alpha(X) = X$ ; no permutation invariance.
- ② data augmentation:  $\alpha(X) = X$  BUT the training data set has been augmented with 4 random permutatons of each graph.
- ③ ordering:  $\alpha(X) = \downarrow (XA)$ ,  $A = [I \ 1]$
- ④ kernels:  $\alpha(X) = (\sum_{k=1}^n \exp(-\|x_k - a_j\|^2))_{1 \leq j \leq m=5nd}$
- ⑤ sumpooling:  $\alpha(X) = 1^T X$
- ⑥ sort-pooling: sorted by last column
- ⑦ set-to-set: introduced in [Vinyals&al.]<sup>25</sup>

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# Enzyme Classification Example

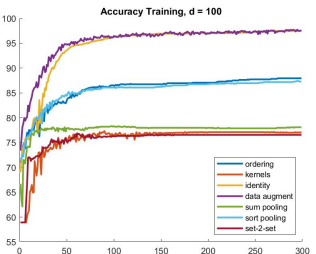
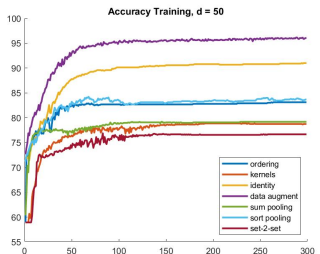
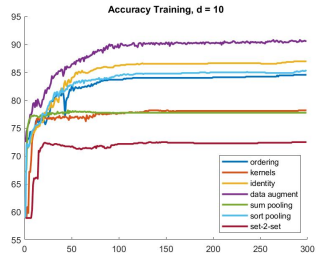
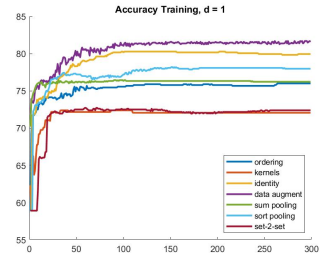
Training Loss: X Entropy





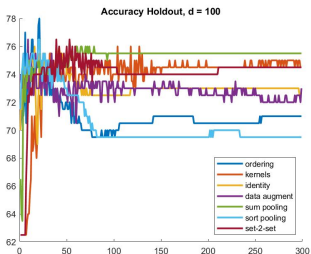
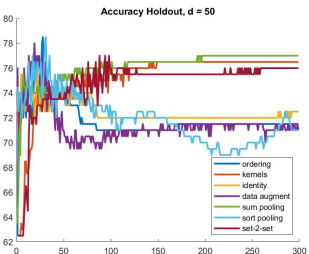
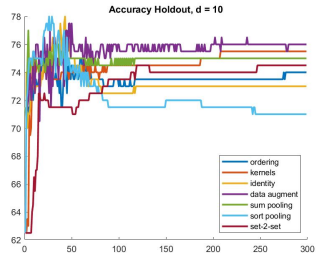
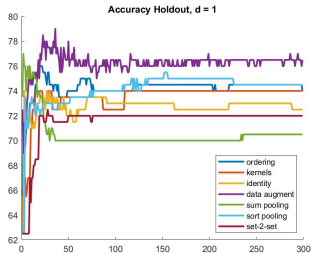
# Enzyme Classification Example

Accuracy on Training set



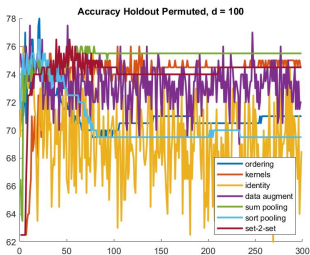
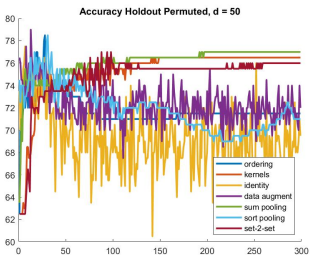
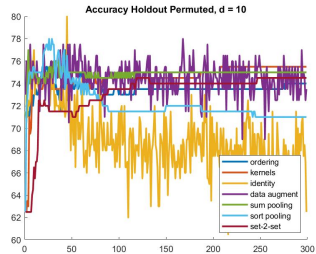
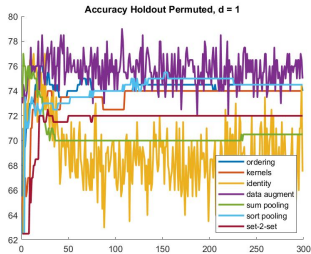
# Enzyme Classification Example

Accuracy on Holdout data



# Enzyme Classification Example

Accuracy on Holdout data with nodes randomly permuted



# Performance Results: Accuracy

d = 50	ordering	kernels	identity	data augment	sum- pooling	sort- pooling	set-2- set
Training	83.1	78.8	91	96	79.2	83.7	76.7
Holdout	71.5	76.5	72.5	71	77	71	76
Holdout Perm	71.5	76.5	69.5	72	77	71	76

**Table:** Accuracy ACC(%) for enzyme/non-enzyme classification of the seven algorithms on PROTEINS\_FULL dataset after 300 epochs for embedding dimension  $d = 50$

For comparison: [Dobson&al.]<sup>26</sup> obtains an accuracy of 77-80% using an SVM based classifier.

<sup>26</sup>P.D. Dobson, A.J. Doig, "Distinguishing Enzyme Structures from Non-enzymes without Alignments", J. Mol. Biol. 330, 771-783, 2003.

# The QM9 Dataset

**Dataset:** QM9<sup>27</sup> consists of about 134,000 isomers of organic molecules made up of CHONF, each containing 10-29 atoms. see <http://quantum-machine.org/datasets/> Nodes corresponds to atoms; each feature vector contains geometry (x,y,z coordinates), partial charge per atom (Mulliken charge), and atom type.

**Task:** the task is regression: predict a physical feature (electron energy gap  $\Delta\epsilon$ ) computed for each molecule.

**Architecture:** ReLU activation and

- GCN with  $L = 3$  layers and 50 hidden nodes in each layer; no dropouts, no batch normalization; zero padding to  $m = 29$  number of rows. output of GCN:  $d = 1, 10, 50, 100$ .
- Mid-layer component:  $\alpha$
- Fully connected NN with dense 3-layers and 150 internal units in each of the two hidden layers; no dropouts, with batch normalization.

<sup>27</sup>R. Ramakrishnan, P.O. Dral, M. Rupp, and O.A. von Lilienfeld. Quantum chemistry structures and properties of 134 kilo molecules. Scientific data. 1(1):1-7. 2014.

# The Network

Training has been done over 300 epochs with a batch size of 128. Loss function: Mean-Square Error (MSE).

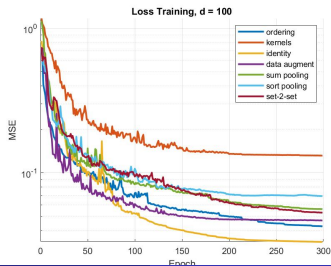
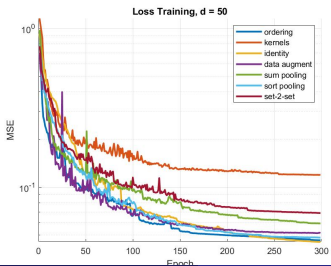
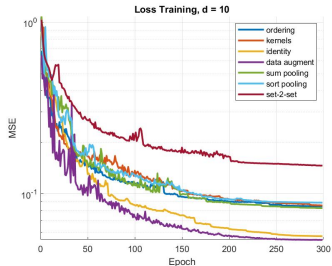
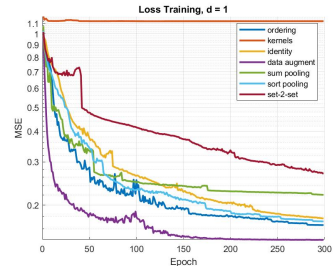
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- ⑦ set-to-set: introduced in [Vinyals&al.]<sup>28</sup>

<sup>28</sup>Vinyals, O., Bengio, S. Kudlur, M., Order Matters: Sequence to sequence for sets, ICLR 2016

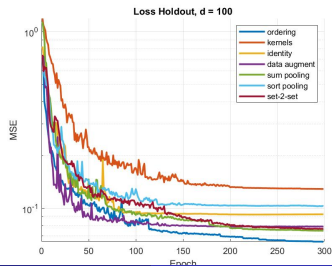
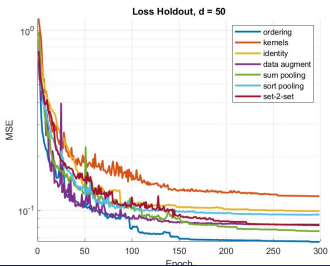
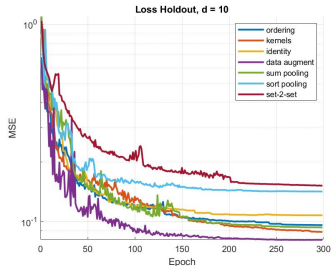
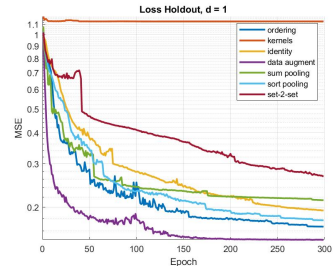
# QM9 Regression Example

## Training MSE



# QM9 Regression Example

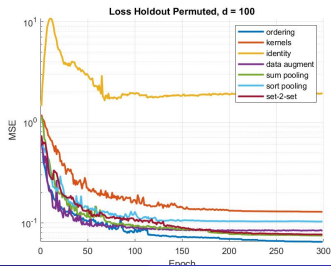
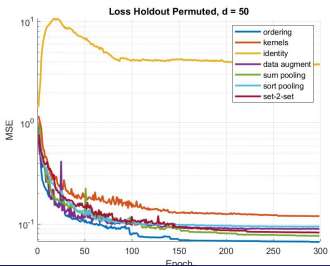
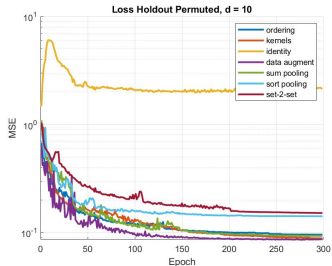
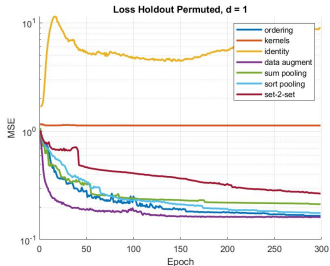
## Validation MSE





# QM9 Regression Example

## Validation MSE with Random Permutations



# Performance Results: MAE

$d = 100$	ordering	kernels	identity	data augment	sum- pooling	sort- pooling	set-2- set
Training	0.155	0.269	0.139	0.164	0.178	0.199	0.173
Holdout	0.187	0.267	0.227	0.206	0.201	0.239	0.201
Holdout Perm	0.187	0.267	1.086	0.213	0.201	0.239	0.201

**Table:** Mean Absolute Error (MAE) for regression of the electron energy gap  $\Delta\epsilon = LUMO - HOMO$  (eV) of the seven algorithms on QM9 dataset after 300 epochs for embedding dimension  $d = 100$

For comparison:

- chemical accuracy is 0.043eV
- the best ML method [Gilmer&al.] achieves MAE of 0.053eV
- Coulomb method [Rupp&al.] achieves MAE of 0.229eV

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# 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  $P \in \mathcal{S}_n$ .

The Wasserstein-2 distance is equivalent to the natural metric:

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

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

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

# 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:

- ① Polynomial embeddings:  $\mathbb{R}[X]^{\mathcal{S}_n}$ , ring of invariant polynomials; [Lipman&al.],[Peyré&al.],[Sanay&al.],[Kemper book] ...
- ② Gaussian kernels:  $f_j(x) = \exp(-\|x - a_j\|^2/\sigma_j^2)$ ; [Gilmer&al.],[Zaheer&al.], [Vinyals&al.],...
- ③ 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.]. Ok on (some) compacts.

# The Embedding Problem

## Notations (2)

### Definition

Fix  $X \in \mathbb{R}^{n \times d}$ . A matrix  $A \in \mathbb{R}^{d \times D}$  is called **admissible** for  $X$  if  $\beta_A^{-1}(\beta_A(X)) = \hat{X}$ . In other words, if  $Y \in \mathbb{R}^{n \times d}$  so that  $\downarrow(XA) = \downarrow(YA)$  then there is  $\Pi \in \mathcal{S}_n$  so that  $Y = \Pi X$ .

We denote by  $\mathcal{A}_{d,D}(X)$  (or  $\mathcal{A}(X)$ ) the set of admissible keys for  $X$ .

### Definition

Fix  $A \in \mathbb{R}^{d \times D}$ . A data matrix  $X \in \mathbb{R}^{n \times d}$  is said **separated by  $A$**  if  $A \in \mathcal{A}(X)$ .

We let  $\mathcal{S}(A)$  denote the set of data matrices separated by  $A$ .

The key  $A$  is universal iff  $\mathcal{S}(A) = \mathbb{R}^{n \times d}$ .

# Genericity Results for $d \geq 2$

Admissible keys

## Theorem

Let  $X \in \mathbb{R}^{n \times d}$ . For any  $D \geq d + 1$  the set  $\mathcal{A}_{d,D}(X)$  of admissible keys for  $X$  is dense in  $\mathbb{R}^{d \times D}$  with respect to Euclidean topology, and it is generic with respect to Zariski topology. In particular,  $\mathbb{R}^{d \times D} \setminus \mathcal{A}_{d,D}(X)$  has Lebesgue measure 0, i.e., almost every key is admissible for  $X$ .

## Proof

It is sufficient to consider the case  $D = d + 1$ . Also, it is sufficient to analyze the case  $A = [I_d \ b]$  and to show that a generic  $b \in \mathbb{R}^d$  defines an admissible key. The vector  $b \in \mathbb{R}^d$  does **not** define an admissible key if there are  $\Xi, \Pi_1, \dots, \Pi_d \in S_n$  so that for  $Y = [\Pi_1 x_1, \dots, \Pi_d x_d]$ ,

$$Yb = \Xi Xb \quad \text{but} \quad Y - \Pi X \neq 0, \quad \forall \Pi \in S_n$$

Define the linear operator



# Genericity Results for $d \geq 2$

Admissible keys

## Proof - cont'd

Let

$$\mathcal{P} = \left\{ (\Pi_1, \dots, \Pi_d) \in (\mathcal{S}_n)^d \mid \forall \Pi \in \mathcal{S}_n, \exists k \in [d] \text{ s.t. } (\Pi - \Pi_k)x_k \neq 0 \right\}$$

Then

$$\{b \in \mathbb{R}^d : [I_d \ b] \text{ not admissible for } X\} = \bigcup_{(\Xi; \Pi_1, \dots, \Pi_d) \in \mathcal{S}_n \times \mathcal{P}} \ker(B(\Xi; \Pi_1, \dots, \Pi_d))$$

It is now sufficient to show that each null space has dimension less than  $d$ . Indeed, the alternative would mean  $B(\Xi; \Pi_1, \dots, \Pi_d) = 0$  but this would imply  $(\Pi_1, \dots, \Pi_d) \notin \mathcal{P}$ .  $\square$

# Non-Universality of vector keys

## Insufficiency of a single vector key

The following is a no-go result, which shows that there is no universal single vector key for data matrices tall enough.

### Proposition

If  $d \geq 2$  and  $n \geq 3$ ,

$$\bigcup_{X \in \mathbb{R}^{n \times d}} \{b \in \mathbb{R}^d : A = [I_d \ b] \text{ not admissible for } X\} = \mathbb{R}^d.$$

Consequently,

$$\bigcap_{X \in \mathbb{R}^{n \times d}} \mathcal{A}_{d,d+1}(X) = \emptyset.$$

On the other hand, for  $n = 2$ ,  $d = 2$ , any vector  $b \in \mathbb{R}^2$  with  $b_1 b_2 \neq 0$  defines a universal key  $A = [I_2 \ b]$ .

# Non-Universality of vector keys

## Insufficiency of a single vector key - cont'd

### Proof

To show the result, it is sufficient to consider a counterexample for  $n = 3$ ,  $d = 2$ , with key  $b = [1, 1]^T$ .

$$X = \begin{bmatrix} 1 & -1 \\ -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad Y = \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{bmatrix}$$

Then  $Xb = [0, -1, 1]^T$  and  $Yb = [1, 0, -1]^T$ , yet  $X \not\sim Y$ . Thus  $[I_2 \ b]$  is not admissible for  $X$ .

Then note if  $a \in \mathbb{R}^d$  so that  $[I_d \ a]$  is admissible for  $X$  then for any  $P \in S_d$  and  $L$  an invertible  $d \times d$  diagonal matrix,  $L^{-1}P^T A \in \mathcal{A}_{d,1}(XPL)$ . This shows how for any  $b \in \mathbb{R}^2$ , one can construct  $X \in \mathbb{R}^{3 \times 2}$  so that  $b \notin \mathcal{A}_{2,1}(X)$ .

For  $n > 3$  or  $d > 2$ , proof follows by embedding this example.

# Genericity Results for $d \geq 2$

## Admissible Data Matrices

### Theorem

*Assume  $a \in \mathbb{R}^d$  is a vector with non-vanishing entries, i.e.,  $a_1 a_2 \cdots a_d \neq 0$ . Then for any  $n \geq 1$ ,  $\mathcal{S}([I_d \ a])$  is dense in  $\mathbb{R}^{n \times d}$  and includes an open dense set with respect to Zariski topology. In particular,  $\mathbb{R}^{n \times d} \setminus \mathcal{S}([I_d \ a])$  has Lebesgue measure 0, i.e., almost every data matrix  $X$  is separated by the vector key  $a$ .*

# Genericity Results for $d \geq 2$

## Admissible Data Matrices

### Theorem

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### Corollary

Assume  $A \in \mathbb{R}^{d \times (D-d)}$  is a matrix such that at least one column has non-vanishing entries. Then for any  $n \geq 1$ ,  $\mathcal{S}([I_d \ A])$  is dense in  $\mathbb{R}^{n \times d}$  and is generic with respect to Zariski topology. In particular,  $\mathbb{R}^{n \times d} \setminus \mathcal{S}([I_d \ A])$  has Lebesgue measure 0, i.e., almost every data matrix  $X$  is separated by the matrix key  $[I_d \ A]$ .

# Proof that $\mathcal{S}([I_d \ A])$ is generic

The case  $D > d$

Assume  $A \in \mathbb{R}^{d \times (D-d)}$  satisfies  $A_{1,k} A_{2,k} \cdots A_{d,k} \neq 0$  for some  $k \in [D-d]$ . The set of non-separated data matrices  $X \in \mathbb{R}^{n \times d}$  (i.e., the complement of  $\mathcal{S}([I_d \ A])$ ) factors as follows:

$$\mathbb{R}^{n \times d} \setminus \mathcal{S}([I_d \ A]) = \bigcup_{(\Xi_1, \dots, \Xi_{D-d}; \Pi_1, \dots, \Pi_d) \in (\mathcal{S}_n)^D} \left( \ker L(\Xi_1, \dots, \Xi_{D-d}; \Pi_1, \dots, \Pi_d; A) \setminus \bigcup_{\Pi \in \mathcal{S}_n} \ker M(\Pi, \Pi_1, \dots, \Pi_d) \right) \quad (*)$$

where, with  $A = [a_1, \dots, a_{D-d}]$ ,  $X = [x_1, \dots, x_d]$ :

$$L(\Xi_1, \dots, \Xi_{D-d}; \Pi_1, \dots, \Pi_d; A): \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^{n \times D-d}, \quad (L((\dots)X))_k = [(\Xi_k - \Pi_1)x_1, \dots, (\Xi_k - \Pi_d)x_d] a_k, \quad k \in [D-d]$$

$$M(\Pi, \Pi_1, \dots, \Pi_d): \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^{n \times d}, \quad M(\Pi, \Pi_1, \dots, \Pi_d)X = [(\Pi - \Pi_1)x_1, \dots, (\Pi - \Pi_d)x_d]$$

# Proof that $\mathcal{S}(A)$ is generic

cont'd

1. The outer union can be reduced by noting that on the "diagonal"  $\Delta$ ,

$$\Delta = \{(\Xi_1, \dots, \Xi_{D-d}; \Pi_1, \dots, \Pi_d) \in (\mathcal{S}_n)^D, \Pi_1 = \Pi_2 = \dots = \Pi_d\}$$

$$M(\Pi_1, \Pi_1, \dots, \Pi_d) = 0 \rightarrow \bigcup_{\Pi \in \mathcal{S}_n} \ker M(\Pi, \Pi_1, \dots, \Pi_d) = \mathbb{R}^{n \times d}$$

2. If  $(\Xi_1, \dots, \Xi_{D-d}; \Pi_1, \dots, \Pi_d) \in (\mathcal{S}_n)^D \setminus \Delta$  then for every  $k \in [D-d]$  there is  $j \in [d]$  such that  $\Xi_k - \Pi_j \neq 0$ . In particular choose the  $k$  column of  $A$  that is non-vanishing. Let  $x_j \in \mathbb{R}^n$  so that  $(\Xi_k - \Pi_j)x_j \neq 0$ . Consider the matrix  $X = [0, \dots, 0, x_j, 0, \dots, 0]$  where  $x_j$  is the only non identically 0 column. Claim:  $X \notin \ker L(\Xi_1, \dots, \Pi_d; A)$ . Indeed, the resulting  $k$  column of  $L()X$  is  $A_{j,k}(\Xi_k - \Pi_j)x_j \neq 0$ . It follows that

$$\dim \ker L(\Xi_1, \dots, \Xi_{D-d}; \Pi_1, \dots, \Pi_d; A) < nd$$

Hence  $\mathbb{R}^{n \times d} \setminus \mathcal{S}([I_d A])$  is a finite union of subsets of closed linear spaces properly included in  $\mathbb{R}^{n \times d}$ . This proves the theorem.  $\square$

# Additional Relations

Note the following relationship and matrix representation of  $X$  when matrices are column-stacked:

$$M(\Pi, \Pi_1, \dots, \Pi_d) = L(\Pi, \dots, \Pi; \Pi_1, \dots, \Pi_d; I)$$

$$L \equiv \begin{bmatrix} A_{1,1}(\Xi_1 - \Pi_1) & A_{2,1}(\Xi_1 - \Pi_2) & \cdots & A_{d,1}(\Xi_1 - \Pi_d) \\ A_{1,2}(\Xi_2 - \Pi_1) & A_{2,2}(\Xi_2 - \Pi_2) & \cdots & A_{d,2}(\Xi_2 - \Pi_d) \\ \vdots & \vdots & \ddots & \vdots \\ A_{1,D-d}(\Xi_{D-d} - \Pi_1) & A_{2,D-d}(\Xi_{D-d} - \Pi_2) & \cdots & A_{d,D-d}(\Xi_{D-d} - \Pi_d) \end{bmatrix}$$

a  $n(D-d) \times nd$  matrix.



# 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  $\mathbb{R}^{d \times D}$  ?

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