

ADVANCED DEEP LEARNING

Lab 1: Symmetry in Deep Learning Representations

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This handout includes theoretical introductions, [coding tasks](#) and [questions](#). Before **Tuesday 13th January at 1pm**, you should submit a **.zip** file named `Lab<x>_lastname.firstname.pdf` containing a `/code/` folder (itself containing your scripts with the gaps filled) and an answer sheet containing your answers to the questions on moodle. Your answers should be well constructed and well justified. They should not repeat the question or generalities in the handout. When relevant, you are welcome to include figures, equations and tables derived from your own computations, theoretical proofs or qualitative explanations. **One submission is required for each student**. No deadline extension will be granted.

1 Learning objective

The goal of this lab is to introduce you to machine learning models for data represented as sets. Specifically, we will implement the DeepSets model. We will evaluate the model in the task of computing the sum of sets of digits and compare it against traditional models such as LSTMs.

2 DeepSets

Typical machine learning algorithms, such as the Logistic Regression classifier or Multi-layer Perceptrons, are designed for fixed dimensional data samples. Thus, these models cannot handle input data that takes the form of sets. The cardinalities of the sets are not fixed, but they are allowed to vary. Therefore, some sets are potentially larger in terms of the number of elements than others. Furthermore, a model designed for data represented as sets needs to be invariant to the permutations of the elements of the input sets. Formally, it is well-known that a function f transforms its domain \mathcal{X} into its range \mathcal{Y} . If the input is a set $X = \{x_1, \dots, x_M\}$, $x_m \in \mathfrak{X}$, i.e., the input domain is the power set $\mathcal{X} = 2^{\mathfrak{X}}$, and a function $f : 2^{\mathfrak{X}} \rightarrow Y$ acting on sets must be permutation invariant to the order of objects in the set, i.e., for any permutation $\pi : f(\{x_1, \dots, x_M\}) = f(\{x_{\pi(1)}, \dots, x_{\pi(M)}\})$. Learning on sets emerges in several real-world applications, and has attracted considerable attention in the past years.

2.1 Dataset Generation

For the purposes of this lab, we consider the task of finding the sum of a given set of digits, and we will create a synthetic dataset as follows: Each sample is a multiset of digits and its target is the sum of its elements. For instance, the target of the sample $X_i = \{8, 3, 5, 1\}$ is $y_i = 17$. We will generate 100,000 training samples by randomly sampling between 1 and 10 digits ($1 \leq M \leq 10$) from $\{1, 2, \dots, 10\}$. With regards to the test set, we will generate 200,000 test samples of cardinalities from 5 to 100 containing again digits from $\{1, 2, \dots, 10\}$. Specifically, we will create 10,000 samples with cardinalities exactly 5, 10,000 samples with cardinalities exactly 10, and so on.

Task 1

Fill in the body of the `create_train_dataset()` function in the `utils.py` file to generate the training set (consisting of 100,000 samples) as discussed above. Each sample should be a multiset of a length that is uniformly at random sampled from $\{1, 2, \dots, 10\}$. Further, each element of the multisets should also be uniformly at random sampled from $\{1, 2, \dots, 10\}$. To train the models, it is necessary that all training samples have identical cardinalities. Therefore, we pad multisets with cardinalities smaller than 10 with zeros. For instance, the multiset $\{4, 5, 1, 7, 5\}$ is represented as $\{0, 0, 0, 0, 0, 4, 5, 1, 7, 5\}$ (Hint: use the `randint()` function of NumPy to generate random integers from $\{1, 2, \dots, 10\}$).

Task 2

Fill in the body of the `create_test_dataset()` function in the `utils.py` file to generate the test set (consisting of 200,000 samples) as discussed above. Each set contains from 5 to 100 digits again drawn from $\{1, 2, \dots, 10\}$. Specifically, the first 10,000 samples will consist of exactly 5 digits, the next 10,000 samples will consist of exactly 10 digits, and so on. Note that here we would like you to return a list of numpy arrays, where the first list element contains a numpy array containing 10,000 samples with cardinality 5, the second list element should contain a numpy array with 10,000 samples of cardinality 10, and the final list element should contain 10,000 samples with cardinality 100.

2.2 Implementation of DeepSets

It can be shown that if \mathcal{X} is a countable set and $\mathcal{Y} = \mathbb{R}$, then a function $f(X)$ operating on a set X having elements from \mathcal{X} is a valid set function, i.e., invariant to the permutation of instances in X , if and only if it can be decomposed in the form $\rho(\sum_{x \in X} \phi(x))$, for suitable transformations ϕ and ρ .

DeepSets achieves permutation invariance by replacing ϕ and ρ with multi-layer perceptrons (universal approximators). Specifically, DeepSets consists of the following two steps [1]:

- Each element x_i of each set is transformed (possibly by several layers) into some representation $\phi(x_i)$.
- The representations $\phi(x_i)$ are added up and the output is processed using the ρ network in the same manner as in any deep network (e.g., fully connected layers, nonlinearities, etc.).

An illustration of the DeepSets model is given in Figure 1.

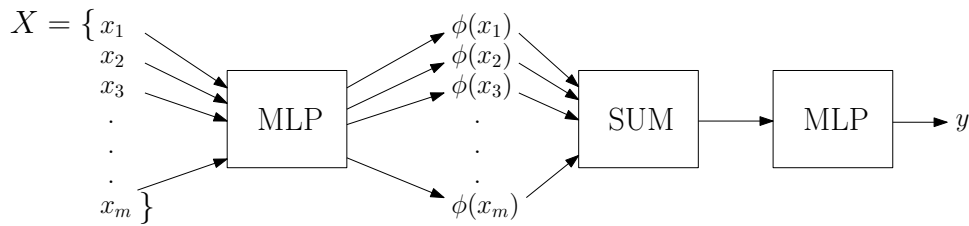


Figure 1: The DeepSets model.

Task 3

Implement the DeepSets architecture in the `models.py` file. More specifically, add the following layers:

- an embedding layer which projects each digit to a latent space of dimensionality h_1
- a fully-connected layer with h_2 hidden units followed by a tanh activation function
- a sum aggregator which computes the sum of the elements of each set
- a fully-connected layer with 1 unit since the output of the model needs to be a scalar (i.e., the prediction of the sum of the digits contained in the set)

Question 1 (5 points)

For the task that we perform here, i.e., determining the sum of a set of integers, what are the optimal MLP parameters (weights and bias) that we expect the DeepSets architecture learn? When answer please assume that we are working with a ReLU instead of a tanh activation function in the first fully connected layer in the model.

We have now defined the DeepSets model. We will compare the DeepSets model against an LSTM, an instance of the family of recurrent neural networks. The next step is thus to define the LSTM model. Given an input set, we will use the LSTM hidden state output for the last time step as the representation of entire set.

Task 4

Implement the LSTM architecture in the `models.py` file. More specifically, add the following layers:

- an embedding layer which projects each digit to a latent space of dimensionality h_1
- an LSTM layer with h_2 hidden units
- a fully-connected layer which takes the LSTM hidden state output for the last time step as input and outputs a scalar

2.3 Model Training

Next, we will train the two models (i.e., DeepSets and LSTM) on the dataset that we have constructed. We will store the parameters of the trained models in the disk and retrieve them later on to make predictions.

Task 5

Fill in the missing code in the `train.py` file, and then execute the script to train the two models. Specifically, you need to generate all the necessary tensors for each batch.

2.4 Predicting the Sum of a Set of Digits

We will now evaluate the two models on the test set that we have generated. We will compute the accuracy and mean absolute error of the two models on each subset of the test set separately. We will

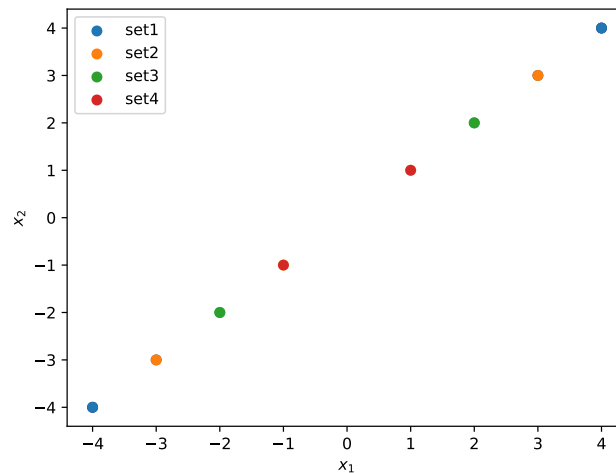


Figure 2: A synthetic example consisting of four sets.

store the obtained accuracies and mean absolute errors in a dictionary.

Task 6

In the `eval.py` file, for each batch of the test set, generate the necessary tensors for making predictions. Compute the output of two models. Compute the accuracy and mean absolute error achieved by the two models and append the emerging values to the corresponding lists of the `results` dictionary (Hint: use the `accuracy_score()` and `mean_absolute_error()` functions of `scikit-learn`. When calculating the accuracy of our models you may want to use `numpy's round()` function to set all predictions to integer values.).

We will next compare the performance of DeepSets against that of the LSTM. Specifically, we will visualize the accuracies of the two models with respect to the maximum cardinality of the input sets.

Task 7

Visualize the accuracies of the two models with respect to the maximum cardinality of the input sets (Hint: you can use the `plot()` function of `Matplotlib`).

Question 2 (5 points)

Consider the dataset shown in Figure 2 which consists of four sets of 2-dimensional vectors. The cardinality of all sets is equal to 2, while for all sets, the sum of their elements is equal to $[0, 0]$. Can the DeepSets model learn different representations for the four sets?

References

- [1] Manzil Zaheer, Satwik Kottur, Siamak Ravanbakhsh, Barnabás Póczos, Ruslan Salakhutdinov, and Alexander J Smola. Deep Sets. In *Advances on Neural Information Processing Systems*, pages 3394–3404, 2017.