On the neural approximation of set functions: A survey from permutation-invariant perspective

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Abstract

Conventional machine learning algorithms have traditionally been designed under the assumption that input data follows a vector-based format, with an emphasis on vector-centric paradigms. However, as the demand for tasks involving set-based inputs has grown, there has been a paradigm shift in the research community towards addressing these challenges. In recent years, the emergence of neural network architectures such as Deep Sets and Transformers has presented a significant advancement in the treatment of set-based data. These architectures are specifically engineered to naturally accommodate sets as input, enabling more effective representation and processing of set structures. Consequently, there has been a surge of research endeavors dedicated to exploring and harnessing the capabilities of these architectures for various tasks involving the approximation of set functions. This comprehensive survey aims to provide an overview of the diverse problem settings and ongoing research efforts pertaining to neural networks that approximate set functions. By delving into the intricacies of these approaches and elucidating the associated challenges, the survey aims to equip readers with a comprehensive understanding of the field. Through this comprehensive perspective, we hope that researchers and practitioners can gain valuable insights into the potential applications, inherent limitations, and future directions of set-based neural networks.

1 Introduction

In recent years, machine learning has achieved significant success in many fields, and many typical machine learning algorithms handle vectors as their input and output (Zhou, 2021; Islam, 2022; Erickson et al., 2017; Jordan & Mitchell, 2015; Mitchell, 1997). For example, some of these applications include image recognition (Sonka et al., 2014; Minaee et al., 2021; Guo et al., 2016), natural language processing (Strubell et al., 2019; Young et al., 2018; Otter et al., 2020; Deng & Liu, 2018), and recommendation systems (Portugal et al., 2018; Melville & Sindhwani, 2010; Zhang et al., 2019b).

However, with the advancement of the field of machine learning, there has been a growing emphasis on the research of algorithms that handle more complex data structures in recent years. In this paper, we consider machine learning algorithms that deal with sets (Hausdorff, 2021; Levy, 2012; Enderton, 1977) as one of such data structures. Here are some examples of set data structures:

- **Set of vector data.** For example or a set of image vectors.
- **Graph data.** We can represent graph data as a pair of node set and edge set.
- **Point cloud data.** Point cloud data consists of a set of data points, each represented by its spatial coordinates in a multi-dimensional space.

Considering machine learning algorithms that handle sets allows us to leverage the representations of these diverse types of data. Certainly, the goal here is to utilize machine learning models to approximate set functions. Set functions, in this context, are mathematical functions that operate on sets of elements or

data points. These functions capture various properties, relationships, or characteristics within a given set. However, when dealing with complex data and large sets, it can be challenging to directly model or compute these set functions using traditional model architectures. Therefore, we need to consider a specialized model architecture specifically designed for the approximation of set functions.

In particular, a notable characteristic of set functions, when compared to vector functions, is their permutation invariance. Permutation invariance, in the context of set functions or set-based data, means that the output of the function remains the same regardless of the order in which elements of the set are arranged. In other words, if you have a set of data points and apply a permutation (rearrangement) to the elements within the set, a permutation-invariant function will produce the same result. This property is crucial when dealing with sets of data where the order of elements should not affect the function's evaluation. In Section 2 we introduce a more formal definition. Popular conventional neural network architectures like VGG (Simonyan & Zisserman, 2014) and ResNet (He et al., 2016) do not inherently possess the permutation-invariant property. Hence, the primary research interest lies in determining what neural network architectures can be adopted to achieve the permutation-invariant property while maintaining the performance and expressive capabilities similar to those achieved by conventional models. In Section 3, we introduce such model architectures, and provide the overview of the objective tasks in Section 4. Furthermore, there have been several theoretical analyses of neural network approximations for such permutation-invariant functions, and Section 5 introduces them. Finally, to evaluate such research, datasets for performance assessment of approximate set functions are essential. In Section 6, we list some of the well-known datasets for this purpose.

The following outlines the organization of this paper.

- In Section 2, we introduce the notation and background knowledge necessary for this paper.
- In Section 3, we introduce the neural network architectures used to approximate set functions.
- In Section 4, we provide an overview of the tasks that can be addressed by approximating set functions.
- In Section 5, we present several theoretical analyses of approximating set functions.
- In Section 6, we list commonly used datasets for approximating set functions.
- Finally, in Section 7, we provide a summary of the survey, discuss the challenges in existing research, and explore potential future research directions.

2 Preliminaries

First, we introduce the necessary definitions and notation.

Definition 2.1. The ground set is denoted as $\mathcal{V} \coloneqq \{1, \dots, |\mathcal{V}|\}$.

Definition 2.2. Let $\varphi : [1, |\mathcal{V}|] \to \mathbb{R}^d$ be the mapping from each element of the ground set $\mathcal{V}$ to the corresponding d-dimensional vector with respect to the indices as $\varphi(s_i) = \boldsymbol{s}_i \in \mathbb{R}^d$ for all $s_i \in \mathcal{S}$. Furthermore, when it is clear from the context, we identify $\mathcal{S} \subseteq \mathcal{V}$ with the set of vectors obtained by this mapping as $\mathcal{S} = \{s_1, \dots, s_{|\mathcal{S}|}\} = \{\varphi(s_1), \dots, \varphi(s_{|\mathcal{S}|})\} = \{\boldsymbol{s}_1, \dots, \boldsymbol{s}_{|\mathcal{S}|}\}$.

Definition 2.3. Let $\Pi_{\mathcal{S}}$ be the set of all permutations of $\mathcal{S} \subseteq \mathcal{V}$

Definition 2.4. Denote the set of all subsets of a set $\mathcal{V}$, known as the power set of $\mathcal{V}$, by $2^{\mathcal{V}}$.

2.1 What do we need to approximate set functions?

There are several key differences between functions that take general vectors as inputs and functions that take sets as inputs.

Definition 2.5 (Permutation invariant)**.** A set function $f : 2^{\mathcal{V}} \to \mathbb{R}$ is said to be permutation invariant if $f(\mathcal{S}) = f(\pi_{\mathcal{S}}\mathcal{S})$ for any set $\mathcal{S} \subseteq \mathcal{V}$ and its arbitrary permutation $\pi_{\mathcal{S}} \in \Pi_{\mathcal{S}}$.

Architecture	Novelties and Contributions	Applied tasks
Deep Sets (Zaheer et al., 2017)	The universality result for permutation-invariance and sum-decomposability.	General set function approximation Point cloud classification Set expansion Set retrieval Image tagging Set anomaly detection
PointNet (Qi et al., 2017a)	The max-decomposition architecture.	Point cloud classification Point cloud segmentation
PointNet++ (Qi et al., 2017b)		
SetNet (Zhong et al., 2018)	Utilizing NetVLAD layer for the set retrieval task.	Set retrieval
Set Transformer (Lee et al., 2019)	Utilizing Transformer architecture for permutation-invariant inputs.	General set function approximation Point cloud classification Set anomaly detection
DSPN (Zhang et al., 2019b)	A model that predicts a set of vectors from another vector.	Set reconstruction Bounding box prediction
iDSPN (Zhang et al., 2021)	The concept of exclusive multiset-equivalence.	Class specific numbering Random multisets reconstruction Object property prediction
Set VAE (Kim et al., 2021b)	The VAE-based set generation model.	Set generation
Slot Attention (Locatello et al., 2020)	A new variant of permutation-invariant attention mechanism.	Object discovery Set prediction
Deep Sets++ & Set Transformer++ (Zhang et al., 2022b)	The Set Normalization as the alternative normalization layer.	General set function approximation Point cloud classification Set anomaly detection
PointCLIP (Zhang et al., 2022c)	CLIP for permutation-invariant inputs.	Point cloud classification

Table 1: Neural network architectures for approximating set functions.

Definition 2.6 (Permutation invariant, set-pair input case)**.** A function $f : 2^{\mathcal{V}\times\mathcal{V}} \to \mathbb{R}$ is said to be permutation invariant if $f(\mathcal{S},\mathcal{T}) = f(\pi_{\mathcal{S}}\mathcal{S}, \pi_{\mathcal{T}}\mathcal{T})$ for any sets $\mathcal{S},\mathcal{T} \subseteq \mathcal{V}$ and arbitrary permutations $\pi_{\mathcal{S}} \in \Pi_{\mathcal{S}}$ and $\pi_{\mathcal{T}} \in \Pi_{\mathcal{T}}$.

Neural networks tasked with approximating set functions face unique challenges and requirements compared to conventional vector-input functions. In order to accurately model and capture the characteristics of sets, these networks need to fulfill the aforementioned properties. First, permutation invariance ensures that the output of the network remains consistent regardless of the order in which elements appear in the set. This is crucial for capturing the inherent structure and compositionality of sets, where the arrangement of elements does not affect the overall meaning or outcome. Second, equivariance to set transformations guarantees that the network's behavior remains consistent under operations such as adding or removing elements from the set. This property ensures that the network can adapt to changes in set size without distorting its output. Finally, the output of the network should be invariant to repeated elements, as the presence of duplicate elements should not impact the resulting function approximation. By satisfying these properties, neural networks can effectively model and approximate set functions, enabling them to tackle a wide range of set-based tasks in various domains.

3 Model Architectures for approximating set functions

In this section, we overview the neural network architectures approximating set functions. Table 1 summarizes architectures and corresponding novelties, contributions and applied tasks.

In particular, we focus on architectures following Deep Sets, which demonstrated universality results for permutation-invariant inputs. However, prior to that, several similar studies on related architectures also exist (Gens & Domingos, 2014; Cohen & Welling, 2016). For example, invariance can be achieved by pose normalization using an equivariant detector (Lowe, 2004; Jaderberg et al., 2015), or by averaging a possibly nonlinear function over a group (Reisert, 2008; Manay et al., 2006; Kondor, 2007).

3.1 Deep Sets

One seminal works for approximating set functions by neural networks is Deep Sets (Zaheer et al., 2017). The framework of Deep Sets is written as

$$f(\mathcal{S}) \coloneqq \rho\left(\sum_{\boldsymbol{s}\in\mathcal{S}} \phi(\boldsymbol{s})\right), \tag{1}$$

for set $\mathcal{S}$, and two functions ϕ, ρ. It is obvious that Deep Sets architecture satisfy the permutation-invariant 2.5, and it can approximate the set function by using arbitrary neural networks ϕ and ρ. It is also known that Deep Sets has the universality for permutation-invariant and sum-decomposability (see Section 5.1 for more details).

3.2 PointNet and PointNet++

The most well-known architecture developed for processing point cloud data is Poin tNet (Qi et al., 2017a). One of the important differences between PointNet and Deep Sets is their pooling operation. For instance, PointNet employs global max pooling, while global sum pooling is adopted in Deep Sets. This implies that we can write PointNet architecture as follows:

$$f(\mathcal{S}) \coloneqq \rho\left(\max_{\boldsymbol{s}\in\mathcal{S}} \phi(\boldsymbol{s})\right). \tag{2}$$

Therefore, we can express the architectures of Deep Sets and PointNet in a unified notation.

The function that can be written in the form of Eq. 1 is referred to as sum-decomposable, and the function that can be written in the form of Eq. 2 is called max-decomposable.

The universality result of sum-decomposability in Deep Sets suggests that a similar result holds for max-decomposable functions, as indicated in subsequent studies (Wagstaff et al., 2022).

3.3 Set Transformer

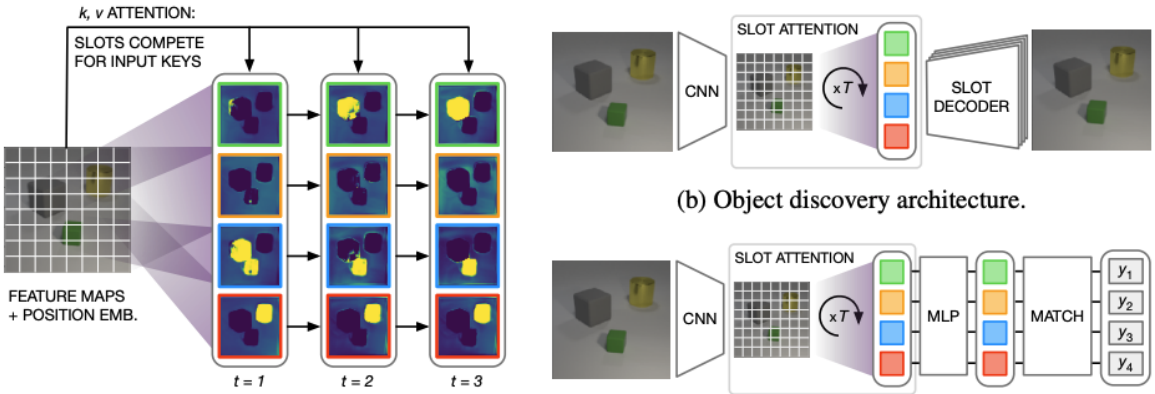
In recent years, the effectiveness of Transformer architectures (Vaswani et al., 2017; Lin et al., 2022) has been reported in various tasks that neural networks tackle, such as natural language processing (Kalyan et al., 2021; Wolf et al., 2019; Kitaev et al., 2020; Beltagy et al., 2020), computer vision (Han et al., 2022b; Khan et al., 2022; Dosovitskiy et al., 2020; Arnab et al., 2021; Zhou et al., 2021a), and time series analysis (Wen et al., 2022; Zhou et al., 2021b; Zerveas et al., 2021). Set Transformer (Lee et al., 2019) utilizes the Transformer architecture to handle permutation-invariant inputs. Similar architectures have also been proposed for point cloud data (Guo et al., 2021; Park et al., 2022; Zhang et al., 2022a; Liu et al., 2023).

The architectures of Deep Sets and PointNet, as evident from Eq. 1 and 2, operate by independently transforming each element of the input set and then aggregating them. However, this approach neglects the relationships between elements, leading to a limitation. On the other hand, Set Transformer addresses this limitation by introducing an attention mechanism, which takes into account the relationships between two elements in the input set. We can write this operation as follows.

$$f(\mathcal{S}) = \rho\left(\frac{1}{\tau(|\mathcal{S}|,2)} \sum_{\mathcal{T}\in\mathcal{S}_{(2)}} \sum_{\boldsymbol{t}\in\mathcal{T}} \phi(\boldsymbol{t})\right), \tag{3}$$

where $\tau(|\mathcal{S}|,2) = \frac{|\mathcal{S}|}{(|\mathcal{S}|-2)!}$. Eq. 3 can be viewed as performing permutation-invariant operations on 2-tuples of permutations of the input set.

As introduced in Section 5.1, recent research has revealed that Deep Sets, PointNet, Set Transformer, and their variants can be regarded as special cases of a function class called Janossy Pooling (Murphy et al., 2018). Moreover, there have been several discussions regarding the generalization of Transformer and Deep Sets (Kim et al., 2021a; Maron et al., 2018).



(a) Slot Attention module.

(b) Object discovery architecture.

(c) Set prediction architecture.

Figure 1: Slot Attention module and example applications to unsupervised object discovery and supervised set prediction with labeled targets, from Figure 1 of Locatello et al. (2020).

3.4 Deep Sets++ and Set Transformer++

Many neural network architectures include normalization layers such as Layer Norm (Ba et al., 2016), BatchNorm (Ioffe & Szegedy, 2015; Bjorck et al., 2018) or others (Wu & He, 2018; Salimans & Kingma, 2016; Huang & Belongie, 2017). SetNorm is used for neural networks that take sets as input, based on the result that normalization layer is permutation-invariant only when the transformation part of the normalization layer deforms all the features with different scales and biases for each feature. Specifically, applying SetNorm to Deep Sets and Set Transformer, referred to as Deep Sets++ and Set Transformer++ respectively, has been shown experimentally to achieve superior performance. Furthermore, this paper also releases a dataset called Flow-RBC, which comprises sets of measurement results of red blood cells of patients, aimed at predicting anemia.

3.5 DSPN and iDSPN

Deep Set Prediction Networks (DSPN) (Zhang et al., 2019b) propose a model for predicting a set of vectors from another set of vectors. The proposed decoder architecture leverages the fact that the gradients of the set functions with respect to the set are permutation-invariant, and it is effective for tasks such as predicting a set of bounding boxes for a single input image. Also, iDSPN (Zhang et al., 2021) introduced the concept of exclusive multiset-equivalence to allow for the arbitrary ordering of output elements with respect to duplicate elements in the input set. They also demonstrated that by constructing the encoder of DSPN using Fspool (Zhang et al., 2019c), the final output for the input set satisfies exclusive multiset-equivalence.

3.6 SetVAE

SetVAE (Kim et al., 2021b) is the set generation model based on Variational Auto-Encoder (VAE) (Kingma & Welling, 2013) that takes into account exchangeability, variable-size sets, interactions between elements, and hierarchy. Here, hierarchy refers to the relationships between subsets within a set, such as the hierarchical structure of elements in the set. The concept of the Hierarchical VAE was introduced in the context of high-resolution image generation (Sønderby et al., 2016; Vahdat & Kautz, 2020), and this study utilizes it for set generation.

3.7 PointCLIP

One of the learning strategies that has garnered significant attention in the field of machine learning in recent years is Contrastive Language-Image Pre-training (CLIP) (Radford et al., 2021; Shen et al., 2021; Luo et al.,

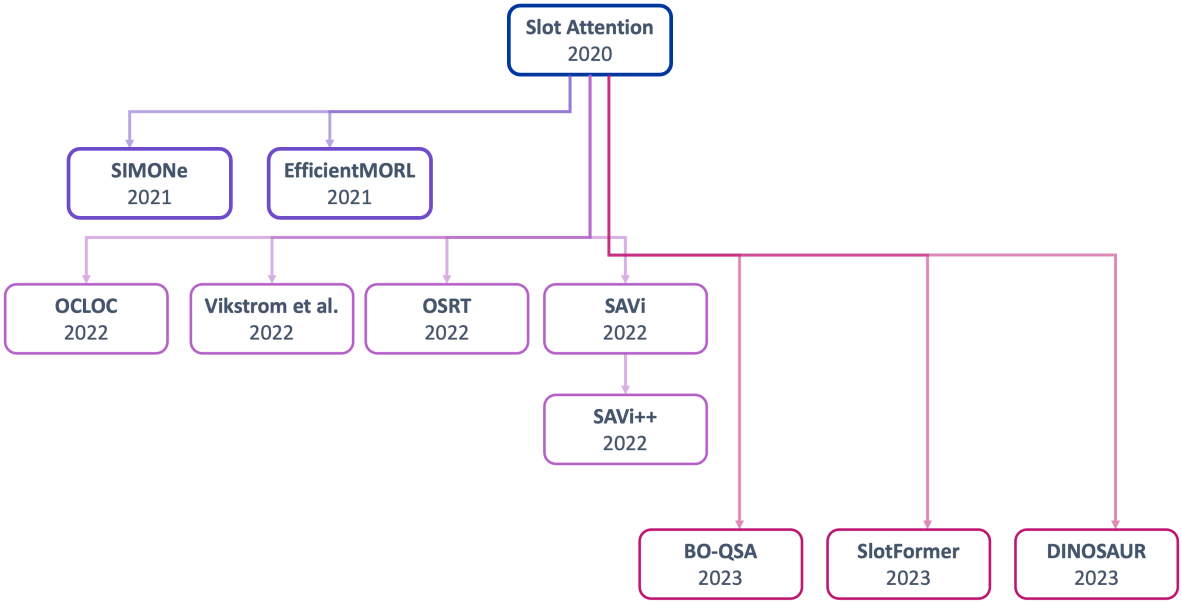


Figure 2: Slot Attention and its variants.

2022). PointCLIP (Zhang et al., 2022c) adopts CLIP for permutation-invariant neural networks. PointCLIP encodes point cloud data using CLIP and achieves category classification for 3D data by examining their positional relationships with category texts. Furthermore, PointCLIPv2 (Zhu et al., 2023) is an improvement of PointCLIP, achieved through a dialogue system.

3.8 Slot Attention

The Slot Attention (Locatello et al., 2020) mechanism was proposed to obtain representations of arbitrary objects in images or videos in an unsupervised manner. Slot Attention employs an iterative attention mechanism to establish a mapping from its inputs to the slots (see Fig. 1). The slots are initially set at random and then refined at each iteration to associate with specific parts or groups of the input features. The process involves randomly sampling initial slot representations from a common probability distribution. It is proven that Slot Attention is

i) permutation invariance with respect to the input;

ii) permutation equivariance with respect to the order of the slots.

Zhang et al. (2022d) pointed out two issues with slot attention: the problem of single objects being bound to multiple slots (soft assignments) and the problem of multiple slots processing similar inputs, resulting in multiple slots having averaged information about the properties of a single object (Lack of tiebreaking). To address these issues, they leverage the observation that part of the slot attention processing can be seen as one step of the Sinkhorn algorithm (Sinkhorn, 1964), and they propose a method to construct slot attention to be exclusive multiset-equivalent without sacrificing computational efficiency.

Chang et al. (2022) argue that slot attention suffers from the issue of unstable backward gradient computation because it performs sequential slot updates during the forward pass. Specifically, as training progresses, the spectral norm of the model increases. Therefore, they experimentally demonstrated that by replacing the iterative slot updates with implicit function differentiation at the fixed points, they can achieve stable backward computation without the need for ad hoc learning stabilization techniques, including gradient

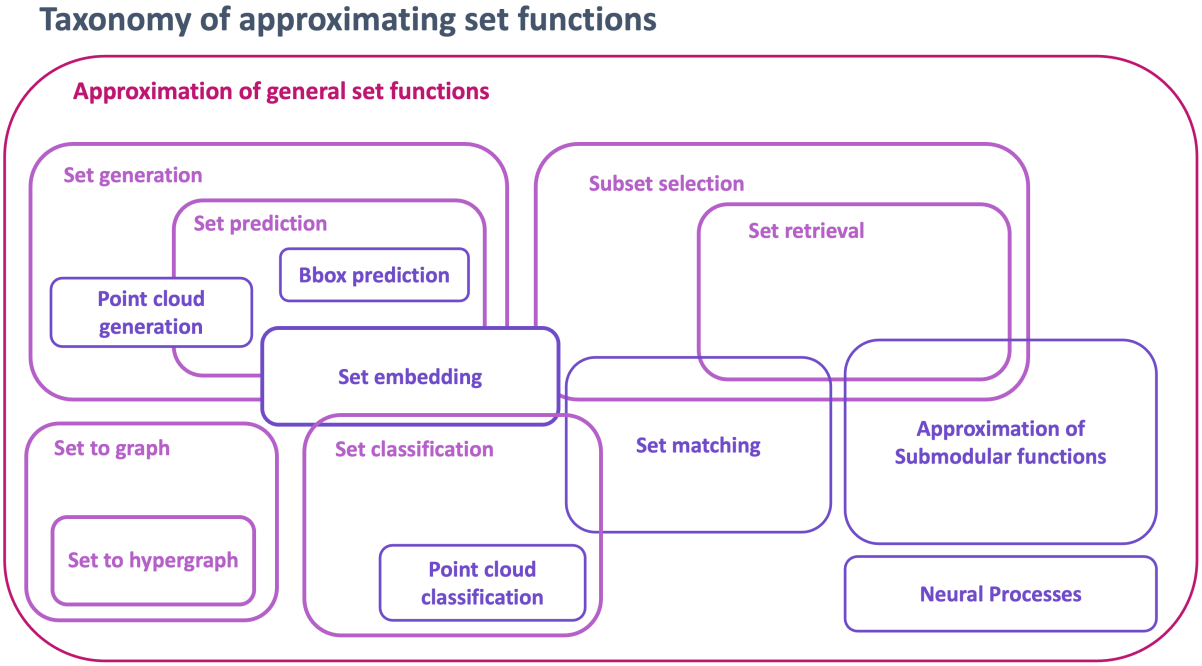


Figure 3: Taxonomy of approximating set functions.

clipping (Pascanu et al., 2013; Zhang et al., 2019a), learning rate warmup (Goyal et al., 2017; Liu et al., 2019) or adjustment of the number of iterative slot updates. Kipf et al. (2021) point out that initializing slots through random sampling from learnable Gaussian distributions during the sequential updating process may lead to instability in behavior. Based on this, Jia et al. (2022) propose stabilizing the behavior by initializing slots with fixed learnable queries, namely BO-QSA. Vikström & Ilin (2022) propose the ViT architecture and a corresponding loss function within the framework of Masked Auto Encoder to acquire object-centric representations. Furthermore, DINOSAUR (Seitzer et al., 2022) learns object-centric representations based on higher-level semantics by optimizing the reconstruction loss with ViT features. Slotformer (Wu et al., 2022) is proposed as a transformer architecture that predicts slots autoregressively, and it has been reported to achieve high performance. There are many other variants of slot attention along with their respective applications, such as SIMONe (Kabra et al., 2021), EfficientMORL (Emami et al., 2021), OSRT (Sajjadi et al., 2022), OCLOC (Yuan et al., 2022), SAVi (Kipf et al., 2021) or SAVi++ (Elsayed et al., 2022).

4 Tasks of approximating set functions

In this section, we organize the tasks addressed by neural networks that approximate set functions. Figure 3 shows the taxonomy of approximating set functions.

4.1 Point cloud processing

Deep Sets, PointNet, and Set Transformer can be generalized in terms of the differences in the aggregation operations of elements within a set. However, specific aggregation operations are also proposed when the input set consists of point clouds. CurveNet (Xiang et al., 2021) proposes to treat point clouds as undirected graphs and represent curves as walks within the graph, thereby aggregating the points.

4.2 Set retrieval and subset selection

There exists a set retrieval task that generalizes the image retrieval task (Datta et al., 2008; Smeulders et al., 2000; Rui et al., 1999) to sets. The goal of the set retrieval system is to search and retrieve sets from the large pool of sets (Zhong et al., 2018).

Subset selection Subset selection is the task of selecting a subset of elements from a given set in a way that retains some meaningful criteria or properties. Ou et al. (2022) introduced the low-cost annotation method for subset selection and demonstrate its effectiveness.

SetNet (Zhong et al., 2018) is an architecture designed for set retrieval, which uses NetVLAD layer (Jin et al., 2021) instead of conventional pooling layers. In this paper, Celebrity Together dataset is proposed specifically for set retrieval.

4.3 Set generation and prediction

Methods for set prediction can be broadly categorized into the following two approaches:

- distribution matching: approximates $P(\mathcal{Y}|\boldsymbol{x})$ for a set $\mathcal{Y}$ and an input vector $\boldsymbol{x}$;
- minimum assignment: calculates loss function between the assigned pairs.

Distribution matching Deep Set Prediction Networks (DSPN) (Zhang et al., 2019b) propose a model for predicting a set of vectors from another set of vectors. The proposed decoder architecture leverages the fact that the gradients of the set functions with respect to the set are permutation-invariant, and it is effective for tasks such as predicting a set of bounding boxes for a single input image. Also, iDSPN (Zhang et al., 2021) introduced the concept of exclusive multiset-equivalence to allow for the arbitrary ordering of output elements with respect to duplicate elements in the input set. PointGlow (Sun et al., 2020) applies the flow-based generative model for point cloud generation.

Minimum assignment In the minimum assignment approach, there is freedom in choosing the distance function, but LSP (Preechakul et al., 2021) relaxes this and ensures convergence. SetVAE (Kim et al., 2021b) is the set generation model based on VAE (Kingma & Welling, 2013) that takes into account exchangeability, variable-size sets, interactions between elements, and hierarchy.

Carion et al. (2020) consider object detection as a bounding box set prediction problem and propose an assignment-based method using a transformer, called Detection Transformer (DETR). Inspired by this identification of object detection and set prediction, many studies have been conducted using similar strategies (Hess et al., 2022; Carion et al., 2020; Ge et al., 2021; Misra et al., 2021). It has been reported that DETR can achieve SOTA performance, but its long training time is known to be a bottleneck. Sun et al. (2021) reconsidered the difficulty of DETR optimization and pointed out two causes of slow convergence: Hungarian loss and Transformer cross attention mechanism. They also proposed several methods to solve these problems and showed their effectiveness through experiments.

Zhang et al. (2020) pointed out that methods optimizing assignment-based set loss inadvertently restrict the learnable probability distribution during the loss function selection phase and assume implicitly that the generated target follows a unimodal distribution on the set space, and proposed techniques to address these limitations.

4.4 Set matching

The task of estimating the degree of matching between two sets is referred to as the set matching.

Set matching can be categorized into two cases: the homogeneous case and the heterogeneous case. In the homogeneous case, both input sets consist of elements from the same category or type. On the other hand, in the heterogeneous case, the input sets contain elements from different categories or types. Saito et al. (2020) proposes a novel approach for the heterogeneous case, which has not been addressed before.

To solve set matching problems, it often relies on learning with negative sampling, and Kimura (2022) provide theoretical analyses for such problem settings. Furthermore, recent research has also reported the task-specific distribution shift in set matching tasks (Kimura, 2023).

4.5 Neural Processes

The Neural Process family (Garnelo et al., 2018b;a; Jha et al., 2022), which is an approximation of probabilistic processes using neural networks, has been studied extensively. Garnelo et al. (2018a) first introduced the idea of conditional Neural Processes which model the conditional predictive distribution $p(f(T)|T, C)$, where C is the labeled dataset and T is the unlabeled dataset. One of the necessary conditions for defining a probabilistic process is permutation invariance. In the case of CNPs, to fulfill this condition, the encoder-decoder parts employ the architecture of Deep Sets. However, the output of CNPs consists of a pair of prediction mean and standard deviation, and it is not possible to sample functions like in actual probabilistic processes. Neural Processes (NPs) (Garnelo et al., 2018b) enable function sampling by introducing latent variables into the framework of CNPs.

Kim et al. (2018) showed that NPs is prone to under fitting. They argued that this problem can be solved by introducing attention mechanism, and proposed Attentive Neural Processes.

4.6 Approximating submodular functions

Submodular set function (Fujishige, 2005; Lovász, 1983; Krause & Golovin, 2014) is one of the important class of set functions, and there exists many applications. First, we introduce the definitions and known results for the submodular set function.

Definition 4.1. A function f is called submodular if it satisfies

$$f(\mathcal{S}) + f(\mathcal{T}) \geq f(\mathcal{S} \cup \mathcal{T}) + f(\mathcal{S} \cap \mathcal{T}), \tag{4}$$

for any $\mathcal{S}, \mathcal{T} \subseteq \mathcal{V}$.

Definition 4.2. A function f is supermodular if $-f$ is submodular.

Definition 4.3. A function that is both submodular and supermodular is called modular.

If f is a modular function, we have

$$f(\mathcal{S}) + f(\mathcal{T}) = f(\mathcal{S} \cap \mathcal{T}) + f(\mathcal{S} \cup \mathcal{T}), \tag{5}$$

for any $\mathcal{S}, \mathcal{T} \subseteq \mathcal{V}$.

Proposition 4.1. If f is modular, it may be written as

$$f(\mathcal{S}) = f(\emptyset) + \sum_{\boldsymbol{s} \in \mathcal{S}} (f(\{\boldsymbol{s}\}) - f(\emptyset)) \tag{6}$$

$$= c + \sum_{\boldsymbol{s} \in \mathcal{S}} \phi(\boldsymbol{s}), \tag{7}$$

for some ψ.

From the above definitions and results, we have the following proposition for permutation-invariant neural networks.

Proposition 4.2. For permutation-invariant neural networks, we have

i) Deep Sets is the modular function;

ii) PointNet is the submodular function,

with $\rho(\boldsymbol{x}) = \boldsymbol{x}$ and $\phi(\boldsymbol{x}) \geq 0$ for all $\boldsymbol{x} \in \mathcal{V}$.

Proof. i) is obvious from the definition.

For ii), we consider the following inequality equivalent to the definition of submodularity.

$$f(\mathcal{S} \cup \{\boldsymbol{x}\}) - f(\mathcal{S}) \geq f(\mathcal{T} \cup \{\boldsymbol{x}\}) - f(\mathcal{T}), \tag{8}$$

for any $\boldsymbol{x} \in \mathcal{V}$ and $\mathcal{S} \subseteq \mathcal{T} \subseteq \mathcal{V}$. Then, it suffices to show that $f(\mathcal{S}) = \max_{\boldsymbol{s} \in \mathcal{S}} \phi(\boldsymbol{s})$ satisfies Eq. 8.

First, if $\phi(\boldsymbol{x}) \leq \max_{\boldsymbol{s} \in \mathcal{S} \cup \mathcal{T}} \phi(\boldsymbol{s})$, we have

$$\begin{aligned} f(\mathcal{S} \cup \{\boldsymbol{x}\}) - f(\mathcal{S}) &= f(\mathcal{S}) - f(\mathcal{S}) \\ &= 0 = f(\mathcal{T}) - f(\mathcal{T}) = f(\mathcal{T} \cup \{\boldsymbol{x}\}) - f(\mathcal{T}), \end{aligned} \tag{9}$$

and it satisfy Eq. 8 with equality.

Next, we assume that $\phi(\boldsymbol{x}) \geq \max_{\boldsymbol{s} \in \mathcal{S} \cup \mathcal{T}} \phi(\boldsymbol{s})$. In this case, if $\boldsymbol{x} \notin \mathcal{S} \cup \mathcal{T}$, we have

$$\begin{aligned} f(\mathcal{S} \cup \{\boldsymbol{x}\}) - f(\mathcal{S}) - \{f(\mathcal{T} \cup \{\boldsymbol{x}\}) - f(\mathcal{T})\} &= \phi(\boldsymbol{x}) - f(\mathcal{S}) - \phi(\boldsymbol{x}) + f(\mathcal{T}) \\ &= f(\mathcal{T}) - f(\mathcal{S}) \\ &\geq 0. \quad (\because \mathcal{S} \subseteq \mathcal{T}) \end{aligned} \tag{10}$$

Also, if $\boldsymbol{x} \notin \mathcal{S}$ and $\boldsymbol{x} \in \mathcal{T}$,

$$f(\mathcal{S} \cup \{\boldsymbol{x}\}) - f(\mathcal{S}) - \{f(\mathcal{T} \cup \{\boldsymbol{x}\}) - f(\mathcal{T})\} = \phi(\boldsymbol{x}) - f(\mathcal{S}) \geq 0. \tag{11}$$

Moreover, since $\mathcal{S} \subseteq \mathcal{T}$ we have $\boldsymbol{x} \in \mathcal{S} \Rightarrow \boldsymbol{x} \in \mathcal{T}$. Then, we have the proof. □

Deep Submodular Functions (Dolhansky & Bilmes, 2016) is one of the seminal works on learning-based submodular functions. Furthermore, Tschiatschek et al. (2016) propose a probability model where the energy function is represented by a parametric submodular function.

4.7 Person re-identification

Person re-identification (Zheng et al., 2015; Liao et al., 2015; Zheng et al., 2017) can be viewed as an approximation problem of set functions since it involves selecting the target element from a set of person images as input. The HAP2S loss (Yu et al., 2018) is proposed with the aim of efficient point-to-set metric learning for the Person re-identification task.

As a variant task of person re-identification, there is also group re-identification (Wei-Shi et al., 2009; Zheng et al., 2014; Lisanti et al., 2017), which involves identifying groups of individuals in images or videos. Lisanti et al. (2017) introduced a visual descriptor that achieves invariance both to the number of subjects and to their displacement within the image in this task.

4.8 Other tasks

Metric learning In traditional video-based action recognition methods, task recognition often involves extracting subtasks and performing temporal alignment. However, Wang et al. (2022) suggests that, in some cases, the order of subtasks may not be crucial, and there could be alternative approaches that can achieve similar results. To perform distance learning between the query video and the contrastive videos, a set matching metric is introduced (Wang et al., 2022).

Sinha & Fleuret (2023) propose the permutation-invariant transformer-based model that can estimate the Earth Mover's Distance in quadratic order with respect to the number of elements. They report the effectiveness of the sinkhorn algorithm in cases where there are constraints on computational costs, as increasing the number of iterations in the Sinkhorn algorithm improves accuracy compared to their proposed algorithm. Cuturi (2013) propose a parallelizable Sinkhorn algorithm operating on multiple pairs of histograms that functions within the GPU environment.

XAI Explainable Artificial Intelligence (XAI) aims to explain the behavior of machine learning models (Gunning et al., 2019; Tjoa & Guan, 2020). Several studies are exploring the combination of approximating set functions and XAI techniques. Cotter et al. (2018) and Cotter et al. (2019) introduce an architecture for approximating interpretable set functions that maintains performance comparable to Deep Sets.

5 Theoretical analysis of approximating set functions

5.1 Sum-decomposability and Janossy pooling

One fundamental property for approximating set function is the sum-decomposability.

Definition 5.1. We say that a function f is sum-decomposable if there are functions ρ and ϕ such that

$$f(\mathcal{S}) = \rho\left(\sum_{\boldsymbol{s}\in\mathcal{S}} \phi(\boldsymbol{s})\right) \tag{12}$$

for any $\mathcal{S} \subseteq \mathcal{V}$. In this case, we say that (ρ, ϕ) is a sum-decomposition of f. Given a sum-decomposition (ρ, ϕ), we write $\Phi(\mathcal{S}) \coloneqq \sum_{\boldsymbol{s}\in\mathcal{S}} \phi(\boldsymbol{s})$. With this notation, we can write Eq. 12 as $f(\mathcal{S}) = \rho(\Phi(\mathcal{S}))$. We may also refer to the function $\rho \circ \Phi$ as a sum-decomposition.

Definition 5.2. Let (ρ, ϕ) be a sum-decomposition. Write $\mathcal{Z}$ for the domain of ρ (which is also the codomain of ϕ, and the space in which the summation happens in Eq. 12. We refer to $\mathcal{Z}$ as the latent space of the sum-decomposition (ρ, ϕ).

Definition 5.3. Given a space $\mathcal{Z}$, we say that f is sum-decomposable via $\mathcal{Z}$ if f has a sum-decomposition whose latent space is $\mathcal{Z}$.

Definition 5.4. We say that f is continuously sum-decomposable when there exists a sumdecomposition (ρ, ϕ) of f such that both ρ and ϕ are continuous. (ϕ, ρ) is then a continuous sum-decomposition of f.

Achieving permutation invariance poses a fundamental challenge in the design of models, as it requires finding the right trade-off between expressive power and maintaining the desired property. The objective is to construct models that can effectively represent diverse functions, while ensuring that the output remains unchanged when the input elements are permuted. This delicate equilibrium guarantees that the models can capture the inherent complexities of the problem at hand, while upholding the crucial aspect of permutation invariance.

One unifying framework of methods that learn either strictly permutation-invariant functions or suitable approximations is Janossy pooling (Murphy et al., 2018). Janossy pooling is renowned for its remarkable expressiveness, and its universality can be readily illustrated. It is capable of representing any permutation-invariant function, making it a highly versatile framework. This exceptional property highlights the ability of Janossy pooling to capture intricate relationships and patterns within sets. With its flexibility and effectiveness, Janossy pooling serves as a valuable tool for modeling and analyzing permutation-invariant functions, offering a broad spectrum of applications across diverse domains.

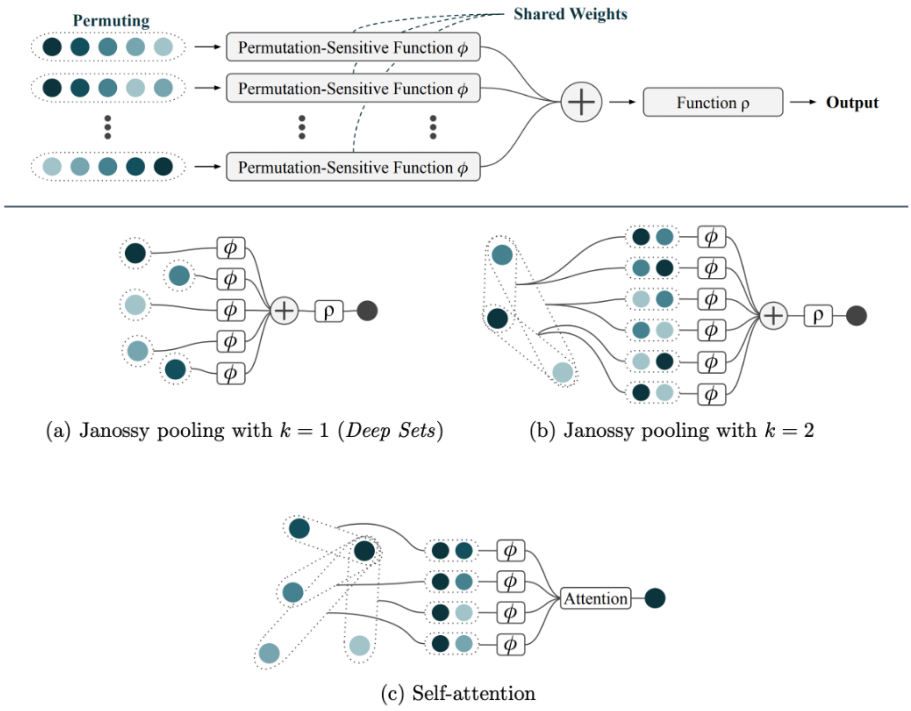
Definition 5.5 (Janossy pooling (Murphy et al., 2018))**.** For any set $\mathcal{S} \subseteq \mathcal{V}$ and its permutations $\Pi_{\mathcal{S}}$, Janossy pooling is defined as the aggregation of outputs of permutation-sensitive function $\Phi(\mathcal{S})$ for all possible permutations:

$$\hat{f}(\mathcal{S}) = \frac{1}{|\Pi_{\mathcal{S}}|} \sum_{\pi_{\mathcal{S}}\in\Pi_{\mathcal{S}}} \Phi(\pi_{\mathcal{S}}(\mathcal{S})). \tag{13}$$

We can also consider the post-process ρ as

$$f(\mathcal{S}) = \rho\left(\hat{f}(\mathcal{S})\right), \tag{14}$$

and this is the form of sum-decomposable 5.1, and permutation-invariant 2.5.



(a) Janossy pooling with $k = 1$ (*Deep Sets*)

(b) Janossy pooling with $k = 2$

(c) Self-attention

Figure 4: Top panel: The Janossy pooling framework with the same permutation-sensitive network to each possible permutation of the input set, from Figure 1 of Wagstaff et al. (2022). Bottom panel: Different versions and variants of Janossy pooling, from Figure 2 of Wagstaff et al. (2022).

Theorem 5.1. Let $f : \mathbb{R}^M \to \mathbb{R}$ be continuous and permutation invariant. Then f has a continuous k-ary Janossy representation via $\mathbb{R}^M$ for any choice of k.

Theorem 5.2. Let $f : \mathbb{R}^M \to \mathbb{R}$ be continuous and permutation invariant. Then f has a continuous M-ary Janossy representation via $\mathbb{R}$.

It is obvious that the computational complexity of Janossy pooling scales at least linearly in the size of $\Pi_{\mathcal{S}}$, which is $|\mathcal{S}|!$. To address this problem, the following strategies are discussed (Murphy et al., 2018):

i) sorting: considering only a single canonical permutation, which is obtained by sorting the inputs;

ii) sampling: aggregating over a randomly-sampled subset of permutations;

iii) restricting permutation to k-tuples: for some $k < |\mathcal{S}|$, let $\mathcal{S}_{\{k\}}$ denote the set of all k-tuples from $\mathcal{S}$, and

$$\hat{f}(\mathcal{S}) = \frac{1}{\tau(|\mathcal{S}|, k)} \sum_{\mathcal{T} \in \mathcal{S}_{\{k\}}} \Phi(\mathcal{T}), \tag{15}$$

where $\tau(|\mathcal{S}|, k) = \frac{|\mathcal{S}|}{(|\mathcal{S}|-k)!}$.

The computational complexity of Eq. 15 is $\mathcal{O}(|\mathcal{S}|^k)$, and for sufficiently small k this gives far fewer that $|\mathcal{S}|!$. Note that third strategy is the generalization of many practical models (Zaheer et al., 2017; Qi et al., 2017a;b; Lee et al., 2019). Indeed, the case of $k = 1$ is equivalent to Deep Sets Zaheer et al. (2017), and many other current neural network architectures resembles the case of $k = 2$.

5.2 Expressive power of Deep Sets and PointNet

Recall that the network architectures of PointNet f_{PointNet} and Deep Sets f_{DeepSets} are given as

$$f_{\text{PointNet}} = \rho\left(\max_{\boldsymbol{s}\in\mathcal{S}} \phi(\boldsymbol{s})\right), \tag{16}$$

$$f_{\text{DeepSets}} = \rho\left(\sum_{\boldsymbol{s}\in\mathcal{S}} \phi(\boldsymbol{s})\right). \tag{17}$$

In addition, we can consider the normalized version of Deep Sets $f_{\text{Normalized}-\text{DeepSets}}$ as

$$f_{\text{N-DeepSets}} = \rho\left(\frac{1}{|\mathcal{S}|}\sum_{\boldsymbol{s}\in\mathcal{S}} \phi(\boldsymbol{s})\right). \tag{18}$$

Bueno & Hylton (2021) provide the comparison of representation power and universal approximation theorems of PointNet and Deep Sets. Briefly,

- PointNet (normalized Deep Sets) has the capability to uniformly approximate functions that exhibit uniform continuity in relation to the Hausdorff (Wasserstein) metric.
- When input sets are allowed to be of arbitrary size, only constant functions can be uniformly approximated by both PointNet and normalized Deep Sets simultaneously.
- Even when the cardinality is fixed to a size of k, there exists a significant disparity in the approximation capabilities. Specifically, PointNet is unable to uniformly approximate averages of continuous functions over sets, such as the center-of-mass or higher moments, for $k \geq 3$. Furthermore, an explicit lower bound on the error for the learnability of these functions by PointNet is established.

5.3 Sufficient and necessary conditions for Deep Sets to be universal

First, we give the reproduction of the key statements of Deep Sets (Zaheer et al., 2017).

Theorem 5.3. Let $f : 2^{\mathcal{V}} \to \mathbb{R}$ where $\mathcal{V}$ is countable. Then, f is sum-decomposable.

Proof. Since $\mathcal{V}$ is countable, each $s \in \mathcal{V}$ can be mapped to a unique element in $\mathbb{N}$ by a bijective function $c : \mathcal{V} \to \mathbb{N}$. If we can choose ϕ so that Φ is invertible, then we can write $\rho = f \circ \Phi^{-1}$, and $f = \rho \circ \Phi$. Then f is sum-decomposable via $\mathbb{R}$. □

Theorem 5.4. Let $M \in \mathbb{N}$, and $f : [0,1]^M \to \mathbb{R}$ be a continuous permutation-invariant function. Then f is continuously sum-decomposable via $\mathbb{R}^{M+1}$.

Theorem 5.5. Deep Sets can represent any continuous permutation-invariant function of M elements if the dimension of the latent space is at least $M + 1$.

In addition, later work (Han et al., 2022a) gives the explicit bounds on the number of parameters with respect to the dimension and the target accuracy ϵ.

Theorem 5.6 (Han et al. (2022a))**.** Let $f : 2^{\mathcal{V}} \to \mathbb{R}$ be a continuously-differentiable, permutation-invariant function. Let $0 < \epsilon < \|\nabla f\|_2 \sqrt{|\mathcal{S}|d}\mathcal{S}^{-\frac{1}{d}}$, for any $\mathcal{S} \subseteq \mathcal{V}$ with the mapping $\varphi : [1, |\mathcal{V}|] \to \mathbb{R}^d$, where $\|\nabla f\|_2 = \max_{\mathcal{S}} \|f(\mathcal{S})\|_2$. Then, there exists $\phi : \mathbb{R}^d \to \mathbb{R}^M$, $\rho : \mathbb{R}^M \to \mathbb{R}$, such that

$$\left| f(\mathcal{S}) - \rho\left(\sum_{\boldsymbol{s}\in\mathcal{S}} \phi(\boldsymbol{s})\right)\right| = \left| f(\mathcal{S}) - \rho\left(\sum_{i=1}^{|\mathcal{S}|} \phi(\varphi(s_i))\right)\right| < \epsilon, \tag{19}$$

where M, the number of feature variables, satisfies the bound

$$M \leq \frac{2^N (\|\nabla f\|_2^2 |\mathcal{S}| d)^{|\mathcal{S}|d/2}}{\epsilon^{|\mathcal{S}|d} |\mathcal{S}|!}. \tag{20}$$

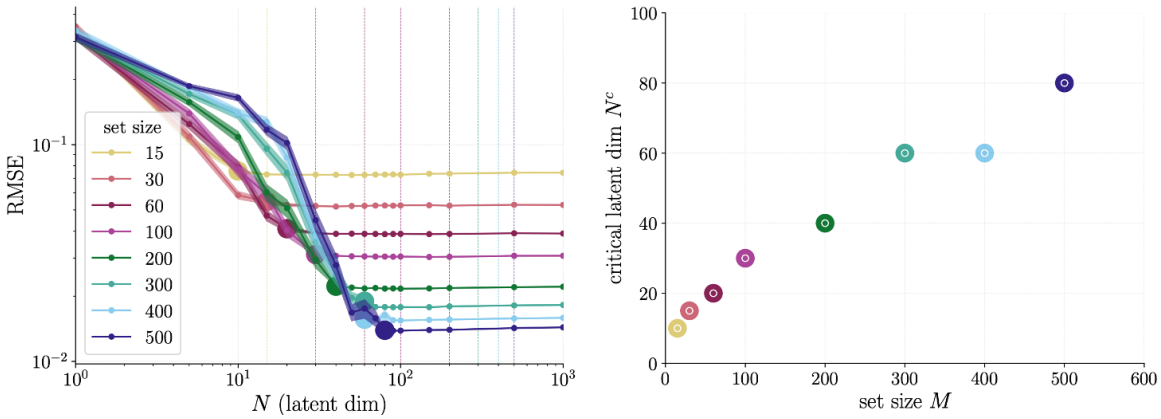


Figure 5: Illustrative toy example, from Figure 3 of Wagstaff et al. (2019). Top panel: Test performance on median estimation depending on latent dimension, and dashed lines indicate $N = M$. Bottom panel: Extracted critical points, and the coloured data points depict minimum latent dimension for optimal performance for different set sizes.

Furthermore, Wagstaff et al. (2022) provides more precise analysis.

Theorem 5.7 (Wagstaff et al. (2022))**.** Let $M, N \in \mathbb{N}$, with $M > N$. Then, there exists continuous permutation-invariant functions $f : \mathbb{R}^M \to \mathbb{R}$ which are not continuously sum-decomposable via $\mathbb{R}^N$.

This implies that for Deep Sets to be capable of representing arbitrary continuous functions on sets of size M, the dimension of the latent space N must be at least M. A similar statement is also true for models based on max-dexomposition, such as PointNet (Qi et al., 2017a).

Definition 5.6. We say that a function f is $max - decomposable$ if there are functions ρ and ϕ such that

$$f(\mathcal{S}) = \rho\left(\max_{\boldsymbol{s}\in\mathcal{S}}(\phi(\boldsymbol{s}))\right), \tag{21}$$

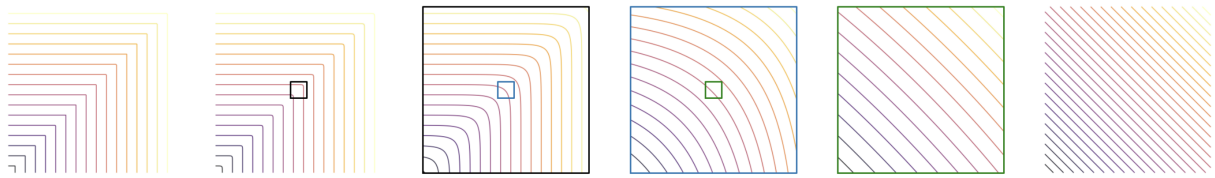
where max is taken over each dimension independently in the latent space.

Theorem 5.8. Let $M > N \in \mathbb{N}$. Then there exist continuous permutation-invariant functions $f : \mathbb{R}^M \to \mathbb{R}$ which are not max-decomposable via $\mathbb{R}^N$.

Figure 5 shows the illustrative example for the above theorems. Theorem 5.7 implies that the number of input elements M to have an influence on the required latent dimension N. The neural network, which has the architecture of Deep Sets, is trained to predict the median of a set of values. The input sets are randomly drawn from either a uniform, a Gaussian, or a Gamma distribution. This figure shows the relationship between different latent dimension N, the input set size M and the predictive performance, and it can be seen that

- The error monotonically decreases with the latent space dimension for every set size;
- Once a specific point is surpassed (referred to as the critical point), enlarging the dimension of the latent space no longer leads to a further reduction in error;
- As the set size increases, the latent dimension at the critical point also grows.

It should be noted that the critical points are observed when $N < M$. The reason behind this phenomenon lies in the fact that the models do not acquire an algorithmic solution for computing the median. Instead, they learn to estimate it based on samples drawn from the input distribution encountered during training.



(a) max on $[-10, 10]^2$ (b) LΣE on $[-100, 100]^2$ (c) LΣE on $[-10, 10]^2$ (d) LΣE on $[-1, 1]^2$ (e) LΣE on $[-.1, .1]^2$ (f) sum on $[-10, 10]^2$

Figure 6: Contour plots for max (left), sum (right), and logsumexp ($L\Sigma E$) on two inputs, from Figure 2 of Soelch et al. (2019). For large ranges, $L\Sigma E$ acts like max, shifting towards sum with decreasing input range. Matching square boxes indicate zoom between plots.

5.3.1 The Choice of Aggregation

The Deep Set architecture exhibits invariance due to the inherent invariance of the aggregation function). Theoretical justification for summing the embeddings $\phi(\boldsymbol{s})$ is provided by the sum-decomposability (see Section 5.1 for more details). In practice, mean or max-pooling operations are commonly employed, offering simplicity and invariance as well as numerical advantages for handling varying population sizes and controlling input magnitude for downstream layers. This section explores alternative approaches and their respective properties.

Proposition 5.9 (Sum Isomorphism (Soelch et al., 2019))**.** Theorem 5.3 can be extended to aggregations of the form $\alpha_g = g \circ \sum \circ g^{-1}$, i. e. summations in an isomorphic space.

Proof. From $\rho \circ \sum \circ \phi = (\rho \circ g^{-1}) \circ g \circ \sum \circ g^{-1} \circ (g \circ \phi)$, sum decompositions can be constructed from α_g-decompositions and vice versa. □

This class includes mean (with $g((s_1, \ldots, s_{n+1})) = (s_1, \ldots, s_n)/s_{n+1}$, $g^{-1}(\boldsymbol{s}) = (\boldsymbol{s}^\top, 1)^\top$) and logsumexp ($L\Sigma E$) with $g = \ln$. Interestingly, $L\Sigma E$ can behave as max or linear function of summation.

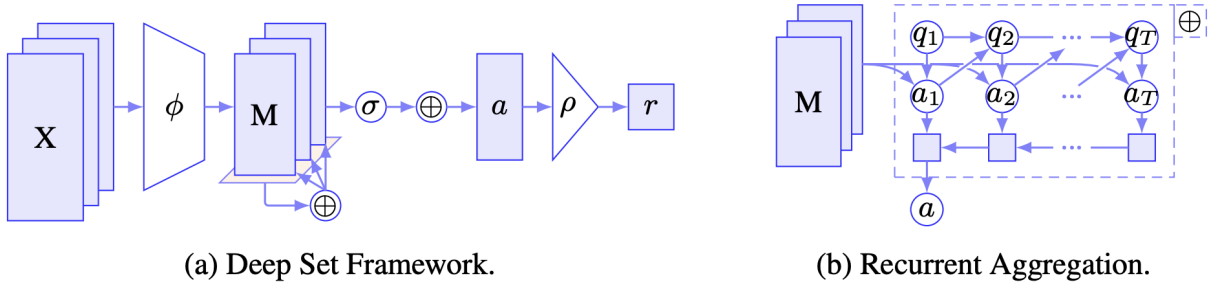
We can observe that divide-and-conquer operations also yield invariant aggregations. In the context of aggregation, order invariance is equivalent to the conquering step remaining invariant to division. This concept extends beyond the realm of basic arithmetic operations and includes logical operators such as any or all, as well as sorting operations that generalize max, min, and percentiles like the median. While these sophisticated aggregations may not be practical for typical first-order optimization, it is worth noting that aggregation techniques can encompass a wide range of complexities. Soelch et al. (2019) propose the learnable aggregation functions, namely recurrent aggregations.

Definition 5.7 (Recurrent and Query Aggregation (Soelch et al., 2019))**.** A recurrent aggregation is a function $f(\mathcal{S}) = \boldsymbol{a}$ that can be written recursively as:

$$
\begin{aligned}
\boldsymbol{q}_t &= \text{query}(\boldsymbol{q}_{t-1}, \boldsymbol{a}_{t-1}) \\
\hat{w}_{i,t} &= \text{attention}(\boldsymbol{m}_i, \boldsymbol{q}_t) \\
\boldsymbol{w}_t &= \text{normalize}(\hat{\boldsymbol{w}}_t) \\
\boldsymbol{a}_t &= \text{reduce}(\{w_{i,t}, \boldsymbol{m}_i\}) \\
\boldsymbol{a} &= g(\boldsymbol{a}_{1:T}),
\end{aligned}
$$

where $\boldsymbol{m}_i = \phi(\boldsymbol{s}_i)$ is an embedding of the input population $\{\boldsymbol{s}_i\}$ and $\boldsymbol{q}_1$ is a constant.

If the reduce operation remains invariant and the normalize operation is equivariant, both recurrent and query aggregations maintain invariance (see Figure 7). Empirical studies show that learnable aggregation functions introduced in this work are more robust in their performance and more consistent in their estimates with growing population sizes.



(a) Deep Set Framework. (b) Recurrent Aggregation.

Figure 7: Deep Set architecture and Recurrent aggregation function from Figure 1 of Soelch et al. (2019).

6 Datasets

In this section, we introduce some commonly used datasets for evaluating the performance of neural networks that approximate set functions.

Flow-RBC (Zhang et al., 2022b): The Flow-RBC dataset comprises 98,240 training examples and 23,104 test examples. Each input set represents the distribution of 1,000 red blood cells (RBCs). Each RBC is characterized by volume and hemoglobin content measurements. The task involves regression, aiming to predict the corresponding hematocrit level measured on the same blood sample. In a blood sample, there are various components, including red blood cells, white blood cells, platelets, and plasma. The hematocrit level quantifies the percentage of volume occupied by red blood cells in the blood sample.

Celebrity Together dataset (Zhong et al., 2018): The Celebrity Together dataset consists of images depicting multiple celebrities together, making it a suitable choice for evaluating set retrieval methods. Unlike other face datasets that only include individual face crops, Celebrity Together comprises full images with multiple labeled faces. The dataset contains a total of 194k images and 546k faces, with an average of 2.8 faces per image.

SHIFT15M (Kimura et al., 2023) SHIFT15M is a dataset designed specifically for assessing models in set-to-set matching scenarios, considering distribution shift assumptions. It allows for evaluating model performance across different levels of dataset shifts by adjusting the magnitude. The dataset contains a total of 2.5m sets and 15m fashion items.

CLEVR (Johnson et al., 2017): CLEVR dataset is a synthetic Visual Question Answering dataset. It contains images of 3D-rendered objects; each image comes with a number of highly compositional questions that fall into different categories. Those categories fall into 5 classes of tasks: Exist, Count, Compare Integer, Query Attribute and Compare Attribute. The CLEVR dataset consists of: a training set of 70k images and 700k questions, a validation set of 15k images and 150k questions, a test set of 15k images and 150k questions about objects, answers, scene graphs and functional programs for all train and validation images and questions. Each object present in the scene, aside of position, is characterized by a set of four attributes: 2 sizes: large, small, 3 shapes: square, cylinder, sphere, 2 material types: rubber, metal, 8 color types: gray, blue, brown, yellow, red, green, purple, cyan, resulting in 96 unique combinations.

ShapeNet (Chang et al., 2015): ShapeNet is a large scale repository for 3D CAD models. The repository contains over 300M models with 220,000 classified into 3,135 classes arranged using WordNet hypernym-hyponym relationships. ShapeNet Parts subset contains 31,693 meshes categorised into 16 common object classes (i.e. table, chair, plane etc.). Each shapes ground truth contains 2-5 parts (with a total of 50 part classes).

ModelNet40 (Wu et al., 2015): ModelNet40 dataset contains 12,311 pre-aligned shapes from 40 categories, which are split into 9,843 for training and 2,468 for testing.

7 Conclusion and discussion

Unlike typical machine learning models that handle vector data, when dealing with set data, it is crucial to ensure permutation-invariance. In this survey, we introduced various neural network architectures that satisfy permutation-invariance and how they are beneficial for a range of tasks. Permutation-invariant architectures not only enhance the ability of model to learn from and make predictions on set data but also open the door to more sophisticated handling of complex structures in machine learning, such as graph. As we delve deeper into the potential of permutation-invariant neural networks and explore their adaptations for specific tasks, future research will likely focus on refining these models, addressing challenges, and uncovering novel applications. This dynamic landscape promises further advancements in machine learning, bridging the gap between vector and set data to unlock new opportunities for understanding and processing complex information structures.

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