Low-Dimensional Lipschitz Embeddings Invariant to Permutations

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Joint work with:
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arXiv preprint: 2203.07546 [math.FA], [cs.LG]
In this talk, we discuss Euclidean embeddings of metric spaces induced by representations of permutation (sub)groups $S_n$ on linear spaces $V$.

Problem: Construct bi-Lipschitz embeddings of the metric space $\hat{V} = V/\sim$ of orbits, $\alpha : \hat{V} \to \mathbb{R}^m$, where $d(\hat{x}, \hat{y}) = \min_{u \in \hat{x}, v \in \hat{y}} \|u - v\|_V$.

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Today we focus on the case $V = \mathbb{R}^{n \times d}$, $X \sim Y \iff Y = PX$ for some $P \in S_n$.
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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 $f : (A, X) \to f(A, X)$ that performs:

1. classification: $f(A, X) \in \{1, 2, \cdots, c\}$
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 $P \in S_n$. 
Graph Convolution Networks (GCN), Graph Neural Networks (GNN)

General architecture of a GCN/GNN

$$Y_1 = \sigma(\tilde{A}XW_1 + B_1)$$
$$Y_2 = \sigma(\tilde{A}Y_1W_2 + B_2)$$
$$\vdots$$
$$Y_L = \sigma(\tilde{A}Y_{L-1}W_L + B_L)$$

GCN (Kipf and Welling ('16)) choses $\tilde{A} = I + A$; GNN (Scarselli et.al. ('08), Bronstein et.al. ('16)) choses $\tilde{A} = p_l(A)$, a polynomial in adjacency matrix. $L$-layer GNN has parameters $(p_1, W_1, B_1, \ldots, p_L, W_L, B_L)$. 

Note the covariance (or, equivariance) property: for any $P \in O(n)$ (including $S_n$), if $(A, X) \mapsto (PA^T, PX)$ and $B_i \mapsto PB_i$ then $Y \mapsto PY$. 
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Note the covariance (or, equivariance) property: for any \( P \in O(n) \) (including \( S_n \)), if \((A, X) \leftrightarrow (PAP^T, PX)\) and \( B_i \leftrightarrow PB_i \) then \( Y \leftrightarrow PY \).
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.
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The metric space $\hat{V}$ when $V = \mathbb{R}^{n \times d}$

Recall the equivalence relation $\sim$ on $V = \mathbb{R}^{n \times d}$ induced by the group of permutation matrices $S_n$ acting on $V$ by left multiplication: for any $X, X' \in \mathbb{R}^{n \times d}$,

$$X \sim X' \iff X' = PX,$$

for some $P \in S_n$

Let $\hat{\mathbb{R}^{n \times d}} = \mathbb{R}^{n \times d}\!/\sim$ be the quotient space endowed with the natural distance induced by Frobenius norm $\| \cdot \|_F$

$$d(\hat{X}_1, \hat{X}_2) = \min_{P \in S_n} \| X_1 - PX_2 \|_F,$$

$\hat{X}_1, \hat{X}_2 \in \hat{\mathbb{R}^{n \times d}}$. 

The metric space $\hat{V}$ when $V = \mathbb{R}^{n \times d}$

Recall the equivalence relation $\sim$ on $V = \mathbb{R}^{n \times d}$ induced by the group of permutation matrices $S_n$ acting on $V$ by left multiplication: for any $X, X' \in \mathbb{R}^{n \times d}$,

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$$d(\hat{X}_1, \hat{X}_2) = \min_{P \in S_n} \| X_1 - PX_2 \|_F , \quad \hat{X}_1, \hat{X}_2 \in \hat{\mathbb{R}}^{n \times d}.$$ 

The computation of the minimum distance is performed by solving the Linear Assignment Problem (LAP) whose convex relaxation is exact:

$$\max_{P \in S_n} \text{trace}(PX_2X_1^T) = \max_{W \in DS(n)} \text{trace}(WX_2X_1^T)$$

where $DS(n) = \{W \in [0, 1]^{n \times n} : W1 = 1, W^T1 = 1\}$ is the convex set of doubly stochastic matrices.
The embedding problem

**Problem**: Construct a bi-Lipschitz embedding \( \hat{\alpha} : \mathbb{R}^{n \times d} \to \mathbb{R}^m \), i.e., an integer \( m = m(n,d) \), a map \( \alpha : \mathbb{R}^{n \times d} \to \mathbb{R}^m \) with constants \( 0 < a \leq b < \infty \) so that for any \( X, X' \in \mathbb{R}^{n \times d} \),

1. If \( X \sim X' \) then \( \alpha(X) = \alpha(X') \).
2. If \( \alpha(X) = \alpha(X') \) then \( X \sim X' \).
3. \( a \cdot d(\hat{X}, \hat{X}') \leq \|\alpha(X) - \alpha(X')\|_2 \leq b \cdot d(\hat{X}, \hat{X}') \).

where \( d(\hat{X}, \hat{X}') = \min_{P \in S_n} \|X - PX'\|_F \).
A Universal Embedding

Consider the map

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

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 equivalent to the natural metric:

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

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

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 $f_1, \cdots, f_m$ and consider:

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

Possible choices:

1. **Polynomial embeddings**: \( \mathbb{R}[X]^{S_n} \), 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.
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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 $x \mapsto \downarrow x = \Pi x$, $\Pi \in S_n$, so that $(\Pi x)_1 \geq (\Pi x)_2 \geq \cdots \geq (\Pi x)_n$. 

Lemma $\downarrow$: $\hat{\mathbb{R}}^n \rightarrow \mathbb{R}^n$ is an isometry (hence bi-Lipschitz): $\|\downarrow (x) - \downarrow (y)\| = \min_{P \in S_n} \|x - Py\|$, 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 $\mathbb{R}^n \times \mathbb{R}^d$. 

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The Max Pool approach

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\[
(\Pi x)_1 \geq (\Pi x)_2 \geq \cdots \geq (\Pi x)_n.
\]

**Lemma**

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

\[
\| \downarrow (x) - \downarrow (y) \| = \min_{P \in S_n} \| x - Py \|, \quad \text{for all } x, y \in \mathbb{R}^n.
\]

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 \( \mathbb{R}^{n \times d} \).
The Encoder $\beta_A$

Notations

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

$$X \sim Y \iff \exists \Pi \in S_n, \ Y = \Pi X$$

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

$$d : \hat{\mathbb{R}}^{n \times d} \times \hat{\mathbb{R}}^{n \times d} \to \mathbb{R}, \ d(X, Y) = \min_{\Pi \in S_n} \|X - \Pi Y\|_F$$

In the following we look for an Euclidean embedding of the form

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

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 $\hat{\beta}_A : \hat{\mathbb{R}}^{n \times d} \to \mathbb{R}^{n \times D}$ is injective.
Intuition behind universality of keys

Consider the case
\[ n = 2, \ d = 3 \]

\[ X = \begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \end{bmatrix} \]
Intuition behind universality of keys

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

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\[ Y = \begin{bmatrix} Y_{11} & Y_{12} & Y_{13} \\ Y_{21} & Y_{22} & Y_{23} \end{bmatrix} \]

Information lost!
Intuition behind universality of keys

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

\[ Y = \downarrow X \]

\[ Y = \begin{bmatrix} Y_{11} & Y_{12} & Y_{13} \\ Y_{21} & Y_{22} & Y_{23} \end{bmatrix} \]
Intuition for this encoder

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

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

\[
Y = \downarrow \begin{bmatrix}
X & Xa
\end{bmatrix}
\]
Three results (1)
Existence of Universal Keys

Theorem

Consider the metric space $(\hat{\mathbb{R}}^{n\times d}, d)$. 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 $\hat{\beta}_A : \hat{\mathbb{R}}^{n\times d} \to \mathbb{R}^{n \times D}$, $\hat{\beta}_A(\hat{X}) = \downarrow (XA)$ is injective. Furthermore, $\hat{\beta}_A$ is bi-Lipschitz with constants $a_0 = \min_{J \subseteq [D], |J| = d} s_d(A[J])$ 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 $d^{th}$ singular value (in this case, the smallest) of $A[J]$. Specifically, for any $X, Y \in \mathbb{R}^{n \times d}$,

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

where all norms are Frobenius norms.
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

$$\hat{\beta}_A : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times D}, \quad X \mapsto \hat{\beta}_A(X) = \downarrow (XA)$$

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 $X, Y \in \mathbb{R}^{n \times d}$,

$$a_0 d(\hat{X}, \hat{Y}) \leq \|\hat{\beta}_A(X) - \hat{\beta}_A(Y)\| \leq b_0 d(\hat{X}, \hat{Y}) \quad (3.2)$$

where all are Frobenius norms. Furthermore, an estimate for $b_0$ is provided by the largest singular value of $A$, $b_0 = s_1(A)$. 
Three results (3)

Dimension Reduction

**Theorem**

Assume $A \in \mathbb{R}^{d \times D}$ is a universal key for $\hat{\mathbb{R}}^{n \times d}$ 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

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

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 $\hat{\mathbb{R}}^{n \times d}$ is not a manifold.
Highlights of proofs

Universal keys

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

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

$$\Pi_k := Q_k^T P_k \sum_{k=1}^{D} \|\Pi_k X - Y) a_k\|_2^2$$
The upper bound is immediate. For lower bound, fix $X, Y \in \mathbb{R}^{n \times d}$:

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

Let $\Pi_k := Q_k^T P_k$ then:

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

so that $\Pi_{k_1} = \cdots = \Pi_{k_d} = \Pi_0$ (pigeonhole principle: needs $D > (d - 1)n!$).
The upper bound is immediate. For lower bound, fix \( X, Y \in \mathbb{R}^{n \times d} \):

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

\[
\prod_k := Q_k^T P_k \sum_{k=1}^{D} \| (\prod_k X - Y) a_k \|_2^2 \geq \sum_{j=1}^{d} \| (\prod_{k_j} X - Y) a_k \|_2^2
\]

so that \( \prod_{k_1} = \cdots = \prod_{k_d} = \prod_0 \) (pigeonhole principle: needs \( D > (d - 1)n! \)). Then:

\[
\| \beta_A(X) - \beta_A(Y) \|_2^2 \geq \sum_{j=1}^{d} \| (\prod_0 X - Y) a_k \|_2^2 \overset{\text{full spark}}{\geq} s_d(A[J])^2 \| \prod_0 X - Y \|_2^2 \\
\geq s_d(A[J])^2 \min_{\Pi \in S_n} \| \Pi X - Y \|_2^2 = s_d(A[J])^2 d(\hat{X}, \hat{Y})^2
\]
Highlights of proofs
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.
The proof follows the approach in [Cahill&al.], [Dufresne]:

\[ 0 = B(\beta_A(X)) - B(\beta_A(Y)) \implies \beta_A(X) - \beta_A(Y) \in \ker(B) \]

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

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

In the polynomial case, [Cahill&al.] exploit arguments from algebraic geometry. Here the problem is simpler since \( \text{Ran}(\Delta) \) 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, \( \text{Ran}(\Delta) \) and \( \ker(B) \) intersect transversally.
Motivation

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)):

<table>
<thead>
<tr>
<th>n</th>
<th>d</th>
<th>D-d</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>(\geq 4)</td>
</tr>
</tbody>
</table>

**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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**Motivation**

\[ V = R^{n \times d} \]

**Sorting**

**Numerics**

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**The Protein Dataset**

**Protein Dataset**: 663 non-enzymes and 450 enzymes out of 1113 proteins. 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 os size \( r = 29 \).

**Task**: the task is classification of each protein into *enzyme* or *non-enzyme*.
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 permutations of each graph.
3. ordering: $\alpha(X) = (XA)_\downarrow$, $A = [I \ 1]$
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.]
Enzyme Classification Example

Training Loss: X Entropy
Enzyme Classification Example

Accuracy on Training set

Accuracy Training, $d = 1$

Accuracy Training, $d = 10$

Accuracy Training, $d = 50$

Accuracy Training, $d = 100$
Enzyme Classification Example

Accuracy on Holdout data

Motivation

\[ V = R^{n \times d} \]

Sorting

Numerics

Permutation Invariant Embeddings

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Enzyme Classification Example

Accuracy on Holdout data with nodes randomly permuted

Accuracy Holdout Permuted, $d = 1$

Accuracy Holdout Permuted, $d = 10$

Accuracy Holdout Permuted, $d = 50$

Accuracy Holdout Permuted, $d = 100$
Performance Results: Accuracy

<table>
<thead>
<tr>
<th>d = 50</th>
<th>ordering</th>
<th>kernels</th>
<th>identity</th>
<th>data augment</th>
<th>sum-pooling</th>
<th>sort-pooling</th>
<th>set-2-set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Training</td>
<td>83.1</td>
<td>78.8</td>
<td>91</td>
<td>96</td>
<td>79.2</td>
<td>83.7</td>
<td>76.7</td>
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<tr>
<td>Holdout</td>
<td>71.5</td>
<td>76.5</td>
<td>72.5</td>
<td>71</td>
<td>77</td>
<td>71</td>
<td>76</td>
</tr>
<tr>
<td>Holdout Perm</td>
<td>71.5</td>
<td>76.5</td>
<td>69.5</td>
<td>72</td>
<td>77</td>
<td>71</td>
<td>76</td>
</tr>
</tbody>
</table>

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.] obtain an accuracy of 77-80% using an SVM based classifier.
The QM9 Dataset

**Dataset:** 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 $\Delta \varepsilon$) 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.
The Network

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

The same 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 permutations 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.]
QM9 Regression Example

Training MSE
QM9 Regression Example

Validation MSE

### Loss Holdout, $d = 1$

- ordering
- kernels
- identity
- data augment
- sum pooling
- sort pooling
- set-2-set

### Loss Holdout, $d = 10$

### Loss Holdout, $d = 50$

### Loss Holdout, $d = 100$
QM9 Regression Example
Validation MSE with Random Permutations

Loss Holdout Permuted, $d = 1$

Loss Holdout Permuted, $d = 10$

Loss Holdout Permuted, $d = 50$

Loss Holdout Permuted, $d = 100$
Performance Results: MAE

<table>
<thead>
<tr>
<th>(d = 100)</th>
<th>ordering</th>
<th>kernels</th>
<th>identity</th>
<th>data augment</th>
<th>sum-pooling</th>
<th>sort-pooling</th>
<th>set-2-set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Training</td>
<td>0.155</td>
<td>0.269</td>
<td>0.139</td>
<td>0.164</td>
<td>0.178</td>
<td>0.199</td>
<td>0.173</td>
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<tr>
<td>Holdout</td>
<td>0.187</td>
<td>0.267</td>
<td>0.227</td>
<td>0.206</td>
<td>0.201</td>
<td>0.239</td>
<td>0.201</td>
</tr>
<tr>
<td>Holdout Perm</td>
<td>0.187</td>
<td>0.267</td>
<td>1.086</td>
<td>0.213</td>
<td>0.201</td>
<td>0.239</td>
<td>0.201</td>
</tr>
</tbody>
</table>

Table: Mean Absolute Error (MAE) for regression of the electron energy gap \(\Delta \varepsilon = LUMO - HOMO\) (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
Bibliography

Bibliography

Bibliography


Thank you!

Questions?
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 $\Pi \in S_n$ so that $Y = \Pi X$.

We denote by $A_{d,D}(X)$ (or $A(X)$) 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 $A \in A(X)$.

We let $S(A)$ denote the set of data matrices separated by $A$. The key $A$ is universal iff $S(A) = \mathbb{R}^{n \times d}$.
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 $A_{d,D}(X)$ 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, $\mathbb{R}^{d \times D} \setminus A_{d,D}(X)$ 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 $\Xi, \Pi_1, \cdots, \Pi_d \in S_n$ so that for $Y = [\Pi_1 x_1, \cdots, \Pi_d x_d]$,

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

Define the linear operator
Genericity Results for $d \geq 2$

Admissible keys

**Proof - cont’d**

Let

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

Then

$$
\{ b \in \mathbb{R}^d : [l_d \ b] \text{ not admissible for } X \} = \bigcup_{(\Xi; \Pi_1, \cdots, \Pi_d) \in S_n \times P} \ker(B(\Xi; \Pi_1, \cdots, \Pi_d))
$$

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

\[
\bigcap_{X \in \mathbb{R}^{n \times d}} A_{d,d+1}(X) = \emptyset.
\]

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, $L^{-1}P^TA \in A_{d,1}(XPL)$. This shows how for any $b \in \mathbb{R}^2$, one can construct $X \in \mathbb{R}^{3\times2}$ so that $b \notin A_{2,1}(X)$.

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 $n \geq 1$, $S([I_d \ a])$ is dense in $\mathbb{R}^{n \times d}$ and includes an open dense set with respect to Zariski topology. In particular, $\mathbb{R}^{n \times d} \setminus S([I_d \ a])$ 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**

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 $n \geq 1$, $S([I_d \ a])$ is dense in $\mathbb{R}^{n \times d}$ and includes an open dense set with respect to Zariski topology. In particular, $\mathbb{R}^{n \times d} \setminus S([I_d \ a])$ has Lebesgue measure 0, i.e., almost every data matrix $X$ is separated by the vector key $a$.

**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 $n \geq 1$, $S([I_d \ A])$ is dense in $\mathbb{R}^{n \times d}$ and is generic with respect to Zariski topology. In particular, $\mathbb{R}^{n \times d} \setminus S([I_d \ A])$ has Lebesgue measure 0, i.e., almost every data matrix $X$ is separated by the matrix key $[I_d \ A]$.
Proof that $S([I_d A])$ 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 $S([I_d A])$) factors as follows:

$$\mathbb{R}^{n \times d} \backslash S([I_d A]) = \bigcup_{(\Xi_1, \cdots, \Xi_{D-d}; \Pi_1, \cdots, \Pi_d) \in (S_n)^D} \left( \ker L(\Xi_1, \cdots, \Xi_{D-d}; \Pi_1, \cdots, \Pi_d; A) \right)$$

$$\bigg\backslash \bigcup_{\Pi \in S_n} \ker M(\Pi, \Pi_1, \cdots, \Pi_d) \bigg)$$

$\hspace{1cm}$ (*)

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

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

$M(\Pi, \Pi_1, \cdots, \Pi_d): \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^{n \times d}$, $M(\Pi, \Pi_1, \cdots, \Pi_d)X = [(\Pi-\Pi_1)x_1, \cdots, (\Pi-\Pi_d)x_d]$
Proof that $S(A)$ is generic

cont’d

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

$$\Delta = \{(\Xi_1, \cdots, \Xi_{D-d}; \Pi_1, \cdots, \Pi_d) \in (S_n)^D, \quad \Pi_1 = \Pi_2 = \cdots = \Pi_d \}$$

$$M(\Pi_1, \Pi_1, \cdots, \Pi_d) = 0 \to \bigcup_{\Pi \in S_n} \ker M(\Pi, \Pi_1, \cdots, \Pi_d) = \mathbb{R}^{n \times d}$$

2. If $(\Xi_1, \cdots, \Xi_{D-d}; \Pi_1, \cdots, \Pi_d) \in (S_n)^D \setminus \Delta$ 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 $X = [0, \cdots, 0, x_j, 0, \cdots, 0]$ where $x_j$ is the only non identically 0 column. Claim: $X \notin \ker L(\Xi_1, \cdots, \Pi_d; A)$. Indeed, the resulting $k$ column of $L()X$ is $A_{j,k}(\Xi_k - \Pi_j)x_j \neq 0$. It follows that

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

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

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

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

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

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