REPRESENTATION LEARNING WITH MULTISETS

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ABSTRACT

We study the problem of learning permutation invariant representations that can capture containment relations. We propose training a model on a novel task: predicting the size of the symmetric difference between pairs of multisets, sets which may contain multiple copies of the same object. With motivation from fuzzy set theory, we formulate both multiset representations and how to predict symmetric difference sizes given these representations. We model multiset elements as vectors on the standard simplex and multisets as the summations of such vectors, and we predict symmetric difference as the ℓ_1-distance between multiset representations. We demonstrate that our representations more effectively predict the sizes of symmetric differences than DeepSets-based approaches with unconstrained object representations. Furthermore, we demonstrate that the model learns meaningful representations, mapping objects of different classes to different standard basis vectors.

1 INTRODUCTION

Tasks for which the input is an unordered collection, i.e. a *set*, are ubiquitous and include multiple-instance learning Ilse et al. (2018), point-cloud classification Zaheer et al. (2017); Qi et al. (2017), estimating cosmological parameters Zaheer et al. (2017); Ravanbakhsh et al. (2016), collaborative filtering Hartford et al. (2018), and relation extraction Verga et al. (2017); Rossiello et al. (2019). Recent work has demonstrated the benefits of permutation invariant models that have inductive biases well aligned with the set-based input of the tasks (Ilse et al., 2018; Qi et al., 2017; Zaheer et al., 2017; Lee et al., 2019).

The the containment relationship between sets — and intersection more generally — is often considered as a measure of relatedness. For instance, when comparing the keywords for two documents, we may wish to model that $\{\texttt{currency}, \texttt{equilibrium}\}$ describes a more specific set of topics than (i.e. is "contained" in) $\{\texttt{money}, \texttt{balance}, \texttt{economics}\}$. The containment order is a natural partial order on sets. However, we are often interested not in sets, but *multisets*, which may contain multiple copies of the same object; examples include bags-of-words, geo-location data over a time period, and data in any multiple-instance learning setting (Ilse et al., 2018). The containment order can be extended to multisets. Learning to represent multisets in a way that respects this partial order is a core representation learning challenge. Note that this may require modeling not just exact containment, but relations that consider the relatedness of individual objects. We may want to learn representations of the multisets' *elements* which induce the desired multiset relations. In the aforementioned example, we may want $\texttt{money} \approx \texttt{currency}$ and $\texttt{balance} \approx \texttt{equilibrium}$.

Previous work has considered modeling hierarchical relationships or orderings between pairs of individual items (Ganea et al., 2018; Lai and Hockenmaier, 2017; Nickel and Kiela, 2017; Suzuki et al., 2019; Vendrov et al., 2015; Vilnis et al., 2018; Vilnis and McCallum, 2015; Li et al., 2019; Athiwaratkun and Wilson, 2018). However, this work does not naturally extend from representing individual items to modeling relations between multisets via the elements' learned representations. Furthermore, we may want to consider richer information about the relationship between two multisets beyond containment, such as the size of their intersection.

In this paper, we present a method for learning representations of multisets and their elements, given the relationships between pairs of multisets — in particular, we propose to use the sizes of their symmetric differences. We learn these representations with the goal of predicting the relationships between unseen pairs of multisets (whose elements may themselves have been unseen during training).

We model multiset elements as vectors on the standard simplex and multisets as the summations of such vectors, and we predict symmetric difference as the ℓ_1-distance between multiset representations. Both our representations and how we predict symmetric difference size are theoretical rooted in fuzzy set theory. We show empirically that both these aspects of our model are important to predicting symmetric difference sizes, comparing our approach to DeepSets-based approaches (Zaheer et al., 2017) with unconstrained item representations. Furthermore, we demonstrate that our model learns meaningful representations, mapping objects of different classes to different standard basis vectors.

2 Related work

2.1 Set representation

Qi et al. (2017) and Zaheer et al. (2017) both explore learning functions on sets. Importantly, they arrive at similar theoretical statements about the approximation of such functions, which rely on permutation invariant pooling functions. In particular, Zaheer et al. (2017) show that any set function $f(A)$ can be approximated by a model of the form $\rho\left(\sum_{a\in A}\phi(a)\right)$ for some learned ρ and ϕ, which they call DeepSets. They note that the sum can be replaced by a max-pool (which is essentially the formulation of Qi et al. (2017)), and observe empirically that this leads to better performance.[1] More recently, there has been some very interesting work on leveraging the relationship between sets. Probst (2018) proposes a set autoencoder, while Skianis et al. (2019) learn set representations with a network that compares the input set to trainable "hidden sets." However, both these approaches require solving computationally expensive matching problems at each iteration.

2.2 Orders and hierarchies

Vendrov et al. (2015) and Ganea et al. (2018) seek to model partial orders on objects via geometric relationships between their embeddings — namely, using cones in Euclidean space and hyperbolic space, respectively. Nickel and Kiela (2017) use a similar idea to embed hierarchical network structures in hyperbolic space, simply using the hyperbolic distance between embeddings. These approaches are unified under the framework of "disk embeddings" by Suzuki et al. (2019). The idea is to map each object to the product space $X \times \mathbb{R}$, where X is a metric space. This mapping can be expressed as $A \mapsto (f(A), r(A))$, and it is trained with the objective that $A \preceq B$ if and only if $d_X(f(A), f(B)) \leq r(B) - r(A)$. An equivalent statement can be made for multisets (see Theorem 3.3.1).

Other work has taken a probabilistic approach to the problem of representing hierarchical relationships. Lai and Hockenmaier (2017) attempt to formulate the Order Embeddings of Vendrov et al. (2015) probabilistically, modeling joint probabilities as the volumes of cone intersections. Vilnis et al. (2018) represent entities as "box embeddings," or rectangular volumes, where containment of one box inside another models order relationships between the objects. (Marginal and conditional probabilities can be computed from intersections of boxes.) Vilnis and McCallum (2015) propose modeling words as Gaussian distributions in order to capture notions of entailment and generality, and this work has been extended to mixtures of Gaussians by Athiwaratkun and Wilson (2017).

2.3 Fuzzy- and multi- sets

The theory of fuzzy sets can be traced back to Zadeh (1965). A fuzzy set A of objects from a universe $\mathcal{U}$ is defined via its *membership function* $\mu_A : \mathcal{U} \to [0, 1]$. Fuzzy set operations — such as intersection — are then defined in terms of this function. In modern fuzzy set theory, intersection is usually defined via a *t-norm*, which is a function $T : [0, 1]^2 \to [0, 1]$ satisfying certain properties. The intersection of two fuzzy sets A and B is defined via the membership function $\mu_{A\cap B}(x) = T(\mu_A(x), \mu_B(x))$. (More in-depth background, including the defining properties of t-norms, is provided in 3.1.) There is also more recent literature on extending fuzzy set theory to multisets (Casasnovas and Mayor, 2008;

[1] We believe there is an interesting theoretical distinction worth noting here, which may help explain this observation. Namely, max-pooling is *idempotent*, meaning that repeatedly pooling a representation with itself does not change the result. On the other hand, summation does not have this property, and so repeated copies of an element are reflected in the result. In this way, DeepSets (with the sum rather than max-pool) is in fact modeling *multisets* rather than sets, which depending on the application may be undesirable.

Miyamoto, 2000), using a membership function of the form $\mu_A : \mathcal{U} \times [0, 1] \to \mathbb{N}$, where $\mu_A(x, \alpha)$ is the number of appearances in A of an object x with membership α.

3 REPRESENTATION OF MULTISETS

Let $\mathcal{U} = \{x_1, \ldots, x_n\}$ be the universe of possible objects. We will denote by $\mathcal{U}^*$ the set of all multisets with elements from $\mathcal{U}$. We are interested in formulating a learnable function $\Psi : \mathcal{U}^* \to \mathbb{R}^d$ mapping such multisets to vectors. Our contributions are: (1) formulating fuzzy multiset operations in a way that is amenable to machine learning, and (2) proposing to learn representations by predicting the sizes of the symmetric differences between pairs of multisets. Furthermore, both the formulation of how we predict symmetric difference size and the actual representations we use to do so are crucial components of (1).

3.1 BACKGROUND: FUZZY SETS

We begin with some background in fuzzy set theory. It is useful to begin by noting a canonical function of the form above for sets: $\Psi(A) = [\mathbf{1}_{x_1 \in A}, \ldots, \mathbf{1}_{x_n \in A}]$. Each coordinate of the vector is 1 if x_i is in A, 0 otherwise. Fuzzy sets generalize this idea, letting $\Psi(A) = [\mu_A(x_1), \ldots, \mu_A(x_n)]$, where $\mu : \mathcal{U} \to [0, 1]$ is the *membership function*. Intuitively, μ_A maps each $x \in \mathcal{U}$ to "how much of a member" x is of A, on a scale from 0 to 1. With this simple generalization, fuzzy set operations can be defined. This is traditionally done by leveraging element-wise fuzzy logical operations, which we define below.

Definition 3.1.1 *A* t-norm *is a function $T : [0, 1]^2 \to [0, 1]$, satisfying the following properties:*

- *Commutativity: $T(a, b) = T(b, a)$*
- *Monotonicity: If $a \leq c$ and $b \leq d$, then $T(a, b) \leq T(c, d)$*
- *Associativity: $T(a, T(b, c)) = T(T(a, b), c)$*
- *1 is the identity: $T(a, 1) = a$*

T-norms generalize the notion of conjunction. Note that the above conditions imply that for any a, $T(a, 0) = 0$, and that $T(1, 1) = 1$. These two observations show that t-norms are "compatible" with classical, non-fuzzy logic — where we identify 0 with "false" and 1 with "true." The standard t-norm is $T(a, b) = \min\{a, b\}$.

Definition 3.1.2 *A* strong negator *is a strictly monotonic, decreasing function $n : [0, 1] \to [0, 1]$ such that $n(0) = 1$, $n(1) = 0$ and $n(n(x)) = x$.*

Unsurprisingly, strong negators generalize logical negation. The standard strong negator is $n(x) = 1 - x$.

Definition 3.1.3 *An* S-norm *(also called a* t-conorm*) is a function with the same properties as a t-norm, except that the identity element is 0.*

S-norms generalize disjunction. For every t-norm (and a given negator), we can define a *complementary s-norm*: $S(a, b) = n(T(n(a), n(b)))$. This is a generalization of De Morgan's laws. The standard s-norm, complementary to the $\min$ t-norm, is $S(a, b) = \max\{a, b\}$.

The membership function for the intersection of two fuzzy sets A and B is naturally defined as $\mu_{A \cap B}(x) = T(\mu_A(x), \mu_B(x))$ for a t-norm T. Similarly, the complement of a fuzzy set is given by $\mu_{\overline{A}}(x) = n(x)$ for a strong negator n, and the union of two fuzzy sets is given by $\mu_{A \cup B}(x) = S(\mu_A(x), \mu_B(x))$ for an s-norm S. Usually, we want T and S to be complementary with respect to n. Then, we can generalize all the usual set operations to fuzzy sets by combining the three basic operations above.

3.2 GENERALIZING TO FUZZY MULTISETS

Our function Ψ above can easily be extended to (non-fuzzy) multisets by letting $\Psi(A) = [m_A(x_1), \ldots, m_A(x_n)]$, where $m_A(x_i) \in \mathbb{N}$ is the multiplicity of x in A. This function m_A should immediately remind us of fuzzy sets. Indeed, if we simply let m_A map to any non-negative real number — that is, $m_A(x_i) \in \mathbb{R}_+$ — we obtain a representation of a version of fuzzy multisets. Note that this is not the same formulation of "fuzzy multisets" usually given in literature (Casasnovas and Mayor, 2008; Miyamoto, 2000). However, this formulation is much more easily amenable to the machine-learning setting. Intuitively, the benefit of "fuzzifying" our multisets is the ability to optimize via backpropagation.

With this definition of fuzzy multisets, we now define fuzzy multiset operations. Furthermore, we require that these operations be compatible both with their equivalents for non-fuzzy multisets and plain old sets (i.e. when $m_A(x_i) \in \mathbb{N}$ and $m_A(x_i) \in \{0, 1\}$, respectively). This will in fact essentially force us to adopt the following definitions:

- Size: $|A| = \sum_{i=1}^{n} m_A(x_i)$
- Intersection: $m_{A \cap B}(x_i) = \min\{m_A(x_i), m_B(x_i)\}$
- Union: $m_{A \cup B}(x_i) = \max\{m_A(x_i), m_B(x_i)\}$
- Multiset addition: $m_{A+B}(x_i) = m_A(x_i) + m_B(x_i)$
- Multiset difference: $m_{A \setminus B}(x_i) = \max\{m_A(x_i) - m_B(x_i), 0\}$
- Symmetric difference: $m_{A \triangle B}(x_i) = |m_A(x_i) - m_B(x_i)|$

It should stand out that our fuzzy multiset intersection and union are in fact the element-wise applications of the standard t-norm and s-norm, respectively. However, our requirement of compatibility with non-fuzzy multiset operations means that we cannot use general t-norms and s-norms, and as we will now argue, makes the operations above the only reasonable choices.

Consider the two (non-fuzzy) multisets, $A = \{1, 1, 1, 2, 2\}$ and $B = \{1, 1, 2, 3\}$. Their intersection should contain all their elements in common: $A \cap B = \{1, 1, 2\}$. That is, we take the minimum number of times each element appears in either A or B, and that is the number of times the element appears in $A \cap B$. This straightforwardly gives us $m_{A \cap B}(x) = \min\{m_A(x), m_B(x)\}$. Requiring that our notion of fuzzy multiset intersection be compatible with non-fuzzy multisets means for whole-number inputs, the membership function must be equivalent to the $\min$ t-norm. As there is no clear gain from letting the membership function deviate for fractional inputs, we define fuzzy multiset intersection as such.

Following similar reasoning, we can convince ourselves that multiset union should be defined as $m_{A \cup B}(x) = \max\{m_A(x), m_B(x)\}$. It is important to differentiate this from "multiset addition," which simply combines two multisets directly: $A + B = \{1, 1, 1, 1, 1, 2, 2, 2, 3\}$ for our example above, and in general $m_{A+B} = m_A(x) + m_B(x)$.

Multiset difference is a little harder to define. The main problem is that we cannot rely on a notion of "complement" for multisets. Instead, let us again try to reason by example. For our example multisets above, we have $A \setminus B = \{1, 2\}$. To arrive at this result, we remove from A each copy of an element which also appears in B. Note that if B had more of a certain element than A, that element would not appear in the final result. In other words, we are performing a subtraction of counts which is "glued" to a minimum value of zero. That is, $m_{A \setminus B}(x) = \max\{m_A(x) - m_B(x), 0\}$. We can further convince ourselves of the correctness of this expression by noting that we recover the identity $A \setminus (A \setminus B) = A \cap B$.

Finally, symmetric multiset difference can be defined using our expression for multiset difference, combined with either multiset addition or union. In particular, note that $A \triangle B = (A \setminus B) + (B \setminus A) = (A \setminus B) \cup (B \setminus A)$ — addition and union both work because $(A \setminus B)$ and $(B \setminus A)$ are necessarily disjoint. This gives us:

$$m_{A \triangle B}(x) = \max\{m_A(x) - m_B(x), 0\} + \max\{m_B(x) - m_A(x), 0\} = |m_A(x) - m_B(x)|.$$

(The equation still holds if we replace the addition with a maximum.)

3.3 MODELING THE RELATIONSHIP BETWEEN MULTISETS

We can now justify our choice of the size of the symmetric difference to capture the relationship between two multisets. First, note that given $|A|$ and $|B|$, and any one of $|A \cap B|$, $|A \setminus B|$, or $|A \triangle B|$, we can tell what fraction of elements of A are in B and vice-versa. In particular, we can also tell whether $A \subseteq B$ and whether $B \subseteq A$. In fact, we can formulate this relationship between containment and symmetric difference as a disk embedding inequality, where the metric space is that induced on $\mathcal{U}^*$ by the counting measure:

Theorem 3.3.1 *For two fuzzy multisets A and B, $A \subseteq B$ if and only if $|A \triangle B| \leq |B| - |A|$.*

Proof. We will in fact show that the inequality above can be replaced with an equality! First, note that $A \subseteq B$ is equivalent to the statement that for any $x \in \mathcal{U}$, $m_A(x) \leq m_B(x)$.

Suppose that $A \subseteq B$. Then, for all $x \in \mathcal{U}$, $m_B(x) \geq m_A(x)$, and the desired result follows:

$$|A \triangle B| = \sum_{x \in \mathcal{U}} m_{A \triangle B}(x) = \sum_{x \in \mathcal{U}} |m_B(x) - m_A(x)| = \sum_{x \in \mathcal{U}} m_B(x) - m_A(x) = |B| - |A|.$$

Suppose on the other hand that $|A \triangle B| \leq |B| - |A|$. We first note that this in fact means that $|A \triangle B| = |B| - |A|$, since we are given

$$\sum_{x \in \mathcal{U}} |m_B(x) - m_A(x)| \leq \sum_{x \in \mathcal{U}} m_B(x) - m_A(x),$$

but it must be that

$$\sum_{x \in \mathcal{U}} |m_B(x) - m_A(x)| \geq \sum_{x \in \mathcal{U}} m_B(x) - m_A(x).$$

Now, suppose for the sake of contradiction that for some $x^* \in \mathcal{U}$, it is the case that $m_A(x^*) > m_B(x^*)$. Then, $m_B(x^*) - m_A(x^*) < 0 \leq |m_B(x^*) - m_A(x^*)|$. But this implies that

$$\sum_{x \in \mathcal{U}} |m_B(x) - m_A(x)| > \sum_{x \in \mathcal{U}} m_B(x) - m_A(x),$$

which is a contradiction. ■

This theoretical connection is by itself a compelling reason to use symmetric difference over intersection or non-symmetric difference. In the context of backpropagation, however, our expression for fuzzy symmetric difference also has the advantage of having derivatives depending both on $m_A(x_i)$ and $m_B(x_i)$ for each i, unless $m_A(x_i) = m_B(x_i)$.

We are now ready to formulate our learning model. To do so, we must formulate Ψ and our loss function. Our loss function will penalize error in predicting $|A \triangle B|$ for input multisets A and B. We will use $\Delta(A, B)$ to denote our predicted symmetric difference size. Given a training distribution D of pairs of multisets, our loss is $\mathcal{L} = \mathbb{E}_{A,B \sim D}\left[(\Delta(A, B) - |A \triangle B|)^2\right]$.

We formulate Ψ with the DeepSets expression in mind: $\Psi(A) = \rho\left(\sum_{a \in A} \phi(a)\right)$, where $\phi : \mathcal{U} \to \mathbb{R}^d$ is some given object-featurization function. To make a perfect analogy to the fuzzy multiset representation above, we would require that each $\phi(a)$ be a standard basis vector. We want to be a little more general, however. For example, we may want to allow $\phi(a) \in \mathbb{R}^d$ with $d < n$. More importantly, we need to be able to learn ϕ. We do this by relaxing from standard basis vectors, allowing $\phi(a)$ to be any non-negative vector such that $||\phi(a)||_1 = 1$. That is, $\phi(a)$ can be a weighted combination of each of the standard bases with non-negative weights summing to 1 (which for $d = n$ can be interpreted as a weighted combination each of the elements of $\mathcal{U}$). The normalization guarantees that $\phi(a)$ has the same scale as any of the basis elements. Importantly, if the norm $|| \cdot ||_1$ is invariant under ρ, then we are guaranteed that $||\Psi(A)||_1 = |A|$. In practice, we guarantee the restrictions above by replacing $\phi(a)$ with $\frac{f(\phi(a))}{||f(\phi(a))||_1}$, where $f : \mathbb{R} \to \mathbb{R}_+$ is a function applied element-wise. For differentiability, we choose the softplus function $f(x) = \log(1 + e^x)$. To guarantee the invariance of $|| \cdot ||_1$ under ρ, we simply let ρ be the identity. We thus obtain: $\Psi(A) = \sum_{a \in A} \frac{f(\phi(a))}{||f(\phi(a))||_1}$, and $\Delta(A, B) = ||\Psi(A) - \Psi(B)||_1$.

Table 1: Mean absolute errors in symmetric difference size prediction on MNIST

	sizes $\in [2, 5]$	sizes $\in [2, 10]$	sizes $\in [2, 20]$
Multisets (restr. ϕ), training sizes $\in [2, 5]$	0.0722	0.1264	0.2061
Multisets (restr. ϕ), training sizes $\in [2, 10]$	0.0595	0.1059	0.1756
Multisets (unrestr. ϕ), training sizes $\in [2, 5]$	0.5614	0.7693	1.1813
Multisets (unrestr. ϕ), training sizes $\in [2, 10]$	0.6349	0.7740	0.9859
DeepSets, training sizes $\in [2, 5]$	1.2152	1.9386	5.2831
DeepSets, training sizes $\in [2, 10]$	1.2227	1.5358	3.0340

4 EXPERIMENTS

We compare our model above with two reasonable alternatives. For the first, we simply relax the restrictions on object representations — which by abuse of notation we will call the restriction of ϕ (to the standard simplex) — letting $\Psi(A) = \sum_{a \in A} \phi(a)$, and Δ as before. The second alternative is to simply replace both Ψ and Δ (which should itself permutation invariant) with DeepSets functions, letting $\Psi(A) = \rho_1 \left(\sum_{a \in A} \phi(a) \right)$ and $\Delta(A, B) = \rho_2 \left(\Psi(A) + \Psi(B) \right)$. We compare these models both on the task of predicting symmetric difference size, and in terms of their learned representations.

4.1 TRAINING AND EVALUATION PROCEDURES

We use MNIST (LeCun, 1998) as our dataset. The training set consists of 60,000 handwritten images of digits, and the test set of 10,000.

We train all the models on 3×10^5 training pairs of multisets. Both of the multisets in each pair are generated randomly at each iteration, as follows. First a size is uniformly sampled in the chosen range — in our experiments, either $[2, 5]$ or $[2, 10]$.[2] That many images are then chosen uniformly at random (with replacement) from the training set. The symmetric difference to be predicted is calculated directly from the image labels. All models are optimized using Adam (Kingma and Ba, 2015) with the default parameters $\beta_1 = 0.9$ and $\beta_2 = 0.999$, and a learning rate of 5×10^{-5}. The learning rate was chosen by logarithmic grid search from 1 down to 5×10^{-6}, training on up to 10^4 pairs during the search. (All models performed best with the chosen learning rate — or at least no worse than any of the other learning rates.) Given this learning rate, we chose to train the models for 3×10^5 iterations, finding that almost all of the models converged by this point.[3]

Evaluation is performed similarly to training, with the addition of multiset sizes uniform on $[2, 20]$, and with images sampled from the test set. Importantly, this means that the none of the images seen during training appear during evaluation. For symmetric difference size prediction, each model is evaluated on 3×10^4 such multiset pairs, and we let $\phi : \mathcal{U} \to \mathbb{R}^n$ (that is, $d = n = 10$).

For the object featurizing function ϕ, we use a variant of the LeNet-5 neural network (LeCun, 1998). Specifically, we adopt the same architecture as used by Ilse et al. (Ilse et al., 2018). (See Appendix A for network architectures.)

4.2 SYMMETRIC DIFFERENCE SIZE PREDICTION

Our results on the MNIST test-set are presented in Table 1. We report the mean absolute errors in symmetric difference size prediction, i.e. by how many elements on average is a model off from the true size. We observe that including the restriction on ϕ greatly improves performance when the symmetric difference is predicted as $\Delta(A, B) = ||\Psi(A) - \Psi(B)||_1$. Furthermore, when ϕ is restricted to the standard simplex, training on larger multisets leads to slightly better performance. It is unclear, however, whether training on larger multisets helps the multiset models "generalize" to multisets with sizes larger than those seen in training. Finally, we see that the using the fuzzy symmetric multiset difference was also important to learning, as the pure DeepSets model struggles

[2] We exclude singleton sets to ensure that the models aren't just learning from comparing pairs of singletons.

[3] The multiset model with restricted ϕ appeared as though further training could still slightly improve performance, but this model already outperformed the others.

to predict the correct value. (We note that rounding the models' predictions to whole numbers only slightly improved performance, if at all.)

4.3 EXAMINING LEARNED REPRESENTATIONS

With $\phi(a) \in \mathbb{R}^n$ restricted to the standard $(n-1)$-simplex, we find empirically that learned representations of objects are approximately the standard basis vectors (as shown in Figure 1 for $n = 3$). This makes sense intuitively, since this is exactly the fuzzy multiset representation on which we base our symmetric difference and size operations. This is an interesting property; we note that, given the mapping from coordinate to class, 98.9% classification accuracy is achieved just by picking the maximum-valued coordinate of the representation of each object. We also examine the case $d < n$, when the dimension of our representations is smaller than the number of possible objects. Here, the "pinched" nature of the restricted representations may be undesirable (Figure 2a). This problem, of course, gets worse with the discrepancy between number of objects and dimension (Figure 2b). On the other hand, the unrestricted multiset model is able to learn more balanced-looking clusters. However, the clusters for $d = n$ appear slightly less well-separated (Figures 3 and 4). The DeepSets model didn't learn interpretable representations (Figure 4c).

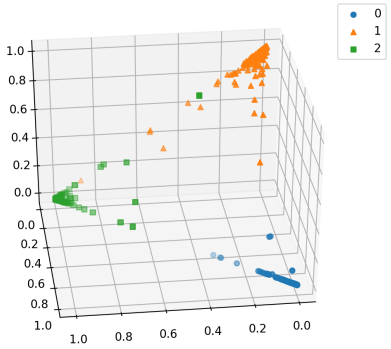
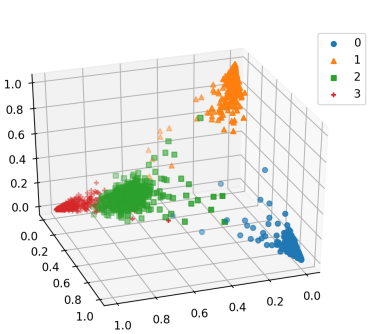
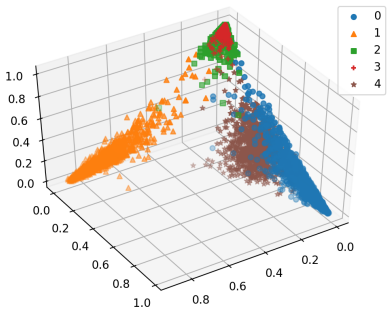


Figure 1: Three-dimensional representations of test-set MNIST images generated by the restricted multiset model trained on multisets of sizes $\in [2, 5]$; the model is trained on images of zeros, ones, twos.

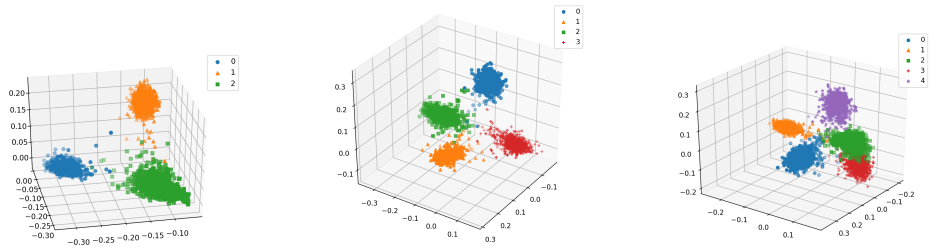


(a) Model trained on zeros, ones, twos, and threes.



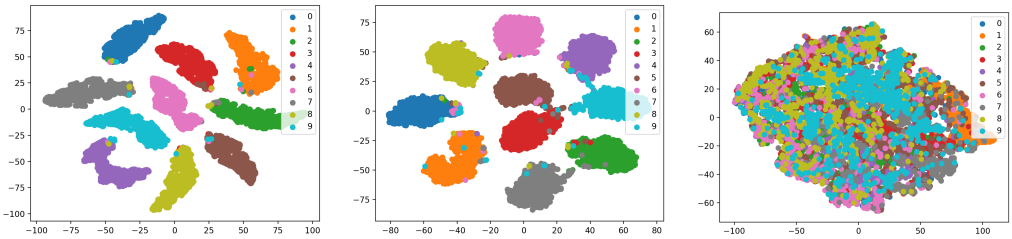
(b) Model trained on zeros, ones, twos, threes, and fours.

Figure 2: Three-dimensional representations of test-set MNIST images generated by the restricted multiset model trained on multisets of sizes $\in [2, 5]$. Note that in (b) the representations of twos and threes are essentially inseparable.



(a) Model trained on zeros, ones, and twos. (b) Model trained on zeros, ones, twos, and threes. (c) Model trained on zeros, ones, twos, threes, and fours.

Figure 3: Three-dimensional representations of test-set MNIST images generated by the unrestricted multiset model trained on multisets of sizes $\in [2, 5]$. Note that in (c), the clusters essentially form a tetrahedron, with one of the vertices being the combination of twos and threes.



(a) Multiset model, restricted ϕ. (b) Multiset model, unrestricted ϕ. (c) Pure DeepSets model.

Figure 4: Two dimensional TSNE (van der Maaten and Hinton, 2008) "projections" of the ten-dimensional representations of test-set MNIST images generated by the models; the models were trained on multisets of sizes $\in [2, 5]$.

5 Conclusion

We propose a novel task: predicting the size of the symmetric difference between pairs of multisets. We demonstrate the utility of this idea, developing a model that given only the sizes of symmetric differences between pairs of multisets, learns representations of such multisets and their elements. Our model learns to map each type of object to a standard basis vector, thus essentially performing semi-supervised clustering. One interesting area for future theoretical work is understanding a related problem: clustering n objects given multiset difference sizes. As a first step, we show in Appendix B that $n - 1$ specific multiset comparisons are sufficient to recover the clusters. We would also be curious to see if our model can learn meaningful representations even if the given labels are not exactly the sizes of symmetric differences — for example, human judgements of how different two bags-of-words are. Finally, we believe it may be interesting in future work to explore using multiset symmetric difference size prediction as an auxiliary or pre-training task, when representations of objects need to be learned.

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A NETWORK ARCHITECTURES

Given input images with c channels, and an output dimension d, the function ϕ is parametrized by the network:

1. A two-dimensional convolution layer with c input channels, 20 output channels, kernel size 5, and stride 1 (no padding)
2. A ReLU activation
3. A two-dimensional max-pooling layer with kernel size 2 and stride 2
4. A two-dimensional convolution layer with 20 input channels, 50 output channels, kernel size 5, and stride 1 (no padding)
5. A ReLU activation
6. A two-dimensional max-pooling layer with kernel size 2 and stride 2
7. A fully-connected linear layer with output size d (the input size is determined by c)

For the DeepSets model, we used for ρ_1 the architecture:

1. A fully-connected linear layer with input size d and output size 100
2. A hyperbolic tangent activation
3. A fully-connected linear layer with input and output size 100

For ρ_2 we used:

1. A fully-connected linear layer with input and output size 100
2. A hyperbolic tangent activation
3. A fully-connected linear layer with input size 100 and output size 1

B CLUSTERING n OBJECTS GIVEN $n-1$ SYMMETRIC SET DIFFERENCE SIZES

We are interested in the following problem. Suppose we have a set of n objects $\mathcal{U}$, each of which belongs to one of k clusters, $C_1, \ldots, C_k$. Let $M : 2^{\mathcal{U}} \to \{1, \ldots, k\}^*$ be the function which takes any subset of $\mathcal{U}$, and gives the multiset of cluster labels represented in that subset. We are given oracle access to the function $\Delta : 2^{\mathcal{U}} \times 2^{\mathcal{U}} \to \mathbb{N}$ which gives the size of the symmetric set difference between the cluster-label multisets: $\Delta(A, B) = |M(A) \triangle M(B)|$. How many queries are required to determine the clusters $C_1, \ldots, C_k$ (up to permutation)?

We show that the clusters can be determined with $n-1$ specific queries. (Another way to think of this is as a training data problem, rather than an oracle querying problem; we show $n-1$ training examples can be sufficient.) We do this in two steps. The step lets us identify k disjoint subsets of $\mathcal{U}$, such that no two of these subsets contain objects from the same cluster. The second step confirms that these subsets are in fact the clusters $C_1, \ldots, C_k$.

The first step consists of logarithmically "splitting" $\mathcal{U}$. The very first query in this step is $\Delta\left(\bigcup_{i=1}^{\lceil k/2 \rceil} C_i, \bigcup_{i=\lceil k/2 \rceil}^{k} C_i\right)$, which tells us that $\bigcup_{i=1}^{\lceil k/2 \rceil} C_i$ and $\bigcup_{i=\lceil k/2 \rceil}^{k} C_i$ are disjoint in terms of represented clusters. We proceed recursively, each query "splitting" the sets in half (in terms of which clusters they contain). The number of such steps required is $k-1$ (which is the number of internal nodes in a balanced binary search tree for k objects). We'll call the resulting disjoint sets $\tilde{C}_1, \ldots, \tilde{C}_k$ (since we technically don't yet know they correspond to the true clusters).

For the second step, we must verify that the objects in each of our sets resulting from step one all belong to the same cluster. This can be done by ordering the objects within each set, and comparing each consecutive pair as singletons. For each of our sets $\tilde{C}_i$, we thus make $|\tilde{C}_i| - 1$ such queries. Across all such sets, we thus make $\sum_{i=1}^{k} |\tilde{C}_i| - 1 = n - k$ queries.

So, the total number of queries made is $(k-1) + (n-k) = n - 1$.