Invariant machine learning on point clouds and other varying-size objects

(including PDEs)

Soledad Villar

Johns Hopkins University

Statistical and computational challenges in probabilistic scientific machine learning @ IMSI

Symmetries in the physical sciences

2 types of symmetries:

ACTIVE

- Symmetries that come from observed regularities of physics

Emmy Noether

conservation of energy — time translation symmetry

conservation of momentum — translation symmetry

conservation of angular momentum — rotation symmetry

PASSIVE

- Symmetries that come from choice of mathematical representation of physical objects

coordinate freedom

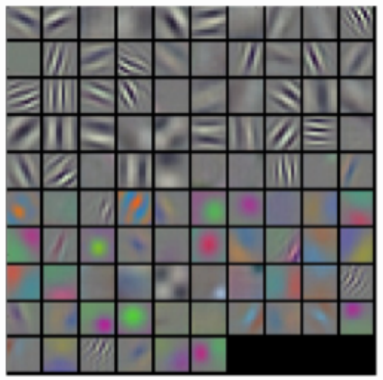
units equivariances

gauge invariances / equivariances

Example

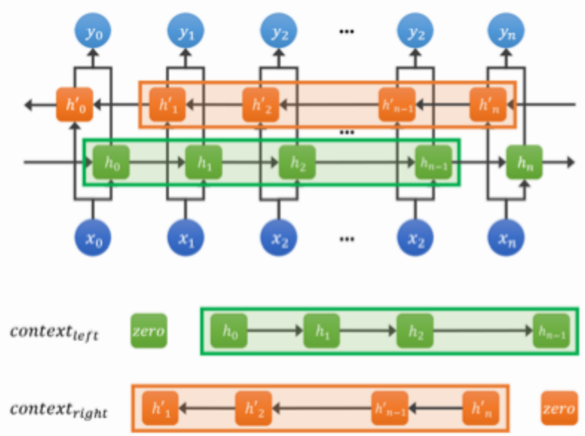
CLAIM: ML / data science methods should be consistent with these

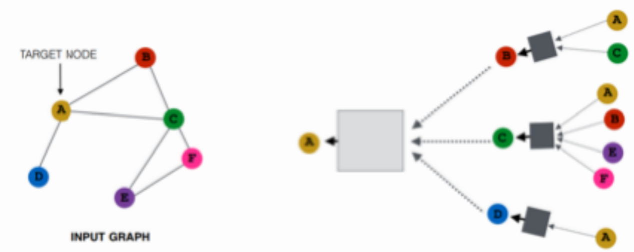
Deep learning archictectures have symmetries



CNN
spatial translation symmetry

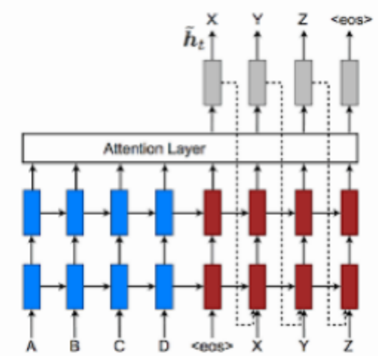
RNN
time translation symmetry





GNN
graph permutation symmetry

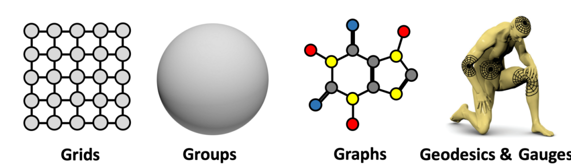
Transformers
flexible symmetries



(permutation and more!)

They exploit symmetries or approximate symmetries
[or more generally the physical structure of problems]

Related with geometric deep learning (Bronstein, Bruna, Cohen, Veličković)

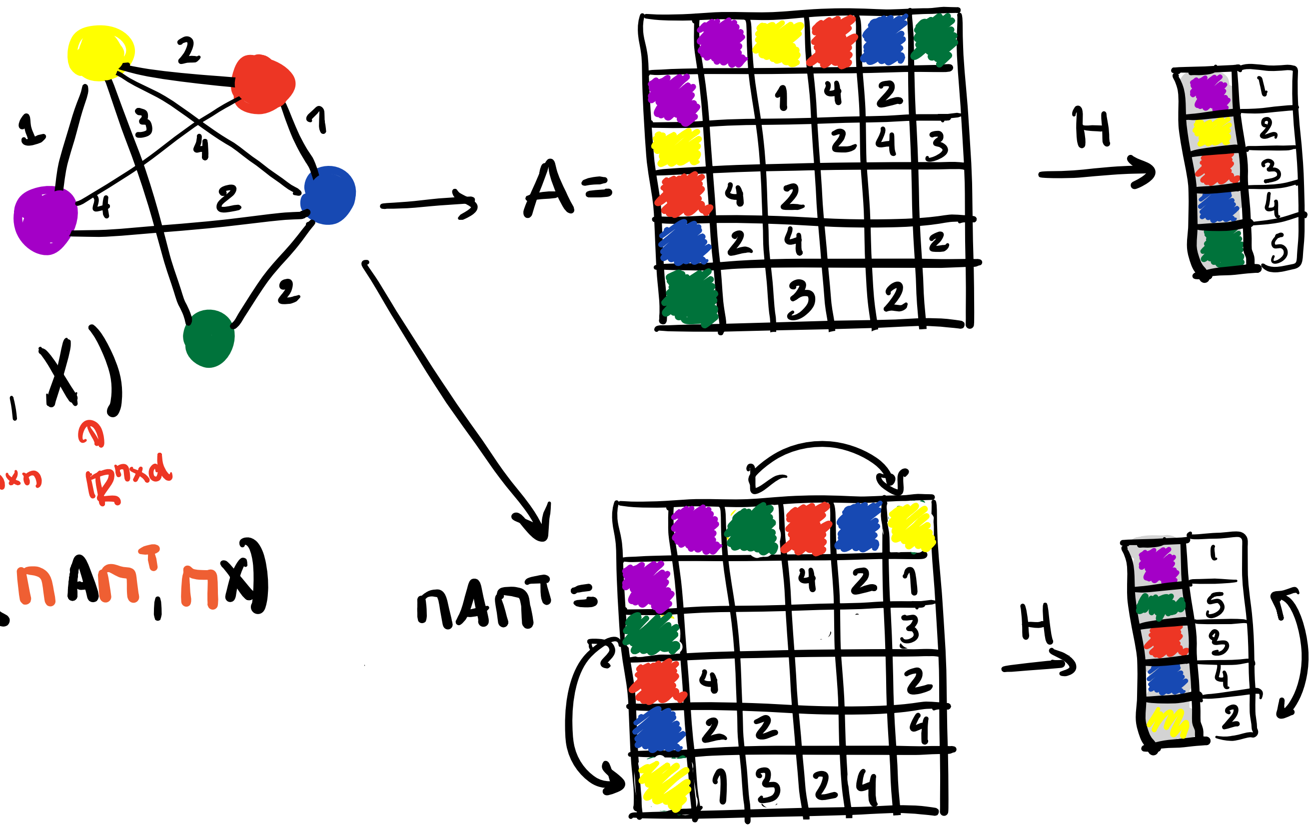


Example: passive symmetries in graph learning

G graph

$G = (A, X)$, $A \in \mathbb{R}^{n\times n}$, $X \in \mathbb{R}^{n\times d}$

$\Pi G = (\Pi A \Pi^T, \Pi X)$



Example: shortest path starting at

- length (invariant)
- path (equivariant)

Node embedding: $G \mapsto \mathbb{R}^{n\times d}$

$$H(\Pi A \Pi^T, \Pi X) = \Pi \cdot H(A, X)$$ equivariant

Graph classification / regression: $G \to \mathbb{R}$

$$F(\Pi A \Pi^T, \Pi X) = F(A, X)$$ invariant

$\forall\ A \in \mathbb{R}^{n\times n}$, $\Pi \in$ permutation

- Permutation symmetry is huge $|S_n| = n!$
- All graph processing methods satisfy this symmetry (eigenvectors are equivariant!)
- Implementing this symmetry translates into explicit (huge) sample complexity gains

This talk

- Invariant functions on point clouds via Galois theory
  with B. Blum Smith, T. Huang, M. Cuturi

- Theoretical framework for ML models on varying-size objects with M. Diaz, E. Levin, Y. Ma
  (transferability on GNNs & beyond) with M. Velasco, K O'Hare, B. Rychtenberg

- Applications to any-dimensional, coordinate-free PDE solvers with T. Phan, G & Y Kevrekidis, J Bello-Rivas

Machine learning on point clouds

Applications:
- Chemistry
- Astronomy
- Material science

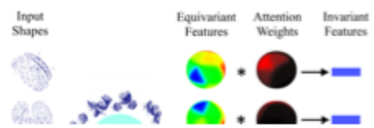
Equivariant Point Network for 3D Point Cloud Analysis

Haiwei Chen[1,2], Shichen Liu[1,2], Weikai Chen[2,3], Hao Li[4], Randall Hill[1,2]
[1]University of Southern California
[2]USC Institute for Creative Technologies
[3]Tencent Game AI Research Center
[4]Pinscreen
{chenh,lshichen,hill}@ict.usc.edu chenwk891@gmail.com hao@hao-li.com

Sep 2019

Abstract

Features that are equivariant to a larger group of symmetries have been shown to be more discriminative and powerful in recent studies [5, 48, 6]. However, higher-order equivariant features often come with an exponentially-growing computational cost. Furthermore, it remains rel-



PointNet++: Deep Hierarchical Feature Learning on Point Sets in a Metric Space

Charles R. Qi Li Yi Hao Su Leonidas J. Guibas
Stanford University

Abstract

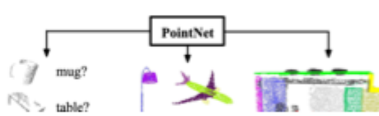
Few prior works study deep learning on point sets. PointNet [20] is a pioneer in this

PointNet: Deep Learning on Point Sets for 3D Classification and Segmentation

Charles R. Qi* Hao Su* Kaichun Mo Leonidas J. Guibas
Stanford University

Abstract

Point cloud is an important type of geometric data structure. Due to its irregular format, most researchers transform such data to regular 3D voxel grids or collections



Effective Rotation-invariant Point CNN with Spherical Harmonics Kernels

Adrien Poulenard
LIX, Ecole Polytechnique
adrien.poulenard@inria.fr

Marie-Julie Rakotosaona
LIX, Ecole Polytechnique
mrakotos@lix.polytechnique.fr

Yann Ponty
LIX, Ecole Polytechnique
yann.ponty@lix.polytechnique.fr

Maks Ovsjanikov
LIX, Ecole Polytechnique
maks@lix.polytechnique.fr

Abstract

We present a novel rotation invariant architecture oper-

require maintaining complex and expensive data-structur compared to volumetric or mesh-based methods. As a sult, starting from the seminal works of PointNet [22] a

IEEE TRANSACTIONS ON VISUALIZATION AND COMPUTER GRAPHICS

A Rotation-Invariant Framework for Deep Point Cloud Analysis

Xianzhi Li, Ruihui Li, Guangyong Chen, Chi-Wing Fu, Daniel Cohen-Or and Pheng-Ann Heng

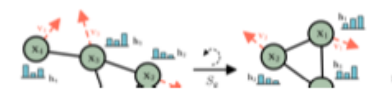
Abstract—Recently, many deep neural networks were designed to process 3D point clouds, but a common drawback is that rotation invariance is not ensured, leading to poor generalization to arbitrary orientations. In this paper, we introduce a new low-level purely

E(n) Equivariant Graph Neural Networks

Victor Garcia Satorras[1] **Emiel Hoogeboom**[1] **Max Welling**[1]

Abstract

This paper introduces a new model to learn graph neural networks equivariant to rotations, translations, reflections and permutations called E(n)-



A simple and universal rotation equivariant point-cloud network

Ben Finkelshtein[1] **Chaim Baskin**[1] **Haggai Maron**[2] **Nadav Dym**[1]

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TECHNICAL ARTICLE

Check for updates

Material Property Prediction Using Graphs Based on Generically Complete Isometry Invariants

Jonathan Balasingham[1] · Viktor Zamaraev[1] · Vitaliy Kurlin[1]

Complete Neural Networks for Euclidean Graphs

Snir Hordan[1] **Tal Amir**[1] **Steven J. Gortler**[2] **Nadav Dym**[1,3]

Abstract

We propose a 2-WL-like geometric graph isomor-

performance is complemented by the theoretical study of these networks and their approximation power. These typi-

Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds

Nathaniel Thomas*
Stanford University
Stanford, California, USA
ncthomas@stanford.edu

Tess Smidt*
University of California, Berkeley
Berkeley, California, USA
Lawrence Berkeley National Lab
Berkeley, California, USA
tsmidt@berkeley.edu

Steven Kearnes
Google
Mountain View, California, USA
kearnes@google.com

Lusann Yang
Google
Mountain View, California, USA
lusann@google.com

Li Li
Google
Mountain View, California, USA
leeley@google.com

Kai Kohlhoff
Google
Mountain View, California, USA
kohlhoff@google.com

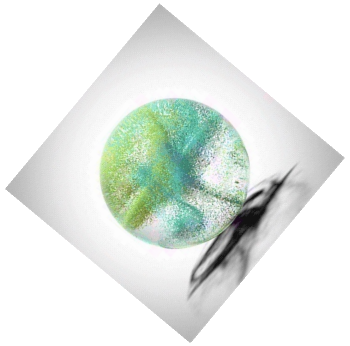
Patrick Riley

Three iterations of $(d-1)$-WL test distinguish non isometric clouds of d-dimensional points.

Valentino Delle Rose[1,2] Alexander Kozachinskiy[1,2,3] Cristóbal Rojas[1,2]
Mircea Petrache[1,2,4] Pablo Barceló[1,2,3]

Motivation

Invariant functions on point clouds

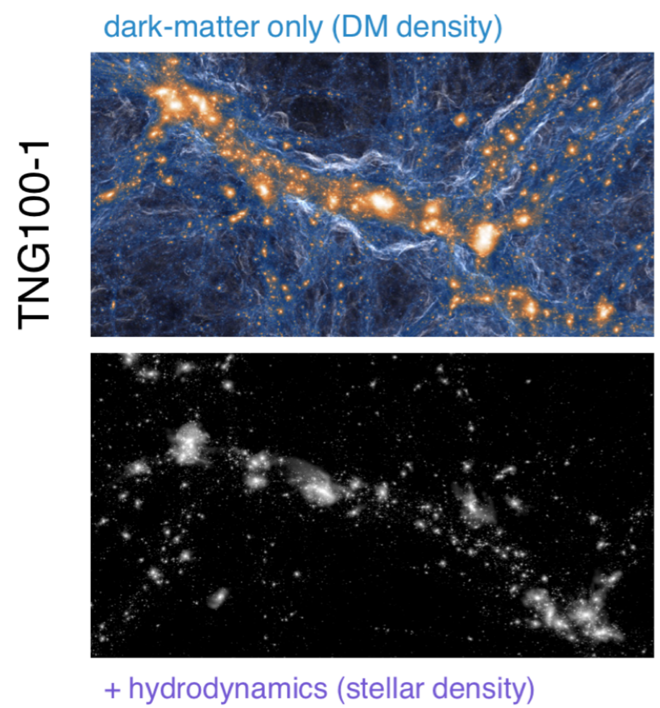


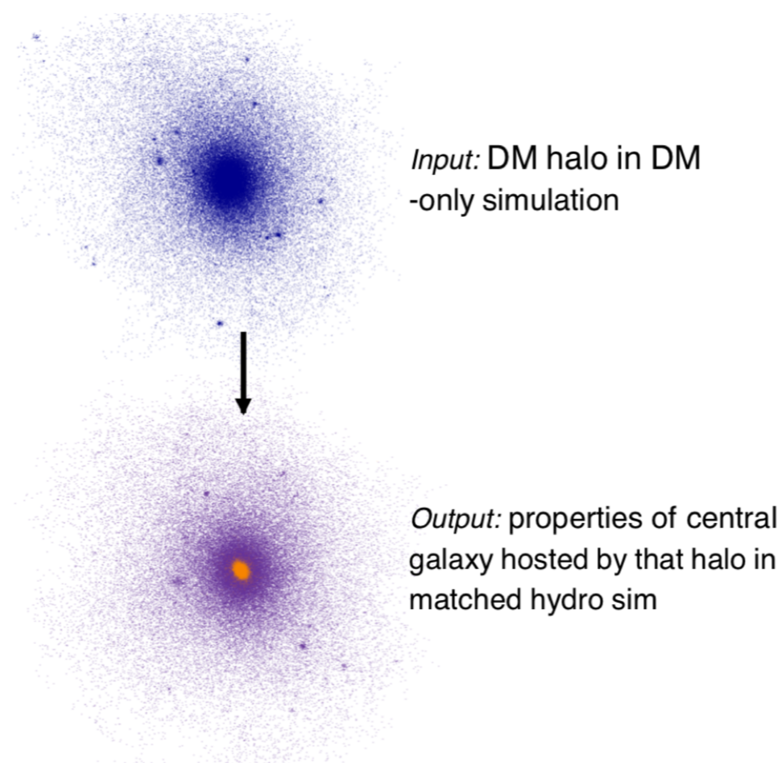
$O(d)$ + permutation symmetry
or $E(d)$

Kate Storey-Fisher

Motivation:
Emulation of cosmological simulations

Galaxy properties predictions from dark-matter only sims:





Based on conversations with
Storey-Fisher, Hogg, Genel, Hattori

Setting: $V = \begin{pmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{pmatrix} \in \mathbb{R}^{d \times n}$ n points in dimension d

$f : \mathbb{R}^{d\times n} \to \mathbb{R}$ - E(d) invariant (translations, rotations, reflections)

$V \mapsto f(V)$ - permutation invariant

- Translations $f\left(V + \begin{bmatrix} | & & | \\ h & \cdots & h \\ | & & | \end{bmatrix} \right) = f(V)$

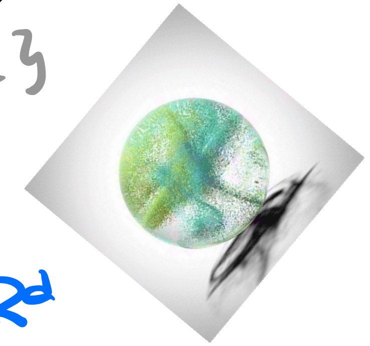
"canonicalization" $V \leftarrow \begin{pmatrix} | & | & & | \\ v_1 - \bar{v} & v_2 - \bar{v} & \cdots & v_n - \bar{v} \\ | & | & & | \end{pmatrix}$ where $\bar{v} = \frac{1}{n} \sum_{i=1}^{n} v_i$ center of mass

define $f(V) = \tilde{f}(V - \bar{v})$ unconstrained

• Rotations and reflections

O(d) Orthogonal group

$\{R \in \mathbb{R}^{d\times d} : RR^T = R^TR = I\}$



$\xrightarrow{f} \mathbb{R}$

O(d)- invariant functions $f : (\mathbb{R}^d)^n \to \mathbb{R}$

$$f(Rv_1, \dots Rv_n) = f(v_1, \dots v_n) \quad \forall\ R \in O(d) \quad v_1 \dots v_n \in \mathbb{R}^d$$

(Weyl 1946) **first fundamental theorem of invariant theory**

$f : (\mathbb{R}^d)^n \to \mathbb{R}$ is $O(d)$-invariant if and only if

$$f(v_1, \dots v_n) = \tilde{f}\Big(\underbrace{(v_i^T v_j)_{i,j=1}^n}_{\text{inner products}} \Big)$$

• Similar characterizations for
- Lorentz
- Rotations
- Symplectic group
- Unitary group

$$\begin{tikzcd}
(\mathbb{R}^d)^n \arrow[r, "f"] \arrow[d, "\Phi"'] & \mathbb{R} \\
\mathbb{R}^{n\times n} \arrow[ur, dashed, "\tilde{f}"'] \arrow[u, dashed, bend left] &
\end{tikzcd}$$

$(v_1, \dots v_n)$

$M \quad M_{ij} = v_i^T v_j$

Extension to equivariance

(Villar et al '21)
Neurips '21

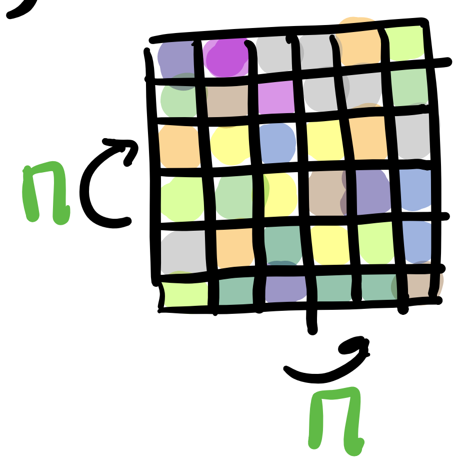
• **Permutations**

$$V = \begin{pmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{pmatrix} \in \mathbb{R}^{d \times n} \qquad O(d) \backslash V / S_n$$

$$f : V \to \mathbb{R} \quad O(d)\text{-invariant} \iff f(V) = \tilde{f}(\underbrace{V^T V}_{\text{Gram matrix}}) \quad X$$

$$f(V\Pi) = f(V) \Rightarrow \tilde{f}(\Pi^T V^T V \Pi) = \tilde{f}(V^T V)$$

($\tilde{f}$ invariant by permutations acting by conjugation)

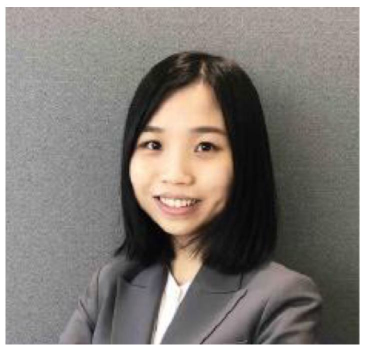


Symmetry of GNNs!

Spoiler: We are not gonna use GNNs

Why invariant theory instead of GNNs?

Ben Blum-Smith



Teresa Huang

Marco Cuturi

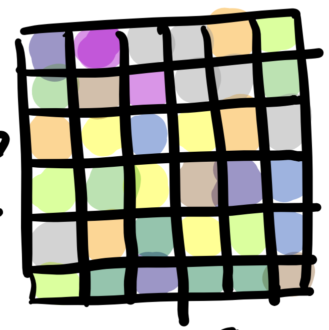
① Constructing the graph has $O(n^2)$ complexity

We'll be able to learn invariant functions with $O(nd)$ complexity

② Improved expressive power over vanilla MPNN ?

③ Interesting mathematical tools that could potentially be used more broadly (Galois theory)

Galois theory (setup)

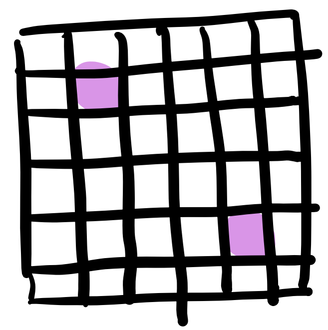
S_n acting by conjugation $\pi \circlearrowleft$  π (permuting rows and columns)

Λ ← is a subgroup of

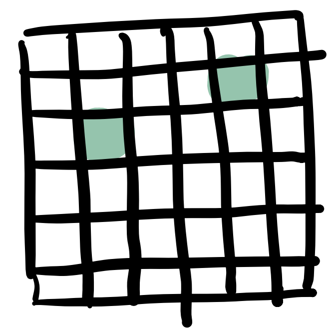
Recall
$X = V^T V \in \mathbb{R}^{n\times n}$, $V \in \mathbb{R}^{d\times n}$

$S_n \times S_{\binom{n}{2}}$ acting by permuting

independently { diag ↔ diag
off diag ⟷ off diag



$X_{ii} \to X_{jj}$



$X_{ij} \to X_{k\ell}$
$i \neq j$
$k \neq \ell$

f is S_n invariant
↑ $\cup$
f is $S_n \times S_{\binom{n}{2}}$ invariant

f^d, f^o → elementary symmetric polynomials
characterize set(X_{ii}) set(X_{ij} $i \neq j$)

Galois theory approach [informal]

Évariste Galois
(1811 - 1832)

If we construct a set of invariants that are only fixed by the desired group (aka no other bigger group fixes all the invariants) then those invariants generate the field of invariant functions

Rosenlicht (1956) the orbits that the field generators fail to uniquely identify (the "bad set") has to satisfy a finite set of equations (⇒ the bad set is an invariant measure zero set)

Galois theory

Id rational functions $\mathbb{R}^{n\times n} \to \mathbb{R}$ (symmetric) $\leftrightarrow \mathbb{R}(x_{ij})$

$\wedge$ $\leftarrow\cdots\rightarrow$ $\cup$ $\uparrow$

S_n field invariant functions by conjugation $\leftrightarrow \mathbb{R}(f^d, f^o, f^*)$

Field extension

$\mathbb{R}[f^* = \sum_{i\neq j} x_{ii} x_{ij}]$

$\wedge$ $\leftarrow\cdots\rightarrow$ $\cup$ (GALOIS correspondence)

$S_n \times S_{\binom{n}{2}}$ field invariant functions $\leftrightarrow \mathbb{R}(f^d, f^o)$

permuting diag → diag

off-diag → off-diag

More work is needed for

$X = V^T V \in \mathbb{R}^{n\times n}$, $V \in \mathbb{R}^{d\times n}$

Deep Sets

(Zaheer et al '19)

$f: \mathbb{R}^{k\times n} \to \mathbb{R}^s$ S_n-invariant $\Rightarrow \exists$ $\phi: \mathbb{R}^k \to \mathbb{R}^\ell$, $\rho: \mathbb{R}^\ell \to \mathbb{R}^s$ such that

$$f(V) = \rho\left(\sum_{v_i \in \mathrm{cols}(V)} \phi(v_i) \right)$$

ℓ can be chosen st $\ell \leq 2kn$

Note this formulation is independent of n and S_n-invariant for all n.

$O(n^2)$ features

Theorem (Blum-Smith, Huang, Cuturi, V) [informal]

$X \in \mathbb{R}^{n\times n}$ symmetric $\quad f(X) = h\left(\text{deepset}(X_{ii}), \text{deepset}(X_{ij})_{i\neq j}, f^*\right)$

can universally approximate invariant functions on symmetric matrices outside an invariant, closed, zero-measure "bad set"

From $O(n^2)$ to $O(nd)$ invariant features:

$$V = \begin{pmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{pmatrix} \in \mathbb{R}^{d \times n}$$

consider $C(V) \in \mathbb{R}^{d \times k}$ "centers"
$O(d)$-equivariant
S_n-invariant

eg: k-means centroids ordered by 2-norm

$$[V\,C] = \begin{pmatrix} | & & | & | & & | \\ v_1 & \cdots & v_n & c_1 & \cdots & c_k \\ | & & | & | & & | \end{pmatrix}$$

$$\tilde{X} = [VC]^T [VC] = \begin{bmatrix} V^T V & V^T C \\ C^T V & C^T C \end{bmatrix} \in \mathbb{R}^{(n+k) \times (n+k)}$$

We'll take $k = d$
(rank d symmetric matrix)

<u>Fact</u>: If C is full rank then $[VC]$ can be recovered from last k rows of $\tilde{X}$
(From low-rank matrix completion)

Invariant machine learning model with $O(nd)$ features

$$f : \mathbb{R}^{d \times n} \to \mathbb{R} \qquad O(d) \text{ invariant}, \; S_n \text{ invariant}$$

$$V \longmapsto h\Big(\underbrace{\text{deepset}\big(\underbrace{C^T V}_{\mathbb{R}^{d\times n}} \big)}_{S_n\text{-invariant}}, \underbrace{C^T C}_{\mathbb{R}^{d\times d}} \Big)$$

Theorem (Blum-Smith, Huang, Cuturi, V) [informal]

The machine learning model above can universally approximate invariant functions on point clouds outside an invariant, closed, zero-measure "bad set"

Numerical experiments

Molecular prediction on QM7b

7,211 molecules with 14 regression targets

Each molecule is a $n \times n$ symmetric matrix

$$f(X) = \text{MLP}\left(\text{deepset}(X_{ii}),\ \text{deepset}(X_{ij})_{i \neq j},\ \text{MLP}(f^*)\right)$$

MAE ↓	Atomization PBE0	Excitation ZINDO	Absorption ZINDO	HOMO ZINDO	LUMO ZINDO	1st excitation ZINDO	Ionization ZINDO
KRR [WRF+18]	9.3	1.83	0.098	0.369	0.361	0.479	0.408
DS-CI (Ours)	12.849±0.757	1.776±0.069	0.086±0.003	0.401±0.017	0.338±0.048	0.492±0.058	0.422±0.012
DTNN [WRF+18]	21.5	1.26	0.074	0.192	0.159	0.296	0.214
DS-CI+ (Ours)	7.650±0.399	1.045±0.030	0.069±0.005	0.172±0.009	0.119±0.005	0.160±0.011	0.189±0.011

MAE ↓	Affinity ZINDO	HOMO KS	LUMO KS	HOMO GW	LUMO GW	Polarizability PBE0	Polarizability SCS
KRR [WRF+18]	0.404	0.272	0.239	0.294	0.236	0.225	0.116
DS-CI (Ours)	0.404±0.047	0.302±0.009	0.225±0.01	0.329±0.016	0.213±0.008	0.255±0.015	0.114±0.008
DTNN [WRF+18]	0.174	0.155	0.129	0.166	0.139	0.173	0.149
DS-CI+ (Ours)	0.122±0.002	0.169±0.007	0.135±0.007	0.183±0.005	0.139±0.004	0.139±0.005	0.088±0.004

Numerical experiments

Point cloud regression on ModelNet 10

(a) Class 2 (chair) (b) Class 7 (sofa)

Goal: learn distances between point clouds

Target: Gromov-Wasserstein-lower-bound (V, V') $\quad V, V' \in \mathbb{R}^{3\times 100}$

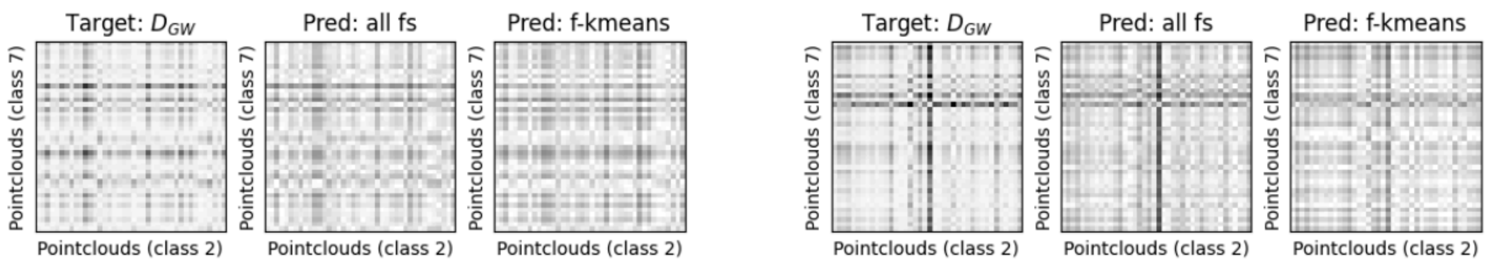
$f(V) = \text{MLP}\left(\text{deepset}\left(C^T V\right), C^T C\right)$

Rank Corr. ↑	ALL fs	K-MEANS
Training set	0.88	0.86
Test set	0.80	0.75

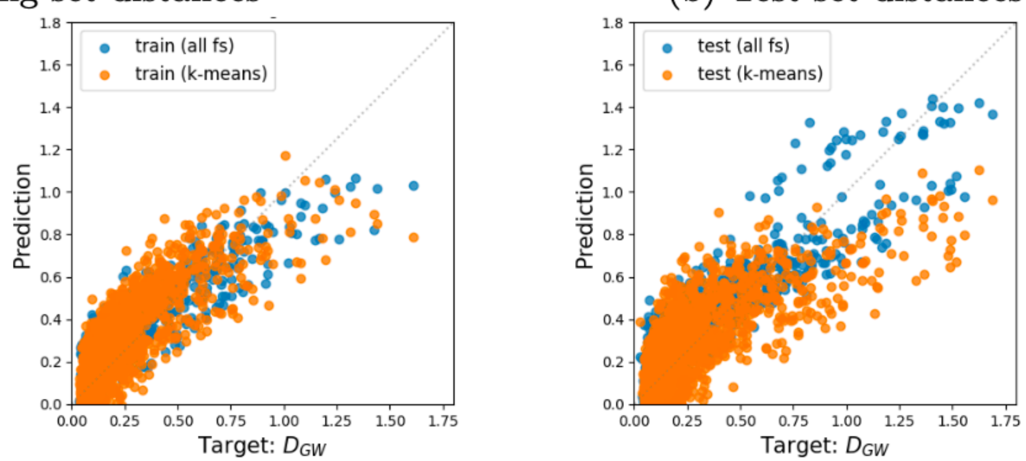
Point cloud regression on ModelNet 10

Goal: learn distances between point clouds

Target: Gromov-Wasserstein-lower-bound (V, V') $\quad V, V' \in \mathbb{R}^{3\times 100}$



(a) Training set distances (b) Test set distances

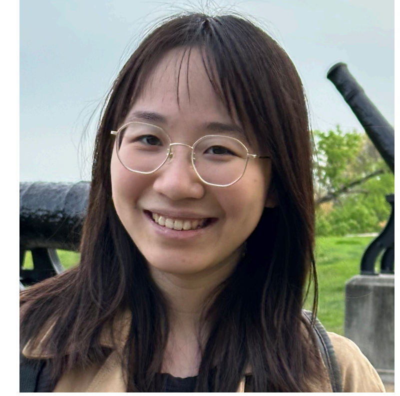


(c) Training set correlation (d) Test set correlation

Machine learning models on objects of varying sizes

Mateo Diaz

Eitan Levin



Yuxin Ma

- Certain ML models are defined on a fixed set of parameters and can be trained/evaluated on inputs of different sizes

<u>Examples</u>

- GNNs

$$f(\overset{n\times n}{A}, \overset{n\times d}{X}) = X_T \qquad X_{t+1} = \rho\left[\sum_{s=1}^{k} \underset{n\times n}{A^s} \overset{n\times d}{X_t} \underset{d\times d}{\theta_{s,t}}\right] \quad X_0 = X$$

- Deep sets

$$f(\underset{n \text{ elements in } \mathbb{R}^k}{X}) = \overset{s\times \ell}{\rho}\left(\sum_{\underset{k}{x_i} \in X} \overset{k\times \ell}{\phi}(x_i)\right)$$

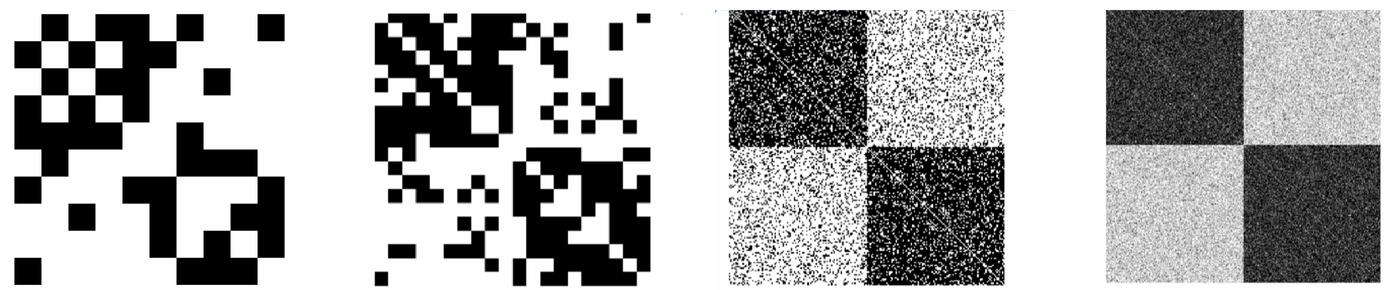
What are the underlying mathematical assumptions?

GNN Transferability

Ruiz et al '20
Levie et al '21
Maskey et al '23

Velasco, O'Hare, Rychtenberg, Villar '24

In GNNs one can consider a sequence of graphs $G_1 \dots G_n \dots$ converging to a graphon G_∞



Kaiying O'Hare

the set of weights of a GNN

A GNN defines functions $f_1 \dots f_n \dots f_\infty$ in each of them

Transferability / size generalization comes from continuity.

Transferability beyond graphs

Levin & Diaz '24

Ma, Diaz, Levin, V '25

$$\begin{tikzcd}
V_n \arrow[r, "\varphi_n"] \arrow[d, "f_n"'] & V_{n+1} \arrow[r, "\varphi_{n+1}"] \arrow[d, "f_{n+1}"] & V_{n+2} \arrow[r, "\varphi_{n+2}"] \arrow[d, "f_{n+2}"] & \cdots \arrow[r] & V_\infty \arrow[d, "f_\infty"] \\
W_n \arrow[r, "\psi_n"] & W_{n+1} \arrow[r, "\psi_{n+1}"] & W_{n+2} \arrow[r, "\psi_{n+2}"] & \cdots \arrow[r] & W_\infty
\end{tikzcd}$$

inputs

ML model

outputs

$f_1, f_2 \ldots f_n, \ldots f_\infty$ are induced by fixed set of weights

- **Compatibility** $\quad f_{n+1} \circ \varphi_n = \psi_n \circ f_n$
- **Continuity** (transferability) $\quad \lim_{n\to\infty} f_n = f_\infty \quad$ all continuous (the choice of topology is important)

Example: sets

consistent sequence	norm	limit space $\overline{V_\infty}$
zero padding $\varphi_n(x) = (x, 0)$	$\lVert x \rVert_p = \left(\sum_n x_i^p\right)^{1/p}$	infinite sequences with ℓ_p metric (symmetrized)
duplication $\varphi_n(x) = (x, x)$	$\lVert x \rVert_{\bar{p}} = \left(\frac{1}{n} \sum x_i^p\right)^{1/p}$	probability measures with Wasserstein p-metric

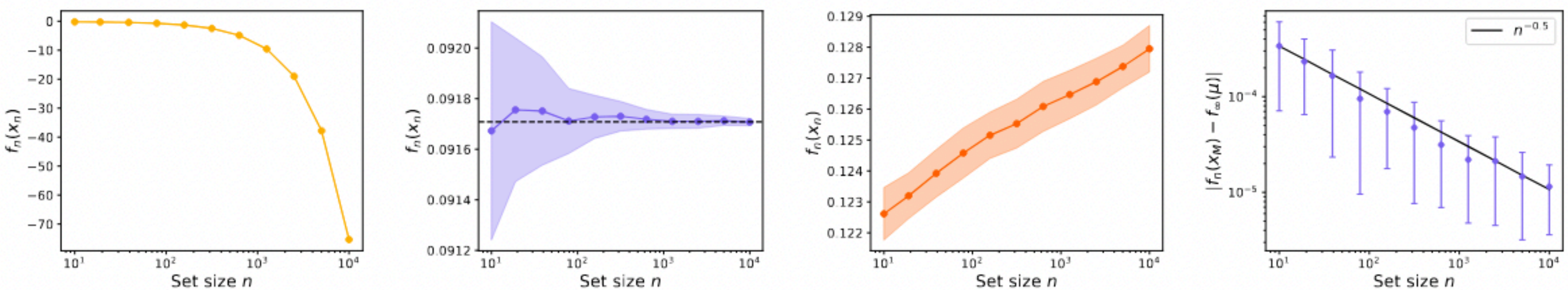
Limits of Models

$$\mathrm{Deepsets}_\infty(X) = \rho\left(\sum_{x \in X} \phi(x_i)\right)$$

$$\overline{\mathrm{Deepsets}_\infty}(\mu) = \rho\left(\int \phi \, d\mu\right)$$

$$\mathrm{PointNet}_\infty(\mu) = \rho\left(\sup_{x \in \mathrm{supp}\,\mu} \phi(x)\right)$$

Model	zero padding $\|\cdot\|_1$	duplication $\|\cdot\|_{\bar{p}}$	duplication $\|\cdot\|_\infty$
Deepset	if $\phi(0)=0 \Rightarrow$ compatible if ϕ, ρ Lipschitz $\Rightarrow$ transferable	incompatible	incompatible
$\overline{\text{Deepset}}$	incompatible	if ϕ, ρ lipschitz $\Rightarrow$ transferable	if ϕ, ρ lipschitz $\Rightarrow$ transferable
PointNets	incompatible	compatible not transferable	if ϕ, ρ lipschitz $\Rightarrow$ transferable



(a) DeepSet [25] output (incompatible)

(b) Normalized DeepSet [3] output (compatible, Lipschitz transferable)

(c) PointNet [20] output (compatible, not transferable)

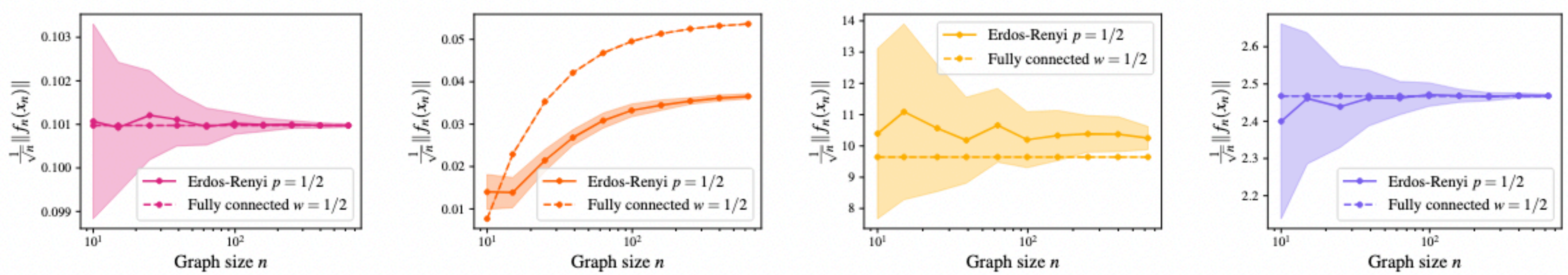
(d) Normalized DeepSet [3] error

Sets models with random weights on growing sets duplication $\|\cdot\|_{\bar{p}}$

The analysis applies to

- GNNs
- ML models on point clouds
- Convergence rates
- Alignment of task → topology → model

Different GNN models with random weights evaluated on seq of graphs with duplication $\|\cdot\|_2$



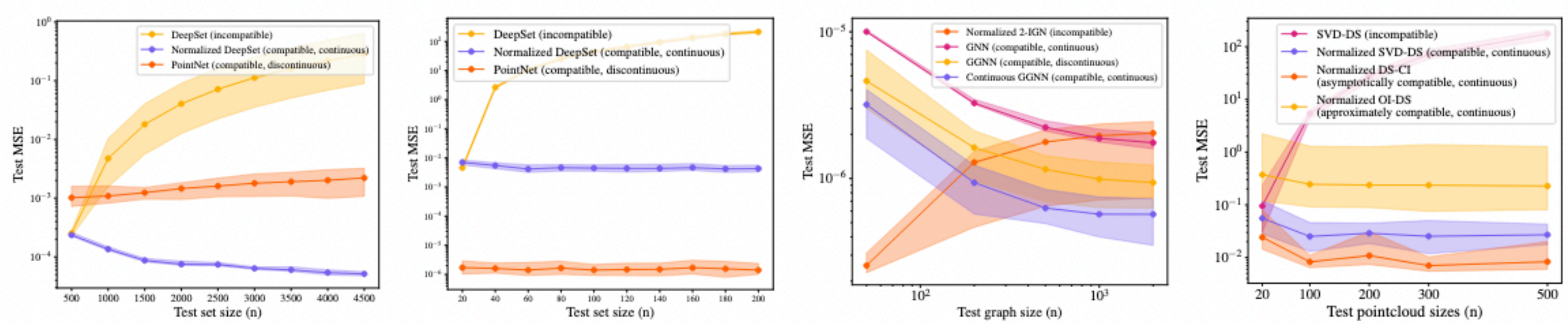
(a) GNN [22] (compatible, transferable)

(b) Normalized 2-IGN [4] (incompatible)

(c) GGNN (compatible, not transferable)

(d) Continuous GGNN (compatible, transferable)

Trained model on fixed size objects evaluated on larger objects for different tasks →



(a) Set: Population statistics

(b) Set: Maximal distance from the origin

(c) GNN: Weighted triangle densities

(d) Point cloud: Gromov-Wasserstein lower bound

Phan, Kevrekidis, V, Kevrekidis, Bello '25

Application: coordinate & dimension-agnostic PDE learning

Given data $(t_i, x_i, u(t_i, x_i))_{i=1}^{N}$

Learn a PDE $\dfrac{\partial u}{\partial t} = \mathcal{F}(u, t, x)$

CLAIM express $\mathcal{F}$ in a $\underbrace{\text{coordinate-free}}_{\text{eg. exterior diff system}}$ dimension-free

& generalize to other domains, dimensions, initial conditions

Example Heat equation $\dfrac{\partial u}{\partial t} = \star d \star d u$

Hodge star encodes domain's geometry

Consider $\Psi_1, \Psi_2 \dots \Psi_K$ scalar fields

PDE

$$\frac{d\Psi_i}{dt} = F_i(\Psi_1, \dots, \Psi_K) \qquad i = 1 \dots K$$

orthogonally symmetric, second order PDE

(to be learned from data)

F_i are functions of $\{\Psi_1 \dots \Psi_K$ (scalar fields)

$\star d \star d \Psi_i$ (laplacians)

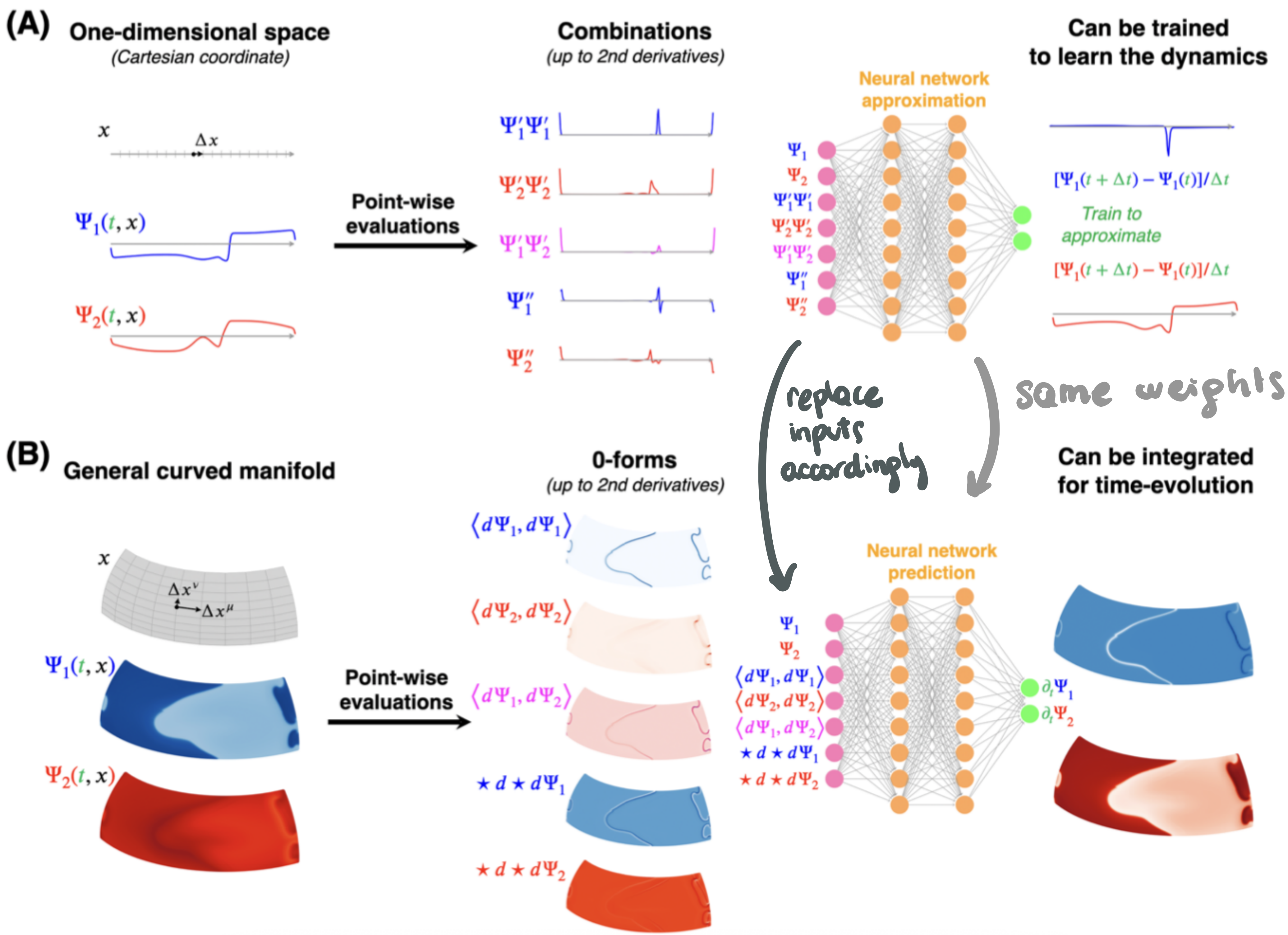
$\langle d\Psi_i, d\Psi_j \rangle$ (inner prod of grad) $\} = B$

$F_i(B)$

$B = \{b_1 \dots b_T\}$

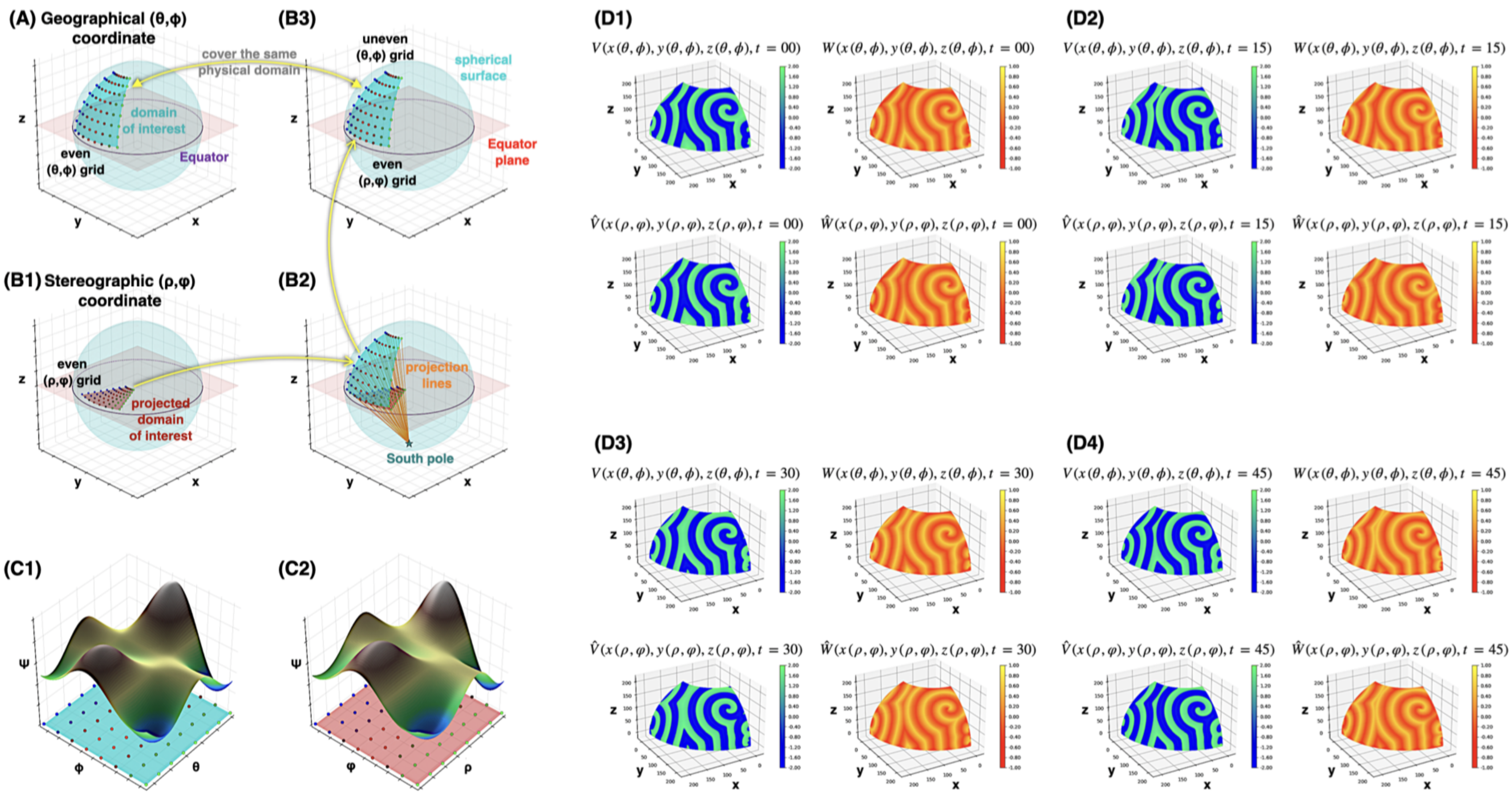
If we change the manifold dimension, initial conditions the learning is consistent

Illustration



Example: FitzHugh - Nagumo system

$$\partial_t V(t) = \star\, d \star dV(t) + V(t) - \frac{1}{3}V^3(t) - W(t)$$
$$\partial_t W(t) = \varepsilon\left[V(t) + \beta - \gamma W(t)\right]\,,$$



Summary

- Invariant functions on point clouds via invariant features
- Galois theory delivers generic universality
- Tricks from low-rank matrix completion and deep sets give information-theoretically optimal complexity
- Theoretical framework for ML models on varying-size objects
  How do objects grow in size? consistent sequences
  Compatibility
  Transferability (aka continuity in the limit $n \to \infty$)
  Alignment of task → topology → model
- Application to PDEs

Thank you!

Villar, Hogg, Storey-Fisher, Yao, Blum-Smith NeurIPS 2021

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Questions?