Understanding Autograd and Neural Network in PyTorch

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In [89]:
```
from datetime import datetime
print(datetime.today().strftime('%Y-%m-%d'))
```

```
2026-01-30
```

Introduction

At Wikipedia, Neural network (NN) is described as a computational model inspired by the structure and functions of biological neural networks. Artificial neuron models that mimic biological neurons have also recently been investigated and shown to significantly improve performance. These are connected by edges, which model the synapses in the brain. Each artificial neuron receives signals from connected neurons, which processes them and sends a signal to other connected neurons. The "signal" is a real number, and the output of each neuron is in this report computed by a linear function of its inputs which is multiplied by an activation function. The strength of the signal at each connection is determined by the weights and biases of the linear function, which are updated during the learning process in order to reduce the loss. The loss is defined as the difference between the predicted output and the correct solution (called the target).

Tensors

Tensor in the computer world simply means a multidimensional array. A scalar is a zero-dimensional tensor, which is a single number.
A leaf tensor is a tensor that is a leaf (in the sense of a graph theory) of a computation graph. I will talk discuss about leafs below.

The requires_grad = True for a tensor tells PyTorch that it should remember how this tensor is used in further computations. For now, think of tensors with requires_grad=True as variables, while tensors with requires_grad=False as constants.

Leafs and requires_grad

Let's start by creating a few tensors and checking their properties requires_grad and is_leaf.

In [ ]:
```
import torch
a = torch.tensor([3.], requires_grad=True)
b = a * a

c = torch.tensor([5.])
d = c * c

print(a.requires_grad)
print(b.requires_grad)
print(c.requires_grad)
print(d.requires_grad,'\n')
print(a.is_leaf)
print(b.is_leaf)
print(c.is_leaf)
print(d.is_leaf)
```

The requires_grad=True statement tells PyTorch to

1. store all mathematical operations (addition, multiplication ...) involving a
2. store the gradient of any new tensor that is created from a

In PyTorch, leaf tensors are either

1. direct input (i.e. not calculated from other tensors) and have requires_grad=True.

Example: neural network weights that are randomly initialized. 2. do not require gradients at all, regardless of whether they are direct input or computed. These are just constants.

Hence, a is a leaf because it is an input variable, and b is not because it is a result of a multiplication. a is set to requires_grad, so b inherits this property.

c is a leaf because it is an input variable

The reason d.is_leaf is True stems from the PyTorch convention that all tensors for which requires_grad is set to False are considered leaf tensors.

All Tensors that have requires_grad = False will be leaf Tensors by convention. Mathematically, d is not a leaf (since it results from another operation, $c * c$), but gradient computation will never extend beyond it. In other words, there will not be any derivative with respect to c. This allows d to be treated as a leaf.

The requires_grad property is inherited, i.e. d has requires_grad = False which is inherited from c.

In [ ]:
```
computinga = torch.tensor([7.], requires_grad=True)
b = torch.tensor([8.], requires_grad=True)
```

In [ ]:

The grad_fn attribute

I create another tensor Q from a and b as

$$Q = a^3 - 4b \tag{1}$$

In [ ]:
```
Q = a**3 - 3*b
```

In PyTorch, tensors can have a grad_fn attribute. When a tensor is created by a mathematical operation, PyTorch keeps track of the operation that created it using the grad_fn. This is part of the computational graph, which is a directed acyclic graph (DAG).

In [ ]:
```
print(a.requires_grad)
print(b.requires_grad)
print(Q.requires_grad)
print(a.grad)
print(b.grad)
print(Q.grad_fn)
```

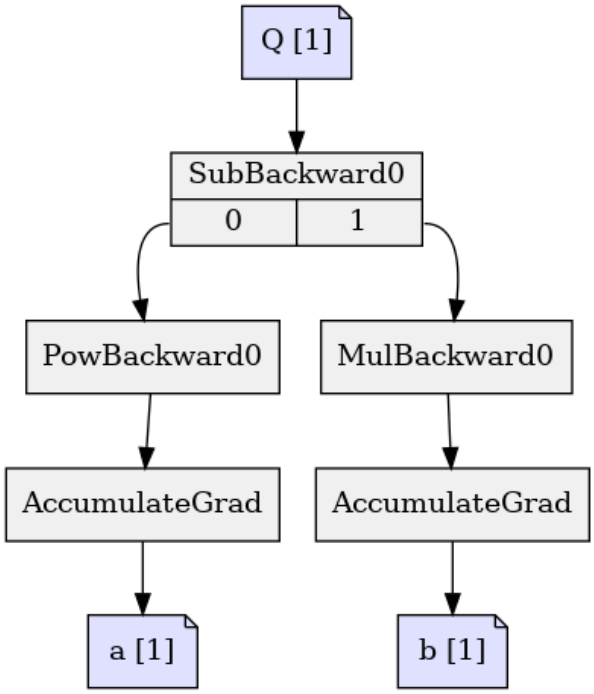
a and b are created with requires_grad=True and that attribute is inherited by Q. The tensors a.grad and b.grad are still not defined because I have not executed the .backward() command.

The grad_fn is an object that represents the operation that created the tensor. It has a backward method, which is used to compute the gradients during the backward pass. If a tensor is created by the user directly (e.g., torch.tensor(2.0, requires_grad=True)}), its grad_fn is None because it is a leaf tensor in the computational graph.

Now I will compute the gradients by a backward pass. Verify that the gradients $\partial Q/\partial a$ and $\partial Q/\partial b$ have been computed

In [ ]:
```
Q.backward()
print('dQ/da',a.grad)
print('dQ/db',b.grad)
```

The .grad_fn attribute is used to analyze the mathematical operations for Q. Below is was used to visualize the autograd graph using the agtree2dot package which can be downloaded at https://fleuret.org/francois/



Autograd graph

The figure above was generated by the code in the cell below.

In [ ]:
```
import agtree2dot
agtree2dot.save_dot(Q,
   {
    a: 'a',
    b: 'b',
    Q: 'Q',
   },
   open('./Q.dot', 'w'))
# dot -T png Q.dot -o Q.png
```

In [ ]:
```
print(Q.grad_fn)
print(Q.grad_fn.next_functions)
```

The first line (object = SubBackward0) of the output shows that Q is obtained by a subtraction i.e. $-3b$. This corresponds to the second box from the top in the graph above

The second line show the two prior operations (object = PowBackward0 and MulBackward0) which correspond to a^3 and the multiplication of 3 and b. They form two branches, 0 and 1. Branch 0 is shown below

In [ ]:
```
print(Q.grad_fn.next_functions[0][0].next_functions)
print(Q.grad_fn.next_functions[0][0].next_functions[0][0].variable)
print(Q.grad_fn.next_functions[0][0].next_functions[0][0].variable is a)
```

Line 1 shows that the variable is accumulated. The value of the variable is printed at the second line and the third line confirms that it is a. Hence, you see that branch 0 is the left branch in the graph above. Next, let's look at branch 1.

In [ ]:
```
print(Q.grad_fn.next_functions[1][0])
print(Q.grad_fn.next_functions[1][0].next_functions)
print(Q.grad_fn.next_functions[1][0].next_functions[0][0].variable)
print(Q.grad_fn.next_functions[1][0].next_functions[0][0].variable is b)
```

The first line says that it is a multiplication (of 3 and b). On the second line you see that the variable has been accumulated. The value of the variable is printed at line 3 and line 4 confirms that the variable is indeed b. Branch 1 corresponds to the right branch in the graph above.

Let's introduce another variable, P

$$Q = a^3 - 3b, \quad P = Q^2 \quad \Rightarrow \quad P = a^6 - 6a^3b + 9b^2 \tag{2}$$

In Python it reads

In [ ]:
```
a = torch.tensor([2.], requires_grad=True)
b = torch.tensor([8.], requires_grad=True)
Q = a**3 - 3*b
P = Q**2
```

The gradient of P with respect to a and b is

$$\partial P/\partial a = \frac{\partial P}{\partial Q}\frac{\partial Q}{\partial a} = 6a^5 - 18a^2b = -384, \quad \partial P/\partial b = \frac{\partial P}{\partial Q}\frac{\partial Q}{\partial b} = -6a^3 + 18b = 96$$

Note that Pytorch uses the chain-rule when computing the gradients above.

Verify that the Pytorch command backward() gives the correct answer.

In [ ]:
```
P.backward()
print('dP/da =',a.grad)
print('dP/db =',b.grad)
```

Note that the command P.backward() deletes all intermediate gradients. If you want the keep $\frac{\partial P}{\partial Q} = 2Q = 2a^3 - 6b = -32$ you must use the command .retain_grad() command, i.e.

In [ ]:
```
Q = a**3 - 3*b
P = Q**2
Q.retain_grad()
a.grad = None # in order to avoid accumulation when  P.backward() is calle
b.grad = None # in order to avoid accumulation when  P.backward() is calle
P.backward()
print('dP/dQ =',Q.grad)
print('dP/da =',a.grad)
print('dP/db =',b.grad)
```

Solve the equation $P = a^6 - 6a^3b + 9b^2 = 0$ using autograd

Let's solve the equation $P = 0$ using autograd.

In [ ]:
```
a = torch.tensor([2.], requires_grad=True)
b = torch.tensor([8.], requires_grad=True)
Q = a**3 - 3*b
P = Q**2
# Define the variables which should be solved for
list_parameters = [a,b]

#under-relaxation
alpha = 0.02

# choose optimizer
optimizer = torch.optim.Adam(params=list_parameters, lr=alpha)

# max number of iterations
max_iter = 200

for n in range(max_iter):

   optimizer.zero_grad()  # set a.grad and b.grad to zero
   P.backward()           # compute dP/da and dP/db (backward step)
   optimizer.step()       # update a and b with gradient descent: a = a -
   Q = a**3 - 3*b         # compute new Q (forward step)
   P = Q**2               # compute new P (forward step)

   if n%50 == 0:
      print(f'iteration no: {n}, P: {P.item():.2e}, a: {a.item():.2e}, b:
```

autograd finds the solution $a = 2.79$ and $b = 7.26$ which gives $P \leq 1.2 \cdot 10^{-4}$.

Find the coefficients of a polynomial satisfying y = sin(x)

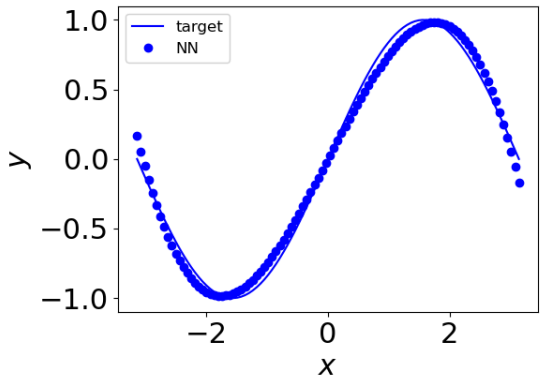
Consider the polynomial $y(x) = ax + bx^2 + cx^3$. I will use autograd to find the coefficients a, b and c that satisfies $y = \sin(x)$. The x vector is set to 100 equidistant points from $-\pi$ to π , and the coefficients are initialized to zero. Note that the coefficients must be defined by requires_grad=True since they will be updated by autograd.

In [ ]:
```
import torch
import math
import matplotlib.pyplot as plt
x = torch.linspace(-math.pi, math.pi, 100)
y = torch.sin(x)

a = torch.tensor(0.,requires_grad=True)
b = torch.tensor(0.,requires_grad=True)
c = torch.tensor(0.,requires_grad=True)
d = torch.tensor(0.,requires_grad=True)
```

I will create a loop as in the cell above

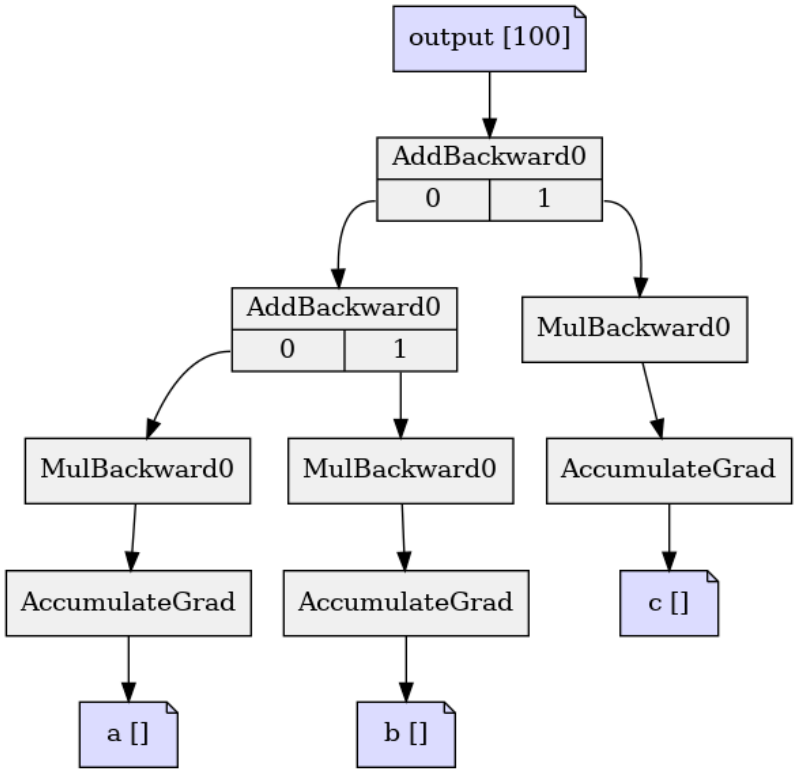
In [ ]:
```
alpha = 1e-5
max_iter = 4000
for n in range(max_iter):
    y_pred = a * x + b * x ** 2 + c * x ** 3 # compute new y (forward step
    L = (y_pred - y).pow(2).sum()            # compute loss
    a.retain_grad()                          # retain a, b and c. This is
    b.retain_grad()                          # since the backward command
    c.retain_grad()                          # delete a.grad, b.grad and c
    L.backward()                             # compute dL/da, dL/db, dL/dc
    if n % 1000 == 0:
        print(f"\nEpoch {n+1}, L: {L.item():.2e}, a.grad: {a.grad:.2e},  b
    # update weights using gradient descent.
    a = a - alpha * a.grad
    b = b - alpha * b.grad
    c = c - alpha * c.grad
    # Set the the gradients after updating weights
    a.grad = None
    b.grad = None
    c.grad = None

print(f'\na = {a.item():.2e}, b = {b.item():.2e}, c = {c.item():.2e}')
```

The figure below shows predicted y v. x



y v. x

The autograd graph is seen below.



Autograd graph for computing a, b and c

Predict the sinus curve with Neural Network (NN)

I will predict the sinus curve with NN. The code is given below.

In [ ]:
```
import torch
import math
import sys
import matplotlib.pyplot as plt
from torch import nn
import agtree2dot

x = torch.linspace(-math.pi, math.pi, 20) # create x
y = torch.sin(x)

X = x.view(-1,1)                          #makes the shape X[N,1]
Y = y.view(-1,1)

# Build the model:
class NN_sinus(nn.Module):
    def __init__(self):
        super().__init__()
        self.input   = nn.Linear(1, 10)  #axis 0: number of inputs
        self.hidden1 = nn.Linear(10, 10)
        self.hidden2 = nn.Linear(10, 1)  #axis 1: number of outputs

    def forward(self, a0):
        a1 = nn.functional.relu(self.input(a0))
        a2 = nn.functional.relu(self.hidden1(a1))
```

```
        a3 = self.hidden2(x2) #output

        return a3

# Create the model
torch.manual_seed(42)  # the same initial weights and seed are created eve
model = NN_sinus()

# Define the loss function and the optimizer
loss_fn = nn.MSELoss()
# learning_rate = 0.0001
learning_rate = 0.001
# choose optimizer
optimizer = torch.optim.Adam(params = model.parameters(), lr = learning_ra

max_iter = 1000
for n in range(max_iter):
  y_pred = model(X)     # predict new y (forward step)
  L = loss_fn(y_pred, Y)# compute the loss, L,  i.e. difference between ta
  optimizer.zero_grad() # set all gradients to zero,  dL/dw_1=0, dL/db_1=0
  L.backward()          # compute the gradient of L w.r.t. all w and b, i.
  optimizer.step()      # update w and b using gradient descent, i.e. w_1=
  if n % 200 == 0:      # print every 200 iteration
     print(f'iter: {n}, L: {round(L.item(), 6)}')
```

1. The grid is created with 20 points
2. The NN_sinus model is created in with two hidden layers (hidden1 and hidden2)
3. and ten neurons (def __init__(self):)
4. A slightly smaller (for visibility)

model with two hidden layers and three neurons is presented below.

5. In the forward step, the nn.functional.relu(a_0) is used. It simply takes the input argument, $a_0 = x_0$, multiplies

it with a weight, w, adds a bias, b, and the ReLU actuator, s, is applied (see the activation functions below). The input, a_1, to the top neural in the first hidden layer is then $a_1 = s\{w_0 a_0 + b_0\}$. The expression in curly parenthesis is the arument in the ReLU activation function. The forward step in the simplified model in the graph below is computed as follows.

First hidden layer.

$$
\begin{aligned}
a_1^{(1)} &= s\left\{w_1^{(0)} a_1^{(0)} + b_1^{(0)}\right\} \\
a_2^{(1)} &= s\left\{w_2^{(0)} a_2^{(0)} + b_2^{(0)}\right\} \\
a_3^{(1)} &= s\left\{w_3^{(0)} a_3^{(0)} + b_3^{(0)}\right\}
\end{aligned}
$$

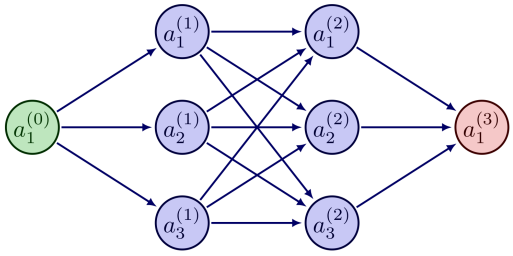
Second hidden layer.

$$a_1^{(2)} = s\left\{w_1^{(1)}a_1^{(1)} + b_1^{(1)} + w_2^{(1)}a_2^{(1)} + b_2^{(1)} + w_3^{(1)}a_3^{(1)} + b_3^{(1)}\right\}$$
$$a_2^{(2)} = s\left\{w_2^{(1)}a_1^{(1)} + b_1^{(1)} + w_2^{(1)}a_2^{(1)} + b_2^{(1)} + w_3^{(1)}a_3^{(1)} + b_3^{(1)}\right\}$$
$$a_3^{(2)} = s\left\{w_3^{(1)}a_1^{(1)} + b_1^{(1)} + w_3^{(1)}a_2^{(1)} + b_2^{(1)} + w_3^{(1)}a_3^{(1)} + b_3^{(1)}\right\}$$

Output.

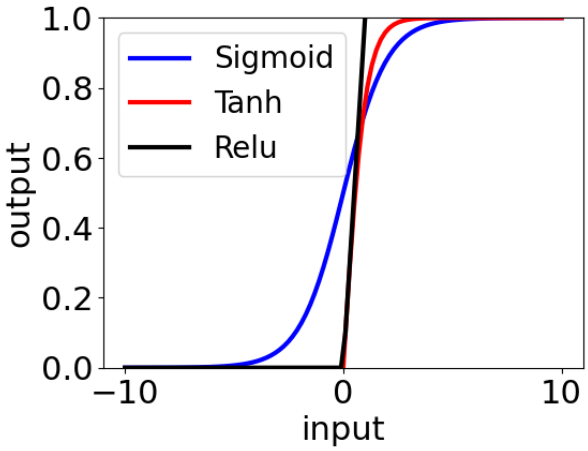
$$a_3^{(3)} = \left\{w_3^{(2)}a_1^{(2)} + b_1^{(2)} + w_3^{(2)}a_2^{(2)} + b_2^{(2)} + w_3^{(2)}a_3^{(2)} + b_3^{(2)}\right\} \equiv Y$$

where $a_3^{(3)}$ is returned as the predicted y, i.e. y_{pred}.



Neural network. Two hidden layer which each have three neurons denoted by circles. The vectors between the neurons represent connections. Input: $a_1^{(0)} = x$; output: $a_1^{(3)} = y$

An activation function is the function which enables neural network to learn complex (non-linear) relationships by transforming the output of the previous layer. Without activation functions, neural network can only learn linear relationships. Three common activation functions are shown below.



Different activation functions. ReLU $= \max(0, x)$; Tanh $= \tanh(x)$; Sigmoid $= (1 + \exp(-x))^{-1}$.

In [ ]:

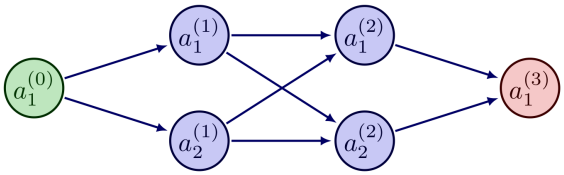
Predict a straight line using NN

In order to better understand the forward step in NN, I will write a Python script without using PyTorch's activators and torch.nn.functional. I start be creating x and y.

In [ ]:
```
import torch
from torch import nn

x = torch.linspace(0, 1, 5)
y = 4*x

X = x.view(-1,1)
Y = y.view(-1,1)
```

Since I will predict a straight line, $y = x$, I don't need any activator. The NN model is built with the code below.

In [ ]:
```
class NN_line(nn.Module):
    def __init__(self):
        super().__init__()
        self.input   = nn.Linear(1, 2)  #axis 0: number of input
        self.hidden1 = nn.Linear(2, 2)
        self.hidden2= nn.Linear(2, 1)  #axis 1: number of output
        self.input.bias.data.normal_(0.,1)
        self.input.weight.data.normal_(0.,1)
        self.hidden1.bias.data.normal_(0.,1)
        self.hidden1.weight.data.normal_(0.,1)
        self.hidden2.bias.data.normal_(0.,1)
        self.hidden2.weight.data.normal_(0.,1)
    def forward(self, x0):
        x1 = model.input.bias.view(-1,1) +  model.input.weight@x0.T
        x2 = model.hidden1.bias.view(-1,1) + model.hidden1.weight@x1
        output_temp = model.hidden2.bias.view(-1,1) + model.hidden2.weight
        output = output_temp.view(-1,1)
        return output
```



Neural network for the straight line. Two hidden layer which each have two neurons denoted by circles.

As can be seen in the figure above, I use two hidden layers and two neurons. All weights and biases are initialized as normal distribution with mean equal to zero and standard deviation equal to 1. There is one input (axis 0 of input) and one output (axis 1 of hidden layer no 2).The forward step is coded as above.

The commands .view(-1,1) and .T are used to reshape vectors between row and column vectors. The symbol '@' denotes matrix multiplication. The shape of

the weights biases are given below.

$$\begin{aligned}\text{input.bias.view}(-1,1) &= \text{torch.Size}([2,5])\\ \text{input.weight} &= \text{torch.Size}([2,1])\\ \text{x0.T} &= \text{torch.Size}([1,5])\\ \text{output, x1} &= \text{torch.Size}([2,5])\end{aligned}$$

Above: input.bias.view(-1,1)[2,5] added to matrix multiplaction of input.weight[2,1] and x0.T[1.5] which gives x1[2.5]. Note that the size of input.bias.view(-1,1) in the Python code really is [2,1] but Python takes care of this.

$$\begin{aligned}\text{x1} &= \text{torch.Size}([2,5])\\ \text{hidden1.bias.view}(-1,1) &= \text{torch.Size}([2,5])\\ \text{hidden1.weight} &= \text{torch.Size}([2,2])\\ \text{output, x2} &= \text{torch.Size}([2,5])\end{aligned}$$

Above: hidden1.bias.view(-1,1)[2,5] added to matrix multiplaction of hidden1.weight[2,2] and x1[2.5] which gives x1[2.5]. Regarding size of hidden1.bias.view(-1,1) in Python code, see comment above.

$$\begin{aligned}\text{x2} &= \text{torch.Size}([2,5])\\ \text{hidden2.bias.view}(-1,1) &= \text{torch.Size}([1,5])\\ \text{hidden2.weight} &= \text{torch.Size}([1,2])\\ \text{output} &= \text{torch.Size}([1,5])\end{aligned}$$

Above: hidden2.bias.view(-1,1)[1,5] added to matrix multiplaction of hidden1.weight[1,2] and x2[2.5] which gives output[1.5]. Regarding size of hidden2.bias.view(-1,1) in Python code, see comment above.

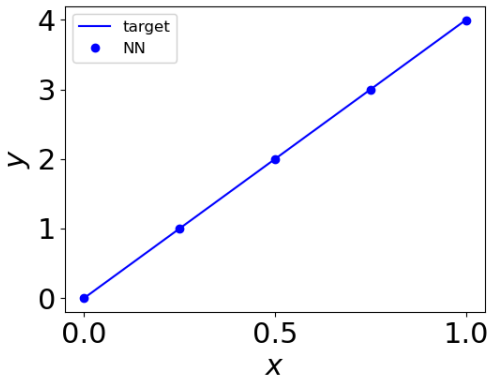
Note that the weights and biases have the same values at all x points.

The iteration loop to converge the NN model is given below (it is the same as above).

In [ ]:
```
# Create the model
torch.manual_seed(42)
model = NN_line()
# Define the loss function and the optimizer
loss_fn = nn.MSELoss()
# under-relaxation
alpha = 0.001
optimizer = torch.optim.Adam(params = model.parameters(), lr = alpha)

max_iter = 1000
for n in range(max_iter):
    y_pred = model(X)
    loss = loss_fn(y_pred, Y)
    optimizer.zero_grad()
    loss.backward()
```

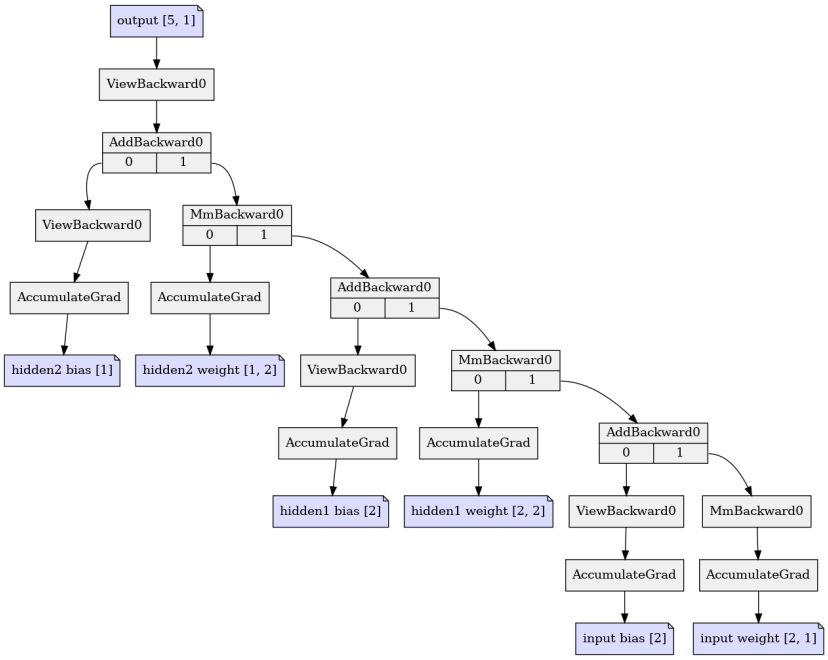
```
    optimizer.step()
    if n % 200 == 0:
      print(f'Iteration: {n}, loss: {round(loss.item(), 6)}')
```

The figure below shows predicted $y = 4$



$$y = 4x$$

The autograd graph is seen below.



Autograd graph for $y = 4x$

References

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