Methodology for Predictive calculator

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0.1 Brief Summary of the Project

This Matura project investigates and evaluates the arithmetic capabilities of different neural networks.

The project began with a literature review to generate a hypothesis regarding the weaknesses of neural networks in performing simple arithmetic. This literature review was submitted as the Zwischenprodukt, alongside a proof-of-concept notebook featuring a comparison of Feed-forward Neural Networks (FNNs) of different sizes.

The next step was to build a Recurrent Neural Network (RNN) and similar attention-based RNNs to investigate their arithmetic capabilities and compare them to those of the FNN using a benchmark.

The benchmark's baseline was defined to be the performance of a basic FNN's performance on different, but roughly still similar arithmetic tasks.

Afterwards, the same was done for the transformer type of neural network model. Here, their exact functionality was thuroughly investigated, because of their unique architectures.

Lastly a simillar workflow was repeated for some bigger, pre-trained models. And finally all the findings were collected and evaluated as a whole.

0.2 Introduction to this document

The goal of this document is assisting reproducability and showing how the findings discussed in the other document have been obtained.

All of the code written for this project is available in the github reporsitory: https://github.com/AntonStantan/matura

In this project all of the code is written in Python-notebooks (Jupyter Lab). The preffered library used was tensorflow keras.

Most of the models were trained locally on a Nvidia GPU device: *Nvidia Jetson Orin Nano Super Developer Kit*

Figure 1: You can see the aformentioned Nvidia Jetson device booting up.

Contents

1 Feed-forward Neural Networks (FNN)

For details on how a FNN works please refer to the section two in the literature study.
This section refers to the /FNN directory in the github reporsitory.
There are two notebooks here: FNN1 and FNN2.

1.1 Train and Test data

Defining the train data; The decision was made to only use subtraction and addition. The arithmetic expressions were defined to consist of two operators (+ or -) and three integers $[-5, 5]$
The reason for these definitions are: + and - are the 2 simplest operators. And the decision to introduce the model to 3 numbers, in place of the more commonly used 2, was made in hopes of simplifying the transition to more numbers later on.
e.g., the first three entries are:

$$1 - -2 + 3 \qquad -2 + -3 - -5 \qquad 3 - 1 - 0$$

In total there are 1907 expressions like this in the train data.

The test data is also defined in a slightly unconventional manner. It is split up into three categories.

- Inside of the number range: Expressions just like in the train data but not inside of train data.

- Outside of the number range: The same expressions, but with numbers in the ranges $[-8, -5]$ and $[5, 8]$ e.g.,

$$-6 + 6 + 8 \qquad -7 + 6 + 7 \qquad 5 - -6 - 6$$

- Longer expressions: Expressions of different lengths. Specifically, there are between 2 and 8 numbers inside of the $[-5, 5]$ range. e.g.,

$$-5 + 1 \qquad 3 + -1 + 4 + -2 + -4 \qquad -2 + 1 + 5 + -5 - -2 + -1 - 2 - 5$$

1.2 Training a Neural Network Using Tensorflow

This subsection will show how the models used in this project were first defined and then trained with tensorflow on the example of a simple FNN.

To start of we will import the necessary libraries.

```
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras.layers import Dense, Layer, Dropout
from tensorflow.keras import layers, Sequential
from tensorflow.keras.layers import PReLU
```

And then we have to make a dataset out of the train and validation data discussed in the previous subsection. Let's use batches of 32. Validation data is like the In-Range-test-data, except there aren't as many expressions.

```
batch_size = 32
train_dataset = tf.data.Dataset.from_tensor_slices((x_train, y_train))
.shuffle(len(x_train)).batch(batch_size)
val_dataset = tf.data.Dataset.from_tensor_slices((x_val, y_val))
.batch(batch_size)
```

We can now define the model using tf.keras.Sequential. The model's architecture is clearly visible. In this example the model has two dense layers with 64 neurons each.
The activation function used is PReLU, as this is the one, which was the most promising in Trask et al., 2018.
Drop-out is included to prevent overfitting. In most models used in this project it wasn't necessary.
As you can see, the input-shape has to be defined, when defining the model.
Additionally, please notice how the output layer only consists of a single neuron with a linear activation function. This means the model we just created is a regression model. This is similar to not having a decoder.

```
input_shape = (15,)
model = Sequential([
    keras.Input(shape = input_shape),      #input

    Dense(64),                             #first dense layer
    PReLU(),                               #PReLU activation function
    Dropout(0.1),                          #dropout layer

    Dense(64),                             #second dense layer
    PReLU(),
    Dropout(0.1),

    Dense(1, activation='linear')          #output layer
])
```

The next step is to compile the model, by choosing an optimizer and loss calculation e.g., in our case Mean Squared Error (MSE)

```
model.compile(optimizer="adam", loss="mse")
```

The last step remaining is to fit the model on some data. We will be fitting our model on the previously defined train and validation data. The training process will take 200 epochs to complete or it might be aborted preemtively if the model starts to overfit and early_stopping is triggered.

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```
model.fit(
    train_dataset,
    validation_data=val_dataset,
    epochs=200,
    callbacks=[early_stopping],
    verbose=1
)
```

1.3   FNN1 and FNN2 Notebooks

In this project two notebooks with FNNs have been created. FNN1 and FNN2.
In FNN1 a simple FNN was created, it's performance was evaluated and FNNs
of different sizes have been compared against eachother in a heatmap. It is
noteworthy, that the models here have been used with a bootstrap, meaning
multiple models with the same sizes were trained and then used to give one
combined prediction. This was done to reduce noise. In later notebooks this
will not be the case, as this makes it more difficult to accurately evaluate a
model.

FNN2 includes a model with hyperparameters (in this case the number of neu-
rons, the number of layers and whether or not to use dropout) chosen by the
keras-tuner. This is simply put an automatization: It picks out models with
different hyperparameters, trains them and compares their performance on val-
idation data. The model with the best-performing hyperparameters will be
chosen as the best model.
The model in FNN2 is evaluated inside of that notebook and it's benchmark is
calculated.

1.4   The Benchmark

To calculate the benchmark a model is evaluated on 4 categories: The test data
inside of the number range, outside of the number range, longer expressions and
a relative MSE of the test data with numbers outside of the range. Refer to the
code below:

```
benchmark = 0
benchmark += baseline_deviation / (meanDiff_InRange**2) / 4
benchmark += baseline_out_deviation / (meanDiff_OutRange**2) / 4
benchmark += baseline_long_deviation / (meanDiff_LongRange**2) / 4
benchmark += baseline_relError / (meanDiff_OutRelRange**2) / 4
print(f"Benchmark: {benchmark}")
```

The usage of a relative error punishes mistakes on "simpler" expressions and
is less harsh on more "difficult". Expressions whose absolute result is small,
are easier for a neural network to solve, while a larger absolute result is more
difficult to calculate.

For the same reason two more adjustments have been made: Not all expressions outside the number range, and not all longer expressions were used.
For longer expressions only expressions with 4 numbers were used.
For expressions with numbers outside of the range, the expression was only used if the absolute values of all three numbers added up to 22.
These subsets were chosen because of their reasonable MSE of around 10 each. This, aswell as the inlusion of the relative MSE is done in hopes of bringing the benchmarks of different models closer together and to increase the linearity between them. This makes the benchmark more comfortable to work with.
The baseline values are defined to be of a FNN model with 30 neurons and two dense layers. It is trained over the period of 200 epochs with early_stopping enabled.
As clearly observable in the code for calculating the benchmark, using this formula defines a model with the same performance as the baseline model to have a benchmark of 1. Models performing worse or better on the test data yield scores below or above 1, respectively.

1.5   Drop-Out

When introducing a Drop-Out with an industry standard value of 0.3; contrary to the expectation of reducing over-fitting, which in some way is present, as the models aren't able to generalize beyond the training range, this has a negative effect on the model. The MSEs of models with Drop-out are higher then, the ones of the previous models without drop-out.

2   Recurrent Neural Network (RNN)

Recurrent Neural Networks (RNNs) work similar to FNNs with one key difference: There is a vector called the hidden-state. This vector contains information about previous inputs. The hidden-state of the previous time-step, in addition to the input of the current time-step, is fed into a model which computes the hidden-state of the present time-step. The output of each time-step is calculated by feeding the respective hiddenstate to a model.

2.1   Numerical Visualization of a RNN:

Let:

- x_t: Input at time step t

- h_t: Hidden state at time step t

- y_t: Output at time step t

- W_{xh}: Weight matrix connecting input to hidden state

- W_{hh}: Weight matrix connecting previous hidden state to current hidden state (recurrent weights)

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- W_{hy}: Weight matrix connecting hidden state to output

- b_h: Bias vector for the hidden layer

- b_y: Bias vector for the output layer

- σ: Activation function (commonly tanh or ReLU for the hidden state)

- σ_{out}: Activation function for the output (e.g. softmax for classification, or linear in our case of regression)

$$h_t = \sigma(W_{xh}x_t + W_{hh}h_{t-1} + b_h)$$

$$y_t = \sigma_{out}(W_{hy}h_t + b_y)$$

2.2 RNN0

The RNN0 notebook includes a model built with the aforementioned architecture. A RNN model consisting of 2 dense layers with 50 neurons each:

```
model = keras.Sequential([
    keras.Input(shape=(input_shape, 1)),
    keras.layers.SimpleRNN(50, return_sequences=True),
    keras.layers.PReLU(),
    keras.layers.SimpleRNN(50),
    keras.layers.PReLU(),
    keras.layers.Dense(1, activation = "linear")
])
```

Notice return_sequences = True. This is necessary for a subsequent layer. By default this is set to false, because RNNs are frequently used with just one layer, for applications like Natural Language Processing (NLP) or Time series analysis like the stock market.
Useful sources for the creation of the first RNN prototype:

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References

Trask, A., Hill, F., Reed, S., Rae, J., Dyer, C., & Blunsom, P. (2018). Neural arithmetic logic units. https://arxiv.org/abs/1808.00508