Deep Set Prediction Networks

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Abstract

We study the problem of predicting a set from a feature vector with a deep neural network. Existing approaches ignore the set structure of the problem and suffer from discontinuity issues as a result. We propose a general model for predicting sets that properly respects the structure of sets and avoids this problem. With a single feature vector as input, we show that our model is able to auto-encode point sets, predict bounding boxes of the set of objects in an image, and predict the attributes of these objects in an image.

1 Introduction

You are given a rotation angle and your task is to draw the four corner points of a square that is rotated by that amount. This is a structured prediction task where the output is a *set*, since there is no inherent ordering to the four points. Such sets are a natural representation for many kinds of data, ranging from the set of points in a point cloud, to the set of objects in an image (object detection), to the set of nodes in a molecular graph (molecular generation). Yet, existing machine learning models often struggle to solve even the simple square prediction task [23].

The main difficulty in predicting sets comes from the ability to permute the elements in a set freely, which means that there are $n!$ equally good solutions for a set of size n. Models that do not take this set structure into account properly (such as MLPs or RNNs) result in discontinuities, which is the reason why they struggle to solve simple toy set prediction tasks [23]. We give background on what the problem is in section 2.

How can we build a model that properly respects the set structure of the problem so that we can predict sets without running into discontinuity issues? In this paper, we aim to address this question. Concretely, we contribute the following:

1. We propose a model that can predict a set from a feature vector while properly taking the structure of sets into account (section 3). We explain what properties we make use of that enables this. Our model uses backpropagation through a set encoder to decode a set and works for variable-size sets. The model is applicable to a wide variety of set prediction tasks since it only requires a feature vector as input.

2. We evaluate our model on several set prediction datasets (section 5). First, we demonstrate that the auto-encoder version of our model is sound on a set version of MNIST. Next, we use the CLEVR dataset to show that this works for general set prediction tasks. We predict the set of bounding boxes of objects in an image and we predict the set of object attributes in an image, both from a single feature vector. Our model is a completely different approach to usual anchor-based object detectors because we pose the task as a set prediction problem, which does not need complicated post-processing techniques such as non-maximum suppression.

2 Background

Representation   We are interested in sets of feature vectors with the feature vector describing properties of the element, for example the 2d position of a point in a point cloud. A set of size n wherein each feature vector has dimensionality d is represented as a matrix $\boldsymbol{Y} \in \mathbb{R}^{d \times n}$ with the elements as columns in an arbitrary order, $\boldsymbol{Y} = [\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n]$. To properly treat this as a set, it is important to only apply operations with certain properties to it [22]: *permutation-invariance* or *permutation-equivariance*. In other words, operations on sets should not rely on the arbitrary ordering of the elements.

Set encoders (which turn such sets into feature vectors) are usually built by composing permutation-equivariant operations with a permutation-invariant operation at the end. A simple example is the model in [22]: $f(\boldsymbol{Y}) = \sum_i g(\boldsymbol{y}_i)$ where g is a neural network. Because g is applied to every element individually, it does not rely on the arbitrary order of the elements. We can think of this as turning the set $\{\boldsymbol{y}_i\}_{i=1}^n$ into $\{g(\boldsymbol{y}_i)\}_{i=1}^n$. This is permutation-equivariant because changing the order of elements in the input set affects the output set in a predictable way. Next, the set is summed to produce a single feature vector. Since summing is commutative, the output is the same regardless of what order the elements are in. In other words, summing is permutation-invariant. This gives us an encoder that produces the same feature vector regardless of the arbitrary order the set elements were stored in.

Loss   In set prediction tasks, we need to compute a loss between a predicted set $\hat{\boldsymbol{Y}} = [\hat{\boldsymbol{y}}_1, \ldots, \hat{\boldsymbol{y}}_n]$ and the target set $\boldsymbol{Y}$. The main problem is that the elements of each set are in an arbitrary order, so we cannot simply compute a pointwise distance. The usual solution to this is an assignment mechanism that matches up elements from one set to the other set. This gives us a loss function that is permutation-invariant in both its arguments.

One such loss is the $O(n^2)$ Chamfer loss, which matches up every element of $\hat{\boldsymbol{Y}}$ to the closest element in $\boldsymbol{Y}$ and vice versa:

$$L_{\text{cha}}(\hat{\boldsymbol{Y}}, \boldsymbol{Y}) = \sum_i \min_j ||\hat{\boldsymbol{y}}_i - \boldsymbol{y}_j||^2 + \sum_j \min_i ||\hat{\boldsymbol{y}}_i - \boldsymbol{y}_j||^2 \tag{1}$$

Note that this does not work well for multi-sets: the loss between $[\boldsymbol{a}, \boldsymbol{a}, \boldsymbol{b}]$, $[\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{b}]$ is 0. A more sophisticated loss that does not have this problem involves the linear assignment problem with the pairwise losses as assignment costs:

$$L_{\text{hun}}(\hat{\boldsymbol{Y}}, \boldsymbol{Y}) = \min_{\pi \in \Pi} ||\hat{\boldsymbol{y}}_i - \boldsymbol{y}_{\pi(i)}||^2 \tag{2}$$

where Π is the space of permutations, which can be solved with the Hungarian algorithm in $O(n^3)$ time. This has the benefit that every element in one set is associated to exactly one element in the other set, which is not the case for the Chamfer loss.

Responsibility problem   A widely-used approach is to simply ignore the set structure of the problem. A feature vector can be mapped to a set $\hat{\boldsymbol{Y}}$ by using an MLP that takes the vector as input and directly produces $\hat{\boldsymbol{Y}}$ with $d \times n$ outputs. Since the order of elements in $\hat{\boldsymbol{Y}}$ does not matter, it appears reasonable to always produce them in a certain order based on the weights of the MLP.

While this seems like a promising approach, [23] point out that this results in a discontinuity issue: there are points where a small change in set space requires a large change in the neural network outputs. The model needs to "decide" which of its outputs is responsible for producing which element, and this responsibility must be resolved discontinuously.

The intuition behind this is as follows. Consider an MLP that detects the colour of two otherwise identical objects present in an image, so it has two outputs with dimensionality 3 (R, G, B) corresponding to those two colours. We are given an image with a blue and red object, so let us say that output 1 predicts blue and output 2 predicts red; perhaps the weights of output 1 are more attuned to the blue channel and output 2 is more attuned to the red channel. We are given another image with a blue and green object, so it is reasonable for output 1 to again predict blue and output 2 to now predict green. When we now give the model an image with a red and green object, or two red

Algorithm 1 Forward pass of set prediction algorithm

1: $\boldsymbol{z} = F(x)$ ▷ encode input with a model
2: $\hat{\boldsymbol{Y}}^{(0)} \leftarrow$ init   ▷ initialise set
3: **for** t $\leftarrow 1, T$ **do**
4:      $l \leftarrow L_{\mathrm{repr}}(\hat{\boldsymbol{Y}}, \boldsymbol{z})$ ▷ compute representation loss
5:      $\hat{\boldsymbol{Y}}^{(t)} \leftarrow \hat{\boldsymbol{Y}}^{(t-1)} - \eta \frac{\partial l}{\partial \hat{\boldsymbol{Y}}^{(t-1)}}$ ▷ gradient descent step on the set
6: **end for**
7: predict $\hat{\boldsymbol{Y}}^{(T)}$
8: $\mathcal{L} = \frac{1}{T} \sum_{t=0}^{T} L_{\mathrm{set}}(\hat{\boldsymbol{Y}}^{(t)}, \boldsymbol{Y}) + \lambda L_{\mathrm{repr}}(\boldsymbol{Y}, \boldsymbol{z})$ ▷ compute loss of outer optimisation

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objects, it is unclear which output should be responsible for predicting which object. Output 2 "wants" to predict both red and green, but has to decide between one of them, and output 1 now has to be responsible for the other object while previously being a blue detector. This responsibility must be resolved discontinuously, which makes modeling sets with MLPs difficult [23].

The main problem is that there is a notion of output 1 and output 2 – an ordered output representation – in the first place, which forces the model to give the set an order. Instead, it is preferable if the outputs of the model themselves are freely interchangeable – in the same way the elements of the set are interchangeable – to not impose an order on the outputs.

3 Deep Set Prediction Networks

This section contains our primary contribution: a model for decoding a feature vector into a set of feature vectors. As we have previously established, it is important for the model to properly respect the set structure of the problem to avoid the responsibility problem.

Our main idea is based on the observation that the gradient of a set encoder with respect to the input set is permutation-equivariant (see proof in Appendix A): *to decode a feature vector into a set, we can use gradient descent to find a set that* encodes *to that feature vector*. Since each update of the set using the gradient is permutation-equivariant, we always properly treat it as a set and avoid the responsibility problem. This gives rise to a nested optimisation: an inner loop that changes a set to encode more similarly to the input feature vector, and an outer loop that changes the weights of the encoder to minimise a loss over a dataset.

With this idea in mind, we build up models of increasing usefulness for predicting sets. We start with the simplest case of auto-encoding fixed-size sets (subsection 3.1), where a latent representation is decoded back into a set. This is modified to support variable-size sets, which is necessary for most sets encountered in the real-world. Lastly and most importantly, we extend our model to general set prediction tasks where the input no longer needs to be a set (subsection 3.2). This gives us a model that can predict a set of feature vectors from a single feature vector. We give the pseudo-code of this method in Algorithm 1.

3.1 Auto-encoding fixed-size sets

In a set auto-encoder, the goal is to turn the input set $\boldsymbol{Y}$ into a small latent space $\boldsymbol{z} = g_{\mathrm{enc}}(\boldsymbol{Y})$ with the encoder g_{enc} and turn it back into the predicted set $\hat{\boldsymbol{Y}} = g_{\mathrm{dec}}(\boldsymbol{z})$ with the decoder g_{dec}. Using our main idea, we define a *representation loss* and the corresponding decoder as:

$$L_{\mathrm{repr}}(\hat{\boldsymbol{Y}}, \boldsymbol{z}) = ||g_{\mathrm{enc}}(\hat{\boldsymbol{Y}}) - \boldsymbol{z}||^2 \tag{3}$$

$$g_{\mathrm{dec}}(\boldsymbol{z}) = \underset{\hat{\boldsymbol{Y}}}{\arg\min}\, L_{\mathrm{repr}}(\hat{\boldsymbol{Y}}, \boldsymbol{z}) \tag{4}$$

In essence, L_{repr} compares $\hat{\boldsymbol{Y}}$ to $\boldsymbol{Y}$ in the latent space. To understand what the decoder does, first consider the simple, albeit not very useful case of the identity encoder $g_{\mathrm{enc}}(\boldsymbol{Y}) = \boldsymbol{Y}$. Solving $g_{\mathrm{dec}}(\boldsymbol{z})$ simply means setting $\hat{\boldsymbol{Y}} = \boldsymbol{Y}$, which perfectly reconstructs the input as desired.

When we instead choose g_{enc} to be a set encoder, the latent representation $\boldsymbol{z}$ is a permutation-invariant feature vector. If this representation is "good", $\hat{\boldsymbol{Y}}$ will only encode to similar latent variables as $\boldsymbol{Y}$ if the two sets themselves are similar. Thus, the minimisation in Equation 4 should still produce a set $\hat{\boldsymbol{Y}}$ that is the same (up to permutation) as $\boldsymbol{Y}$, except this has now been achieved with $\boldsymbol{z}$ as a bottleneck.

Since the problem is non-convex when g_{enc} is a neural network, it is infeasible to solve Equation 4 exactly. Instead, we perform gradient descent to approximate a solution. Starting from some initial set $\hat{\boldsymbol{Y}}^{(0)}$, gradient descent is performed for a fixed number of steps T with the update rule:

$$\hat{\boldsymbol{Y}}^{(t+1)} = \hat{\boldsymbol{Y}}^{(t)} - \eta \cdot \frac{\partial L_{\text{repr}}(\hat{\boldsymbol{Y}}^{(t)}, \boldsymbol{z})}{\partial \hat{\boldsymbol{Y}}^{(t)}} \tag{5}$$

with η as the learning rate and the prediction being the final state, $g_{\text{dec}}(\boldsymbol{z}) = \hat{\boldsymbol{Y}}^{(T)}$. This is the aforementioned inner optimisation loop. In practice, we let $\hat{\boldsymbol{Y}}^{(0)}$ be a learnable $\mathbb{R}^{d \times n}$ matrix which is part of the neural network parameters.

To obtain a good representation $\boldsymbol{z}$, we still have to train the weights of g_{enc}. For this, we compute the auto-encoder objective $L_{\text{set}}(\hat{\boldsymbol{Y}}^{(T)}, \boldsymbol{Y})$ – with $L_{\text{set}} = L_{\text{cha}}$ or L_{hun} – and differentiate with respect to the weights as usual, backpropagating through the steps of the inner optimisation. This is the aforementioned outer optimisation loop.

In summary, each forward pass of our auto-encoder first encodes the input set to a latent representation as normal. To decode this back into a set, gradient descent is performed on an initial guess with the aim to obtain a set that encodes to the same latent representation as the input. The same set encoder is used in encoding and decoding.

Variable-size sets   To extend this from fixed- to variable-size sets, we make a few modifications to this algorithm. First, we pad all sets to a fixed maximum size to allow for efficient batch computation. We then concatenate an additional mask feature m_i to each set element $\hat{\boldsymbol{y}}_i$ that indicates whether it is a regular element ($m_i = 1$) or padding ($m_i = 0$). With this modification to $\hat{\boldsymbol{Y}}$, we can optimise the masks in the same way as the set elements are optimised. To ensure that masks stay in the valid range between 0 and 1, we simply clamp values above 1 to 1 and values below 0 to 0 after each gradient descent step. This performed better than using a sigmoid in our initial experiments, possibly because it allows exact 0s and 1s to be recovered.

3.2   Predicting sets from a feature vector

In our auto-encoder, we used an encoder to produce both the latent representation as well as to decode the set. This is no longer possible in the general set prediction setup, since the target representation $\boldsymbol{z}$ can come from a separate model (for example an image encoder F encoding an image $\boldsymbol{x}$), so there is no longer a set encoder in the model.

When naïvely using $\boldsymbol{z} = F(\boldsymbol{x})$ as input to our decoder, our decoding process is unable to predict sets correctly from it. Because the set encoder is no longer shared in our set decoder, there is no guarantee that optimising $g_{\text{enc}}(\hat{\boldsymbol{Y}})$ to match $\boldsymbol{z}$ converges towards $\boldsymbol{Y}$ (or a permutation thereof). To fix this, we simply add a term to the loss of the outer optimisation that encourages $g_{\text{enc}}(\boldsymbol{Y}) \approx \boldsymbol{z}$ again. In other words, the target set should have a very low representation loss itself. This gives us an additional L_{repr} term in the loss function of the outer optimisation for supervised learning:

$$\mathcal{L} = L_{\text{set}}(\hat{\boldsymbol{Y}}, \boldsymbol{Y}) + \lambda L_{\text{repr}}(\boldsymbol{Y}, \boldsymbol{z}) \tag{6}$$

with L_{set} again being either L_{cha} or L_{hun}. With this, minimising $L_{\text{repr}}(\hat{\boldsymbol{Y}}, \boldsymbol{z})$ in the inner optimisation will converge towards $\boldsymbol{Y}$. The additional term is not necessary in the pure auto-encoder because $\boldsymbol{z} = g_{\text{enc}}(\boldsymbol{Y})$, so $L_{\text{repr}}(\boldsymbol{Y}, \boldsymbol{z})$ is always 0 already.

Practical tricks   For the outer optimisation, we can compute the set loss for not only $\hat{\boldsymbol{Y}}^{(T)}$, but all $\hat{\boldsymbol{Y}}^{(t)}$. That is, we use $\frac{1}{T} \sum_t L_{\text{set}}(\hat{\boldsymbol{Y}}^{(t)}, \boldsymbol{Y})$ as loss. This encourages $\hat{\boldsymbol{Y}}$ to converge to $\boldsymbol{Y}$ quickly and not diverge with more steps, which significantly increases the robustness of our algorithm.

We sometimes observed divergent training behaviour when the outer learning rate is set inappropriately. By replacing the instances of $|| \cdot ||^2$ in L_{set} and L_{repr} with the Huber loss (squared error for differences below 1 and absolute error above 1) – as is commonly done in object detection models – training became less sensitive to hyperparameter choices.

4 Related work

The main approach we compare our method to is the simple method of using an MLP decoder to predict sets. This has been used for predicting point clouds [1; 5], bounding boxes [15; 2], and graphs (sets of nodes and edges) [3; 17]. These predict an ordered representation (list) and treat it as if it is unordered (set). As we previously discussed, this approach runs into the responsibility problem. Some works on predicting 3d point clouds make domain-specific assumptions such as independence of points within a set [11] or grid-like structures [20].

An alternative approach is to use an RNN decoder to generate this list [12; 18; 19]. The problem can be made easier if it can be turned from a set into a sequence problem by giving a canonical order to the elements in the set through domain knowledge [19]. For example, [21] generate the nodes of a graph by ordering the set of nodes based on the node traversal order of a breadth-first search.

The closest work to ours is by Mordatch [13]. They also iteratively minimise a function (their energy function) in each forward pass of the neural network and differentiate through the iteration to learn the weights. They have only demonstrated that this works for modifying small sets of 2d elements in relatively simple ways, so it is unclear whether their approach scales to the harder problems such as object detection that we tackle in this paper. In particular, minimising L_{repr} in our model has the easy-to-understand consequence of making the predicted set more similar to the target set, while it is less clear what minimising their learned energy function $E(\hat{Y}, z)$ does.

Zhang et al. [23] construct an auto-encoder that pools a set into a feature vector where information from the encoder is shared with their decoder. This is done to make their decoder permutation-equivariant, which they use to avoid the responsibility problem. However, this strictly limits their decoder to usage in auto-encoders because it requires an encoder to be present during inference.

Greff et al. [6] construct an auto-encoder for images with a set-structured latent space. They are able to find latent sets of variables to describe an image composed of a set of objects with some task-specific assumptions. While interesting from a representation learning perspective, our model is more immediately useful in practice because it works for general supervised learning tasks.

Our inspiration for using backpropagation through an encoder as a decoder comes from the line of introspective neural networks [9; 10] for image modeling. An important difference is that in these works, their two optimisation loops (generating predictions/samples and learning the network weights) are performed in sequence, while ours are nested. The nesting allows our outer optimisation to differentiate through the inner optimisation. Note that [6] and [13] also differentiate through an optimisation, which suggests that this type of optimisation is of general use when working with sets.

5 Experiments

In the following experiments, we compare our set prediction network to a model that uses an MLP as set decoder. In all experiments, we fix the hyperparameters of our model $T = 10, \eta = 800, \lambda = 0.1$. Further details about the model architectures, training settings, and hyperparameters are given in Appendix B. We provide the source code to reproduce all experiments at `https://github.com/Cyanogenoid/dspn`.

5.1 MNIST

We begin with the task of auto-encoding a set version of MNIST. A set is constructed from each image by including all the pixel coordinates (x and y, scaled to the interval $[0, 1]$) of pixels that have a value above the mean pixel value. The size of these sets varies from 32 to 342 across the dataset.

Model In our model, we use a set encoder that processes each element individually with a 3-layer MLP, followed by FSPool [23] as pooling function to produce 64 latent variables. These are decoded
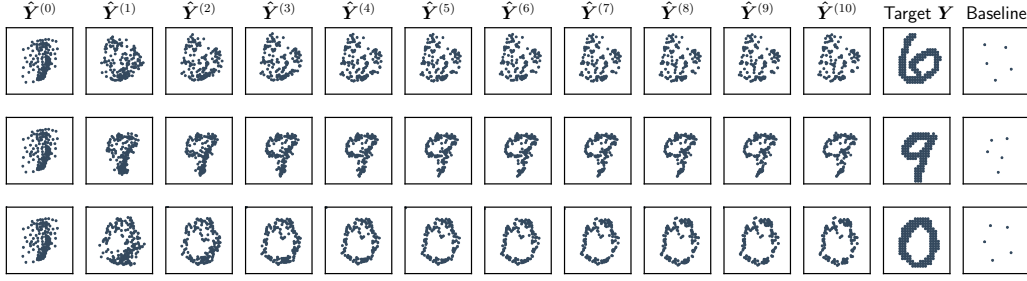
Figure 1: Progression of set prediction algorithm on MNIST ($\hat{Y}^{(t)}$).

with our algorithm to predict the input set. We compare this against a baseline model with the same encoder, but with a traditional MLP as decoder. Note that this baseline has significantly more parameters than our model. For the baseline, we include a mask feature with each element to allow for variable-size sets. Due to the large maximum set size, use of Hungarian matching is too slow. Thus, we use the Chamfer loss to compute the loss between predicted and target set in this experiment.

Results In Figure 1, we show the progression of $\hat{Y}$ throughout the minimisation with $\hat{Y}^{(10)}$ as the final prediction, the ground-truth set, and the baseline prediction. Our model clearly predicts much better sets than the baseline model, which only learned to output very few points in the rough shape of the digit. Observe how every optimisation starts with the same set $\hat{Y}^{(0)}$, but is transformed differently depending on the gradient of g_{enc}. Through this minimisation of L_{repr} by the inner optimisaton, the set is gradually changed into a shape that closely resembles the correct digit.

For the baseline, we tried to tune hyperparameters and network architecture without clear improvements over the shown results. Switching FSPool to a simpler average pooling significantly worsened the performance of both our model and the baseline. We believe that the reason for the poor result of the baseline on this dataset is due to the Chamfer loss not penalising prediction of too many padding elements enough. Most outputs of the MLP get stuck in the local optimum of outputting padding elements because it is an easy way to get a reasonably low loss. Optimisation of L_{repr} in our model prevents this pathological behaviour.

Note that reconstructions shown in [23] for the same auto-encoding task appear much better because their decoder uses additional information outside of the latent space: they copy multiple $n \times n$ matrices from the encoder into the decoder. In contrast, all information about the set is completely contained in our permutation-invariant 64d latent space.

5.2 Bounding box prediction

Next, we turn to the task of object detection on the CLEVR dataset [8], which contains 70,000 training and 15,000 validation images. The goal is to predict the set of bounding boxes for the objects in an image. The target set contains at most 10 elements with 4 dimensions each: the (normalised) x-y coordinates of the top-left and bottom-right corners of each box. As the dataset does not contain bounding box information canonically, we use [4] to calculate approximate bounding boxes. This causes the ground-truth bounding boxes to not always be perfect, which is a source of noise.

Model We encode the image with a ResNet34 [7] into a 512d feature vector, which is fed into the set decoder. The set decoder predicts the set of bounding boxes *from a single feature vector* describing the whole image. This is in contrast to existing region proposal networks [14] for bounding box prediction where the use of the entire feature map is required for the typical anchor-based approach. As the set encoder in our model, we use a 2-layer relation network [16] with FSPool [23] as pooling. We again compare this against a baseline that uses an MLP as set decoder. Since the sets are much smaller compared to our MNIST experiments, we can use the Hungarian loss as set loss. We perform no post-processing (such as non-maximum suppression) on the predictions of the model. The whole model is trained end-to-end.
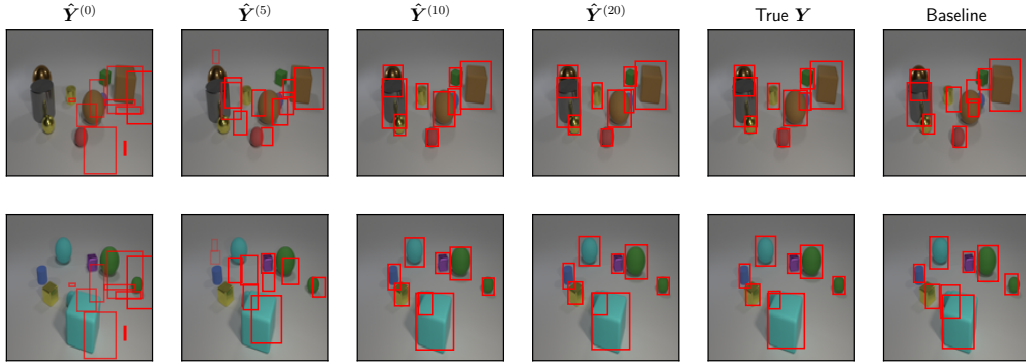
6

Figure 2: Progression of set prediction algorithm for bounding boxes in CLEVR. The baseline sometimes struggles with heavily-overlapping objects and often fails to centre the object in the boxes.

Table 1: Average Precision (AP) for different intersection-over-union thresholds for a predicted bounding box to be considered correct. Mean and standard deviation over 6 runs.

Model	AP_{50}	AP_{90}	AP_{95}	AP_{98}	AP_{99}
Baseline	$99.3_{\pm 0.2}$	$94.0_{\pm 1.9}$	$57.9_{\pm 7.9}$	$0.7_{\pm 0.2}$	$0.0_{\pm 0.0}$
Ours (10 iters)	$98.8_{\pm 0.3}$	$94.3_{\pm 1.5}$	$85.7_{\pm 3.0}$	$\mathbf{34.5}_{\pm 5.7}$	$\mathbf{2.9}_{\pm 1.2}$
Ours (20 iters)	$\mathbf{99.8}_{\pm 0.0}$	$\mathbf{98.7}_{\pm 1.1}$	$\mathbf{86.2}_{\pm 7.2}$	$24.3_{\pm 8.0}$	$1.4_{\pm 0.9}$
Ours (30 iters)	$\mathbf{99.8}_{\pm 0.1}$	$96.7_{\pm 2.4}$	$75.5_{\pm 12.3}$	$17.4_{\pm 7.7}$	$0.9_{\pm 0.7}$

Results We show our results in Table 1 using the standard average precision (AP) metric used in object detection with sample predictions in Figure 2. Our model is able to very accurately localise the objects with high AP scores even when the intersection-over-union (IoU) threshold for a predicted box to match a groundtruth box is very strict. In particular, our model using 10 iterations (the same it was trained with) has much better AP_{95} and AP_{98} than the baseline. The baseline model can predict bounding boxes in the close vicinity of objects, but fails to place the bounding box precisely on the object. This is visible from the decent performance for low IoU thresholds, but bad performance for high IoU thresholds.

We can also run our model with more inner optimisation steps than the 10 it was trained with. Many results improve when doubling the number of steps, which shows that further minimisation of $L_{\mathrm{repr}}(\hat{Y}, z)$ is still beneficial, even if it is unseen during training. The model "knows" that its prediction is still suboptimal when L_{repr} is high and also how to change the set to decrease it. This confirms that the optimisation is stable and does not diverge significantly with more steps. Being able to change the number of steps allows for a dynamic trade-off between prediction quality and inference time depending on what is needed for a given task. The less-strict AP metrics (which measure large mistakes) improve with more iterations, while the very strict AP_{98} and AP_{99} metrics consistently worsen. This is perhaps a sign that the inner optimisation learned to reach its best prediction at exactly 10 steps, but slightly overshoots when run for longer.

Bear in mind that we do not intend to directly compete against traditional object detection methods. Our goal is to demonstrate that our model can accurately predict a set from a single feature vector, which is of general use for set prediction tasks not limited to image inputs.

5.3 State prediction

Lastly, we want to directly predict the full state of a scene from images on CLEVR. This is the set of objects with their position in the 3d scene (x, y, z coordinates), shape (sphere, cylinder, cube), colour (eight colours), size (small, large), and material (metal/shiny, rubber/matte) as features. For example, an object can be a "small cyan metal cube" at position (0.95, -2.83, 0.35). We encode the categorial features as one-hot vectors and concatenate them into an 18d feature vector for each object. Note that we do not use bounding box information, so the model has to implicitly learn which object in the image corresponds to which set element with the associated properties. This makes it different

Table 2: Average Precision (AP) in % for different distance thresholds of a predicted set element to be considered correct. AP_∞ only requires all attributes to be correct, regardless of 3d position. Mean and standard deviation over 6 runs.

Model	AP_∞	AP_1	$AP_{0.5}$	$AP_{0.25}$	$AP_{0.125}$
Baseline	$3.6_{\pm 0.5}$	$1.5_{\pm 0.4}$	$0.8_{\pm 0.3}$	$0.2_{\pm 0.1}$	$0.0_{\pm 0.0}$
Ours (10 iters)	$72.8_{\pm 2.3}$	$59.2_{\pm 2.8}$	$39.0_{\pm 4.4}$	$12.4_{\pm 2.5}$	$1.3_{\pm 0.4}$
Ours (20 iters)	$84.0_{\pm 4.5}$	$80.0_{\pm 4.9}$	$\mathbf{57.0}_{\pm 12.1}$	$\mathbf{16.6}_{\pm 9.0}$	$\mathbf{1.6}_{\pm 0.9}$
Ours (30 iters)	$\mathbf{85.2}_{\pm 4.8}$	$\mathbf{81.1}_{\pm 5.2}$	$47.4_{\pm 17.6}$	$10.8_{\pm 9.0}$	$0.6_{\pm 0.7}$

from usual object detection tasks, since bounding boxes are required for traditional object detection models that rely on anchors.

Model   We use exactly the same model as for the bounding box prediction in the previous experiment with all hyperparameters kept the same. The only difference is that it now outputs 18d instead of 4d set elements. For simplicity, we continue using the Hungarian loss with the Huber loss as pairwise cost, as opposed to switching to cross-entropy for the categorical features.

Results   We show our results in Table 2 and give sample outputs in Appendix C. The evaluation metric is the standard average precision as used in object detection, with the modification that a prediction is considered correct if there is a matching groundtruth object with exactly the same properties and within a given Euclidean distance of the 3d coordinates. Our model clearly outperforms the baseline. This shows that our model is also suitable for modeling high-dimensional set elements.

When evaluating with more steps than our model was trained with, the difference in the more lenient metrics improves even up to 30 iterations. This time, the results for 20 iterations are all better than for 10 iterations. This suggests that 10 steps is too few to reach a good solution in training, likely due to the higher difficulty of this task compared to the bounding box prediction. Still, the representation z that the input encoder produces is good enough such that minimising L_{repr} more at evaluation time leads to better results. When going up to 30 iterations, the result for predicting the state only (excluding 3d position) improves further, but the accuracy 3d position worsens. We believe that this is again caused by overshooting the target due to the bias of training the model with only 10 iterations.

6   Discussion

In this paper we showed how to predict sets with a deep neural network in a way that respects the set structure of the problem. We demonstrated in our experiments that this works for small (size 10) and large sets (up to size 342), as well as low-dimensional (2d) and higher-dimensional (18d) set elements. Our model is consistently better than the baseline across all experiments by predicting sets properly, rather than predicting a list and pretending that it is a set.

The improved results of our approach come at a higher computational cost. Each evaluation of the network requires time for $O(T)$ passes through the set encoder, which makes training take about 75% longer on CLEVR with $T = 10$. Keep in mind that this only involves the set encoder (which can be fairly small), not the input encoder (such as a CNN or RNN) that produces the target z. Further study into representationally-powerful and efficient set encoders such as RN [16] and FSPool [23] – which we found to be critical for good results in our experiments – would be of considerable interest, as it could speed up the convergence and thus inference time of our method. Another promising approach is to better initialise $Y^{(0)}$ – perhaps with an MLP – so that the set needs to be changed less to minimise L_{repr}. Our model would act as a set-aware refinement method of the MLP prediction.

Our algorithm may be suitable for generating samples under other invariance properties. For example, we may want to generate images of objects where the rotation of the object does not matter (such as aerial images). Our model with a rotation-invariant image encoder could predict images without forcing the model to choose a fixed orientation of the image, which could be a useful inductive bias.

In conclusion, we are excited about enabling a wider variety of set prediction problems to be tackled with deep neural networks. Our main idea should be readily extensible to similar domains such as graphs to allow for better graph prediction, for example molecular graph generation or end-to-end

scene graph prediction from images. We hope that our model inspires further research into graph generation, stronger object detection models, and – more generally – a more principled approach to set prediction.

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A Proof of permutation-equivariance

Definition 1. *A function $f : \mathbb{R}^{n \times c} \to \mathbb{R}^d$ is permutation-invariant iff it satisfies:*

$$f(\boldsymbol{X}) = f(\boldsymbol{PX}) \tag{7}$$

for all permutation matrices $\boldsymbol{P}$.

Definition 2. *A function $g : \mathbb{R}^{n \times c} \to \mathbb{R}^{n \times d}$ is permutation-equivariant iff it satisfies:*

$$\boldsymbol{P}g(\boldsymbol{X}) = g(\boldsymbol{PX}) \tag{8}$$

for all permutation matrices $\boldsymbol{P}$.

Theorem 1. *The gradient of a permutation-invariant function $f : \mathbb{R}^{n \times c} \to \mathbb{R}^d$ with respect to its input is permutation-equivariant:*

$$\boldsymbol{P}\frac{\partial f(\boldsymbol{X})}{\partial \boldsymbol{X}} = \frac{\partial f(\boldsymbol{PX})}{\partial \boldsymbol{PX}} \tag{9}$$

Proof. Using Definition 1, the chain rule, and the orthogonality of $\boldsymbol{P}$:

$$\boldsymbol{P}\frac{\partial f(\boldsymbol{X})}{\partial \boldsymbol{X}} = \boldsymbol{P}\frac{\partial f(\boldsymbol{PX})}{\partial \boldsymbol{X}} \tag{10}$$

$$= \boldsymbol{P}\frac{\partial \boldsymbol{PX}}{\partial \boldsymbol{X}}\frac{\partial f(\boldsymbol{PX})}{\partial \boldsymbol{PX}} \tag{11}$$

$$= \boldsymbol{PP}^T\frac{\partial f(\boldsymbol{PX})}{\partial \boldsymbol{PX}} \tag{12}$$

$$= \frac{\partial f(\boldsymbol{PX})}{\partial \boldsymbol{PX}} \tag{13}$$

$\square$

B Details

In our algorithm, η was chosen in initial experiments and we did not tune it beyond that. We did this by increasing η until the output set visibly changed between inner optimisation steps when the set encoder is randomly initialised. This makes it so that changing the set encoder weights has a noticeable effect rather than being stuck with $\hat{\boldsymbol{Y}}^{(T)} \approx \hat{\boldsymbol{Y}}^{(0)}$.

$T = 10$ was chosen because it seemed to be enough to converge to good solutions on MNIST. We simply kept this for the supervised experiments on CLEVR.

In the supervised experiments, we would often observe large spikes in training that cause the model diverge when $\lambda = 1$. By changing around various parameters, we found that reducing λ eliminated most of this issue and also made training converge to better solutions. Much smaller values than 0.1 converged to worse solutions. This is likely because the issue of not having the $L_{\text{repr}}(\boldsymbol{Y}, \boldsymbol{z})$ term in the outer loss in the first place ($\lambda = 0$) is present again – see subsection 3.2.

For all experiments, we used Adam with the default momentum values and batch size 32. The only hyperparameter we tuned in the experiments is the learning rate. Every individual experiment is run on a single 1080 Ti GPU.

We tried an alternative version of the inner optimisation that includes a momentum term. This gave us slightly better results, but we did not use this for any experiments in the paper to keep our method as simple as possible.

B.1 MNIST

For MNIST, we train our model and the baseline model for 100 epochs to make sure that they have converged. Both models have a 3-layer MLP with ReLU activations and 256 neurons in the first two layers and 64 in the third. For simplicity, sets are padded to a fixed size for FSPool. FSPool has 20 pieces in its piecewise linear function. We tried learning rates in

$\{1.0, 0.1, 0.03, 0.01, 0.003, 0.001, 0.0003, 0.0001, 0.00001\}$ and chose 0.01. For the baseline, none of the other learning rates performed significantly better than the one we chose.

The baseline is trained slightly differently to our model. The baseline does not output mask values natively, so we have to train it with the mask values in the training target. In other words, it is trained to predict x coordinate, y coordinate, and the mask for each point. Better results (but still worse than our model) with fewer predicted padding points can be achieved by not including this mask value in the target, but this baseline model no longer predicts variable-sized sets. Our model is trained without mask values in the target and is able to learn the mask values purely through L_{repr} in the inner optimisation.

It is possible to explicitly include the sum of masks as a feature in the representation z for our model. This improves our results on MNIST – likely due to an explicit signal for the model to predict the correct set size – but again, we do not use this to keep our model as simple as possible.

B.2   CLEVR

We train our model and the baseline model for 100 epochs on the training set of CLEVR and evaluate on the validation set, since no ground-truth scene information is available for the test set. The set encoder is a 2-layer Relation Network with ReLU activation between the two layers, wherein the sum pooling is replaced with FSPool. The two layers have 512 neurons each. Because we use the Hungarian loss instead of the Chamfer loss here, including the mask feature in the target set does not worsen results, so we include the mask target for both the baseline and our model for consistency. To tune the learning rate, we started with the learning rate found for MNIST and decreased it similarly-sized steps until the training accuracy after 100 epochs worsened. We settled on 0.0003 as learning rate for both the bounding box and the state prediction task. All other hyperparameters are kept the same as for MNIST. The ResNet-18 that encodes the image is not pre-trained.

C Additional outputs

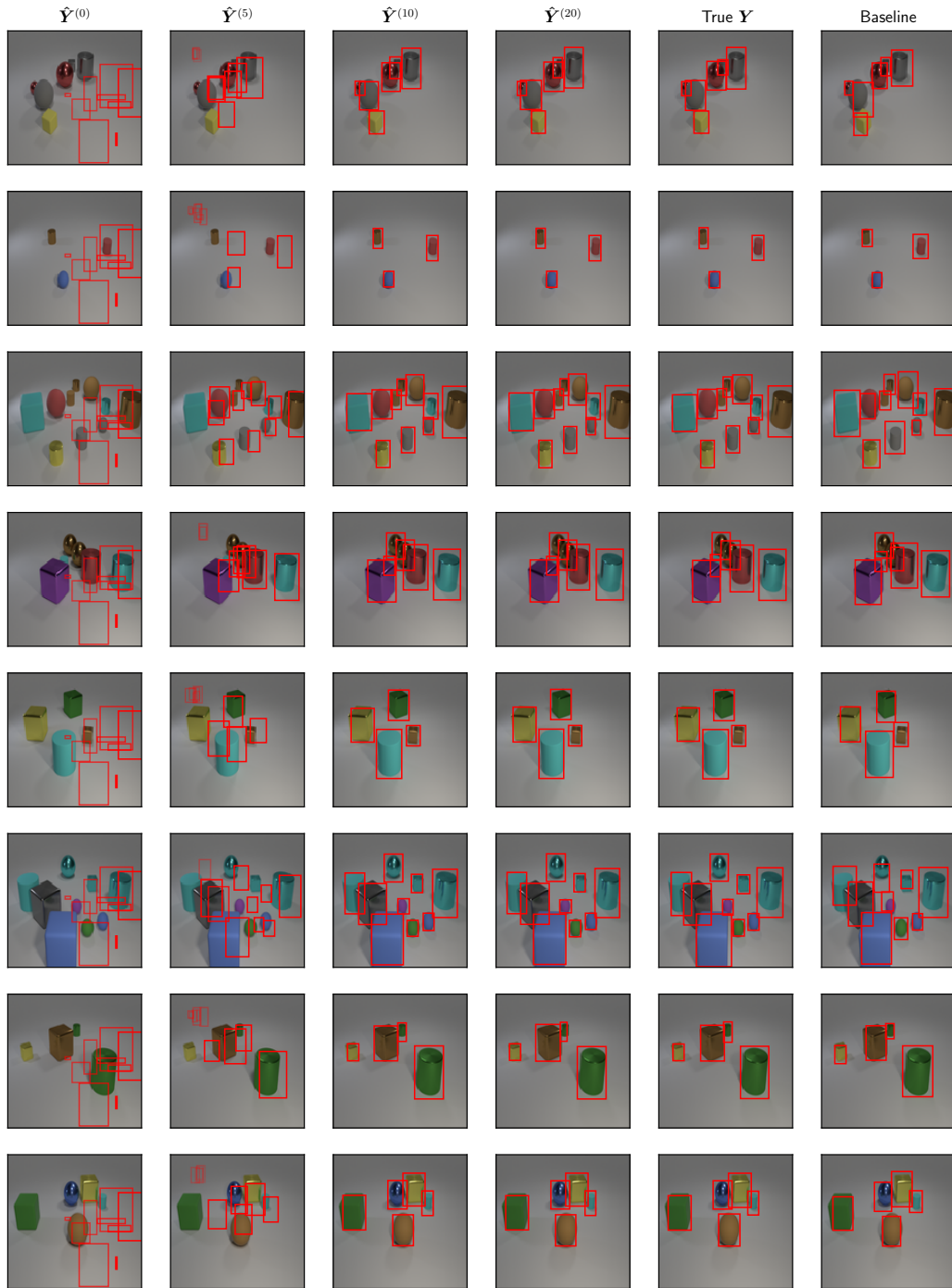Figure 3: Progression of set prediction algorithm on MNIST.

Figure 4: Progression of set prediction algorithm on CLEVR bounding boxes.

Table 3: Progression of set prediction algorithm on CLEVR state prediction. Red text denotes a wrong attribute. Objects are sorted by x coordinate, so they are sometimes misaligned with wrongly-coloured red text (see third example: red entries in $\hat{Y}^{(20)}$ and bottom two red entries in baseline).
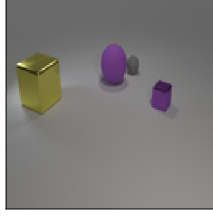
$\hat{Y}^{(5)}$	$\hat{Y}^{(10)}$	$\hat{Y}^{(20)}$	True Y	Baseline
(-0.14, 1.16, 3.57)	(-2.33, -2.41, 0.73)	(-2.33, -2.42, 0.78)	(-2.42, -2.40, 0.70)	(-1.65, -2.85, 0.69)
large purple rubber sphere	large yellow metal cube	large yellow metal cube	large yellow metal cube	large yellow metal cube
(0.01, 0.12, 3.42)	(-1.20, 1.27, 0.67)	(-1.21, 1.20, 0.65)	(-1.18, 1.25, 0.70)	(-0.95, 1.08, 0.68)
large gray metal cube	large purple rubber sphere	large purple rubber sphere	large purple rubber sphere	large green rubber sphere
(0.67, 0.65, 3.38)	(-0.96, 2.54, 0.36)	(-0.96, 2.59, 0.36)	(-1.02, 2.61, 0.35)	(-0.40, 2.14, 0.35)
small purple metal cube	small gray rubber sphere	small gray rubber sphere	small gray rubber sphere	small red rubber sphere
(0.67, 1.14, 2.96)	(1.61, 1.57, 0.36)	(1.58, 1.62, 0.38)	(1.74, 1.53, 0.35)	(1.68, 1.77, 0.35)
small purple rubber sphere	small yellow metal cube	small purple metal cube	small purple metal cube	small brown metal cube
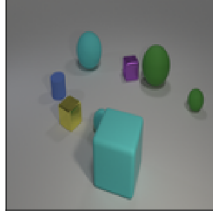
$\hat{Y}^{(5)}$	$\hat{Y}^{(10)}$	$\hat{Y}^{(20)}$	True Y	Baseline
(-0.29, 1.14, 3.73)	(-2.78, 0.86, 0.72)	(-2.62, 0.83, 0.68)	(-2.88, 0.78, 0.70)	(-2.42, 0.63, 0.71)
small purple metal cube	large cyan rubber sphere	large cyan rubber sphere	large cyan rubber sphere	large purple rubber sphere
(-0.11, -0.37, 3.65)	(-2.17, -1.59, 0.38)	(-2.14, -1.63, 0.35)	(-2.14, -1.63, 0.35)	(-2.40, -2.07, 0.35)
small brown metal cube	small blue rubber cylinder	small blue rubber cylinder	small blue rubber cylinder	small green rubber cylinder
(0.08, 0.56, 3.84)	(-0.45, 2.19, 0.40)	(-0.60, 2.23, 0.29)	(-0.78, 1.97, 0.35)	(-0.74, 2.46, 0.33)
large cyan rubber	small purple metal cube	small purple metal cube	small purple metal cube	small cyan metal cube
(0.69, -0.43, 3.55)	(-0.14, -2.15, 0.38)	(-0.30, -1.99, 0.32)	(-0.38, -2.06, 0.35)	(0.30, -1.86, 0.34)
small brown rubber sphere	small yellow metal cube	small yellow metal cube	small yellow metal cube	small gray rubber sphere
(1.12, 0.21, 3.83)	(0.53, 2.56, 0.70)	(0.27, 2.46, 0.72)	(0.42, 2.56, 0.70)	(0.69, -2.10, 0.36)
large cyan rubber cube	large green rubber sphere	large green rubber sphere	large green rubber sphere	small red metal cube
(1.23, -0.25, 3.58)	(0.93, -1.41, 0.35)	(0.86, -1.31, 0.27)	(0.81, -1.30, 0.35)	(1.12, 2.28, 0.70)
small cyan rubber sphere	small cyan rubber sphere	small cyan rubber sphere	small cyan rubber sphere	large cyan rubber sphere
(1.73, 1.04, 3.57)	(2.50, -2.08, 0.76)	(2.64, -2.05, 0.76)	(2.56, -1.94, 0.70)	(2.55, -2.26, 0.73)
small cyan rubber sphere	large cyan rubber cube	large cyan rubber cube	large cyan rubber cube	large yellow rubber cube
(2.06, 1.94, 3.81)	(2.61, 2.59, 0.33)	(2.75, 2.73, 0.35)	(2.74, 2.64, 0.35)	(2.99, 2.59, 0.35)
large brown rubber sphere	small green rubber sphere	small green rubber sphere	small green rubber sphere	small purple rubber sphere
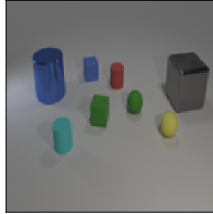
$\hat{Y}^{(5)}$	$\hat{Y}^{(10)}$	$\hat{Y}^{(20)}$	True Y	Baseline
(0.22, 0.12, 3.47)	(-2.76, -1.42, 0.68)	(-2.68, -1.64, 0.77)	(-2.62, -1.76, 0.70)	(-2.47, -1.73, 0.70)
small brown rubber cube	large blue metal cylinder	large blue metal cylinder	large blue metal cylinder	large cyan metal cylinder
(0.41, 0.11, 3.77)	(-1.56, -0.61, 0.35)	(-2.43, 0.03, 0.34)	(-2.29, 0.49, 0.35)	(-2.42, 0.09, 0.36)
large gray metal cube	small blue rubber cylinder	small blue rubber cube	small blue rubber cube	small blue rubber cylinder
(0.50, 0.44, 3.61)	(-1.08, 0.23, 0.33)	(-1.00, 1.18, 0.33)	(-0.93, 1.15, 0.35)	(-1.24, 1.16, 0.36)
small gray rubber cube	small green rubber cube	small red rubber cylinder	small red rubber cylinder	small red rubber cube
(0.83, 0.53, 3.45)	(-0.07, 0.97, 0.36)	(-0.01, -1.00, 0.46)	(0.28, -2.84, 0.35)	(0.39, 0.20, 0.33)
small cyan rubber sphere	small green rubber cylinder	small green rubber cube	small cyan rubber cylinder	small red rubber sphere
(0.86, 0.85, 3.50)	(0.28, -2.44, 0.49)	(0.21, -2.88, 0.40)	(0.29, -0.98, 0.35)	(0.56, -3.11, 0.35)
small gray rubber sphere	small cyan rubber cylinder	small cyan rubber cylinder	small green rubber cube	small yellow rubber cylinder
(1.86, 2.34, 3.80)	(1.36, -0.63, 0.38)	(0.99, 0.17, 0.37)	(0.92, 0.54, 0.35)	(0.90, 0.64, 0.35)
large gray metal cube	small green rubber sphere	small green rubber sphere	small green rubber sphere	small green rubber sphere
(1.97, 0.55, 3.61)	(2.01, 3.07, 0.65)	(1.97, 2.89, 0.39)	(2.04, 2.78, 0.70)	(2.39, 0.27, 0.36)
small green rubber sphere	large gray metal cube	large gray metal cube	large gray metal cube	small yellow rubber sphere
	(2.69, 0.63, 0.34)	(2.87, 0.51, 0.25)	(2.70, 0.67, 0.35)	(2.44, 2.55, 0.68)
	small yellow rubber sphere	small yellow rubber sphere	small yellow rubber sphere	large gray metal cube