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Computational Solid State Physics

Problem 5 - ANN

Description

Create an artificial neural network (ANN) to solve the X-OR problem, using the back-propagation method. The input level consists of 2 nodes, the hidden level also consists of 2 nodes and the output level consists of one node, as in the diagram. The initial weights of the links should be randomly selected from a uniform distribution w ∈(-1.1). The maximum acceptable error in the output ($\frac{1}{2}|output - target|^2$) to be considered 0.01 and the learning rate η= 0.2. The maximum number of training cycles (epochs) will be 10000. After the network training is finished, the computer code should write the final weights of all connections in a file.

Solution

This problem was solved with a `python` script, which implements the XOR gate algorithm required. The code can be found in the appendix or on github.

The python script is discussed below.

Discussion of python script

Initialization

Nodes and layers are implemented as python `dataclass` classes, which facilitate access to automatic activation of nodes/layers, and other features. In this implementation layers consist of nodes, which offers modularity in adding, extending and generally future-proofing the code. An example of the functionality of the above is i.e. when the `u` or `y` value of a Node is changed:

```python
#...
    def __setattr__(self, attr, value):
        # When `u` value is changed, update `y` and `delta`
        if attr == "u":
            self.__dict__[attr] = value
            self.__dict__["y"] = self.actf()
            self.__dict__["delta"] = self.actf2()
        elif attr == "y":
            # When `y` is changed, update `delta`
            self.__dict__["delta"] = self.actf2()
        super().__setattr__(attr, value)
#...
```

The `Neural` class implements the `run` method which initializes the network for a list of inputs. It makes a "forward pass" and then backpropagates until all outputs are "trained" (their mean squared loss is less than the targeted error). The layer initialization method is the following:

```python
#...
    def init_layers(self, in1, in2):
        self.inp = Layer([Node(), Node()])
        self.inp.set("y", in1, in2)
        self.target = np.logical_xor(in1, in2)
        self.hid = Layer([Node(), Node()])
        self.out = Layer([Node()])
#...
```

It would be simple to add layers this way.

Forward pass

The method that implements the forward pass is the following:

```python
#...
    def forward_pass(self):
        # Calculate hidden layer activation
        hid_u = (self.inp.get("y") @ self.hid_w + self.hid_bias).flatten()
        self.hid.set("u", *hid_u)
        # Calculate out layer activation
        out_u = (self.hid.get("y") @ self.out_w.T + self.out_bias).flatten()
        self.out.set("u", *out_u)

        self.error = 0.5 * np.power(self.out.get("y") - self.target, 2)
#...
```

Here, the new `u` values are calculated through multiplying the layer's `y` values with the corresponding weights and adding the biases. The layers are then automatically activated as discussed previously.

Back-propagation

The method that implements back-propagation is the following:

```python
#...
    def backpropagate(self):
        # Calculate deltas
        out_d = (self.out.get("delta") * (self.target - 
self.out.get("y"))).flatten()
        self.out.set("delta", out_d)
        hid_d = (self.hid.get("delta") * (out_d @ self.out_w)).flatten()
        self.hid.set("delta", *hid_d)

        # Update hidden weights and bias
        self.inp.set("delta", [0, 0])
        hid_w_upd = self.inp.get("y").T @ self.hid.get("delta") * self.lr
        self.hid_w += hid_w_upd
        hid_b_upd = self.hid.get("delta") * self.lr
        self.hid_bias += hid_b_upd

        # Update output weights and bias
        out_w_upd = self.hid.get("y") * self.out.get("delta") * self.lr
        self.out_w += out_w_upd
        out_b_upd = self.lr * self.out.get("delta")
        self.out_bias += out_b_upd

#...
```

Deltas are calculated for the output and hidden layer and then the weights are updated. Input layer's deltas are set to 0.

Miscellanous

The class implements a `write_to_file` function which writes the results to a txt file following the convention: `trained_weights<learning_rate>-<max_error>.txt`. Additionaly, a `run_w_check` method is implemented which, after the network is trained makes one forward pass witch each input and outputs the results of the pass (target vs output for each input).

Results

Results and graphs are presented below, showcasing the network's training for different learning rates and max error thresholds.

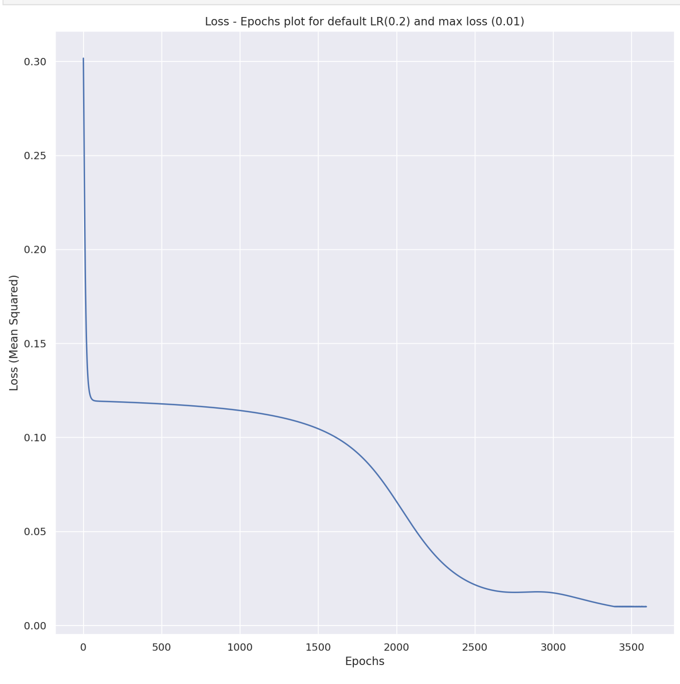
In [1]:

```python
# Basic -> LR = 0.2 ; Max Loss = 0.01
from src.neural_n import Neural
from matplotlib import pyplot as plt
import seaborn as sns

sns.set_theme()

neur = Neural()
neur.run_w_check()
```

```
Trained after 3595 epochs with target mean squared loss 0.0100 and LR=0.20
Checking for [(0, 0)]
Target: 0 Out 0.14119647686790823
Checking for [(0, 1)]
Target: 1 Out 0.8586513363776396
Checking for [(1, 0)]
Target: 1 Out 0.858592445117178
Checking for [(1, 1)]
Target: 0 Out 0.1396240702431677
```

In [2]:

```python
fig, ax = plt.subplots(figsize=(12, 12), dpi=200)

ax.plot(list(neur.track_error))
ax.set_xlabel("Epochs")
ax.set_ylabel("Loss (Mean Squared)")
ax.set_title("Loss - Epochs plot for default LR(0.2) and max loss (0.01)")
plt.show()
```



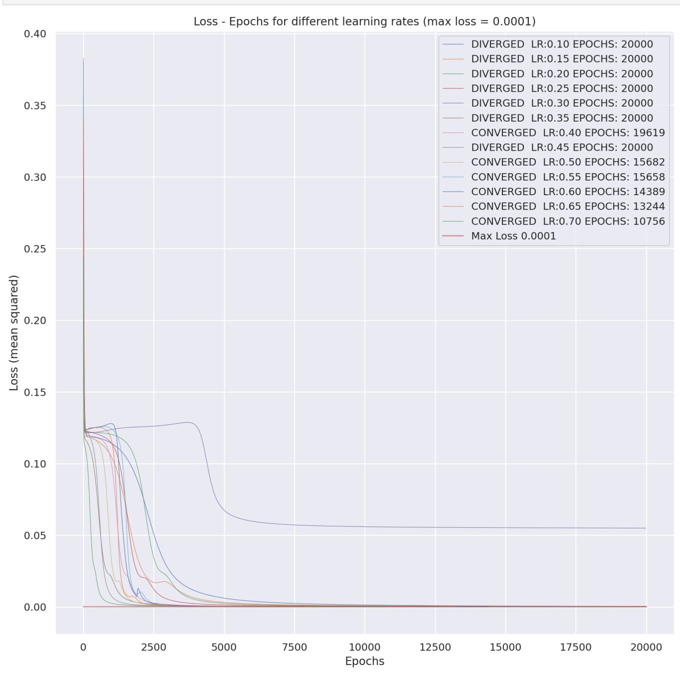
In [3]:

```python
import numpy as np

MAX_EPOCH = 20000
MAX_ERROR = 0.0001
LRs = np.arange(0.1, 0.71, 0.05)
neurs = [Neural(lr=l, max_error=MAX_ERROR, epochs=MAX_EPOCH) for l in LRs]
losses = []
for n in neurs:
    n.run_epochs()
    losses.append(n.track_error)
```

```
Neural Network did not converge after 19999 epochs with LR=0.10  and max squared loss 
0.0001. Current error : 0.1289
Neural Network did not converge after 19999 epochs with LR=0.15  and max squared loss 
0.0001. Current error : 0.0003
Neural Network did not converge after 19999 epochs with LR=0.20  and max squared loss 
0.0001. Current error : 0.0002
Neural Network did not converge after 19999 epochs with LR=0.25  and max squared loss 
0.0001. Current error : 0.0002
Neural Network did not converge after 19999 epochs with LR=0.30  and max squared loss 
0.0001. Current error : 0.0565
Neural Network did not converge after 19999 epochs with LR=0.35  and max squared loss 
0.0001. Current error : 0.0001
Trained after 19618 epochs with target mean squared loss 0.0001 and LR=0.40
Neural Network did not converge after 19999 epochs with LR=0.45  and max squared loss 
0.0001. Current error : 0.1364
Trained after 15681 epochs with target mean squared loss 0.0001 and LR=0.50
Trained after 15657 epochs with target mean squared loss 0.0001 and LR=0.55
Trained after 14388 epochs with target mean squared loss 0.0001 and LR=0.60
Trained after 13243 epochs with target mean squared loss 0.0001 and LR=0.65
Trained after 10755 epochs with target mean squared loss 0.0001 and LR=0.70
```

In [4]:

```python
from matplotlib.pyplot import cm

fig, ax = plt.subplots(figsize=(12, 12), dpi=200)

for idx, lr in enumerate(LRs):
    data = losses[idx]
    if len(data) == MAX_EPOCH:
        txt = "DIVERGED "
    else:
        txt = "CONVERGED "


    ax.plot(data, label=f"{txt} LR:{lr:.2f} EPOCHS: {len(data)}", linewidth=.5)

ax.plot([0, 20000], [MAX_ERROR, MAX_ERROR], label=f"Max Loss {MAX_ERROR}", alpha=0.5)
ax.legend()
ax.set_title(f"Loss - Epochs for different learning rates (max loss = {MAX_ERROR})")
ax.set_ylabel("Loss (mean squared)")
ax.set_xlabel("Epochs")
plt.show()
```



Discussion of graphs

For a much tigher loss threshold of `0.0001` a higher learning rate appears to be more efficient as it converges (faster) to a trained network. Learning rates must be carefully selected, as a big learning rate might converge faster but at the risk of chaotic behaviour which might end up diverging. Small learning rates usually converge but a slower pace than a big one.

Appendix

The python script that implements the ANN: `neural_n.py`

```python
import numpy as np

from dataclasses import dataclass, field
from typing import List

rng = np.random.default_rng(4385)


class Neural:
    def __init__(self, max_error=0.01, lr=0.2, epochs=10000):
        self.max_error = max_error
        self.error = None
        self.target = None
        self.lr = lr  # Learning rate
        self.trained = True
        self.track_error = []
        self.epochs = epochs

        self.hid_w = rng.uniform(size=(2, 2))
        self.out_w = rng.uniform(size=(1, 2))

        self.hid_bias = rng.uniform(size=(1, 2))
        self.out_bias = rng.uniform()

    def init_layers(self, in1, in2):
        self.inp = Layer([Node(), Node()])
        self.inp.set("y", in1, in2)
        self.target = np.logical_xor(in1, in2)
        self.hid = Layer([Node(), Node()])
        self.out = Layer([Node()])

    def forward_pass(self):
        # Calculate hidden layer activation
        hid_u = (self.inp.get("y") @ self.hid_w + self.hid_bias).flatten()
        self.hid.set("u", *hid_u)
        # Calculate out layer activation
        out_u = (self.hid.get("y") @ self.out_w.T + self.out_bias).flatten()
        self.out.set("u", *out_u)

        self.error = 0.5 * np.power(self.out.get("y") - self.target, 2)

    def backpropagate(self):
        # Calculate deltas
        out_d = (self.out.get("delta") * (self.target - 
self.out.get("y"))).flatten()
        self.out.set("delta", out_d)
        hid_d = (self.hid.get("delta") * (out_d @ self.out_w)).flatten()
        self.hid.set("delta", *hid_d)

        # Update hidden weights and bias
        self.inp.set("delta", [0, 0])
        hid_w_upd = self.inp.get("y").T @ self.hid.get("delta") * self.lr
        self.hid_w += hid_w_upd
        hid_b_upd = self.hid.get("delta") * self.lr
        self.hid_bias += hid_b_upd

        # Update output weights and bias
        out_w_upd = self.hid.get("y") * self.out.get("delta") * self.lr
        self.out_w += out_w_upd
        out_b_upd = self.lr * self.out.get("delta")
        self.out_bias += out_b_upd

    def write_to_file(self):
        with open(f"trained_weights{self.lr}-{self.max_error}.txt", "w+") as 
f:
            np.savetxt(f, self.hid_w)
            np.savetxt(f, self.hid_bias)
            np.savetxt(f, self.out_w)
            np.savetxt(f, self.out_bias)

    def run(self):
        inputs = np.array([[0, 0], [0, 1], [1, 0], [1, 1]])
        self.trained = True
        for inpt in inputs:
            self.init_layers(*inpt)
            self.forward_pass()
            # Track [0, 0] input error
            if (inpt == [0, 0]).all():
                self.track_error.append(self.error[0])
            if self.error < self.max_error:
                continue
            self.trained = False
            self.backpropagate()

    def run_epochs(self):
        for i in range(self.epochs):
            self.run()
            if self.trained == True:
                print(
                    f"Trained after {i} epochs with target mean squared loss 
{self.max_error:.4f} and LR={self.lr:.2f}"
                )
                self.write_to_file()
                return
        print(f"Neural Network did not converge after {i} epochs with LR=
{self.lr:.2f} "
              f" and max squared loss {self.max_error}. Current error : 
{self.error[0][0]:.4f}")

    def run_w_check(self):
        self.run_epochs()
        inputs = np.array([[0, 0], [0, 1], [1, 0], [1, 1]])

        for inpt in inputs:
            self.init_layers(*inpt)
            self.forward_pass()
            print(f"Checking for [{(*inpt,)}]")
            print(f"Target: {int(self.target)} Out {self.out.nodes[0].y}")


@dataclass(eq=False)
class Node:
    u: float = 0
    y: float = field(init=False)
    delta: float = field(init=False)

    def __post_init__(self):
        self.y = self.actf()
        self.delta = self.actf2()

    def __setattr__(self, attr, value):
        # When `u` value is changed, update `y` and `delta`
        if attr == "u":
            self.__dict__[attr] = value
            self.__dict__["y"] = self.actf()
            self.__dict__["delta"] = self.actf2()
        elif attr == "y":
            # When `y` is changed, update `delta`
            self.__dict__["delta"] = self.actf2()
        super().__setattr__(attr, value)

    def actf(self):
        # Activation function
        return 1 / (1 + np.exp(-self.u))

    def actf2(self):
        return self.y * (1 - self.y)


@dataclass(eq=False)
class Layer:
    nodes: List[Node]

    def get(self, attr):
        return np.array([getattr(n, str(attr)) for n in self.nodes]).reshape(
            1, len(self.nodes)
        )

    def set(self, attr, *args):
        if type(args[0]) == np.array or type(args[0]) == list:
            # Untuple if np.array or list
            (args,) = args
        for i, arg in enumerate(args):
            setattr(self.nodes[i], str(attr), arg)


if __name__ == "__main__":
    Neural().run_w_check()
```