Low-Dimensional Lipschitz Embeddings Invariant to Permutations

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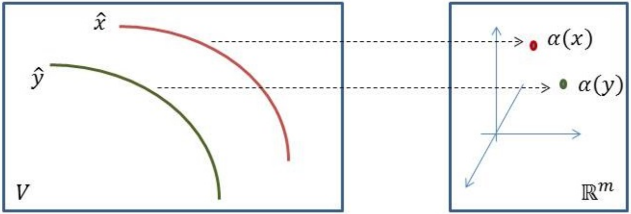
arXiv preprint: 2203.07546 [math.FA] , [cs.LG]

High-Level View

In this talk, we discuss Euclidean embeddings of metric spaces induced by representations of permutation (sub)groups $\mathcal{S}_n$ 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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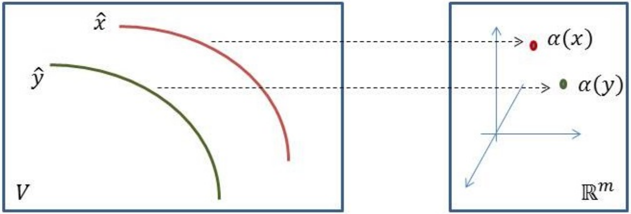

Today we focus on the case $V = \mathbb{R}^{n\times d}$, $X \sim Y \Leftrightarrow Y = PX$ for some $P \in \mathcal{S}_n$.

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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.

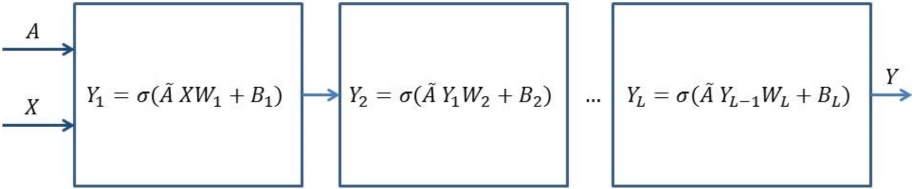
Contruct a map $f : (A, X) \to f(A, X)$ that performs:

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

Graph Convolution Networks (GCN), Graph Neural Networks (GNN)

General architecture of a GCN/GNN



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 $(p_1, W_1, B_1, \cdots, p_L, W_L, B_L)$.

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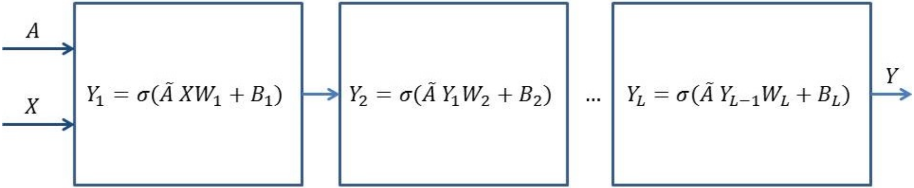

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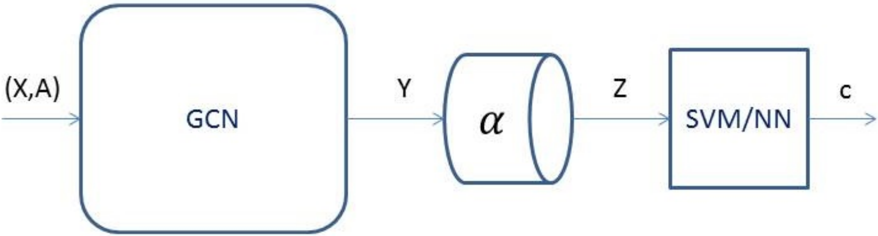
Note the *covariance (or, equivariance) property*: for any $P \in O(n)$ (including $\mathcal{S}_n$), if $(A, X) \mapsto (PAP^T, PX)$ and $B_i \mapsto PB_i$ then $Y \mapsto PY$.

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 α 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 α 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 $\mathcal{S}_n$ acting on V by left multiplication: for any $X, X' \in \mathbb{R}^{n \times d}$,

$$X \sim X' \quad \Leftrightarrow \quad X' = PX \ , \ \text{for some } P \in \mathcal{S}_n$$

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

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

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

$$\max_{P \in \mathcal{S}_n} trace(PX_2X_1^T) = \max_{W \in DS(n)} trace(WX_2X_1^T)$$

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

The embedding problem

Problem: Construct a bi-Lipschitz embedding $\hat{\alpha} : \widehat{\mathbb{R}^{n \times d}} \to \mathbb{R}^m$, 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 $d(\hat{X}, \hat{X}') = \min_{P \in \mathcal{S}_n} \|X - PX'\|_F$.

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 δ 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 $f_1, \cdots, f_m$ and consider:

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

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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.

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The Max Pool approach

The idea is provided by the following observation.
Let $\downarrow: \mathbb{R}^n \to \mathbb{R}^n$ denote the *sorting map* $x \mapsto \downarrow x = \Pi x$, $\Pi \in \mathcal{S}_n$, so that

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

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Lemma

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

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

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 β_A

Notations

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

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

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

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

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

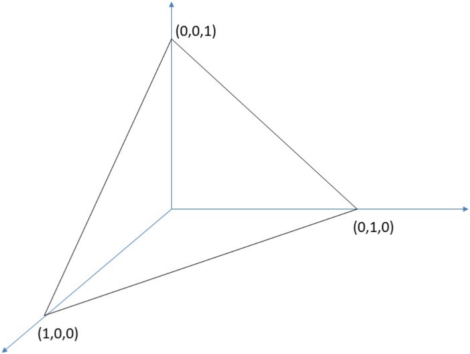
$$\beta_A : \mathbb{R}^{n\times d} \to \mathbb{R}^{n\times D} \quad , \quad \beta_A(X) = \downarrow (XA)$$

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 β_A.
The key is called *universal* if $\widehat{\beta_A} : \widehat{\mathbb{R}^{n\times d}} \to \mathbb{R}^{n\times D}$ is injective.

Intuition behind universality of keys

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

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



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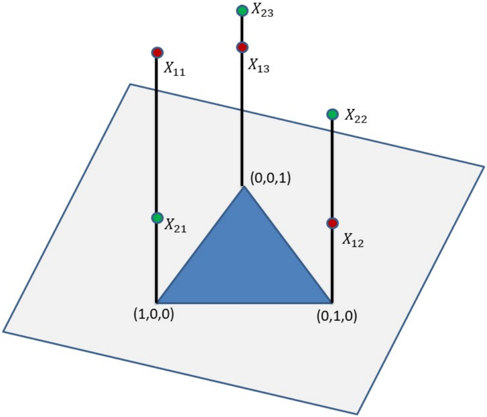

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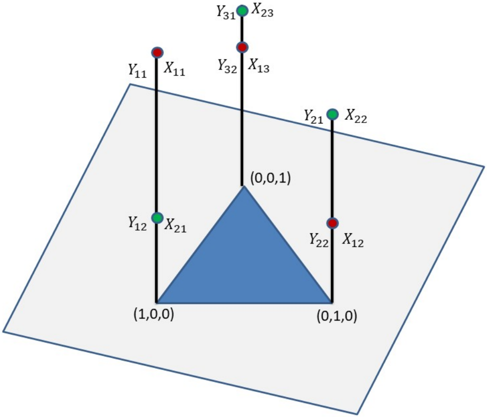
Information lost!



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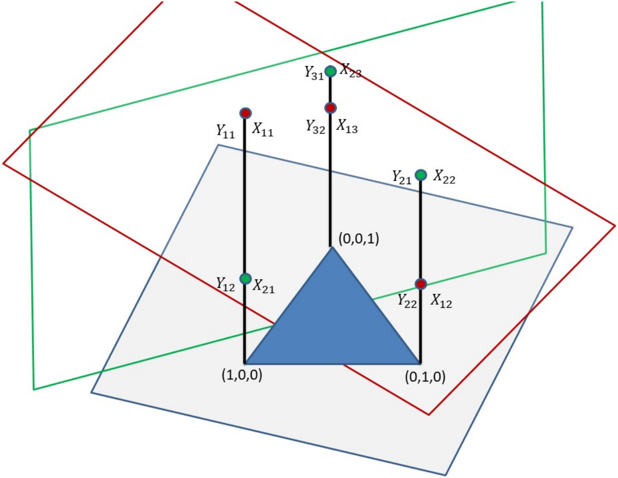
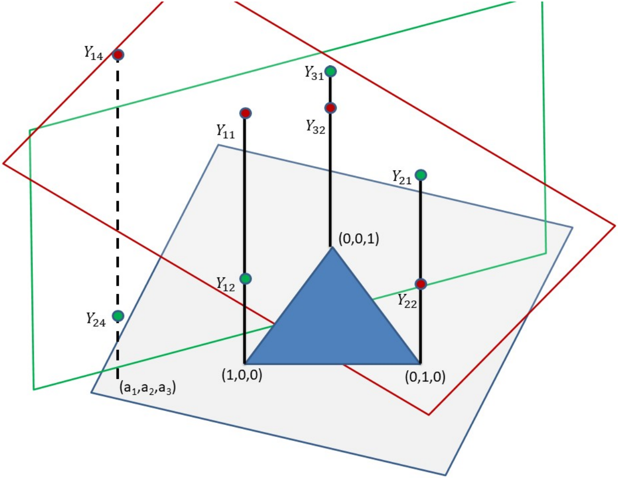


Intuition for this encoder

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

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

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



Three results (1)

Existence of Universal Keys

Theorem

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

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

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

$$a_0\, d(\hat{X}, \hat{Y}) \leq \|\beta_A(X) - \beta_A(Y)\| \leq b_0\, d(\hat{X}, \hat{Y}) \tag{3.2}$$

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

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

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

Highlights of proofs

Universal keys

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

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

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

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

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

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

$$\|\beta_A(X) - \beta_A(Y)\|_2^2 \geq \sum_{j=1}^{d} \|(\Pi_0 X - Y)a_{k_j}\|_2^2 \overset{full\ \ spark}{\geq} s_d(A[J])^2 \|\Pi_0 X - Y\|^2$$

$$\geq s_d(A[J])^2 \min_{\Pi \in \mathcal{S}_n} \|\Pi X - Y\|^2 = s_d(A[J])^2 d(\hat{X}, \hat{Y})^2$$

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.

Highlights of proofs

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

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

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.

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	≥ 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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The Protein Dataset

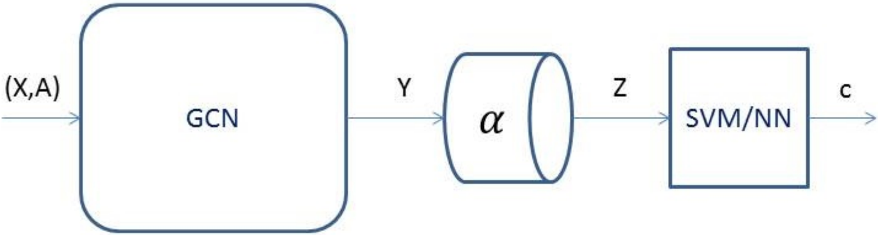
Protein Dataset: 663 non-enzymes and 450 enzymes out of 1113 proteins. Each graph associated to one protein: nodes represent amino acids and edges represent the bonds between them. Number of nodes (aminoacids): varying between 20 and 620 with average of 39. Input feature vectors os size $r = 29$.

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: α
- Fully connected NN with dense 3-layers and 150 internal units; no dropouts, with batch normalization.



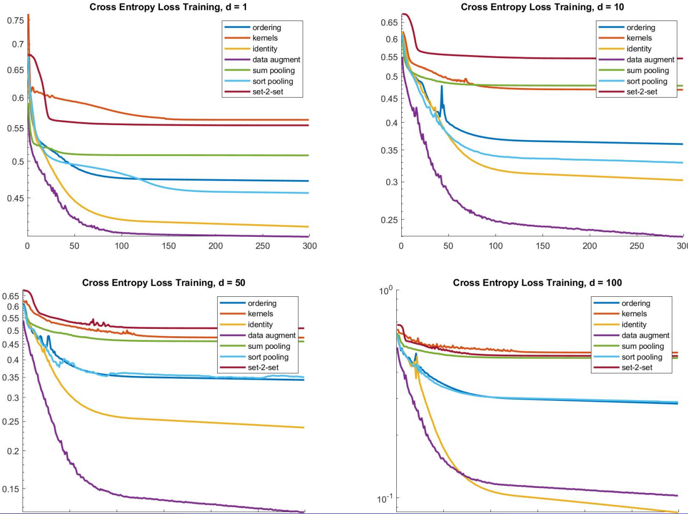
The Network

Training has been done over 300 epochs with a batch size of 128. Loss function: binary cross-entropy.
The following 7 α 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.]

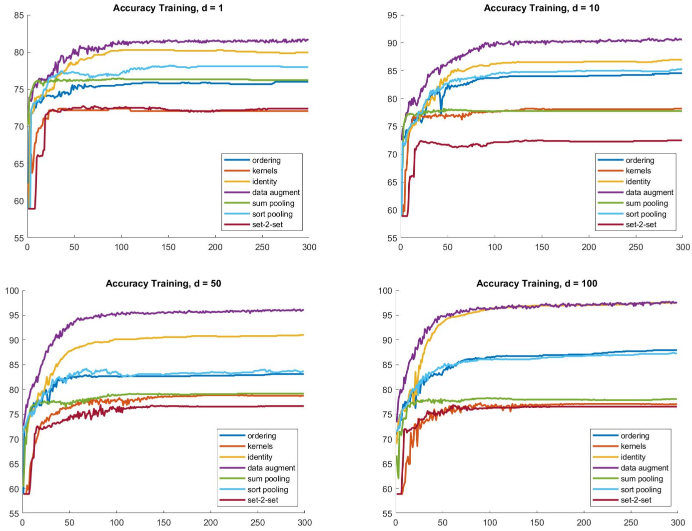
Enzyme Classification Example

Training Loss: X Entropy



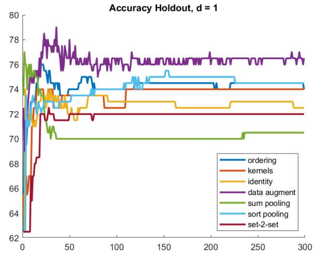
Enzyme Classification Example

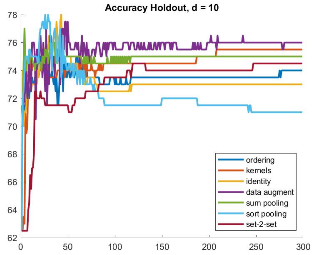
Accuracy on Training set

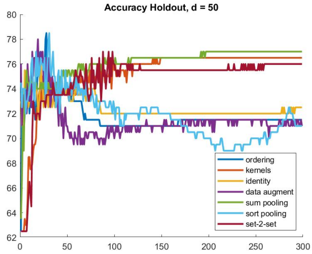


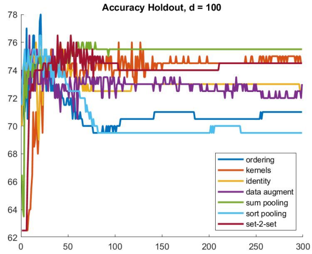
Enzyme Classification Example

Accuracy on Holdout data



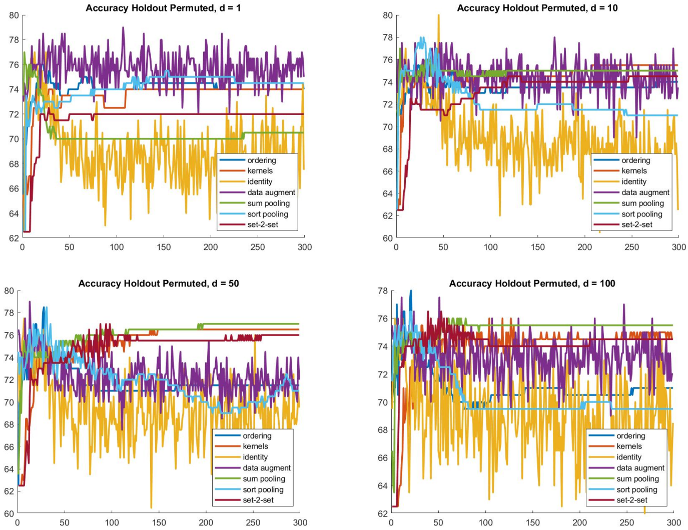






Enzyme Classification Example

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.] 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 containins 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: α
- Fully connected NN with dense 3-layers and 150 internal units in each of the two hidden layers; no dropouts, with batch normalization.

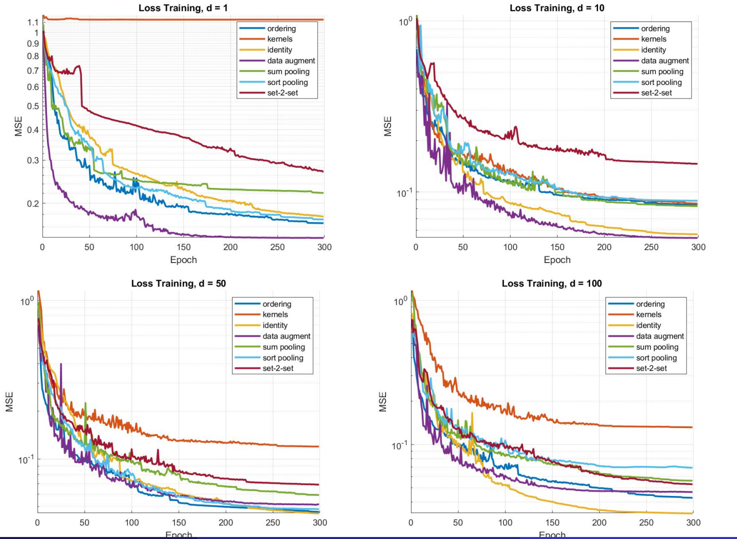
The Network

Training has been done over 300 epochs with a batch size of 128. Loss function: Mean-Square Error (MSE).
The same 7 α 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.]

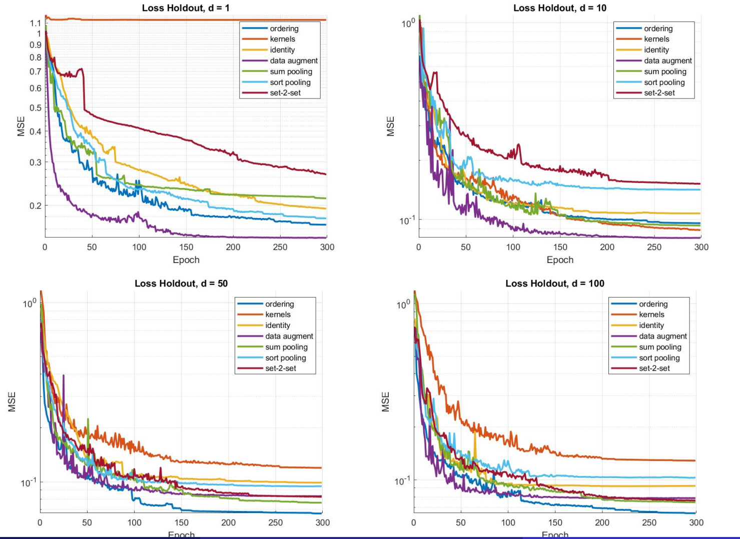
QM9 Regression Example

Training MSE



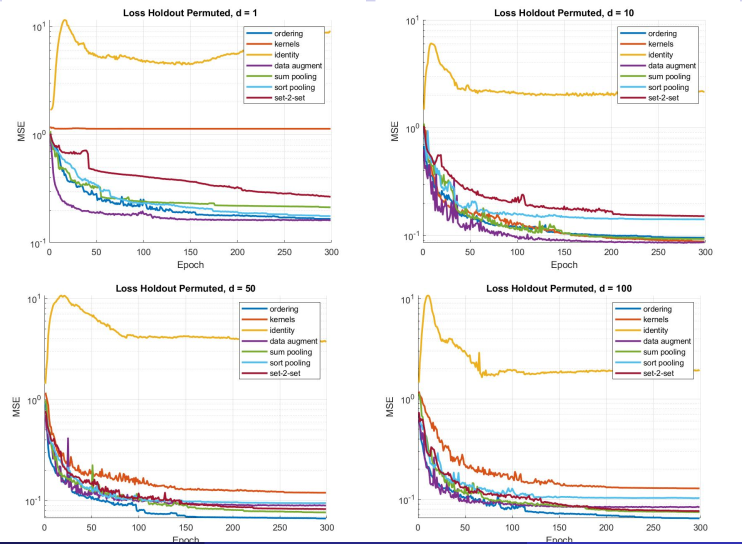
QM9 Regression Example

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 $\Delta\varepsilon = LUMO - HOMO$ (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 $0.229eV$

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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 $\Pi \in \mathcal{S}_n$ sot 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 $\Xi, \Pi_1, \cdots, \Pi_d \in S_n$ so that for $Y = [\Pi_1 x_1, \cdots, \Pi_d x_d]$,

$$Yb = \Xi X b \;\; \text{but} \;\; Y - \Pi X \neq 0 \;,\; \forall \Pi \in \mathcal{S}_n$$

Define the linear operator

Genericity Results for $d \geq 2$

Admissible keys

Proof - cont'd
Let

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

Then

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

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 $(\Pi_1, \cdots, \Pi_d) \notin \mathcal{P}$. $\square$

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 $b = [1, 1]^T$.

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

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, $L^{-1}P^TA \in \mathcal{A}_{d,1}(XPL)$. 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

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.

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:

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

$$\left.\setminus \bigcup_{\Pi\in\mathcal{S}_n} \ker\ M(\Pi,\Pi_1,\cdots,\Pi_d)\right) \quad (*)$$

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

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

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

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

cont'd

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

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

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

2. If $(\Xi_1, \cdots, \Xi_{D-d}; \Pi_1, \cdots, \Pi_d) \in (\mathcal{S}_n)^D \setminus \Delta$ 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 $X = [0, \cdots, 0, x_j, 0, \cdots, 0]$ where x_j is the only non identically 0 column. Claim: $X \notin \ker L(\Xi_1, ..., \Pi_d; A)$. 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 $\mathbb{R}^{n\times d} \setminus \mathcal{S}([I_d \;\; A])$ 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:

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

$$L \equiv \left[\begin{array}{cccc} A_{1,1}(\Xi_1-\Pi_1) & A_{2,1}(\Xi_1-\Pi_2) & \cdots & A_{d,1}(\Xi_1-\Pi_d) \\ A_{1,2}(\Xi_2-\Pi_1) & A_{2,2}(\Xi_2-\Pi_2) & \cdots & A_{d,2}(\Xi_2-\Pi_d) \\ \vdots & \vdots & \ddots & \vdots \\ A_{1,D-d}(\Xi_{D-d}-\Pi_1) & A_{2,D-d}(\Xi_{D-d}-\Pi_2) & \cdots & A_{d,D-d}(\Xi_{D-d}-\Pi_d \end{array}\right.$$

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