Abelian Neural Networks

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Abstract

We study the problem of modeling a binary operation that satisfies some algebraic requirements. We first construct a neural network architecture for Abelian group operations and derive a universal approximation property. Then, we extend it to Abelian semigroup operations using the characterization of associative symmetric polynomials. Both models take advantage of the analytic invertibility of invertible neural networks. For each case, by repeating the binary operations, we can represent a function for multiset input thanks to the algebraic structure. Naturally, our multiset architecture has size-generalization ability, which has not been obtained in existing methods. Further, we present modeling the Abelian group operation itself is useful in a word analogy task. We train our models over fixed word embeddings and demonstrate improved performance over the original word2vec and another naive learning method.

1 Introduction

Thanks to the universal approximation theorem (Cybenko 1989; Leshno et al. 1993; Lu, Pu, Feicheng Wang, et al. 2017; Lu, Pu, F. Wang, et al. 2017), feed-forward neural networks can approximate any continuous functions. However, since available data in the real world is limited, the use of a suitable network architecture that reflects inductive biases behind each problem usually leads to better empirical performance on unseen data. For example, convolutional neural networks (LeCun et al. 1989), which reflect shift invariance of input images, have become the first choice for image recognition; Invertible neural networks (Papamakarios et al. 2019), which are designed to be bijective and be able to compute the inverse, have often been used to model complex probability distributions. When constructing a new architecture, since we often limit the operations of the networks, its expressive power for a target function class matters. This has been studied for each case, such as the universality of the convolutional neural networks for continuous functions (Zhou 2018) and the invertible neural networks for smooth invertible functions (Teshima et al. 2020).

Recently, there has been increasing attention to permutation invariance as an inductive bias. Graph neural networks (Kipf and M. Welling 2017; Gilmer et al. 2017) and neural networks for (multi)sets (Zaheer et al. 2017; Qi et al. 2017)

reflect this and succeeded in many fields such as chemical molecules, combinatorial optimization, and 3D point clouds. A byproduct of these models is that they can handle inputs of different sizes, e.g., graphs or (multi)sets of different sizes. In real-world applications, since annotating label for or training on inputs of large size is computationally expensive, we sometimes try to train a model on smaller data in size and make it generalize to larger test data. Empirically, some studies have reported the size-generalization ability of neural networks for certain tasks (Khalil et al. 2017; Abe et al. 2019). On the other hand, it has been shown that graph neural networks do not naturally generalize to larger graphs than the training graphs (Yehudai et al. 2020).

This work presents the multiset learning setting where we can naturally induce the size generalization. We consider a function over multisets that can be expressed as the composition of binary operations. In order for the function to be well-defined, the binary operation needs to form an Abelian semigroup. For example, $\max(\cdot, \cdot)$, $\min(\cdot, \cdot)$, and + are semigroup operations and they indeed compose well-defined multiset functions: the maximum, minimum, and summation. To model such binary operations, we propose two novel neural network architectures: Abelian group network and Abelian semigroup network that meet the condition of the Abelian group and semigroup, respectively. We show that the Abelian group network is a universal approximator of smooth Abelian group operations. By repeating the binary operations, we can construct two multiset architectures that have the size-generalization ability. Another useful property of the Abelian group network is that it can explicitly compute the inverse element in the Abelian group. Therefore, it is also suitable for learning a better function that is otherwise heuristically modeled by simple operations such as + and -.

2 Preliminaries and Related Work

2.1 Definitions

In this section, let us introduce some basic notations and important definitions that will play a key role in this work.

2.1.1 Notations

By \mathbb{N} , we represent the set of the natural numbers including 0. We denote a vector by a bold symbol, e.g., \boldsymbol{x} . Let $\boldsymbol{x} \in \mathbb{R}^d$ be a d-dimensional vector. We represent the i-th element $(1 \leq i \leq d)$ of \boldsymbol{x} by x_i . For $1 \leq k \leq d$, $\boldsymbol{x}_{\leq k} \in \mathbb{R}^k$ is a k-dimensional vector $(x_1, \ldots, x_k)^T$ and $\boldsymbol{x}_{< k} \in \mathbb{R}^{k-1}$ is a (k-1)-dimensional vector $(x_1, \ldots, x_{k-1})^T$. We denote the elementwise product of two vectors $x, y \in \mathbb{R}^d$ by $x \otimes y$, such that $(x \otimes y)_i = x_i y_i$. We denote the elementwise division of two vectors $x \in \mathbb{R}^d$, $y \in (\mathbb{R} \setminus \{0\})^d$ by $x \otimes y$, such that $(x \otimes y)_i = x_i/y_i$. Unless otherwise noted, $\|\cdot\|$ represents the L^2 (Euclidean) norm.

Let \mathcal{X} be the domain of each element. We denote the set of multisets over \mathcal{X} by $\mathbb{N}^{\mathcal{X}}$. We use $\{x_1, \dots x_n\} \in \mathbb{N}^{\mathcal{X}}$ to describe a multiset composed

of $x_1, \ldots, x_n \in \mathcal{X}$ (any confusion with sets is not problematic in this paper). Addition over multisets is defined as follows: $\{x_1, \ldots, x_n\} + \{x_{n+1}, \ldots, x_N\} = \{x_1, \ldots, x_n, x_{n+1}, \ldots, x_N\}$. The cardinality of a multiset is the number of elements with multiplicity and is expressed by $|\cdot|$ e.g., $|\{1, 2, 2, 3\}| = 4$. A symmetric group S_n is the set of all n! permutations that can be performed on n elements.

2.1.2 Universality

Universality is an important theoretical property of neural networks' expressive power. Let \mathcal{M} be a model and \mathcal{F} be a class of target functions, both of which are sets of functions $\mathcal{X} \to \mathcal{Y}$. The model \mathcal{M} is a sup-universal approximator of \mathcal{F} if for any target function $f^* \in \mathcal{F}$, for any $\epsilon > 0$, and for any compact subset $\mathcal{K} \subset \mathcal{X}$, there exists a function $f \in \mathcal{M}$ such that

$$\sup_{\boldsymbol{x} \in \mathcal{K}} \|f(\boldsymbol{x}) - f^*(\boldsymbol{x})\| < \epsilon. \tag{1}$$

If not noted otherwise, universality refers to the sup-universal property.

For $p \in [1, \infty)$, \mathcal{M} is an L^p -universal approximator of \mathcal{F} if for any target function $f^* \in \mathcal{F}$, for any $\epsilon > 0$, and for any compact subset $\mathcal{K} \subset \mathcal{X}$, there exists a function $f \in \mathcal{M}$ such that

$$\int_{\mathcal{K}} \|f(\boldsymbol{x}) - f^*(\boldsymbol{x})\|^p d\boldsymbol{x} < \epsilon. \tag{2}$$

If \mathcal{M} is sup-universal for \mathcal{F} , \mathcal{M} is L^p -universal for \mathcal{F} . Therefore, L^p -universality is a weaker condition of sup-universality.

2.1.3 Basic Algebra

Here, we introduce the basic definition of important algebraic structures in this study. Let G be a set and $\circ: G \times G \to G$ be a binary operation. Below, we review four properties to define Abelian semigroups and groups.

Associativity For any $x, y, z \in G$, $(x \circ y) \circ z = x \circ (y \circ z)$.

Identity Element There exists an element $e \in G$, called the identity element, such that for any $x \in G$, $x \circ e = e \circ x = x$.

Inverse Element For any $x \in G$, there exists an element $x^{-1} \in G$, called the inverse element of x, such that $x \circ x^{-1} = x^{-1} \circ x = e$.

Commutativity For any $x, y \in G$, $x \circ y = y \circ x$.

Table 1 shows which properties are required in each algebraic structure. A semigroup only requires associativity to the binary operation. A group is a semigroup with an identity element and inverse elements. An Abelian (semi)group is a (semi)group with commutativity.

Table 1: Properties required for each algebraic structure.

	Associativity	Identity	Inverse	Commutativity
Semigroup	✓	-	-	-
Group	✓	\checkmark	\checkmark	-
Abelian Semigroup	\checkmark	-	-	\checkmark
Abelian Group	\checkmark	\checkmark	\checkmark	\checkmark

2.2 Invertible Neural Networks

Invertible neural networks are neural networks that approximate invertible functions $\mathbb{R}^d \to \mathbb{R}^d$. Here, we review some existing studies for multi-dimensional case, i.e., $d \geq 2$, and single-dimensional case, i.e., d = 1.

2.2.1 Normalizing Flows

Multi-dimensional invertible neural networks have been studied mainly in the context of normalizing flows (Tabak and Vanden-Eijnden 2010), which iteratively apply invertible functions to a simple original probability distribution to express complex probability distributions (Kobyzev, Prince, and Brubaker 2020; Papamakarios et al. 2019). There have been many variants proposed including residual flows (Behrmann, Duvenaud, and Jacobsen 2019), neural ODEs (T. Q. Chen et al. 2018), and autoregressive flows (Kingma, Salimans, and M. Welling 2017). Here we review affine coupling flows (Dinh, Krueger, and Y. Bengio 2015), one of the most popular models with parallelizable efficient inverse computation. Each layer of the affine coupling flows maps $\mathbf{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$ to $\mathbf{y} = (y_1, \dots, y_d) \in \mathbb{R}^d$ such that

$$\begin{cases} \boldsymbol{y}_{\leq k} &= \boldsymbol{x}_{\leq k}, \\ \boldsymbol{y}_{>k} &= \boldsymbol{x}_{>k} \otimes \exp(\alpha(\boldsymbol{x}_{\leq k})) + \beta(\boldsymbol{x}_{\leq k}), \end{cases}$$
(3)

where exp is applied elemntwise and $\alpha, \beta : \mathbb{R}^k \to \mathbb{R}^{d-k}$ are trainable functions. The inverse is computed as follows:

$$\begin{cases} \boldsymbol{x}_{\leq k} &= \boldsymbol{y}_{\leq k}, \\ \boldsymbol{x}_{>k} &= (\boldsymbol{y}_{>k} - \beta(\boldsymbol{y}_{\leq k})) \otimes \exp(-\alpha(\boldsymbol{y}_{\leq k})) \end{cases}$$
(4)

They are used in many successful applications such as NICE (Dinh, Krueger, and Y. Bengio 2015), Real NVP (Dinh, Sohl-Dickstein, and S. Bengio 2017), and Glow (Kingma and Dhariwal 2018).

Although the normalizing flows have a limited form of transform, they still admit universalities on certain classes of functions (Teshima et al. 2020). The affine coupling flows are L^p -universal for C^2 -diffeomorphism. Some more complex models including deep sigmoidal flows (Huang et al. 2018) and sum-of-squares polynomial flows (Jaini, Selby, and Yu 2019) are sup-universal for C^2 -diffeomorphism.

2.2.2 Single-dimensional Invertible Neural Networks

For single-dimensional functions, invertibility is equivalent to strict monotonicity. Monotonic networks (Sill 1997) model strictly monotonic functions. Let K be a number of groups and J_k be a number of units for the k-th group. A single-dimensional monotonic network $f: \mathbb{R} \to \mathbb{R}$ is described as follows with parameters $w^{(k,j)}, b^{(k,j)} \in \mathbb{R}$:

$$f(x) = \min_{1 \le k \le K} \max_{1 \le j \le J_k} w^{(k,j)} \cdot x + b^{(k,j)}, \tag{5}$$

where all the weights $w^{(k,j)}$ are constrained to be positive for increasing monotonicity and negative for decreasing monotonicity. For example, the following form is used in practice for the increasingly monotonic case:

$$f(x) = \min_{1 \le k \le K} \max_{1 \le j \le J_k} \exp(\tilde{w}^{(k,j)}) \cdot x + b^{(k,j)}, \tag{6}$$

where $\tilde{w}^{(k,j)} \in \mathbb{R}$. The monotonic networks are a universal approximator for strictly monotonic functions. Monotonic rational-quadratic transforms (Durkan et al. 2019) are another universal model for the single-dimensional case.

2.3 Related Work

Here, we explain related work.

2.3.1 Algebraic Structures in Neural Networks

In the literature of deep learning, algebraic structures mainly appear in the context of group invariant/equivariant neural networks. For image input, some studies tried to incorporate reflection and rotation invariance into convolutional neural networks (Cohen and Max Welling 2016; Worrall et al. 2017). Neural networks for (multi)sets (Zaheer et al. 2017; Qi et al. 2017) adopted invariance/equivariance to symmetric group actions. Recent studies have investigated symmetries invariant/equivariant to more general group actions, such as a subgroup of the symmetric group (Maron, Fetaya, Segol, and Yaron Lipman 2019) and sets of symmetric elements (Maron, Litany, et al. 2020).

On the other hand, our work tries to model an Abelian group/semigroup operation itself.

2.3.2 Inductive Bias and Expressive Power of Neural Networks

Inductive biases are assumptions on the nature of the data-generating process or the space of solutions in machine learning (P. Battaglia et al. 2018). Many studies have constructed special neural networks that reflect the inductive biases of a given problem setting. At the same time, since those networks are often composed of limited forms of neural operations, expressive power including universal approximation properties have been studied.

Convolutional layers of convolutional neural networks (CNN) (LeCun et al. 1989) are designed to be invariant to the small shift of an input image. CNN without fully connected layers has been shown to be universal (Zhou 2018). Forcing the network functions to be bijective (=invertible) is also an inductive bias, which we summarized in Section 2.2. Message passing graph neural networks (Gilmer et al. 2017) such as graph convolutional networks (Kipf and M. Welling 2017) and graph attention networks (Vaswani et al. 2017) are designed under the assumption that neighboring nodes have similar properties. They have been shown to have limited expressive power in terms of graph isomorphism (Xu, Hu, et al. 2019; Morris et al. 2019) and more expressive models have been studied (Sato, Yamada, and Kashima 2019; Maron, Fetaya, Segol, and Y. Lipman 2019; Keriven and Peyré 2019; Maehara and Hoang 2019). For a (multi)set learning problem, DeepSets (Zaheer et al. 2017) are one of the most popular models with universal approximation property.

2.3.3 Size Generalization

Graph neural networks and neural networks for (multi)sets can handle graphs of different sizes, and their size-generalization ability has been empirically shown in some applications such as physical systems (Peter Battaglia et al. 2016) and combinatorial optimization (Khalil et al. 2017; Abe et al. 2019; Veličković et al. 2020). However, from a theoretical perspective, there exist simple tasks on which graph neural networks do not naturally generalize to larger graphs (Yehudai et al. 2020). Recent work has analyzed the extrapolation of graph neural networks trained by gradient descent (Xu, Zhang, et al. 2021). There have been few studies on size generalization of (multi)sets probably because of difficulty in analyzing DeepSets for inputs of different sizes.

3 Proposed Methods

Here, we introduce the proposed methods. First, we describe the motivation for modeling Abelian group and semigroup operations from the perspective of multiset learning. Next, we propose a model for Abelian group operations and show its universality. Then, we extend it for the Abelian semigroup by using the characterization of the associative symmetric polynomials. Finally, we present architectures for multiset input and show the size-generalization ability of the model for Abelian groups.

3.1 Motivation on Multiset Functions

Let \mathcal{X} and \mathcal{Y} be Euclidian spaces, i.e., $\mathcal{X} = \mathbb{R}^{d_1}$ and $\mathcal{Y} = \mathbb{R}^{d_2}$. A function $f: \mathcal{X}^n \to \mathcal{Y}$ is called permutation invariant if for any $\mathbf{X} \in \mathcal{X}^n$ and for any permutation $\sigma \in S_n$, $f(\sigma \cdot \mathbf{X}) = f(\mathbf{X})$ holds. This concept can be extended to functions that take vectors of different dimensions. Namely, a function $f: \bigcup_{k \in \mathbb{N}} \mathcal{X}^k \to \mathcal{Y}$ is called permutation invariant if for any $k \in \mathbb{N}$, for any $\mathbf{X} \in \mathbb{N}$

 \mathcal{X}^k and for any permutation $\sigma \in S_k$, $f(\sigma \cdot \mathbf{X}) = f(\mathbf{X})$ holds. When $f: \bigcup_{k \in \mathbb{N}} \mathcal{X}^k \to \mathcal{Y}$ is permutation invariant, it can be also viewed as a function that takes multisets as input. For notation simplicity, we use the same variable to express the multiset function: $f: \mathbb{N}^{\mathcal{X}} \to \mathcal{Y}$.

In this work, we propose to learn a function over multisets that can be represented as the composition of binary operations. For this function class, size generalization is naturally guaranteed, as we will show in Theorem 3. Below, we present a necessary and sufficient condition for multiset functions that are represented by the composition of binary operations to be well-defined.

Proposition 1 (Permutation Invariant Conditions for Binary Operation). Let $f: \bigcup_{k \in \mathbb{N}} \mathcal{X}^k \to \mathcal{X}$ be a function represented as

$$f(X) = x_1 \circ \cdots \circ x_n, \tag{7}$$

where $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n) \in \mathcal{X}^n$ and $\circ : \mathcal{X} \times \mathcal{X} \to \mathcal{X}$ is a binary operation (left-associative). The function f is invariant if and only if \circ forms an Abelian semigroup, namely, \circ is commutative and associative.

Proof. It is obvious that when \circ is commutative and associative, f is permutation invariant. Let us consider the case when f is permutation invariant. $f((\boldsymbol{x}_1, \boldsymbol{x}_2)) = f((\boldsymbol{x}_2, \boldsymbol{x}_1))$ leads to $\boldsymbol{x}_1 \circ \boldsymbol{x}_2 = \boldsymbol{x}_2 \circ \boldsymbol{x}_1$ (commutativity). From $f((\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)) = f((\boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_1))$, we have $(\boldsymbol{x}_1 \circ \boldsymbol{x}_2) \circ \boldsymbol{x}_3 = (\boldsymbol{x}_2 \circ \boldsymbol{x}_3) \circ \boldsymbol{x}_1$ and commutativity leads to $(\boldsymbol{x}_1 \circ \boldsymbol{x}_2) \circ \boldsymbol{x}_3 = \boldsymbol{x}_1 \circ (\boldsymbol{x}_2 \circ \boldsymbol{x}_3)$ (associativity). \square

When this condition holds, we represent the multiset version of $f: \mathbb{N}^{\mathcal{X}} \to \mathcal{X}$ as follows by denoting a composition of \circ by \bigcirc :

$$f(X) = \bigcup_{x \in X} x, \tag{8}$$

where $X \in \mathbb{N}^{\mathcal{X}}$ is a multiset of \mathcal{X} . On the basis of this proposition, our goal decomposes into learning Abelian semigroup operations over \mathcal{X} . In Section 3.2 and 3.3, we propose neural network architectures for Abelian groups and Abelian semigroups.

3.2 Abelian Group Network

We present the Abelian group network that models Abelian group operations as follows:

$$\boldsymbol{x} \circ \boldsymbol{y} = \phi^{-1}(\phi(\boldsymbol{x}) + \phi(\boldsymbol{y})), \tag{9}$$

where $\phi: \mathcal{X} \to \mathcal{X}$ is a trainable invertible function, typically modeled by an invertible neural network.

First, we check that this binary operation satisfies the four conditions of the Abelian group in Section 2.1.3. Associativity and commutativity follow from the following proposition shown in Appendix A.1.

Proposition 2 (Semigroup Conservation). Let $\rho: \mathcal{X} \to \mathcal{X}$ be a bijective function. When $*: \mathcal{X} \times \mathcal{X} \to \mathcal{X}$ is associative, $\mathbf{x} \circ \mathbf{y} = \rho^{-1}(\rho(\mathbf{x}) * \rho(\mathbf{y}))$ is also assoviative. Similarly, when * is commutative, \circ is commutative.

By this proposition, since + is associative and commutative, the Abelian group network is also associative and commutative. The identity element is

$$e = \phi^{-1}(\mathbf{0}),\tag{10}$$

which satisfies

$$x \circ e = x \circ (\phi^{-1}(\mathbf{0}))$$

= $\phi^{-1}(\phi(x) + \mathbf{0}) = x$. (11)

The inverse element of $x \in \mathcal{X}$ is

$$x^{-1} = \phi^{-1}(-\phi(x)), \tag{12}$$

which satisfies

$$\mathbf{x} \circ \mathbf{x}^{-1} = \mathbf{x} \circ (\phi^{-1}(-\phi(\mathbf{x})))$$

$$= \phi^{-1}(\phi(\mathbf{x}) - \phi(\mathbf{x}))$$

$$= \phi^{-1}(\mathbf{0}) = \mathbf{e}.$$
(13)

It is worth noting that we can analytically compute the inverse function (Equation 12). The experiment in Section 4.3 takes advantage of this quality of the Abelian group network.

Next, we present the universality of the Abelian group network.

Theorem 1 (Universality of Abelian group networks). Let \mathcal{X} be a Euclidean space. Abelian group networks are a universal approximator of Abelian Lie group operations over \mathcal{X} . In other words, for any Abelian Lie group operation \circ : $\mathcal{X} \times \mathcal{X} \to \mathcal{X}$, for any $\epsilon > 0$, and for any compact subset $\mathcal{K} \subset \mathcal{X}$, there exists a binary operation function $*: \mathcal{X} \times \mathcal{X} \to \mathcal{X}$ represented by an Abelian group network such that

$$\sup_{\boldsymbol{x} \in \mathcal{K}, \boldsymbol{y} \in \mathcal{K}} \|(\boldsymbol{x} \circ \boldsymbol{y}) - (\boldsymbol{x} * \boldsymbol{y})\| < \epsilon. \tag{14}$$

Appendix A.2 provides the proof. It is based on the theory of the Lie group and the universality of invertible neural networks.

3.3 Abelian Semigroup Network

Although the Abelian group network proposed in Section 3.2 is universal for smooth group operations, it is not sufficient for approximating an Abelian semi-group operation such as the product over \mathbb{R} , i.e., $x \circ y = xy$. Now we extend the Abelian group network and propose the Abelian semigroup network. Our idea is to extend + of Equation 9 to a polynomial. From Proposition 2, Equation 9 is still a semigroup after we replace + by a polynomial of x and y as long

as the polynomial is associative and symmetric as a binary operation. We call the polynomials with this property associative symmetric polynomials, which are characterized by the following theorem. Since the original paper only gives a brief explanation, we give detailed proof in Appendix A.3.

Theorem 2 (Characterization of Associative Symmetric Polynomials, Commutative Case of (Yoshida 1963)). An associative symmetric polynomial of x and y is one of the following three forms:

$$x * y = \begin{cases} \alpha \\ \alpha + x + y \\ \frac{\beta(\beta - 1)}{\gamma} + \beta(x + y) + \gamma xy \quad (\gamma \neq 0), \end{cases}$$
 (15)

where α, β, γ are coefficients

By applying this theorem to Proposition 2 for \mathcal{X} with elementwise product and division, we obtain the following three kinds of Abelian semigroup operations:

$$\boldsymbol{x} \circ \boldsymbol{y} = \begin{cases} \rho^{-1}(\boldsymbol{\alpha}) & (16) \\ \rho^{-1}(\rho(\boldsymbol{x}) + \rho(\boldsymbol{y}) + \boldsymbol{\alpha}) & (17) \\ \rho^{-1}(\boldsymbol{\beta} \otimes (\boldsymbol{\beta} - \boldsymbol{1}) \oslash \boldsymbol{\gamma} + \boldsymbol{\beta} \otimes (\rho(\boldsymbol{x}) + \rho(\boldsymbol{y})) & +\boldsymbol{\gamma} \otimes \rho(\boldsymbol{x}) \otimes \rho(\boldsymbol{y})), \end{cases}$$
(18)

where $\rho: \mathcal{X} \to \mathcal{X}$ is an invertible function and $\alpha, \beta, \gamma \in \mathcal{X}$ are parameters (γ is nonzero for all elements in Equation 18). Equation 16 is a constant case, on which we do not put a focus due to its trivialness. Equation 17 forms a group where $e = \rho^{-1}(-\alpha)$, $x^{-1} = \rho^{-1}(-\rho(x) - 2\alpha)$. It can be expressed by the Abelian group network with $\phi(x) = \rho(x) + \alpha$ and $\phi^{-1}(x) = \rho^{-1}(x - \alpha)$ in Equation 9. Equation 18 is a semigroup but not a group. Just using this equation is fine, but we propose a simpler form, as the Abelian semigroup network:

$$\boldsymbol{x} \circ \boldsymbol{y} = \phi^{-1}(\phi(\boldsymbol{x}) \otimes \phi(\boldsymbol{y})), \tag{19}$$

where $\phi: \mathcal{X} \to \mathcal{X}$ is a trainable invertible function typically modeled by an invertible neural network. This is a special case of Equation 18 when $\beta = 0, \gamma = 1$ and therefore is a semigroup. Conversely, the Abelian semigroup network can express Equation 18 by

$$\phi(\mathbf{x}) = \gamma \otimes \rho(\mathbf{x}) + \beta, \ \phi^{-1}(\mathbf{x}) = \rho^{-1}((\mathbf{x} - \beta) \otimes \gamma).$$
 (20)

Moreover, the Abelian semigroup network can approximate the Abelian group network: $\phi'^{-1}(\phi'(\boldsymbol{x})+\phi'(\boldsymbol{y}))$. Let $\mathcal{X}_{>0}=\mathbb{R}^d_{>0}$, where $\mathcal{X}=\mathbb{R}^d$. One construction is approximating a bijective function $\pi:\mathcal{X}\to\mathcal{X}_{>0}$,

$$\pi(\mathbf{x}) = \exp(\phi'(\mathbf{x})), \ \pi^{-1}(\mathbf{x}) = \phi'^{-1}(\log(\mathbf{x}))$$
 (21)

by ϕ , where exp and log act elementwise. This is possible in any compact subset of \mathcal{X} . From the previous discussions so far, the Abelian semigroup network can approximate any binary operation which is homeomorphic to an associative symmetric polynomial. We confirm this fact in the experiments.

3.4 Multiset Architecture

So far, we proposed the binary operation architecture of the Abelian group network and Abelian semigroup network represented by Equation 9 and 19. respectively. By calculating Equation 8, we can write the two models for multiset input $X = \{x_1, \dots x_n\} \in \mathcal{X}$ in simple forms:

$$f(\mathbf{X}) = \phi^{-1} \left(\sum_{\mathbf{x} \in \mathbf{Y}} \phi(\mathbf{x}) \right), \tag{22}$$

$$f(\mathbf{X}) = \phi^{-1}(\phi(\mathbf{x}_1) \otimes \cdots \otimes \phi(\mathbf{x}_n)), \tag{23}$$

where the invertible function $\phi: \mathcal{X} \to \mathcal{X}$ is typically modeled by an invertible neural network. We can train this network by usual deep learning strategies. e.g., minimizing a loss function with minibatch stochastic gradiant descent from dataset $\{(\boldsymbol{X}_i, \boldsymbol{y}_i)\}_{i=1}^N$, where $\boldsymbol{X}_i \in \mathbb{N}^{\mathcal{X}}$ and $\boldsymbol{y}_i \in \mathcal{X}$.

Now, we consider the size-generalization ability of the multiset architectures. An intuitive explanation is as follows. If trained only on multisets of two elements, our models can learn the correct binary operation. Therefore, they generalize to multisets of larger size. For the Abelian group network, since the error bound for small multiset propagates in the form of the sum, we can derive the following theorem.

Theorem 3 (Size Generalization of Abelian Group Networks). Let $f^* : \mathbb{N}^{\mathcal{X}} \to \mathbb{N}^{\mathcal{X}}$ \mathcal{X} be a target function expressed by a composition of Abelian semigroup (\mathcal{X}, \circ) : $f^*(X) = \bigcup_{x \in X} x$. Let $f: \mathbb{N}^{\mathcal{X}} \to \mathcal{X}$ be a multiset architecture of the Abelian group network: $f(X) = \phi^{-1} \left(\sum_{x \in X} \phi(x) \right)$. When

$$\phi^{-1}\left(\sum_{x\in X}\phi(x)\right)$$
. When

$$||f(\boldsymbol{X}) - f^*(\boldsymbol{X})|| < \epsilon \tag{24}$$

holds for any $X \in \mathbb{N}^{\mathcal{X}}$ whose size is smaller than $a \geq 2$, then

$$||f(\boldsymbol{X}) - f^*(\boldsymbol{X})|| < \frac{\epsilon \left((aK_1K_2)^{\lceil \log_a b \rceil} - 1 \right)}{aK_1K_2 - 1}$$
(25)

holds for any $X (\in \mathbb{N}^{\mathcal{X}})$ whose size is $b (\geq a)$, under the condition that the Lipschitz constants of ϕ and ϕ^{-1} are K_1 and K_2 , respectively.

Appendix A.4 provides the proof. For the Abelian semigroup network, the error bound for small multiset propagates in the form of the product with the values $\phi(x_i)$, which prevents us from inducing the bound like above. However, it still has the size-generalization ability in most real applications where the values are not too large. We confirm this by an experiment in Section 4.2.

Experiments 4

In this section, we describe two experiments on the effectiveness of the proposed architectures. First, we check the size generalization of our models on synthetic data. Next, we present a real-world problem that the binary operation architecture of the Abelian group network is useful. We train word analogy functions over the fixed vectors of word2vec.

4.1 Common Settings

We implemented the neural networks in the PyTorch framework (Paszke et al. 2019) and optimized them using the Adam algorithm (Kingma and Ba 2015). The hyperparameters for each model in each problem were tuned with validation datasets using the Bayesian optimization of the Optuna framework (Akiba et al. 2019). The experiments were run on Intel Xeon E5-2695 v4 with NVIDIA Tesla P100 GPU. See Appendix B for the detailed settings, such as the model architecture and the range of hyperparameters.

4.2 Learning Synthetic Data

To check the size generalization over semigroup and group operations on multisets, we trained the models on synthetic data. The binary operation forms of the examined functions are $x \circ y = x + y, x + y + 1, \sqrt[3]{x^3 + y^3}$ (group cases) and $x \circ y = xy, x + y + \frac{xy}{2}$ (semigroup cases).

Setup For the single-dimensional invertible neural network of the Abelian group network and Abelian semigroup network, we used monotonic networks (Sill 1997). We tuned the hyperparameters, the number of groups and the number of units for each group. As a baseline, we used DeepSets (Zaheer et al. 2017), one of the most popular models for (multi)set learning. It incorporates two multilayer perceptrons (MLP). We used the same number of hidden layers for the two MLPs and tuned the hyperparameters, the number of layers in each MLP, the middle dimension, and the hidden dimension. Each model was trained to minimize the mean squared error on a training set.

Data Generation As training data, we generated 500 multisets of size $\{2,3,4\}$ (chosen uniformly random). All the elements were single-dimensional and selected uniformly at random from [-5.0,5.0]. A validation data of 100 multisets were generated from the same distribution. We prepared two kinds of test data. One consisted of 100 multisets drawn from the same distribution as the training and validation data, which we refer to by *small*. To see the size-generalization ability, the other consisted of 100 multisets of size $\{10,11,12\}$ (chosen uniformly at random) with the same element distribution, which we refer to by *large*.

Results Table 2 summarizes the results. For the group functions, all models including the Abelian semigroup network performed well. This is consistent with the fact that group operations can be approximated by the Abelian semigroup network, as discussed in Section 3.3. While the Abelian group network was better on the other two cases, DeepSets outperformed the Abelian group network

Table 2: Mean squared error comparison between the models for each function. The upper three operations are groups and the lower two equations are semigroups. Square root of the values are presented. Smaller is better.

$x \circ y$		DeepSets	AGN	ASN
x+y	small	0.00226	3.63e-7	0.0832
	large	0.908	0.0366	0.309
x+y+1	small	0.00772	4.17e-7	0.136
	large	0.0335	0.0132	0.956
$\sqrt[3]{x^3 + y^3}$	small	0.0844	0.284	0.427
	large	0.229	0.636	1.26
\overline{xy}	small	13.0	36.7	0.00000295
	large	28500	28390	31.5
$x+y+\frac{xy}{2}$	small	0.965	7.08	0.000660
	large	194	193	1.22

on $\sqrt[3]{x^3+y^3}$. This is possibly due to the optimization of MLPs in DeepSets being easier than monotonic networks in the Abelian group network and Abelian semigroup network. Invertible neural networks for the single-dimensional case that are easy to optimize are important for future work. For the semigroup operations, as well as DeepSets, the Abelian group network did not work well. This is reasonable because these semigroup operations can not be expressed by the Abelian group network.

On the size generalization, although DeepSets worked fairly well, our models worked better. For example, the Abelian semigroup network was better than DeepSets on *large* of x + y despite being worse on *small*; The Abelian group network had similar results on xy and $x + y + \frac{xy}{2}$.

4.3 Word Analogies

The vector representations of words by word2vec (Mikolov, K. Chen, et al. 2013; Mikolov, Sutskever, et al. 2013) trained only on large unlabeled text data are known to capture linear regularities between words. For example, vec("king") – vec("man") + vec("woman") results in the most similar vector to vec("queen"). Formally, for predicting a word d in a relation a:b=c:d, the word with the most similar vector to b-a+c (we denote the corresponding vector for each word by using a bold symbol) is selected in terms of the cosine similarity:

$$\cos(\mathbf{v_1}, \mathbf{v_2}) = \frac{\mathbf{v_1} \cdot \mathbf{v_2}}{\|\mathbf{v_1}\| \|\mathbf{v_2}\|}.$$
 (26)

Usually, the words a, b, c are excluded from the candidate vocabulary, under the assumption that a common word does not appear in one analogy example. Although this assumption is reasonable in many cases, it prevents us from solving certain problems such as a past tense verb analogy "do": "did" = "split": "split"

or a plural noun analogy "apple": "apples" = "deer": "deer". On the other hand, if we do not exclude the words a,b,c from the candidates, word2vec suffers from severe performance degradation e.g., falling from 73.59% to 20.64% in our preliminary experiment on the Google analogy test set. This is due to the nature of the word2vec algorithm: the result of the simple arithmetic calculation b-a+c has a high probability of being close to b or c in the cosine similarity, especially in a high dimensional space. One approach to mitigate this issue is to use richer functions than addition and subtraction. We propose to model a word analogy function by $b \circ a^{-1} \circ c$ where \circ is a group. Then the original calculation b-a+c can be seen as a special case when $\circ = +$. In this experiment, we trained the Abelian group network from labeled dataset and compared it with the original word2vec and another learning-based approach.

Table 3: Accuracy on bigger analogy test set when we did not exclude a, b, c from the candidates.

	num	WV	WV + MLP	WV + AGN
Overall	3314	177~(5.34%)	565 (17.05%)	$690\ (20.82\%)$
Inflectional	900	100 (11.11%)	317 (35.22%)	435~(48.33%)
Derivational	882	4(0.45%)	15 (1.70%)	20~(2.27%)
Lexicographic	632	52 (8.23%)	154 (24.37%)	$172\ (27.22\%)$
Encyclopedic	900	$21\ (2.33\%)$	79 (8.78%)	63 (7.00%)

Table 4: Accuracy on bigger analogy test set when we excluded a, b, c from the candidates.

	num	WV	WV + MLP	WV + AGN
Overall	3314	864 (26.07%)	569 (17.17%)	$1065\ (32.14\%)$
Inflectional	900	614 (68.22%)	324 (36.00%)	656~(72.89%)
Derivational	882	$103\ (11.68\%)$	17 (1.93%)	98 (11.11%)
Lexicographic	632	83 (13.13%)	151 (23.89%)	205~(32.44%)
Encyclopedic	900	64 (7.11%)	77 (8.56%)	$106\ (11.78\%)$

Word Embedding We used a 300-dimensional word2vec model for 3 billion words trained on Google News corpus of about 100 billion words 1 . We normalized each word embedding by L^{2} norm, following the implementation of the Gensim framework (Řehůřek and Sojka 2010).

Word Analogy Models We compared three different models for a word analogy function $f: \mathbb{R}^{300} \times \mathbb{R}^{300} \times \mathbb{R}^{300} \to \mathbb{R}^{300}$ that takes the vectors of words

¹https://code.google.com/archive/p/word2vec/

a, b, c and predicts the vector of a word d. In the original word2vec,

$$f(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) = \boldsymbol{b} - \boldsymbol{a} + \boldsymbol{c}. \tag{27}$$

As a baseline, we prepared a learning algorithm based on a multilayer perceptron, which we denote by WV + MLP:

$$f(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) = \text{MLP}(\boldsymbol{b} - \boldsymbol{a} + \boldsymbol{c}), \tag{28}$$

where we train MLP : $\mathbb{R}^{300} \to \mathbb{R}^{300}$. In the proposed method (WV + AGN), f is modeled as follows:

$$f(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) = \boldsymbol{b} \circ \boldsymbol{a}^{-1} \circ \boldsymbol{c}$$

= $\phi^{-1}(\phi(\boldsymbol{b} - \boldsymbol{a} + \boldsymbol{c})).$ (29)

For the invertible neural network $\phi: \mathbb{R}^{300} \to \mathbb{R}^{300}$, we adopted the Glow architecture (Kingma and Dhariwal 2018).

Setup For WV + MLP and WV + AGN, we minimized the loss function:

$$loss_f(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{d}) = -cos(f(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}), \boldsymbol{d}), \tag{30}$$

on the training set. We measured the accuracy on the test set by calculating the most similar vector to the model output for each word:

$$\underset{\boldsymbol{d} \in \mathcal{V}}{\arg \max} \cos(f(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}), \boldsymbol{d}), \tag{31}$$

where \mathcal{V} is the set of all word embeddings in the word2vec model. For reference, we also tested the case where we removed the words a, b, c from the candidates:

$$\underset{\boldsymbol{d} \in \mathcal{V} \setminus \{a,b,c\}}{\arg \max} \cos(f(\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}),\boldsymbol{d}), \tag{32}$$

Datasets The bigger analogy test set (BATS) (Rogers, Drozd, and Matsuoka 2016) consists of 4 categories, each of which has 10 smaller subcategories of 50 unique relations. We split the bigger analogy test set into a training set (60%), a validation set (20%), and a test set (20%). First, for each subcategory, we extracted the pairs included in the word2vec vocabularies and randomly split them into the three sets by each ratio. Then for each set, we generated all the combinations of the pairs for each subcategory and concatenated them among all subcategories. Some relations contain multiple acceptable candidates, such as mammal and canine for hypernyms of dog. We used the first candidate for training and accepted any for the test. Table 6 in Appendix B.2 summarizes the explanation and the number of extracted pairs for all subcategories. Also, we conducted a transfer experiment to the Google analogy test set (Mikolov, K. Chen, et al. 2013) in Appendix B.2.

Results Table 3 summarizes the results on the bigger analogy test set when we used the whole vocabulary. The proposed method outperformed WV + MLP in all categories except Encyclopedic. The accuracy comparison when we excluded a,b,c is shown in Table 4. In this setting, WV + MLP performed poorly compared even with the original WV. On the other hand, the proposed method still worked better than WV. We show the full results for each subcategory of the bigger analogy test set in Table 10 and 11 in Appendix B.2. We explain the results on transferring test to the Google analogy test set in Appendix B.2. Overall, we can conclude that while the naive learning approach overfitted to the certain dataset and evaluation criteria, the inductive biases incorporated in the Abelian group network successfully prevented the model from overfitting.

5 Conclusion and Future Work

In this work, we proposed two novel neural network architectures, the Abelian group network and Abelian semigroup network, and showed their theoretical properties. To investigate the effectiveness of our models, we conducted two experiments. The first experiment on synthetic data validated our theories on expressive power and size generalization. In the second experiment, we presented that the binary operation version of the Abelian group network is useful for modeling a word analogy function. Our method improved the performance of word2vec, especially when we searched the whole vocabulary for the candidates.

One of the technical obstacles facing our models when it comes to real-world (multi)set problems is that the dimensions of each element of the input (multi)set and the output should be equal. By direct implementation, our methods can not be used for (multi)set classification problems such as document-category classification, where we need to output a vector of label-number dimension from a (multi)set of high-dimensional vectors. This issue can be mitigated by using some other techniques such as label embedding (Weston, S. Bengio, and Usunier 2011). We believe our models with a theoretical size-generalization guarantee give a new insight into the field of (multi)set learning.

Further, modeling a (multi)set function is a fundamental setting that appears not only in direct real-world applications but also as a component of more complex objects such as graphs (Xu, Hu, et al. 2019). Constructing size-generalizable graph neural networks by using our models as building blocks remains as future research.

Finally, let us summarize some open problems. Although the Abelian group network is universal, the expressive power of the Abelian semigroup network is unknown as yet. Also, the theoretical reason behind the good size-generalization performance of DeepSets in the experiment on learning synthetic data remains a topic of investigation.

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A Proofs

A.1 Proof of Proposition 2

Proof. Associativity:

$$(\boldsymbol{x} \circ \boldsymbol{y}) \circ \boldsymbol{z} = \rho^{-1}(\rho(\rho^{-1}(\rho(\boldsymbol{x}) * \rho(\boldsymbol{y}))) * \rho(\boldsymbol{z}))$$

$$= \rho^{-1}((\rho(\boldsymbol{x}) * \rho(\boldsymbol{y})) * \rho(\boldsymbol{z}))$$

$$= \rho^{-1}(\rho(\boldsymbol{x}) * (\rho(\boldsymbol{y}) * \rho(\boldsymbol{z}))) \; (\because \text{Associativity of } *)$$

$$= \rho^{-1}(\rho(\boldsymbol{x}) * \rho(\rho^{-1}(\rho(\boldsymbol{y}) * \rho(\boldsymbol{z}))))$$

$$= \boldsymbol{x} \circ (\boldsymbol{y} \circ \boldsymbol{z}).$$
(33)

Commutativity:

$$\mathbf{y} \circ \mathbf{x} = \rho^{-1}(\rho(\mathbf{y}) * \rho(\mathbf{x}))$$

$$= \rho^{-1}(\rho(\mathbf{x}) * \rho(\mathbf{y})) \ (\because \text{Commutativity of } *)$$

$$= \mathbf{x} \circ \mathbf{y}.$$
(34)

A.2 Proof of Theorem 1

First, we review the concept of the Lie group. A Lie group is a group over a manifold in which the group operation $(x,y) \mapsto x \circ y$ and the inverse function $x \mapsto x^{-1}$ are both differentiable. An Abelian Lie group is a Lie group that satisfies commutativity. The real numbers \mathbb{R} with the addition + forms a Lie group, which we denote by $(\mathbb{R}, +)$. Also, the torus $\mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$ with the addition + modulo $2\pi\mathbb{Z}$ forms a Lie group, which we denote by $(\mathbb{T}, +)$. It is known that any connected Abelian Lie group is isomorphic to $(\mathbb{R}, +)^k \times (\mathbb{T}, +)^h$ for some $k, h \in \mathbb{N}$ (Section 4.4.2 of (Procesi 2007)).

Now, we give the proof of Theorem 1.

Proof. We use the fact that any connected Abelian Lie group is isomorphic to $(\mathbb{R},+)^k \times (\mathbb{T},+)^h$ for some $k,h \in \mathbb{N}$. The Abelian Lie group over \mathcal{X} is the special cases of this and therefore any \circ can be represented as

$$\boldsymbol{x} \circ \boldsymbol{y} = \pi^{-1}(\pi(\boldsymbol{x}) + \pi(\boldsymbol{y})), \tag{35}$$

where $\pi: \mathcal{X} \to \mathcal{X}$ is a homeomorphic function in terms of Lie groups, i.e., $\pi(\cdot)$ and $\pi^{-1}(\cdot)$ are analytic. Take any $\epsilon > 0$ and a compact subset $\mathcal{K} \subset \mathcal{X}$. We denote the image of $\mathcal{K} \times \mathcal{K}$ through the function $(\boldsymbol{x}, \boldsymbol{y}) \mapsto \pi(\boldsymbol{x}) + \pi(\boldsymbol{y})$ by $\mathcal{S}' = \{\pi(\boldsymbol{x}) + \pi(\boldsymbol{y}) \mid \boldsymbol{x}, \boldsymbol{y} \in \mathcal{K}\}$. Let

$$S = \{ s \mid \exists s' \in S' \ s.t. \ ||s - s'|| \le 2\epsilon \}$$
(36)

and

$$\mathcal{K}' = \mathcal{K} \cup \pi^{-1}(\mathcal{S}). \tag{37}$$

Then, we have a Lipschitz constant L > 0 of π^{-1} over S since π^{-1} is continuous and S is compact. Also, from the universality of invertible neural networks (Teshima et al. 2020) for the compact set K', there exists an invertible neural network $\phi: \mathcal{X} \to \mathcal{X}$ such that for any $\mathbf{x} \in K'$

$$\|\pi(\boldsymbol{x}) - \phi(\boldsymbol{x})\| < \frac{\epsilon}{2L+1} \tag{38}$$

and for any $x' \in \pi(\mathcal{K}')$

$$\|\pi^{-1}(\mathbf{x}') - \phi^{-1}(\mathbf{x}')\| < \frac{\epsilon}{2L+1}.$$
 (39)

Then, for any $x, y \in \mathcal{K}$, $\phi(x) + \phi(y) \in \mathcal{S}(\subset \pi(\mathcal{K}'))$ because

$$\|(\pi(\boldsymbol{x}) + \pi(\boldsymbol{y})) - (\phi(\boldsymbol{x}) + \phi(\boldsymbol{y}))\| \le \|\pi(\boldsymbol{x}) - \phi(\boldsymbol{x})\| + \|\pi(\boldsymbol{y}) + \phi(\boldsymbol{y})\|$$

$$< \frac{2\epsilon}{2L+1}$$

$$< 2\epsilon.$$
(40)

Therefore, for any $x, y \in \mathcal{X}$, we have from the Lipshitz continuity of π^{-1}

$$\|\pi^{-1}(\pi(x) + \pi(y)) - \pi^{-1}(\phi(x) + \phi(y))\| \le L\|(\pi(x) + \pi(y)) - (\phi(x) + \phi(y))\|$$

$$< L \cdot \frac{2\epsilon}{2L+1}$$

$$= \frac{2L\epsilon}{2L+1}$$
(41)

and from Equation 39

$$\|\pi^{-1}(\phi(x) + \phi(y)) - \phi^{-1}(\phi(x) + \phi(y))\| < \frac{\epsilon}{2L + 1}.$$
 (42)

From Equation 41 and 42, for any $x, y \in \mathcal{K}$, we obtain

$$\|(\boldsymbol{x} \circ \boldsymbol{y}) - (\boldsymbol{x} * \boldsymbol{y})\| = \|\pi^{-1}(\pi(\boldsymbol{x}) + \pi(\boldsymbol{y})) - \phi^{-1}(\phi(\boldsymbol{x}) + \phi(\boldsymbol{y}))\|$$

$$\leq \|\pi^{-1}(\pi(\boldsymbol{x}) + \pi(\boldsymbol{y})) - \pi^{-1}(\phi(\boldsymbol{x}) + \phi(\boldsymbol{y}))\|$$

$$+ \|\pi^{-1}(\phi(\boldsymbol{x}) + \phi(\boldsymbol{y})) - \phi^{-1}(\phi(\boldsymbol{x}) + \phi(\boldsymbol{y}))\|$$

$$\leq \frac{2L\epsilon}{2L+1} + \frac{\epsilon}{2L+1}$$

$$= \epsilon$$
(43)

This concludes that Abelian group networks are universal.

A.3 Proof of Theorem 2

Proof. First, we prove that associative polynomials are at most first-order for each variable. Assume that we have a n-order $(n \ge 2)$ associative polynomial

$$x * y = \sum_{i=0}^{n} \sum_{j=0}^{n} \alpha_{i,j} x^{i} y^{j},$$
(44)

where $\alpha_{i,j} \in \mathbb{R}$ for $0 \le i, j \le n$. Then, we have

$$(x*y)*z = \sum_{i=0}^{n} \sum_{j=0}^{n} \alpha_{i,j} (\sum_{k=0}^{n} \sum_{l=0}^{n} \alpha_{k,l} x^{k} y^{l})^{i} z^{j}$$

$$(45)$$

and

$$x * (y * z) = \sum_{i=0}^{n} \sum_{j=0}^{n} \alpha_{i,j} x^{i} (\sum_{k=0}^{n} \sum_{l=0}^{n} \alpha_{k,l} y^{k} z^{l})^{i}.$$
 (46)

Since * is associative, these two must form an identity. By comparing a coefficient of x^{n^2} , we obtain

$$\sum_{j=0}^{n} \alpha_{n,j} \left(\sum_{l=0}^{n} \alpha_{n,l} y^{l} \right)^{n} z^{j} = 0.$$
 (47)

If we have $0 \le j' \le n$ such that $\alpha_{n,j'} \ne 0$, from the coefficient of $z^{j'}$,

$$\left(\sum_{l=0}^{n} \alpha_{n,l} y^l\right)^n = 0. \tag{48}$$

Recursively, we get $\alpha_{n,0} = \alpha_{n,1} = \cdots = \alpha_{n,n} = 0$, which leads to contradiction. Therefore, we now have

$$\alpha_{n,0} = \alpha_{n,1} = \dots = \alpha_{n,n} = 0. \tag{49}$$

In the same way, we can also prove

$$\alpha_{0,n} = \alpha_{1,n} = \dots = \alpha_{n,n} = 0. \tag{50}$$

From Equation 49 and 50 for $n \ge 2$, now we know that associative polynomials are at most first-order for each variable. Therefore, symmetric associative polynomials have the form:

$$x * y = \alpha + \beta(x+y) + \gamma xy. \tag{51}$$

Then we have

$$(x*y)*z = \alpha + \beta((\alpha + \beta(x+y) + \gamma xy) + z) + \gamma(\alpha + \beta(x+y) + \gamma xy)z$$
 (52)

and

$$x * (y * z) = \alpha + \beta((\alpha + \beta(x+y) + \gamma xy) + z) + \gamma(\alpha + \beta(x+y) + \gamma xy)z.$$
 (53)

By solving this identity, we obtain

$$\alpha \gamma = \beta(\beta - 1). \tag{54}$$

This condition is equivalent to the associativity of *. It decomposes into three cases: $(\gamma = 0, \beta = 0)$, $(\gamma = 0, \beta = 1)$, and $\gamma \neq 0$. For each case, we obtain

$$x * y = \begin{cases} \alpha \\ \alpha + x + y \\ \frac{\beta(\beta - 1)}{\gamma} + \beta(x + y) + \gamma xy \quad (\gamma \neq 0). \end{cases}$$
 (55)

A.4 Proof of Theorem 3

Proof. We prove that for any $X \in \mathbb{N}^{\mathcal{X}}$ of size smaller than $b \geq a$,

$$||f(\boldsymbol{X}) - f^*(\boldsymbol{X})|| < \frac{\epsilon \left((aK_1K_2)^{\lceil \log_a b \rceil} - 1 \right)}{aK_1K_2 - 1}$$
(56)

by induction on size b. Note that $K_1K_2 > 1$ because they are the Lipschitz constants of inverse functions.

Base Case When b = a, Inequality 56 holds.

Inductive Step We assume Inequality 56 holds for size b' = 1, ..., b-1. We divide X of size b into balanced a subsets $X_1, ..., X_a$ so that $X = X_1 + ... X_a$ and each $|X_i| \leq \lceil \frac{b}{a} \rceil$. Then,

$$||f(X) - f^{*}(X)|| = \left\| \phi^{-1} \left(\sum_{x \in X} \phi(x) \right) - \bigcup_{x \in X} x \right\|$$

$$= \left\| \phi^{-1} \left(\sum_{i=1}^{a} \sum_{x \in X_{i}} \phi(x) \right) - \bigcup_{i=1}^{a} \left(\bigcup_{x \in X_{i}} x \right) \right\|$$

$$= \left\| \phi^{-1} \left(\sum_{i=1}^{a} \phi(f(X_{i})) \right) - f^{*} \left(\left\{ f^{*}(X_{1}), \dots, f^{*}(X_{a}) \right\} \right) \right\|$$

$$\leq \left\| \phi^{-1} \left(\sum_{i=1}^{a} \phi(f(X_{i})) \right) - \phi^{-1} \left(\sum_{i=1}^{a} \phi(f^{*}(X_{i})) \right) \right\| +$$

$$\left\| \phi^{-1} \left(\sum_{i=1}^{a} \phi(f^{*}(X_{i})) \right) - f^{*} \left(\left\{ f^{*}(X_{1}), \dots, f^{*}(X_{a}) \right\} \right) \right\|$$

$$\leq K_{2} \left\| \sum_{i=1}^{a} \phi(f(X_{i})) - \phi(f^{*}(X_{i})) \right\| +$$

$$\left\| f \left(\left\{ f^{*}(X_{1}), \dots, f^{*}(X_{a}) \right\} \right) - f^{*} \left(\left\{ f^{*}(X_{1}), \dots, f^{*}(X_{a}) \right\} \right) \right\|$$

$$< K_{2} \left(\sum_{i=1}^{a} \left\| \phi(f(X_{i})) - \phi(f^{*}(X_{i})) \right\| \right) + \epsilon$$

$$\leq K_{2} \left(\sum_{i=1}^{a} K_{1} \left\| f(X_{i}) - f^{*}(X_{i}) \right\| \right) + \epsilon$$

$$= K_{1}K_{2} \left(\sum_{i=1}^{a} \left\| f(X_{i}) - f^{*}(X_{i}) \right\| \right) + \epsilon.$$

$$(57)$$

From the assumption on size $\lceil \frac{b}{a} \rceil$, we obtain

$$||f(\mathbf{X}) - f^{*}(\mathbf{X})|| < aK_{1}K_{2} \cdot \frac{\epsilon((aK_{1}K_{2})^{\lceil \log_{a} \lceil \frac{b}{a} \rceil \rceil} - 1)}{aK_{1}K_{2} - 1} + \epsilon$$

$$< aK_{1}K_{2} \cdot \frac{\epsilon((aK_{1}K_{2})^{\lceil \log_{a} \frac{b}{a} \rceil} - 1)}{aK_{1}K_{2} - 1} + \epsilon$$

$$< \frac{\epsilon((aK_{1}K_{2})^{\lceil \log_{a} b \rceil} - 1)}{aK_{1}K_{2} - 1},$$
(58)

which establishes the inductive step.

B Experimental Details

Here, we explain the detailed setting and further discussion of the experiments that we did not cover in the main part.

B.1 Learning Synthetic Data

Model Architecture For the implementation of the monotonic networks, we basically followed the Equation 5, except that we added a coefficient term $s \in \mathbb{R}$ which automatically learn the sign of the weights:

$$f(x) = \min_{1 \le k \le K} \max_{1 \le j \le J_k} s \cdot \exp(\tilde{w}^{(k,j)}) \cdot x + b^{(k,j)}.$$
 (59)

Hyperparameters All networks were trained by the Adam algorithm of $lr = 10^{-3}$, beta = (0.9, 0.999) for 1000 epochs with the batch size of 32. Hyperparameters of each model were tuned with the validation dataset using the Optuna framework for each function. For DeepSets, the number of layers for each MLP was selected from [2,8] and the middle dimension and hidden dimension were selected from [2,32]. For the Abelian group network and Abelian semigroup network, the number of groups and the number of units in each group were selected from [2,32].

B.2 Word Analogies

Model architecture For the invertible neural network for the Abelian group network and Abelian semigroup network, we implemented Glow architectures based on the FrEIA framework ². We stacked Glow coupling layers and random permutation layers of the dimensions in turn. For each Glow coupling layer, we used three layer feedforward neural networks with a hyperparameter of hidden_dim.

²https://github.com/VLL-HD/FrEIA

Hyperparameters All networks were trained by the Adam algorithm of $lr = 10^{-3}$, beta = (0.9, 0.999) for 100 epochs with the batch size of 32. The hyperparameters of each model were tuned with the validation dataset using the Optuna framework. For MLP, the number of layers was selected from [2, 6] and the hidden dimension was selected from [8, 256]. For the Abelian group network, the number of layers was selected from [2, 6] and the hidden dimension was selected from [8, 256]. Weight_decay was selected from $[0, 10^{-3}]$ for all models.

Table 5 summarizes the selected hyperparameters for each model.

Table 5: Selected hyperparameters in word analogy task.

	layer_num	hidden_dim	weight_decay
W2V	-	-	-
W2V + MLP	4	223	6.43e-4
W2V + AGN	5	151	1.60e-4

Transfer Test Google analogy test set (Mikolov, K. Chen, et al. 2013) includes 19,544 question pairs (8,869 semantic and 10,675 syntactic). The semantic questions are composed of five categories: common capital city, all capital cities, currency, city-in-state, and man-woman. The syntactic questions are composed of 9 categories: adjective to adverb, opposite, comparative, superlative, present participle, nationality adjective, past tense, plural nouns, and plural verbs. Table 7 shows the detailed explanation of the Google analogy test set. All the words were included in the word2vec vocabulary.

To test the transferability to another dataset, we measured the accuracy on the Google analogy test set. We compared the models trained on the bigger analogy test set (Section 4.3). Table 8 summarizes the full results on the Google analogy test set when we used the whole vocabulary as the candidates. The proposed model trained on the bigger analogy test set successfully transferred to the Google analogy test set with the best accuracy on 11 subcategories out of 14. On the other hand, the performance of WV + MLP significantly deteriorated, especially 0% accuracy in 4 subcategories out of 5 in the semantics task. Table 9 shows the results on the Google analogy test set when we excluded a,b,c from the candidates. In this case, the original WV performed the best. This is probably because the word2vec model was highly tuned for the Google analogy test set for this evaluation method.

Detailed Results Table 10 and 11 summarizes the full results for each subcategory in the bigger analogy test set. We can see the performance improvement of the proposed method in most subcategories.

Table 6: Detailed explanation of bigger analogy test set. *pair* refers to the whole relation size and *used* refers to the number included in the word2vec model.

	used refers to the number in			
category	subcategory	example	pair	used
Inflectional	I01 noun - plural_reg	album:albums	50	50
Inflectional	I02 noun - plural_irreg	ability:abilities	50	48
Inflectional	I03 adj - comparative	angry:angrier	50	49
Inflectional	I04 adj - superlative	able:ablest	50	49
Inflectional	$I05 \text{ verb_inf} - 3pSg$	accept:accepts	50	50
Inflectional	I06 verb_inf - Ving	achieve:achieving	50	49
Inflectional	I07 verb_inf - Ved	accept:accepted	50	50
Inflectional	$I08 \text{ verb_Ving - } 3pSg$	adding:adds	50	50
Inflectional	I09 verb_Ving - Ved	adding:added	50	50
Inflectional	I10 verb $_3$ pSg - Ved	adds:added	50	50
Derivational	D01 noun+less_reg	arm:armless	50	48
Derivational	D02 un+adj_reg	able:unable	50	49
Derivational	$D03 adj+ly_reg$	according:accordingl	50	49
Derivational	D04 over+adj_reg	ambitious:overambiti	50	50
Derivational	$D05 \text{ adj+ness_reg}$	amazing:amazingness	50	45
Derivational	D06 re+verb_reg	acquire:reacquire	50	48
Derivational	D07 verb+able_reg	accept:acceptable	50	49
Derivational	D08 verb+er_irreg	achieve:achiever	50	49
Derivational	D09 verb+tion_irreg	accuse:accusation	50	48
Derivational	D10 verb+ment_irreg	accomplish:accomplis	50	47
Encyclopedic	E01 country - capital	abuja:nigeria	50	37
Encyclopedic	E02 country - language	andorra:catalan	50	36
Encyclopedic	E03 UK_city - county	aberdeen:aberdeenshi	50	24
Encyclopedic	E04 name - nationality	aristotle:greek	50	23
Encyclopedic	E05 name - occupation	andersen:writer/poet	50	27
Encyclopedic	E06 animal - young	ape:baby/infant	50	50
Encyclopedic	E07 animal - sound	alpaca:bray	50	50
Encyclopedic	E08 animal - shelter	ant:anthill/insectar	50	50
Encyclopedic	E09 things - color	ant:black/brown/red	50	50
Encyclopedic	E10 male - female	actor:actress	50	48
Lexicographic	L01 hypernyms - animals	allosaurus:dinosaur/	50	50
Lexicographic	L02 hypernyms - misc	armchair:chair/seat/	50	50
Lexicographic	L03 hyponyms - misc	backpack:daypack/kit	50	50
Lexicographic	L04 meronyms - substance	atmosphere:gas/oxyge	50	50
Lexicographic	L05 meronyms - member	acrobat:troupe	50	50
Lexicographic	L06 meronyms - part	academia:college/uni	50	47
Lexicographic	L07 synonyms - intensity	afraid:terrified/hor	50	50
Lexicographic	L08 synonyms - exact	airplane:aeroplane/p	50	50
Lexicographic	L09 antonyms - gradable	able:unable/incapabl	50	50
Lexicographic	L10 antonyms - binary	after:before/earlier	50	50

Table 7: Detailed explanation of Google analogy test set. num refers to the whole relation size and used refers to the number included in the word2vec $\underline{\text{model}}$.

category	subcategory	example	num	used
Semantic	capital-common-countries	Athens:Greece	506	506
Semantic	capital-world	Abuja:Nigeria	4524	4524
Semantic	currency	Algeria:dinar	866	866
Semantic	city-in-state	Chicago:Illinois	2467	2467
Semantic	family	boy:girl	506	506
Syntactic	gram1-adjective-to-adverb	amazing:amazingly	992	992
Syntactic	gram2-opposite	acceptable:unacceptable	812	812
Syntactic	gram3-comparative	bad:worse	1332	1332
Syntactic	gram4-superlative	bad:worst	1122	1122
Syntactic	gram5-present-participle	code:coding	1056	1056
Syntactic	gram6-nationality-adjective	Albania:Albanian	1599	1599
Syntactic	gram7-past-tense	dancing:danced	1560	1560
Syntactic	gram8-plural	banana:bananas	1332	1332
Syntactic	gram9-plural-verbs	decrease:decreases	870	870

Table 8: Model comparison for each subcategory of Google analogy test set when we did not excluded a, b, c from the candidates.

	num	WV	WV + MLP	WV + AGN
Overall	19544	4033 (20.64%)	1346 (6.89%)	5676~(29.04%)
Semantic	8869	1995 (22.49%)	161 (1.82%)	$2260\ (25.48\%)$
Syntactic	10675	$2038 \ (19.09\%)$	1185 (11.10%)	3416~(32.00%)
capital-c	506	225 (44.47%)	0 (0.00%)	$227\ (44.86\%)$
capital-w	4524	$1168 \ (25.82\%)$	0 (0.00%)	$1223\ (27.03\%)$
currency	866	185~(21.36%)	0 (0.00%)	119 (13.74%)
city-in-s	2467	$252\ (10.21\%)$	0 (0.00%)	350~(14.19%)
family	506	165 (32.61%)	161 (31.82%)	341~(67.39%)
gram1-adj	992	15 (1.51%)	86~(8.67%)	84 (8.47%)
$\operatorname{gram} 2$ -opp	812	14 (1.72%)	$200 \ (24.63\%)$	$235\ (28.94\%)$
gram 3- com	1332	329 (24.70%)	$242\ (18.17\%)$	713~(53.53%)
$\operatorname{gram} 4\operatorname{-sup}$	1122	$124\ (11.05\%)$	244 (21.75%)	406~(36.19%)
gram 5-pre	1056	73~(6.91%)	71 (6.72%)	160~(15.15%)
gram 6-nat	1599	1180~(73.80%)	0 (0.00%)	996~(62.29%)
$\operatorname{gram} 7$ - pas	1560	134~(8.59%)	127~(8.14%)	$353\ (22.63\%)$
gram8-plu	1332	$63 \ (4.73\%)$	82~(6.16%)	176~(13.21%)
gram9-plu	870	106 (12.18%)	133 (15.29%)	293 (33.68%)

Table 9: Model comparison for each subcategory of Google analogy test set when we excluded a,b,c from the candidates.

	num	WV	WV + MLP	WV + AGN
Overall	19544	14382 (73.59%)	1427 (7.30%)	11857 (60.67%)
Semantic	8869	$6482 \; (73.09\%)$	$163 \ (1.84\%)$	4918 (55.45%)
Syntactic	10675	7900~(74.00%)	$1264\ (11.84\%)$	6939~(65.00%)
capital-common	506	421 (83.20%)	0 (0.00%)	378 (74.70%)
capital-world	4524	$3580 \; (79.13\%)$	0 (0.00%)	2689 (59.44%)
currency	866	304~(35.10%)	0 (0.00%)	$180 \ (20.79\%)$
city-in-state	2467	1749~(70.90%)	0 (0.00%)	$1223\ (49.57\%)$
family	506	$428 \ (84.58\%)$	163 (32.21%)	448~(88.54%)
gram1-adjective	992	$283\ (28.53\%)$	93 (9.38%)	$283\ (28.53\%)$
gram2-opposite	812	347 (42.73%)	$201\ (24.75\%)$	419~(51.60%)
gram3-comparati	1332	1210~(90.84%)	$248 \ (18.62\%)$	1044~(78.38%)
gram4-superlati	1122	980~(87.34%)	246 (21.93%)	777 (69.25%)
gram 5-present-p	1056	825~(78.12%)	$78 \ (7.39\%)$	729~(69.03%)
gram6-nationali	1599	1438~(89.93%)	0 (0.00%)	$1158 \ (72.42\%)$
gram7-past-tens	1560	1029~(65.96%)	$157 \ (10.06\%)$	1061~(68.01%)
gram8-plural	1332	1197~(89.86%)	$103 \ (7.73\%)$	826 (62.01%)
gram9-plural-ve	870	591 (67.93%)	138 (15.86%)	$642 \ (73.79\%)$

Table 10: Model comparison for each subcategory of bigger analogy test set when we did not exclude a,b,c from the candidates.

	num	WV	WV + MLP	WV + AGN
I01	90	2 (2.22%)	5 (5.56%)	7 (7.78%)
I02	90	0(0.00%)	0(0.00%)	0(0.00%)
I03	90	13 (14.44%)	22 (24.44%)	41~(45.56%)
I04	90	10 (11.11%)	18 (20.00%)	39~(43.33%)
I05	90	26 (28.89%)	58 (64.44%)	60~(66.67%)
I06	90	$14 \ (15.56\%)$	$13 \ (14.44\%)$	57~(63.33%)
I07	90	3(3.33%)	54~(60.00%)	$42 \ (46.67\%)$
I08	90	$11\ (12.22\%)$	40 (44.44%)	54~(60.00%)
I09	90	8 (8.89%)	49 (54.44%)	62~(68.89%)
I10	90	$13\ (14.44\%)$	58 (64.44%)	73 (81.11%)
D01	90	0~(0.00%)	0~(0.00%)	0 (0.00%)
D02	90	0 (0.00%)	1~(1.11%)	0 (0.00%)
D03	90	1 (1.11%)	2(2.22%)	5~(5.56%)
D04	90	0~(0.00%)	0~(0.00%)	$0\;(0.00\%)$
D05	72	0 (0.00%)	2(2.78%)	5~(6.94%)
D06	90	0 (0.00%)	2~(2.22%)	0 (0.00%)
D07	90	0~(0.00%)	0~(0.00%)	0~(0.00%)
D08	90	0 (0.00%)	4~(4.44%)	0 (0.00%)
D09	90	3(3.33%)	0 (0.00%)	7~(7.78%)
D10	90	0 (0.00%)	4~(4.44%)	3 (3.33%)
E01	56	0 (0.00%)	0 (0.00%)	2~(3.57%)
E02	56	4 (7.14%)	$14 \; (25.00\%)$	4 (7.14%)
E03	20	6~(30.00%)	0 (0.00%)	3~(15.00%)
E04	20	2 (10.00%)	3 (15.00%)	4~(20.00%)
E05	30	5 (16.67%)	6~(20.00%)	5 (16.67%)
E06	90	4 (4.44%)	36 (40.00%)	42~(46.67%)
E07	90	3 (3.33%)	18~(20.00%)	7 (7.78%)
E08	90	12 (13.33%)	39 (43.33%)	56~(62.22%)
E09	90	10 (11.11%)	38~(42.22%)	35 (38.89%)
E10	90	6 (6.67%)	0 (0.00%)	14~(15.56%)
L01	90	0 (0.00%)	$52\ (57.78\%)$	38 (42.22%)
L02	90	1 (1.11%)	15~(16.67%)	8 (8.89%)
L03	90	$0\ (0.00\%)$	$0\ (0.00\%)$	$0\ (0.00\%)$
L04	90	0 (0.00%)	4 (4.44%)	4 (4.44%)
L05	90	0 (0.00%)	1 (1.11%)	0 (0.00%)
L06	90	$9\ (10.00\%)$	0 (0.00%)	6 (6.67%)
L07	90	$11\ (12.22\%)$	5 (5.56%)	7 (7.78%)
L08	90	0 (0.00%)	$0\ (0.00\%)$	0 (0.00%)
L09	90	0 (0.00%)	$2\ (2.22\%)$	0 (0.00%)
L10	90	0 (0.00%)	0 (0.00%)	0 (0.00%)

Table 11: Model comparison for each subcategory of bigger analogy test set when we excluded a,b,c from the candidates.

	num	WV	WV + MLP	WV + AGN
I01	90	53 (58.89%)	5 (5.56%)	55 (61.11%)
I02	90	$42\ (46.67\%)$	0 (0.00%)	30 (33.33%)
I03	90	$86 \ (95.56\%)$	22 (24.44%)	73 (81.11%)
I04	90	68~(75.56%)	18 (20.00%)	64 (71.11%)
I05	90	61~(67.78%)	58 (64.44%)	61~(67.78%)
I06	90	69~(76.67%)	$13 \ (14.44\%)$	71~(78.89%)
I07	90	52 (57.78%)	55 (61.11%)	68~(75.56%)
I08	90	56 (62.22%)	42~(46.67%)	69~(76.67%)
I09	90	58 (64.44%)	50 (55.56%)	85~(94.44%)
I10	90	69 (76.67%)	61 (67.78%)	80 (88.89%)
D01	90	0~(0.00%)	0~(0.00%)	0 (0.00%)
D02	90	3~(3.33%)	3~(3.33%)	2(2.22%)
D03	90	26~(28.89%)	2(2.22%)	$15\ (16.67\%)$
D04	90	$11\ (12.22\%)$	0 (0.00%)	3 (3.33%)
D05	72	$21\ (29.17\%)$	2(2.78%)	17 (23.61%)
D06	90	13 (14.44%)	2(2.22%)	19~(21.11%)
D07	90	1 (1.11%)	0 (0.00%)	4 (4.44%)
D08	90	1 (1.11%)	4 (4.44%)	2 (2.22%)
D09	90	21 (23.33%)	0 (0.00%)	$24\ (26.67\%)$
D10	90	6 (6.67%)	4 (4.44%)	12 (13.33%)
E01	56	18 (32.14%)	0 (0.00%)	5 (8.93%)
E02	56	0 (0.00%)	14 (25.00%)	4 (7.14%)
E03	20	0 (0.00%)	0 (0.00%)	0 (0.00%)
E04	20	0 (0.00%)	3 (15.00%)	4 (20.00%)
E05	30	0 (0.00%)	6 (20.00%)	2 (6.67%)
E06	90	5 (5.56%)	33 (36.67%)	47 (52.22%)
E07	90	3 (3.33%)	17 (18.89%)	19 (21.11%)
E08	90	2(2.22%)	40 (44.44%)	53 (58.89%)
E09	90	12 (13.33%)	38 (42.22 %) 0 (0.00%)	33 (36.67%) 38 (42.22%)
E10 L01	90	43 (47.78%) 7 (7.78%)	48 (53.33%)	51 (56.67%)
L01	90	3 (3.33%)	15 (16.67%)	17 (18.89%)
L02	90	3 (3.33%)	0 (0.00%)	2(2.22%)
L03	90	1 (1.11%)	3 (3.33%)	5 (5.56%)
L04	90	1 (1.11%)	1 (1.11%)	$1 \ (1.11\%)$
L05	90	0 (0.00%)	0 (0.00%)	1 (1.11%) $1 (1.11%)$
L07	90	12 (13.33%)	4 (4.44%)	2 (2.22%)
L08	90	27 (30.00%)	0 (0.00%)	17 (18.89%)
L09	90	2 (2.22%)	5 (5.56%)	5 (5.56%)
L10	90	8 (8.89%)	1 (1.11%)	5 (5.56%)
		` '	` /	