PINN Exercise!

How to put boundary condition in a loss funcion...

Solve the following problem with a PINN

$$\begin{cases} u'' = \cos(\pi x) & \text{in } (0,2), \text{ second derivatives} \\ u'(0) = 3 & \text{Neuman boundary condition} \\ u(2) = 0. \end{cases}$$

Take inspiration from the exercises we have done in class.

In this case, the exact solution is

$$u(x) = 3(x-2) - \frac{1}{\pi^2}(\cos(\pi x) - 1).$$

In [1]:
```
#### starting stuff ####

import torch
import torch.nn as nn
from torch.autograd import Variable

import numpy as np
```

In [ ]:
```
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.input_layer = nn.Linear(1,5)
        self.hidden_layer1 = nn.Linear(5,5)
        self.hidden_layer2 = nn.Linear(5,5)
        self.hidden_layer3 = nn.Linear(5,5)
        self.hidden_layer4 = nn.Linear(5,5)
        self.output_layer = nn.Linear(5,1)

    def forward(self, x):
        input = x
        layer1_out = torch.sigmoid(self.input_layer(input))
        layer2_out = torch.sigmoid(self.hidden_layer1(layer1_out))
        layer3_out = torch.sigmoid(self.hidden_layer2(layer2_out))
        layer4_out = torch.sigmoid(self.hidden_layer3(layer3_out))
        layer5_out = torch.sigmoid(self.hidden_layer4(layer4_out))
        output = self.output_layer(layer5_out)

        # We do NOT return the output, but we modify the output in order to,
        # in a strong way, put the condition that u(2)=0
        return (x - 2)*output # Way to avoid boundary condition in the loss because
                    # you set the condition in that way
```

In [3]:
```
### (2) Model
seed = 0
torch.manual_seed(seed)
net = Net()
mse_cost_function = torch.nn.MSELoss() # Mean squared error
optimizer = torch.optim.Adam(net.parameters())
```

In [4]:
```
## PDE as loss function. Thus would use the network which we call as u_theta
def R(x, net):
    u = net(x) # the dependent variable u is given by the network based on independent variables x,t

    ## Based on our R = du/dx - 2du/dt - u, we need du/dx and du/dt
    u_x = torch.autograd.grad(u.sum(), x, create_graph=True)[0]

    u_xx = torch.autograd.grad(u_x.sum(), x, create_graph=True)[0] # We have to compute the second derivatives
                                                          # Notice that here we use the scalar form

    f = torch.Tensor(np.cos(np.pi*x.detach().numpy()))
    pde = u_xx - f

    return pde
```

In [5]:
```
### Neumann Boundary
def Neumann(net):
    x_bc_n = np.zeros((1,1)) # Point of the boundary put as zero
    x_bc_n[0] = 0;

    pt_x_bc = Variable(torch.from_numpy(x_bc_n).float(), requires_grad=True) # I evaluate my net in the point 0

    u = net(pt_x_bc)
    u_x = torch.autograd.grad(u.sum(), pt_x_bc, create_graph=True)[0] # Should work also without u.sum() because this is a scalar value
                                                        # But it is always a good standard to perfome the computation in this way

    neumann = u_x - 3. # Neuman boundary condition -- as another PDE to verify

    return neumann
```

In [6]:
```
## Data from Boundary Conditions -- Definition of the boundary condition points
# u(x,0)=6e^(-3x)
```

```python
## BC just gives us datapoints for training

# BC tells us that for any x in range[0,2] and time=0, the value of u is given by 6e^(-3x)
# Take say 500 random numbers of x
x_bc = np.zeros((1,1)) # x point
x_bc[0] = 2;
u_bc = np.zeros((1,1)) # u point
```

In [ ]:
```python
### (3) Training / Fitting
iterations = 10000
for epoch in range(iterations):
    optimizer.zero_grad() # to make the gradients zero

    # Loss based on boundary conditions
    pt_x_bc = Variable(torch.from_numpy(x_bc).float(), requires_grad=False)
    pt_u_bc = Variable(torch.from_numpy(u_bc).float(), requires_grad=False)
    net_bc_out = net(pt_x_bc) # output of u(x)
    mse_u = mse_cost_function(net_bc_out, pt_u_bc) # Difference between the net evaluation and the boundary condition

    net_neumann = Neumann(net)
    zero_n = np.zeros((1,1))
    pt_zero_n = Variable(torch.from_numpy(zero_n).float(), requires_grad=False)
    mse_n = mse_cost_function(net_neumann, pt_zero_n)

    # Loss based on PDE
    x_collocation = np.random.uniform(low=0.0, high=2.0, size=(500,1)) # Take all the points inside
    all_zeros = np.zeros((500,1))

    # Using the definition of the residual I have to compute the derivatives
    pt_x_collocation = Variable(torch.from_numpy(x_collocation).float(), requires_grad=True)
    pt_all_zeros = Variable(torch.from_numpy(all_zeros).float(), requires_grad=False)
    f_out = R(pt_x_collocation, net) # output of R(x)
    mse_f = mse_cost_function(f_out, pt_all_zeros)

    # Combining the loss functions
    loss =  mse_n + mse_f # + mse_u -- We can retrain with this modification
                # (see the recordings of 15-04-2025 for more details)

    loss.backward()
    optimizer.step()

    with torch.autograd.no_grad():
        if epoch % 1000 == 199:
            print("epoch", epoch, 'loss', loss.item())
            # Loss goes down quite fast
```

```
epoch 199 loss 0.00369077711366117
epoch 1199 loss 0.003172205761075O2
epoch 2199 loss 0.0017516122898086905
epoch 3199 loss 0.0010161682730540633
epoch 4199 loss 6.511950778076425e-05
epoch 5199 loss 3.1326027965405956e-05
epoch 6199 loss 2.31406265811529e-05
epoch 7199 loss 1.7137992472271435e-05
epoch 8199 loss 7.931336767796893e-06
epoch 9199 loss 5.77520177102997e-06
```

💡 Let's recap: what are the three loss components?

In the code you have:

- `mse_u` → penalises the error on the **boundary conditions (Dirichlet)**, i.e. forces the network to respect (u(x) = u_{BC}(x)) at specific points in the domain.
- `mse_n` → penalises the error on the **Neumann conditions**, i.e. forces the derivative of the network to respect certain constraints.
- `mse_f` → penalises the **violation of the PDE** at the **internal points (collocation points)**, i.e. forces the network to satisfy the differential equation.

You are currently training **only with**:

`python loss = mse_n + mse_f`

❓ Why is `mse_u` **commented**?

It is probably to **test how well the network is able to learn the boundary conditions 'on its own '** - that is, without directly forcing (u(x) \approx u_{BC}(x)), but only guiding it with the Neumann + PDE.

This can be useful for:

- **Evaluate the robustness of the PINN**: can the network find the correct solution based *only* on the PDE and the derivative at the edge?
- **Avoid overfitting** on the edge data: if `mse_u` is too dominant, the network may overfitting those points and neglect the interior.

🔁 What happens if you **discard** `mse_u`?

`python loss = mse_u + mse_n + mse_f`

➡️ In this case, **the network will be explicitly penalised if it does not meet the boundary conditions**.

Expected effects:

- The **solution will be more accurate** at the edges, especially if (u(x)) is known there.

- You may get faster and more stable **convergence**.
- But be careful: if the problem domain is large or if you have few collocation points, you might **bias the network** too much towards the initial/edge conditions and neglect the interior.

✅ When is it recommended to include `mse_u` ?

Yes, in **almost all practical cases**, including `mse_u` is **strongly recommended**, because:

- it improves overall accuracy,
- it imposes "certain" information that the network can exploit,
- it allows the trade-off between compliance with PDE and compliance with boundary conditions to be adjusted.

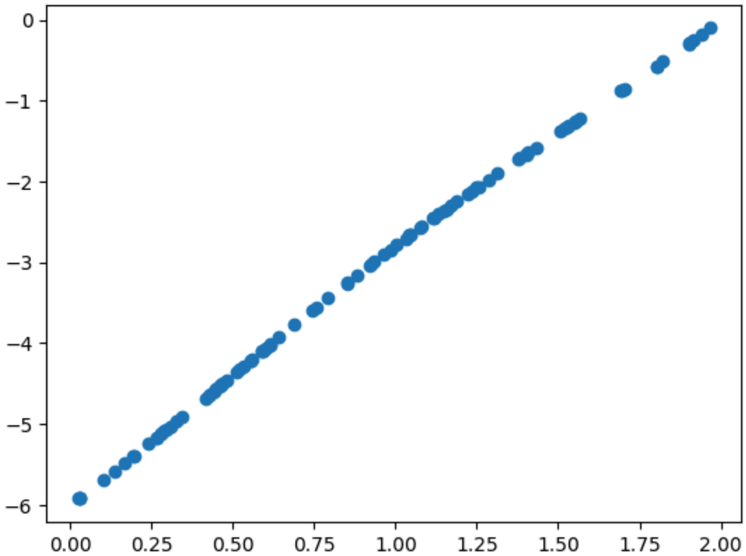
🎯 Conclusion

- `mse_u` **is important**, but is sometimes commented on temporarily to test the network's ability to *generalise*.
- **Commenting it** would give you more accurate solutions at the edges, and it is generally **better to keep it in the loss**.
- If you want to be more flexible, you can also use **weights**:

`python loss = α * mse_u + β * mse_n + γ * mse_f`

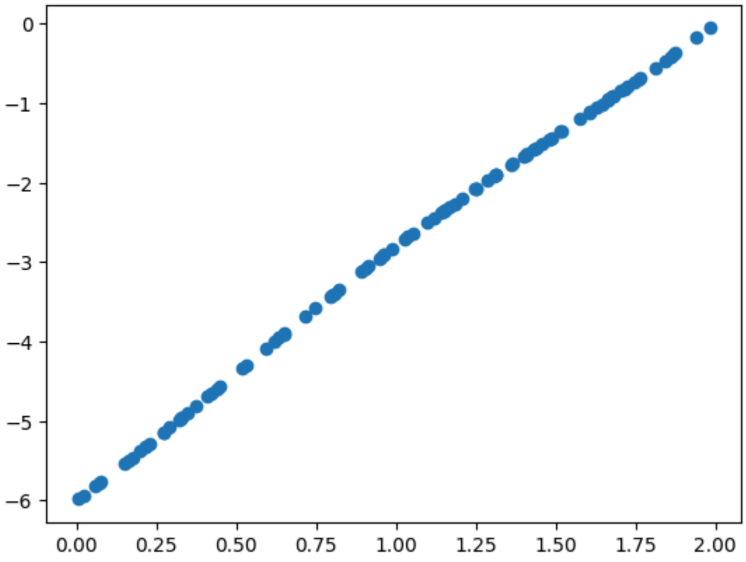
and tune the values of `α, β, γ` to balance the three sources of information.

In [9]:
```
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
from matplotlib import cm
from matplotlib.ticker import LinearLocator, FormatStrFormatter
import numpy as np

x=np.random.uniform(low=0.0, high=2.0, size=(100,1))

pt_x = Variable(torch.from_numpy(x).float(), requires_grad=True)
pt_u = net(pt_x)
u=pt_u.data.cpu().numpy()
plt.scatter(x, u)
plt.show()

# We are a little bit before 0
```



In [10]:
```
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
from matplotlib import cm
from matplotlib.ticker import LinearLocator, FormatStrFormatter
import numpy as np

x=np.random.uniform(low=0.0, high=2.0, size=(100,1))
print(np.cos(np.pi*2))
u=3*(x - 2) - (np.cos(np.pi*x) - 1)*(1/(np.pi**2))
plt.scatter(x, u)
plt.show()
```

```
1.0
```



To impose *directly* the boundary conditions (usually gives better training results) you have to:

- impose the condition directly on the output of the forward law multiplying the output by a function that does the job!

In our case: to make the solution zero at $x = 2$, a good function is $x - 2$. Thus `(x - 2)*output`.

- Get rid of the Dirichlet cost: it is not needed anymore :)

🔍 What these two final plots show

Both are **scatter plots** representing the function:

$$u(x) = 3(x-2) - \frac{\cos(\pi x) - 1}{\pi^2}$$

calculated for **100 random points** in the domain (x \in [0, 2]).

📊 Interpretation

These plots are used to **show the shape of the solution** (u(x)) in a 1D context (without temporal dependence), or to assess **the behaviour of the network over the domain**. The fact that there is **only the function `u(x)`** and no predicted solution (`u_pred`) implies that:

- You are **visually verifying** that the solution has the expected form (continuous, smooth, consistent with the data).
- Or that you are **sampling the ground truth** for later comparisons, or inspecting the network output.

Both plots are identical (the data are regenerated but the shape is the same), so one of the plots may be a control or a duplicate.

✅ Conclusion

These two plots show **the `u(x)` true function**, sampled on random points. The objective seems to be:

- **Visual verification** of the correctness or form of the analytical solution.
- **Preparation** for comparison with the network solution (although not shown here).