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Paper review & Research progress

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Greek philosophy & Stoicism (1)

Aristotle

A human is a **social creature**.

Greek philosophy & Stoicism (2)

Marcus Aurelius

The happiness and unhappiness of the **rational, social animal** depends not on what he feels but on what he does just as his virtue and vice consist not in feeling but in doing.

Greek philosophy & Stoicism (3)

Marcus Aurelius

Here is the rule to remember in future. When anything tempts you to be bitter: not, ‘This is a misfortune’ but **‘To bear this worthily is good fortune.’**.

Set2Graph (1)

Introduction

Many problems in machine learning can be cast as learning functions from sets to graphs, or more generally to hypergraphs; in short, **Set2Graph** functions. Current neural network models that approximate **Set2Graph** functions come from two main ML sub-fields:

- Equivariant learning
- Similarity learning

Set2Graph (2)

Problem

Learning functions mapping sets of vectors in $\mathbb{R}^{d_{in}}$ to graphs, or generally hypergraphs. For example:

- Clustering
- Predicting features on edges and nodes in graphs
- Learning k-edge information in sets

Proposal

Model that can approximate arbitrary continuous **Set2Graph** functions over compact sets.

Set2Graph (3)

We represent each set-to-graph function as a collection of set-to-k-edge functions, where each set-to-k-edge function learns features on k-edges.

Given an input set $\mathcal{X} = \{x_1, .., x_n\} \subset \mathbb{R}^{d_{in}}$, we consider functions F^k attaching feature vectors to k-edges: each k-tuple $(x_{i_1}, .., x_{i_k})$ is assigned with an output vector $F^k(\mathcal{X})_{i_1, i_2, .., i_k} \in \mathbb{R}^{d_{out}}$.

Functions mapping sets to hypergraphs with hyper-edges of size up-to-k are modeled by $(F^1, F^2, .., F^k)$. Functions mapping set to standard graphs are represented by (F^1, F^2). Set-to-graph functions are well-defined if they satisfy a property called **equivariance**.

Set2Graph (4)

(Maron et al., 2019) - Invariant and Equivariant Graph Networks

1. Full equivariant model.
2. Each linear layer is chosen from the space of all linear equivariant layers.
3. Learning F^k would require equivariant layers mapping 1st-order tensor (representing sets) to k-order tensors (representing k-edge hypergraphs).
4. Computationally infeasible $\leftarrow$ **I think it is similar to CCNs (out of PSPACE)!**

Set2Graph (5)

Theoretical question - Universality

- Universality is the ability of the models to approximate any continuous equivariant function.
- Set-to-Set models: universal.
- Graph-to-Graph models (message passing): non-universal.
- High-order equivariant models: universal.

Another machine-learning approach for learning set-to-graph functions is similarity learning: A siamese network ϕ is used to embed each set element independently $y_i = \phi(x_i)$ and pairwise information is extracted from pairs of embeddings $\psi(y_i, y_j)$.

Set2Graph (6)

Proposal

Composition of three networks:

$$F^k = \psi \circ \beta \circ \phi$$

- ϕ: Set-to-Set model.
- β: Non-learnable broadcasting Set-to-Graph layer.
- ψ: Simple Graph-to-Graph network using only a single MLP acting on each k-edge feature vector independently.

Set2Graph (7)

A matrix $X = (x_1, .., x_n)^T \in \mathbb{R}^{n \times d_{in}}$ represents a set of n vectors $x_i \in \mathbb{R}^{d_{in}}$. Reordering the rows of X by the permutation σ:

$$(\sigma \cdot X)_{i,j} = X_{\sigma^{-1}(i),j}$$

X and $\sigma \cdot X$ represent the same set for all $\sigma \in \mathbb{S}_n$.

A tensor $Y \in \mathbb{R}^{n^k \times d_{out}}$ where $Y_{i,:} \in \mathbb{R}^{d_{out}}$ represents the feature vector attached to the k-edge defined by the k-tuple $(x_{i_1}, .., x_{i_k})$, where $i = (i_1, .., i_k) \in [n]^k$ without repeating indices:

$$(\sigma \cdot Y)_{i,j} = Y_{\sigma^{-1}(i),j}$$

$$\sigma^{-1}(i) = (\sigma^{-1}(i_1), .., \sigma^{-1}(i_k))$$

Y and $\sigma \cdot Y$ represent the same k-edge data for all $\sigma \in \mathbb{S}_n$.

Set2Graph (8)

Equivariance

For F^k to represent a well-defined map between sets $X \in \mathbb{R}^{n \times d_{in}}$ and k-edge data $Y \in \mathbb{R}^{n^k \times d_{out}}$, it should be equivariant to permutations:

$$F^k(\sigma \cdot X) = \sigma \cdot F^k(X)$$

Theorem 1

The model F^k is set-to-k-edge universal.

Theorem 2

The model $(F^1, .., F^k)$ is set-to-hypergraph universal.

Set2Graph (10)

1. Partitioning for particle physics
2. Learning Delaunay triangulations
3. Molecular properties prediction
4. 3D convex hull

Set2Graph & CCNs in solving NP-complete & NP-hard problems

NP-hard

Finding the mininum Hamiltonian cycle/path given a set of points is a **Set2Graph** problem.

NP-complete

Can Set2Graph and CCNs estimate/approximate the solution of NP-complete problems (e.g. 3-SAT, Hamiltonian)?