lab10

June 13, 2024

0.1 Lab 10

Kacper Szot, Jakub Rękas ### Zadanie 1 Dane jest równie różniczkowe

$$\frac{du}{dx} = cos(\omega x)$$

dla $x \in \Omega$,

gdzie $x, \omega, u \in \mathbb{R}$

$\Omega = \{x| - 2\pi \leq x \leq 2\pi\}$ to dziedzina szukanego rozwiązania

$u(\cdot)$ to poszukiwana funkcja Warunek początkowy

$$u(0) = 0.$$

Analityczne roziązanie równiania z warunkiem początkowym przybiera następującą postać:

$$u(x) = \frac{1}{\omega} sin(\omega x).$$

[ ]:
```
import torch
import torch.nn as nn
import numpy as np
import matplotlib.pyplot as plt
```

[ ]:
```
def exact_solution(x, w0):
    "Defines the analytical spectral bias problem"
    return (1/w0) * np.sin(w0 * x)
```

[ ]:
```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print(torch.cuda.device_count())
print(torch.cuda.current_device())
print(device)

class FCN(nn.Module):
    "Defines a fully-connected network in PyTorch"
    def __init__(self, N_INPUT, N_OUTPUT, N_HIDDEN, N_LAYERS):
        super().__init__()
        activation = nn.Tanh
```

```
        self.fcs = nn.Sequential(*[
                        nn.Linear(N_INPUT, N_HIDDEN),
                        activation()])
        self.fch = nn.Sequential(*[
                        nn.Sequential(*[
                            nn.Linear(N_HIDDEN, N_HIDDEN),
                            activation()]) for _ in range(N_LAYERS-1)])
        self.fce = nn.Linear(N_HIDDEN, N_OUTPUT)
    def forward(self, x):
        x = self.fcs(x)
        x = self.fch(x)
        x = self.fce(x)
        return x
```

```
1
0
cuda
```

[ ]:
```
torch.manual_seed(123)
```

[ ]: <torch._C.Generator at 0x79c8505c1f70>

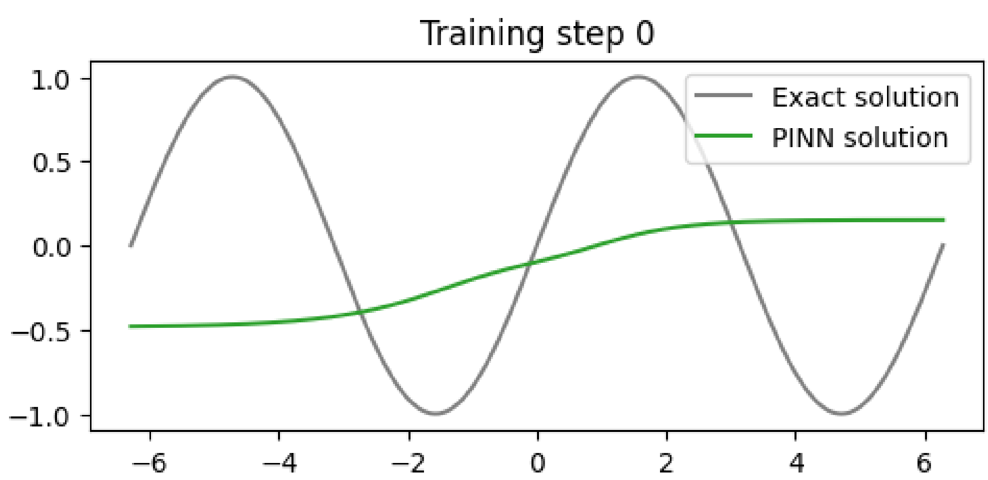
[ ]:
```
# train the PINN
def train(pinn, w0, test_points, train_steps=50001,train_points=3000):
  x_boundary = torch.tensor(0.,device=device).view(-1,1).requires_grad_(True)#
  x_physics = torch.linspace(-2*np.pi,2*np.pi,train_points,device=device).
↪view(-1,1).requires_grad_(True)#
  x_test = torch.linspace(-2*np.pi,2*np.pi,test_points,device=device).view(-1,1)
  u_exact = exact_solution(x_test.cpu(),w0)
  optimiser = torch.optim.Adam(pinn.to(device).parameters(),lr=0.001)
  losses = []
  for i in range(train_steps):
      optimiser.zero_grad()

      # compute boundary loss
      u = pinn(x_boundary)#
      loss1 = (torch.squeeze(u))**2

      # compute physics loss
      u = pinn(x_physics)#
      dudx = torch.autograd.grad(u, x_physics, torch.ones_like(u),␣
↪create_graph=True)[0]#
      loss2 = torch.mean((dudx - torch.cos(x_physics*w0))**2)
      loss =loss1+loss2
      losses.append(loss.cpu().detach().numpy())

      # backpropagate joint loss, take optimiser step
```

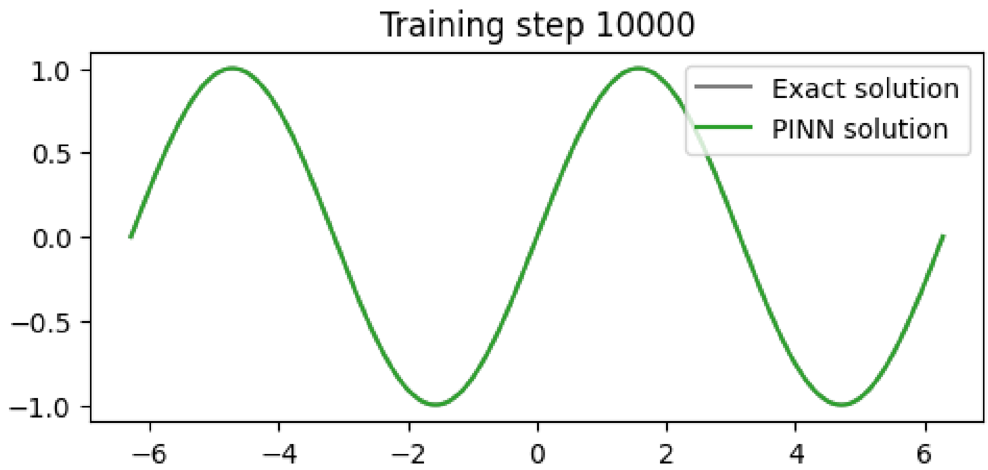
```
        loss.backward()
        optimiser.step()

        #plot the result as training progresses
        if i % 10000 == 0:
            u = pinn(x_test).detach()
            plt.figure(figsize=(6,2.5))
            plt.plot(x_test.cpu()[:,0], u_exact[:,0], label="Exact solution",␣
↪color="tab:grey")
            plt.plot(x_test.cpu()[:,0], u.cpu()[:,0], label="PINN solution",␣
↪color="tab:green")
            plt.title(f"Training step {i}")
            plt.legend()
            plt.show()

    plt.title("loss function")
    plt.yscale("log")
    plt.xlabel('Iteration')
    plt.ylabel('Loss')
    plt.plot(losses)
    plt.show()
```

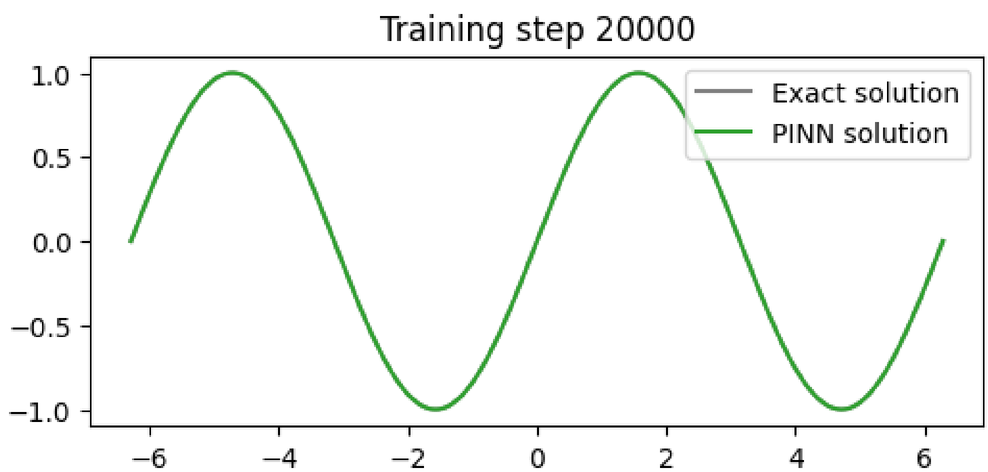
(a) Przypadek $\omega = 1$.

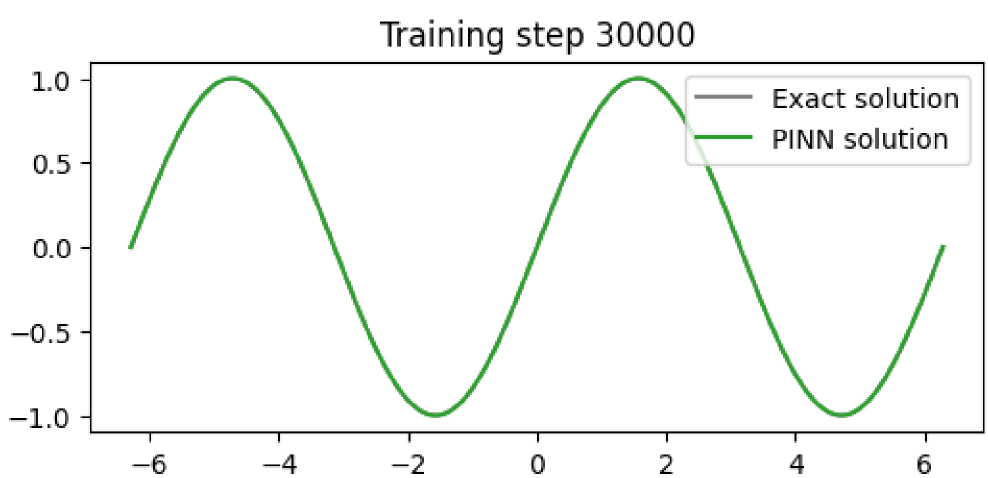
2 warstwy ukryte, 16 neuronów w każdej warstwe
liczba punktów treningowych: 200
liczba punktów testowych: 1000

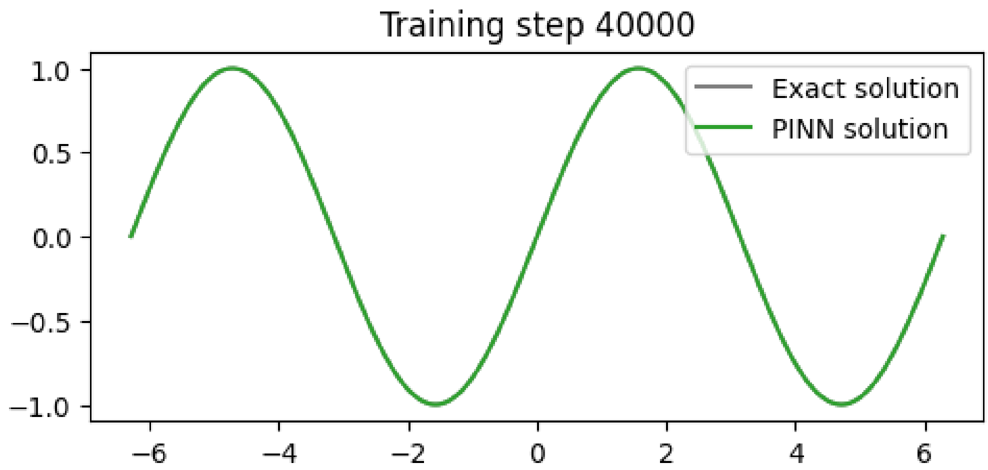
[ ]:
```
#zadanie 1 model a
pinn = FCN(1,1,16,2)
train(pinn=pinn,w0=1,test_points=1000,train_points=200)
```

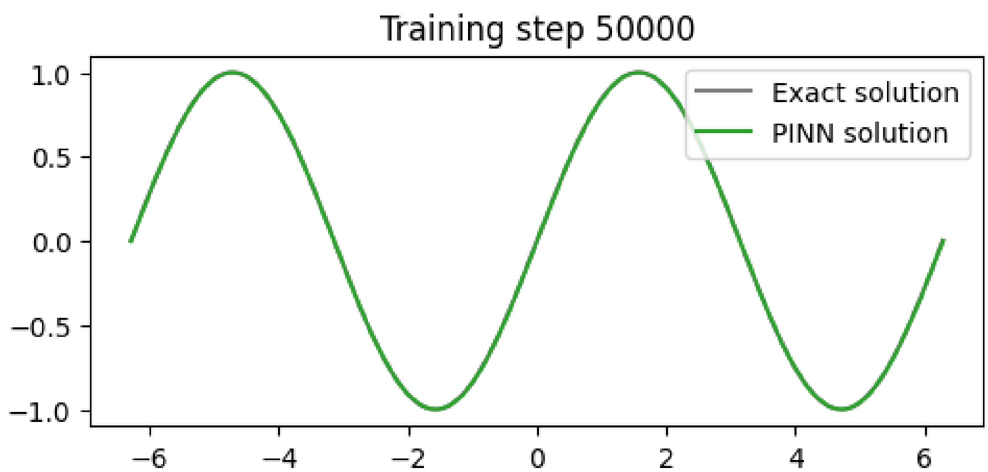


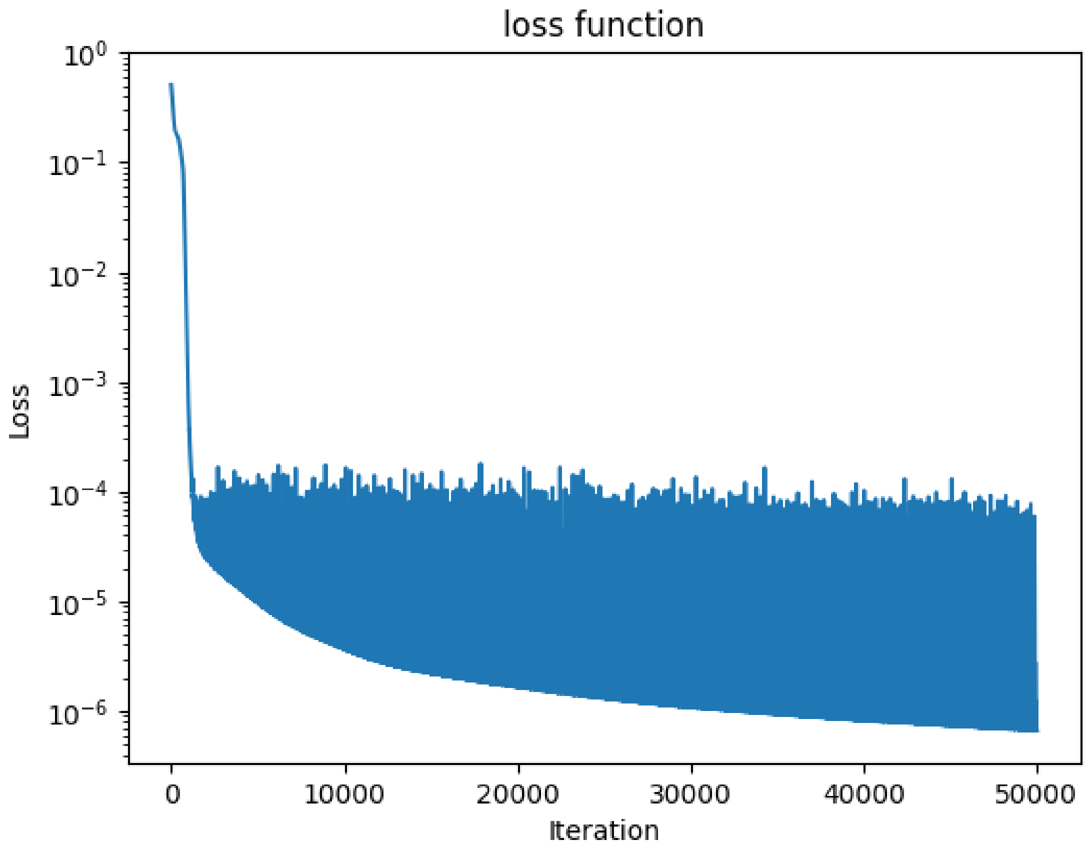

Training step 10000
Exact solution
PINN solution


Training step 20000
Exact solution
PINN solution


Training step 30000
Exact solution
PINN solution


Training step 40000
Exact solution
PINN solution
1.0
0.5
0.0
−0.5
−1.0
−6
−4
−2
0
2
4
6

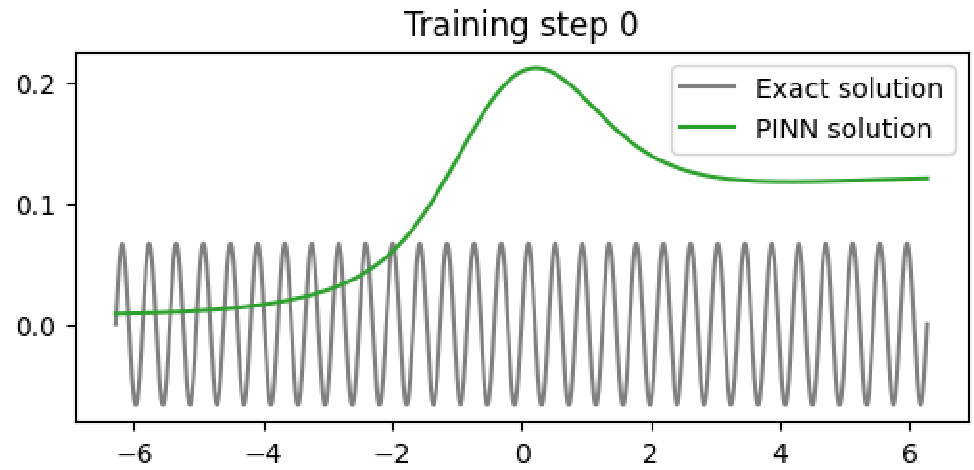

Training step 50000
Exact solution
PINN solution
1.0
0.5
0.0
−0.5
−1.0
−6
−4
−2
0
2
4
6

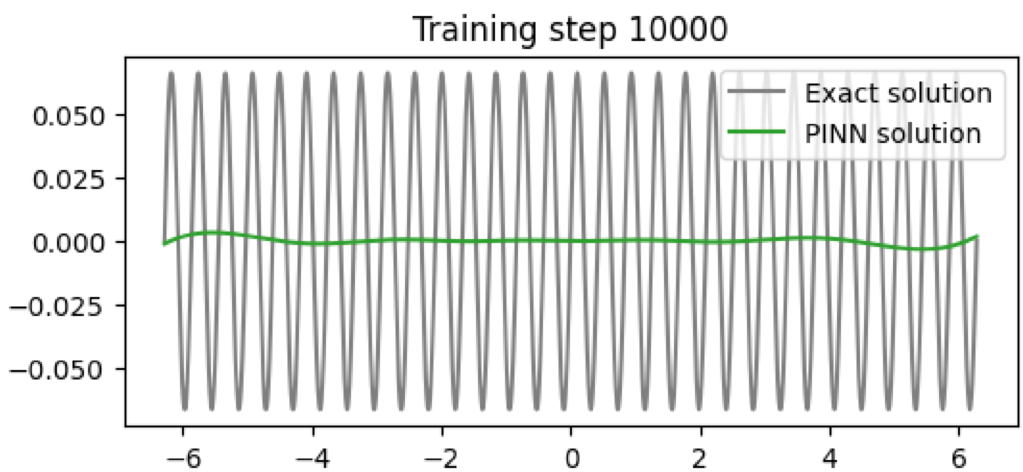


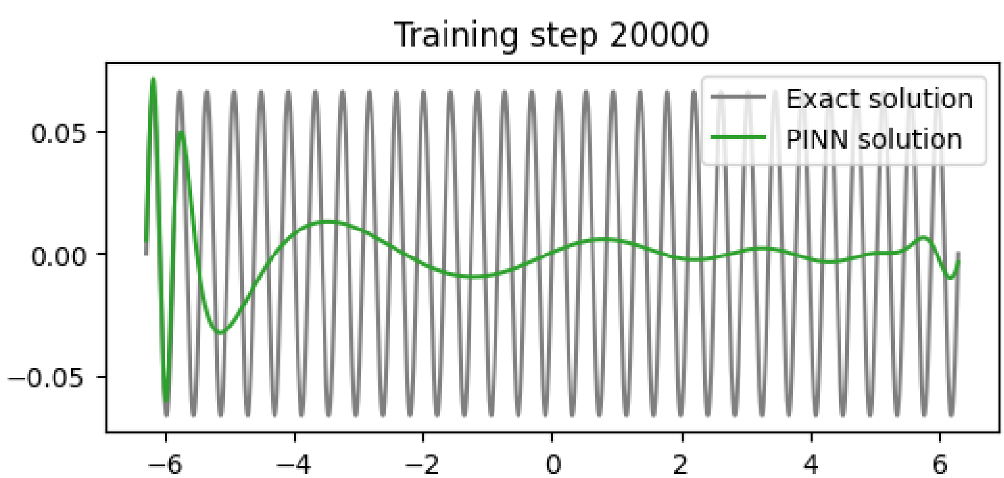
Sieć mimo małych rozmiarów, realatywnie szybko osiąga zbierznośc i dobre wyniki.

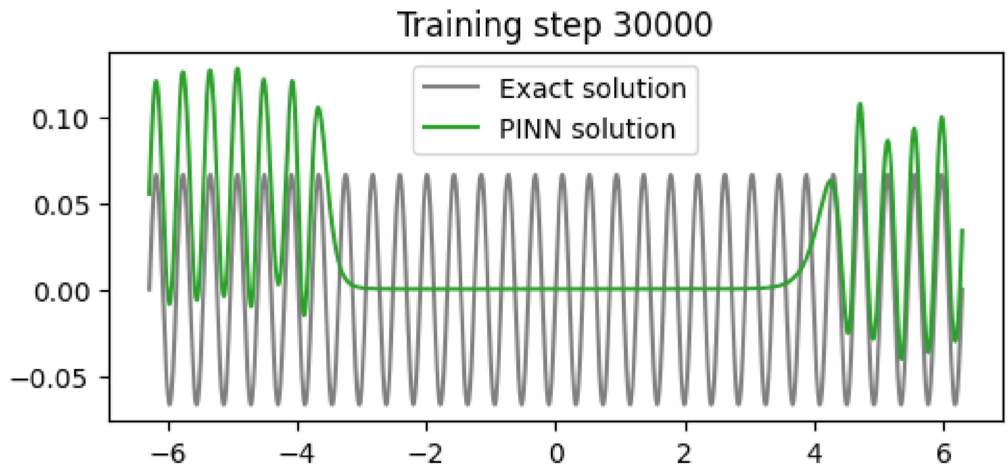
(b) Przypadek $\omega = 15$. 2 warstwy ukryte, 16 neuronów w każdej warstwie
liczba punktów treningowych: 3000
liczba punktów testowych: 5000

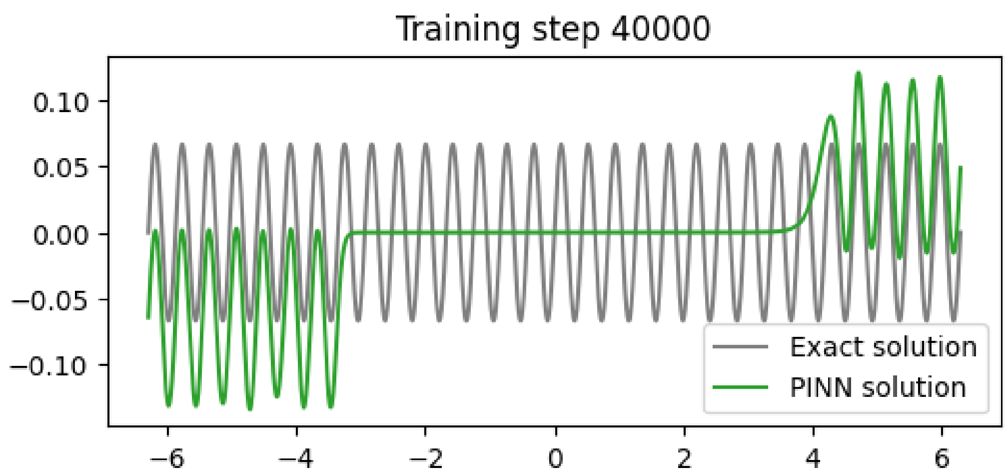
[ ]:
```
#zadanie 1 podpunkt b model b
pinn = FCN(1,1,16,2)
train(pinn=pinn,w0=15,test_points=5000,train_points=3000)
```

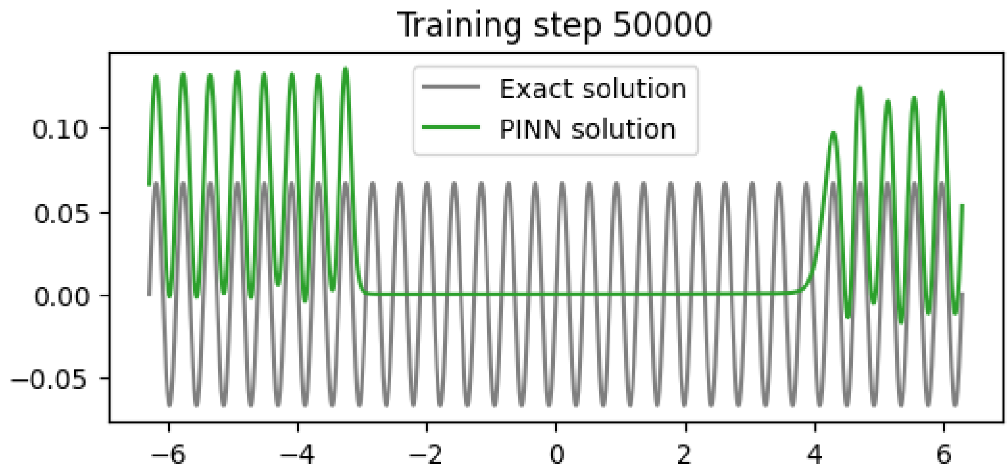

Training step 0
Exact solution
PINN solution
0.2
0.1
0.0
−6
−4
−2
0
2
4
6

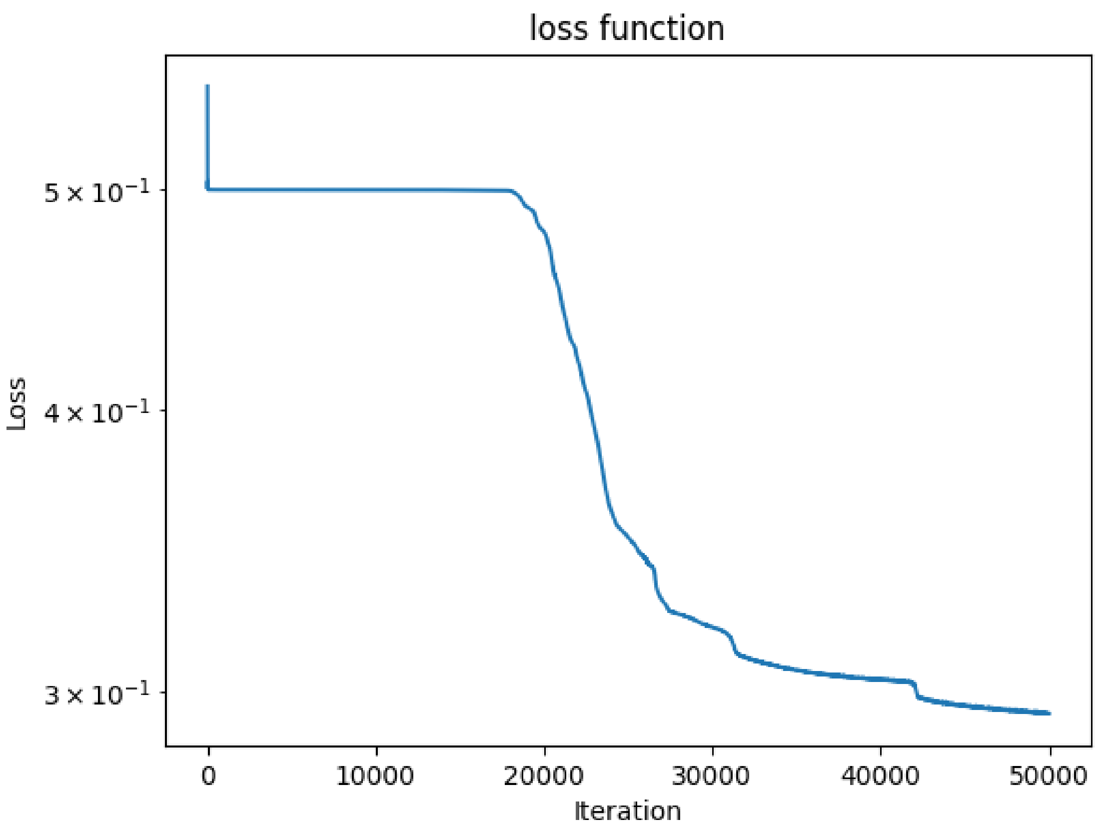

Training step 10000
Exact solution
PINN solution
0.050
0.025
0.000
−0.025
−0.050
−6
−4
−2
0
2
4
6


Training step 20000
Exact solution
PINN solution
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6


Training step 30000
Exact solution
PINN solution
0.10
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6


Training step 40000
Exact solution
PINN solution
0.10
0.05
0.00
−0.05
−0.10
−6
−4
−2
0
2
4
6



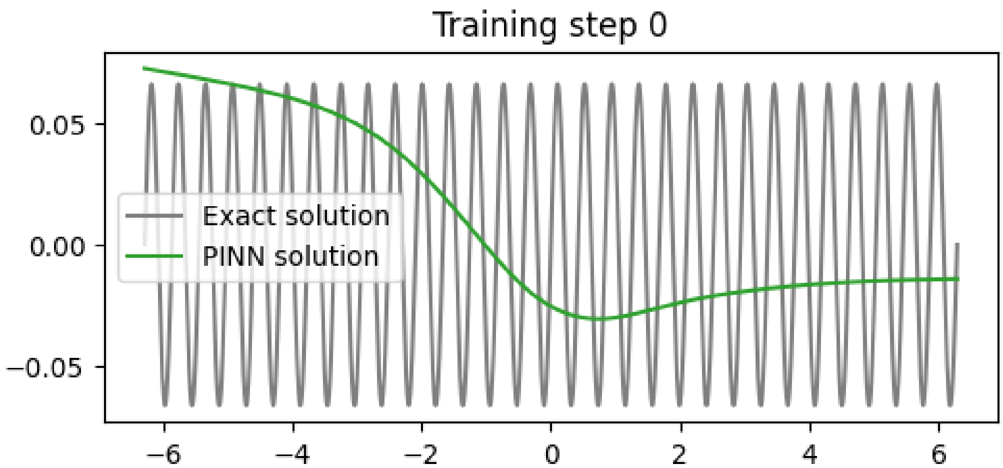


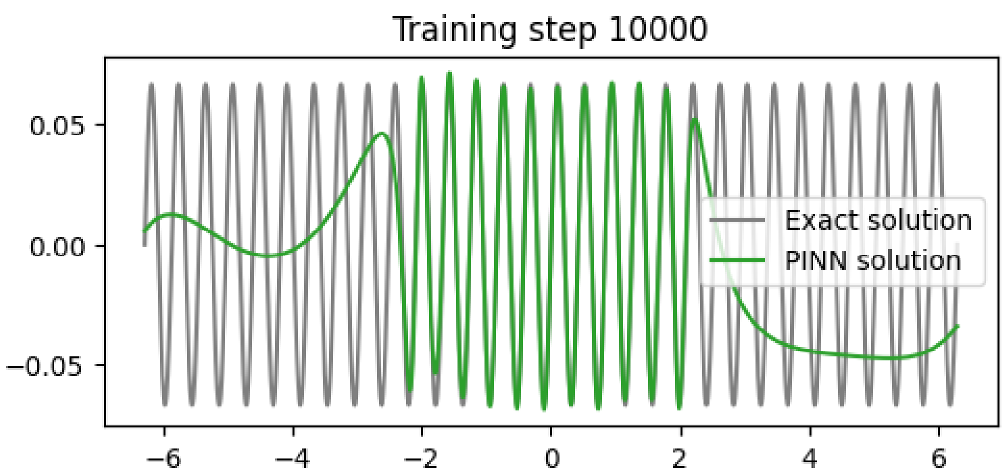
Małej sieci neuronowej nie udaje się osiągnąć zadowalających wyników w trakcie 50000 iteracji dla wysokiej częstotliwości.

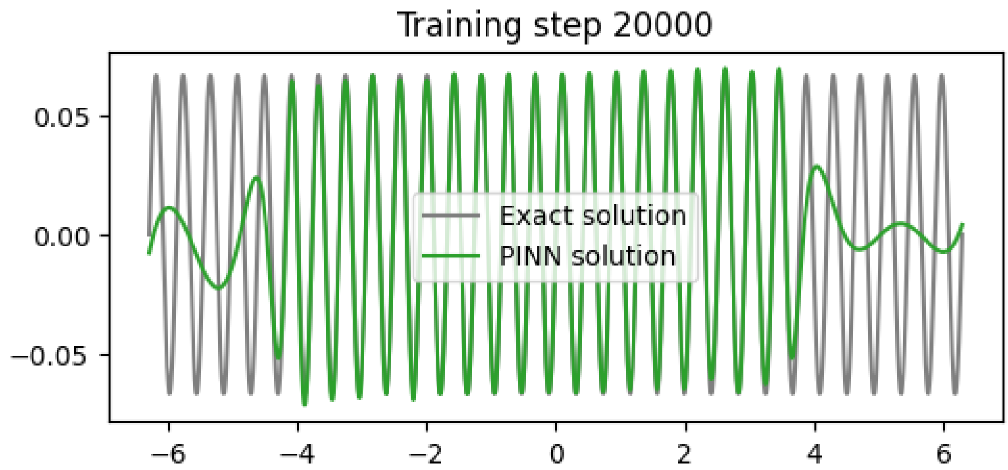
(b) Przypadek $\omega = 15$. 4 warstwy ukryte, 64 neuronów w każdej warstwie
liczba punktów treningowych: 3000

liczba punktów testowych: 5000

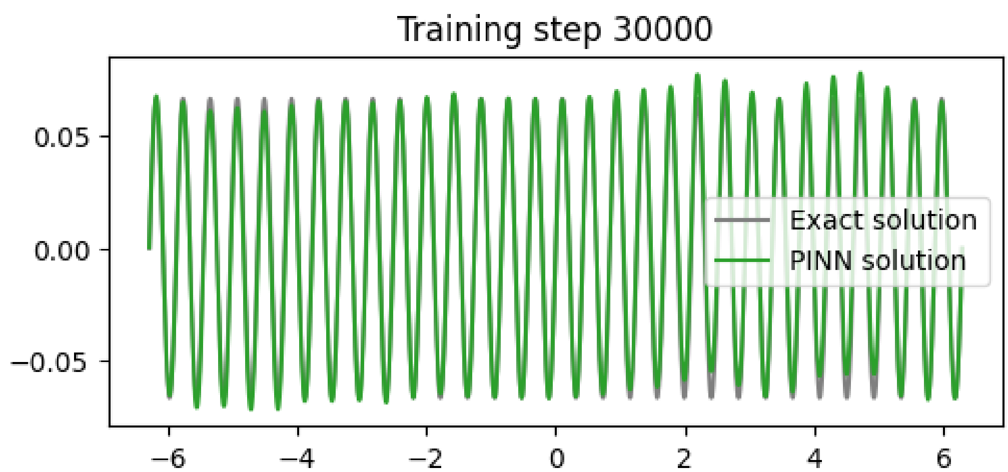
[ ]:
```
#zadanie 1 podpunkt b model c
pinn = FCN(1,1,64,4)
train(pinn=pinn,w0=15,test_points=5000,train_points=3000)
```



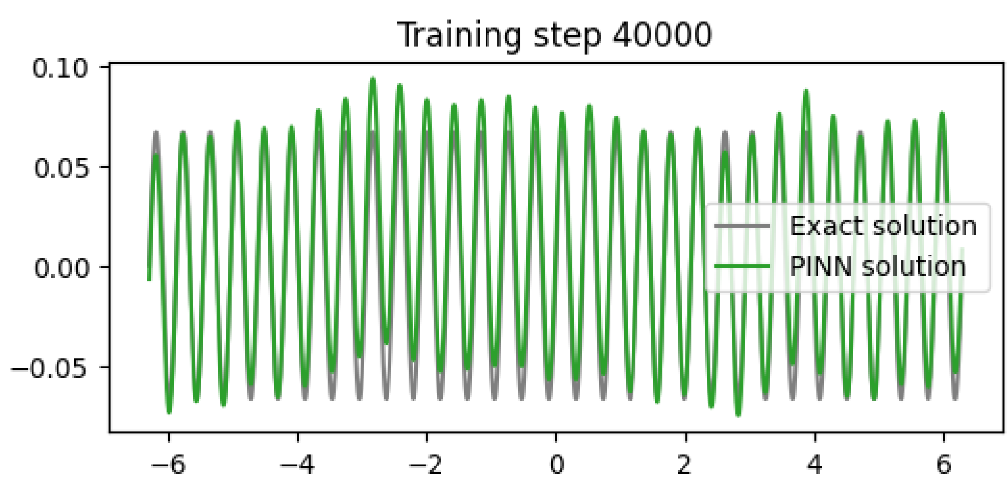




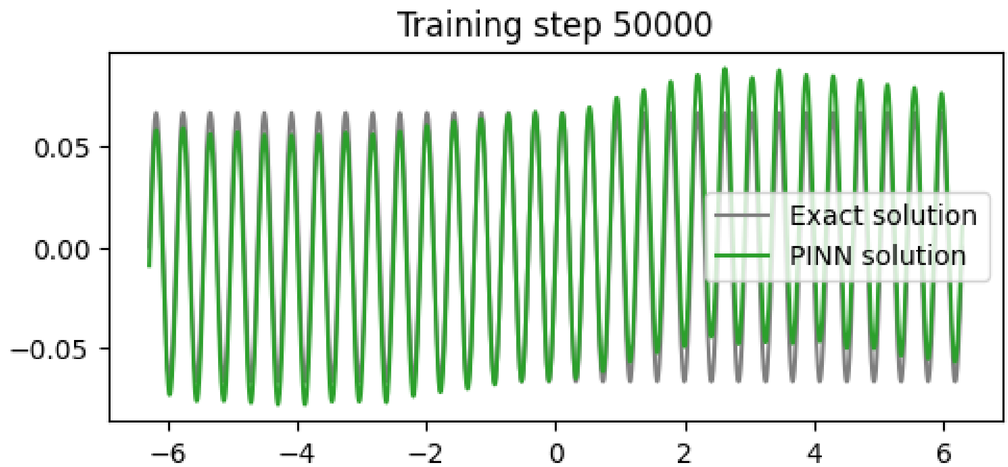
Training step 20000
Exact solution
PINN solution

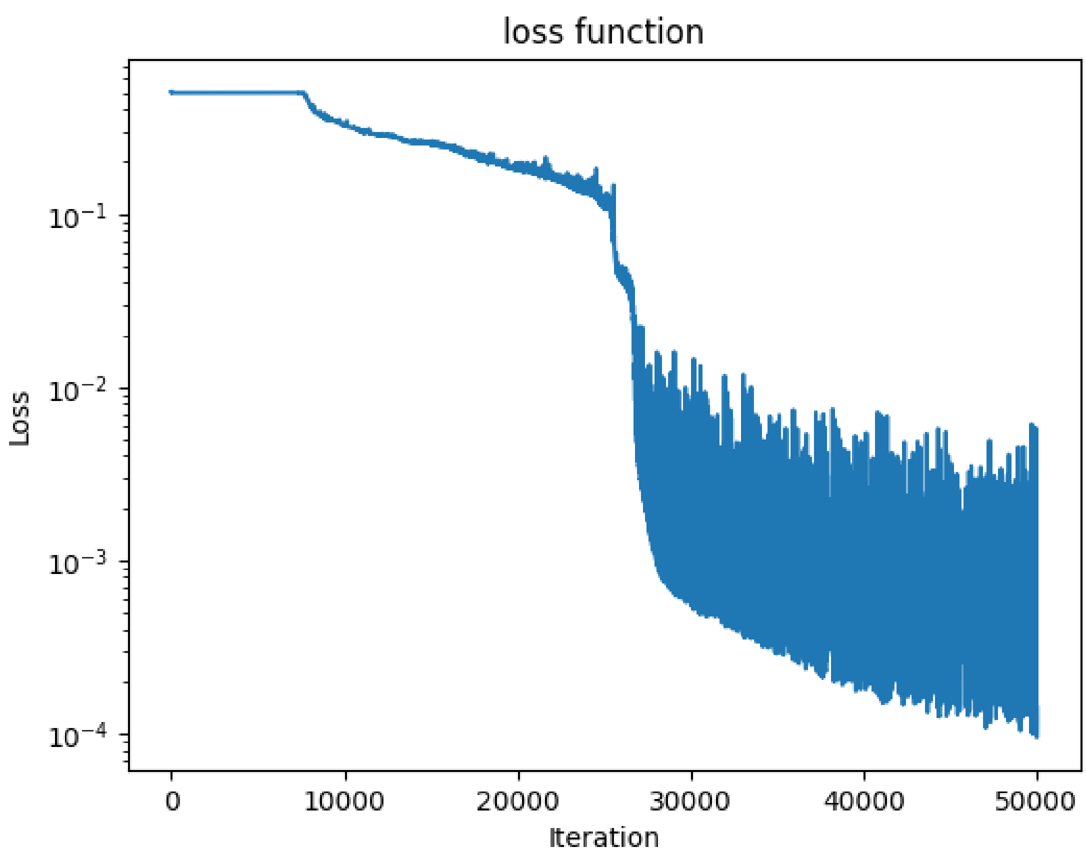


Training step 30000
Exact solution
PINN solution



Training step 40000
Exact solution
PINN solution

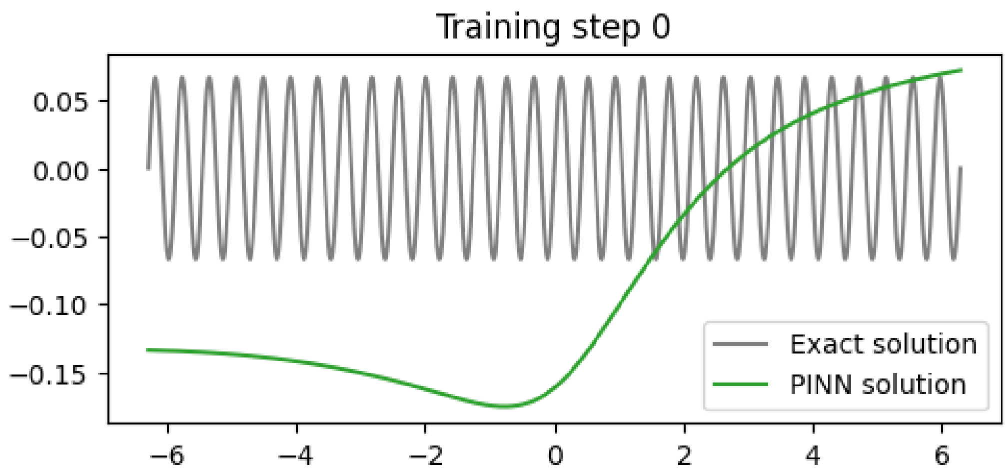


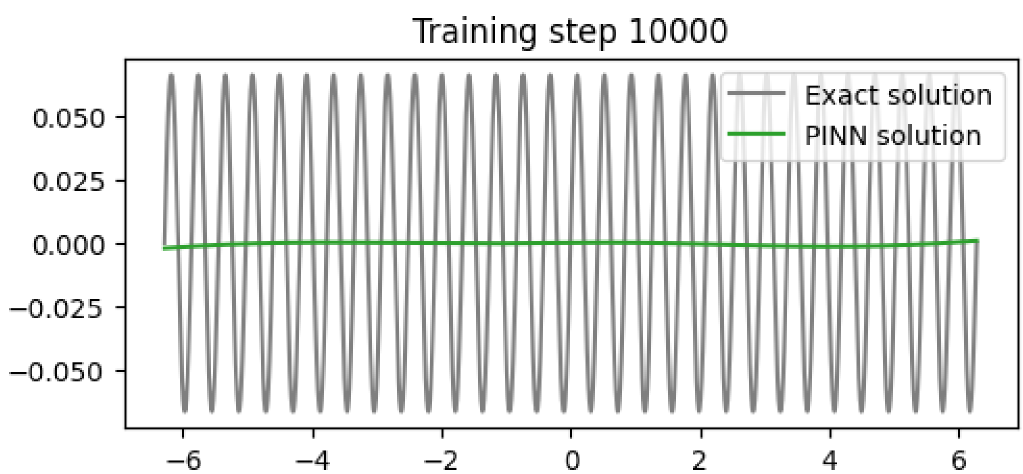


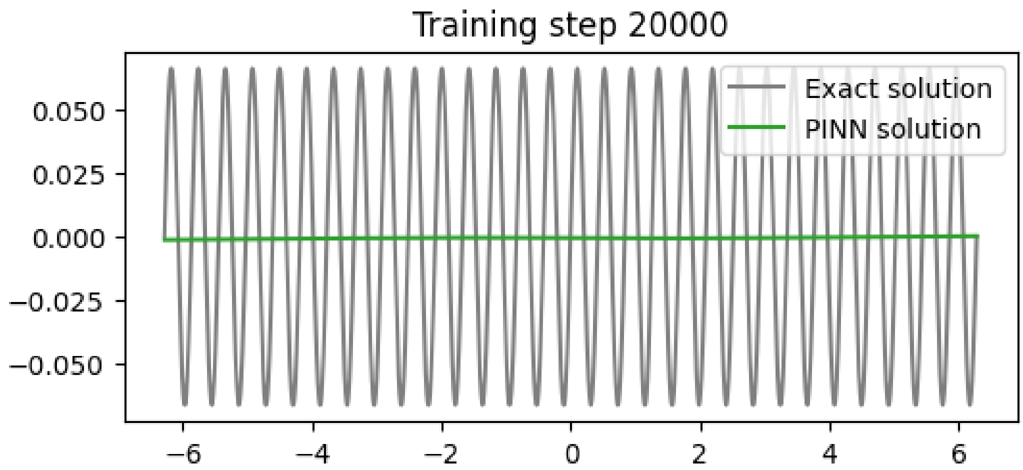
Sieci neuronowej udaje się osiągnąć zadowalających wyników w trakcie 50000 iteracji dla wysokiej częstotliwości.

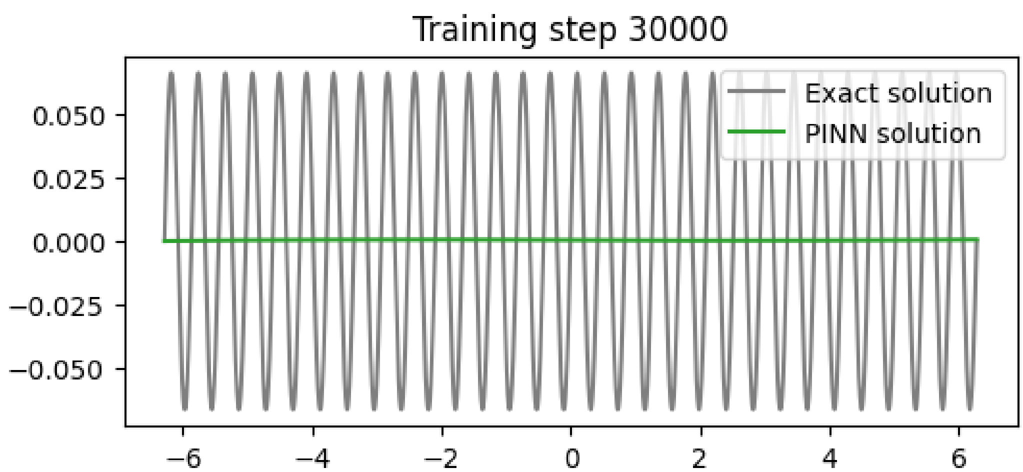
(b) Przypadek $\omega = 15$. 5 warstwy ukryte, 128 neuronów w każdej warstwie
liczba punktów treningowych: 3000
liczba punktów testowych: 5000

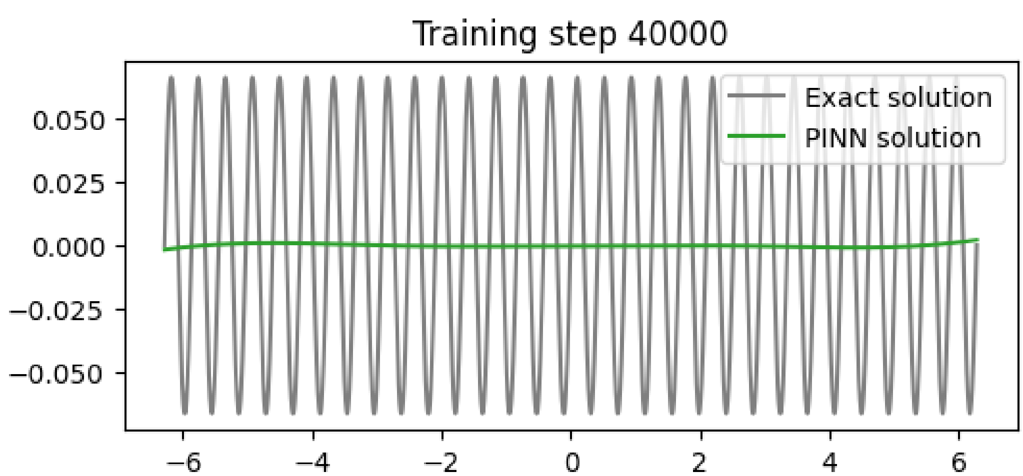
[ ]:
```
#zadanie 1 podpunkt b model c
pinn = FCN(1,1,128,5)
train(pinn=pinn,w0=15,test_points=5000,train_points=3000)
```

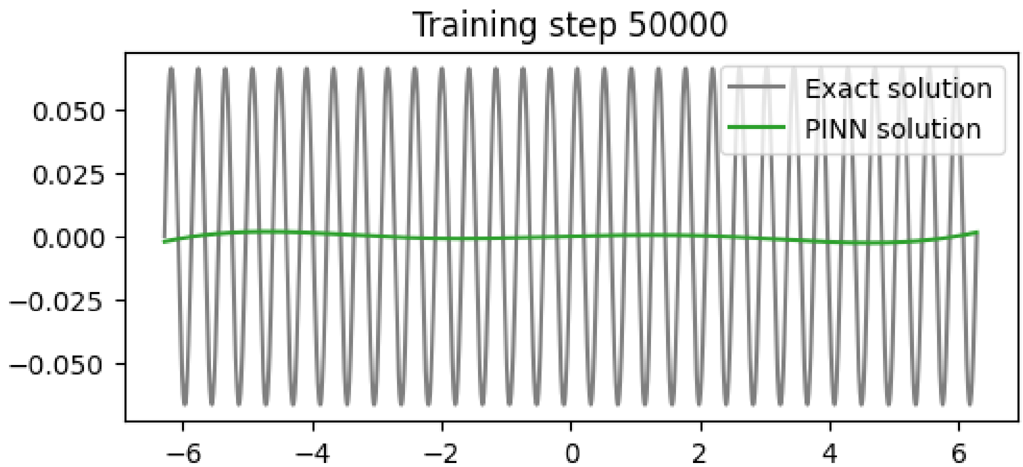


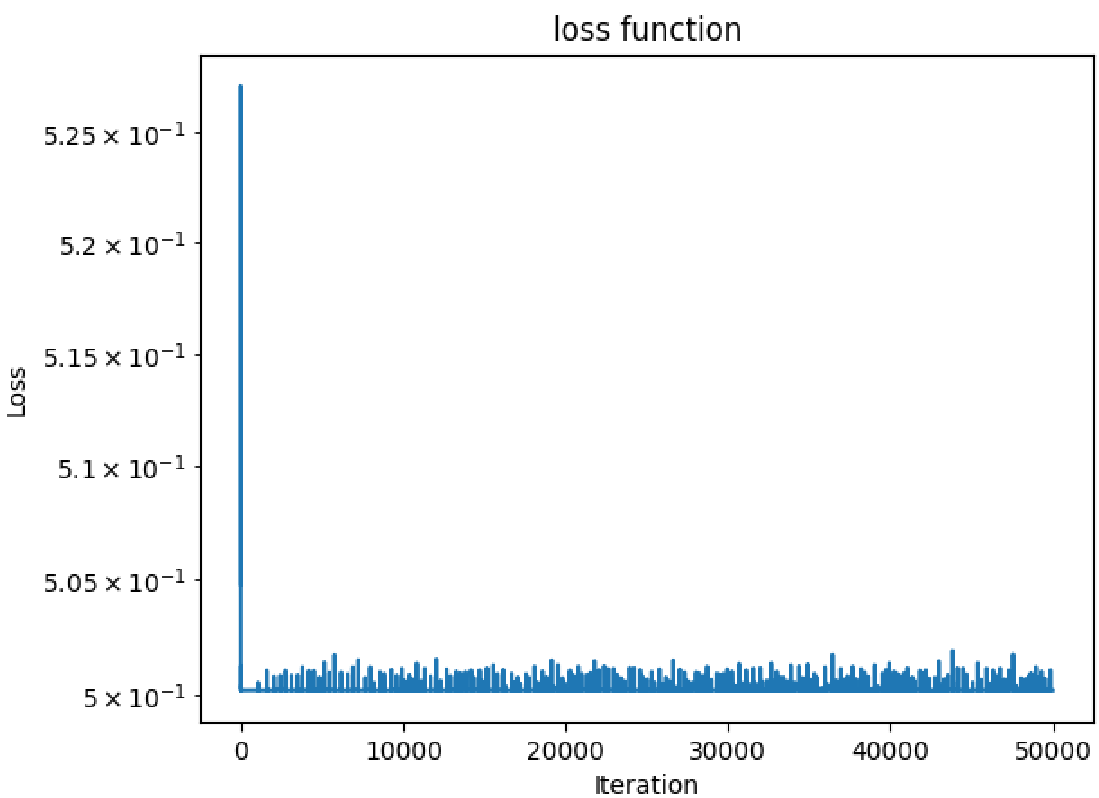



Training step 20000
Exact solution
PINN solution
0.050
0.025
0.000
−0.025
−0.050
−6
−4
−2
0
2
4
6


Training step 30000
Exact solution
PINN solution
0.050
0.025
0.000
−0.025
−0.050
−6
−4
−2
0
2
4
6


Training step 40000
Exact solution
PINN solution
0.050
0.025
0.000
−0.025
−0.050
−6
−4
−2
0
2
4
6



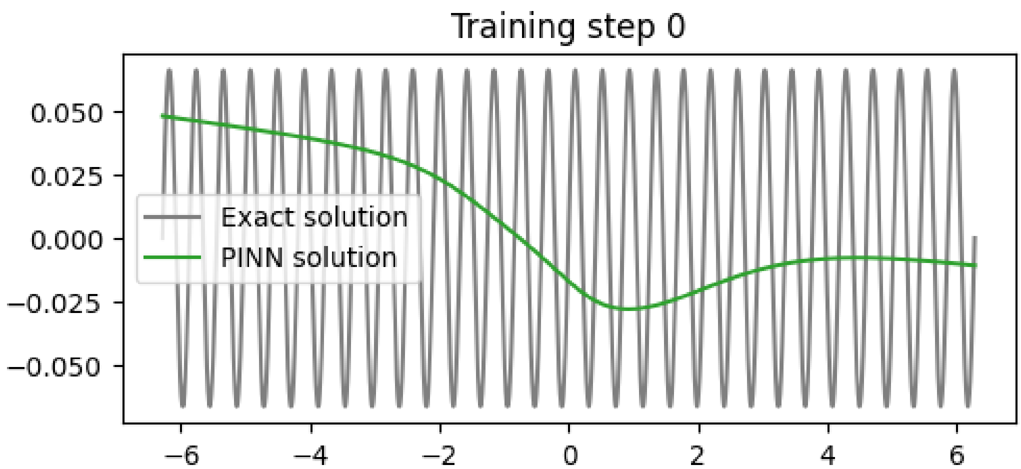


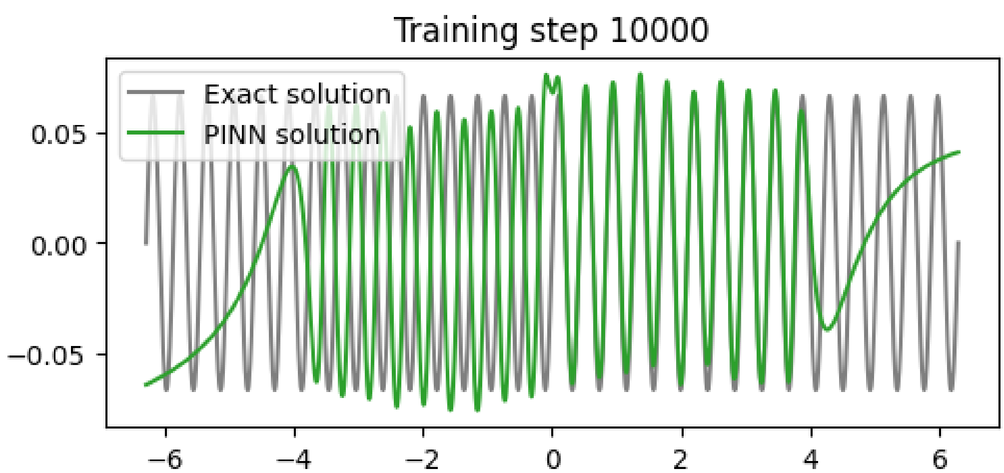
Dużej sieci neuronowej nie udaje się osiągnąć zadowalających wyników w trakcie 50000 iteracji dla wysokiej częstotliwości, prawdopodobnie 50000 to zbyt mało iteracji.

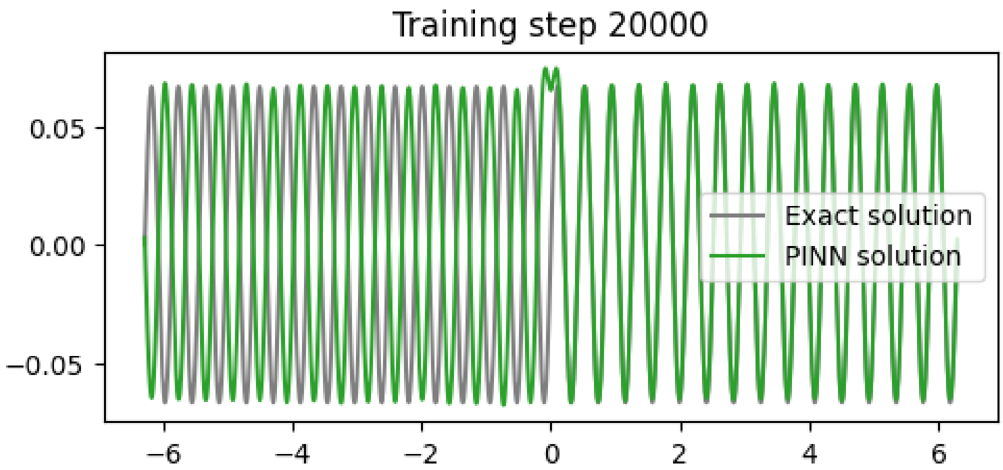
(c) 4 warstwy ukryte, 64 neuronów w każdej warstwie
liczba punktów treningowych: 3000
liczba punktów testowych: 5000
Aby zagwarantować spełnienie warunku $\hat{u}(0) = 0$ wprowadzamy $\hat{u}(x) = tanh(\omega x) \cdot NN(x)$

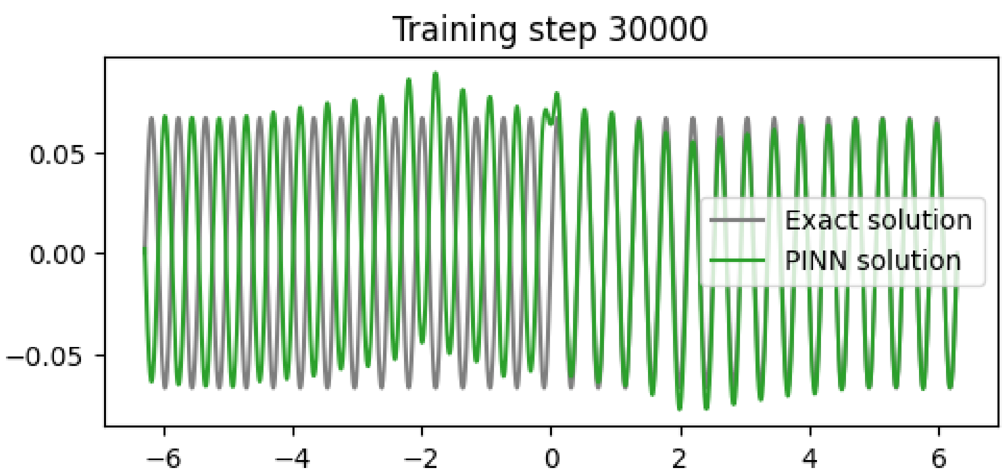
```
[ ]: # zadanie 1 podpunkt c
# zastoswoanie u = tanh(w0, x) * NN(x;0)
def train_using_tanh_in_output(pinn, w0, test_points,␣
↪train_steps=50001,train_points=3000):
    x_boundary = torch.tensor(0.,device=device).view(-1,1).requires_grad_(True)#
    x_physics = torch.linspace(-2*np.pi,2*np.pi,train_points,device=device).
↪view(-1,1).requires_grad_(True)#
    x_test = torch.linspace(-2*np.pi,2*np.pi,test_points,device=device).view(-1,1)
    u_exact = exact_solution(x_test.cpu(),w0)
    losses=[]
    optimiser = torch.optim.Adam(pinn.to(device).parameters(),lr=0.001)
    for i in range(train_steps):
        optimiser.zero_grad()
        # compute physics loss
        u = torch.tanh(x_physics*w0) * pinn(x_physics)#
        dudx = torch.autograd.grad(u, x_physics, torch.ones_like(u),␣
↪create_graph=True)[0]#
        loss2 = torch.mean((dudx - torch.cos(x_physics*w0))**2)
        loss =loss2
        losses.append(loss.cpu().detach().numpy())


        # backpropagate joint loss, take optimiser step
        loss.backward()
        optimiser.step()

        #plot the result as training progresses
        if i % 10000 == 0:
            u = pinn(x_test).detach()
            plt.figure(figsize=(6,2.5))
            plt.plot(x_test.cpu()[:,0], u_exact[:,0], label="Exact solution",␣
↪color="tab:grey")
            plt.plot(x_test.cpu()[:,0], u.cpu()[:,0], label="PINN solution",␣
↪color="tab:green")
            plt.title(f"Training step {i}")
            plt.legend()
            plt.show()
    plt.title("loss function")
    plt.yscale("log")
    plt.xlabel('Iteration')
    plt.ylabel('Loss')
    plt.plot(losses)
```

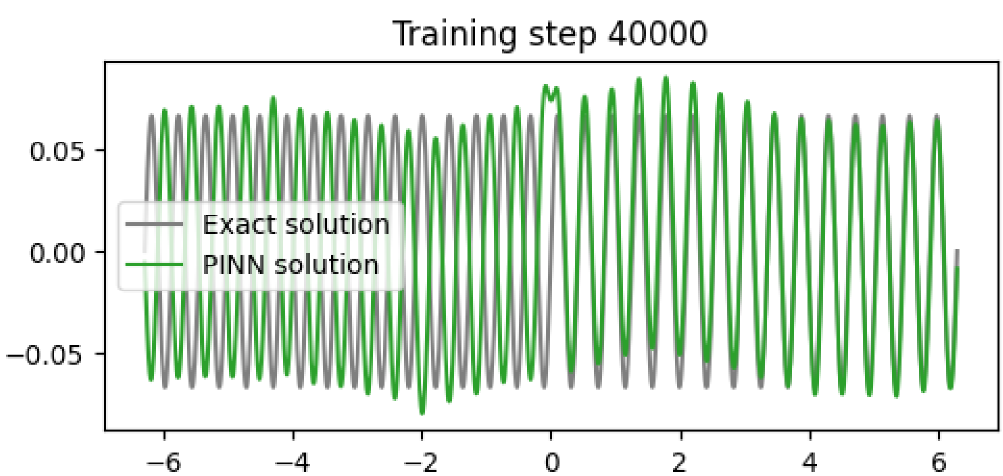
```
  plt.show()

pinn = FCN(1,1,64,4)
train_using_tanh_in_output(pinn=pinn,w0=15,test_points=5000,train_points=3000)
```

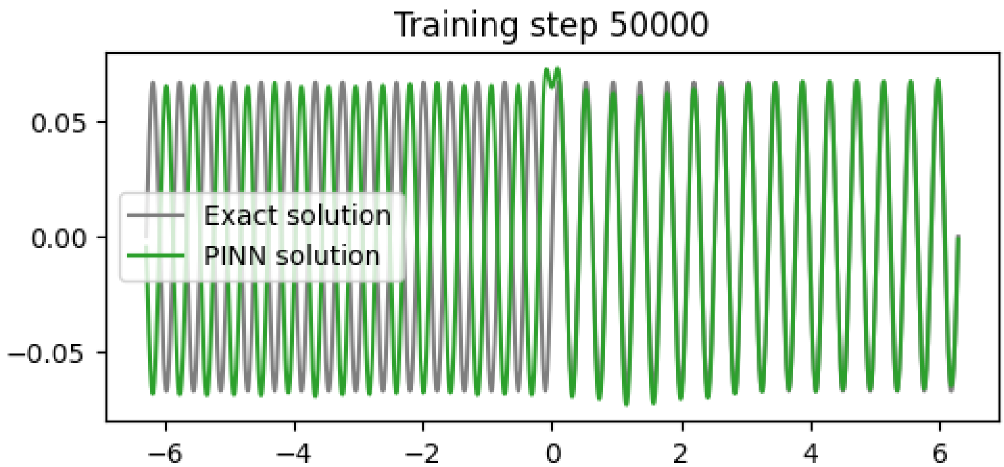


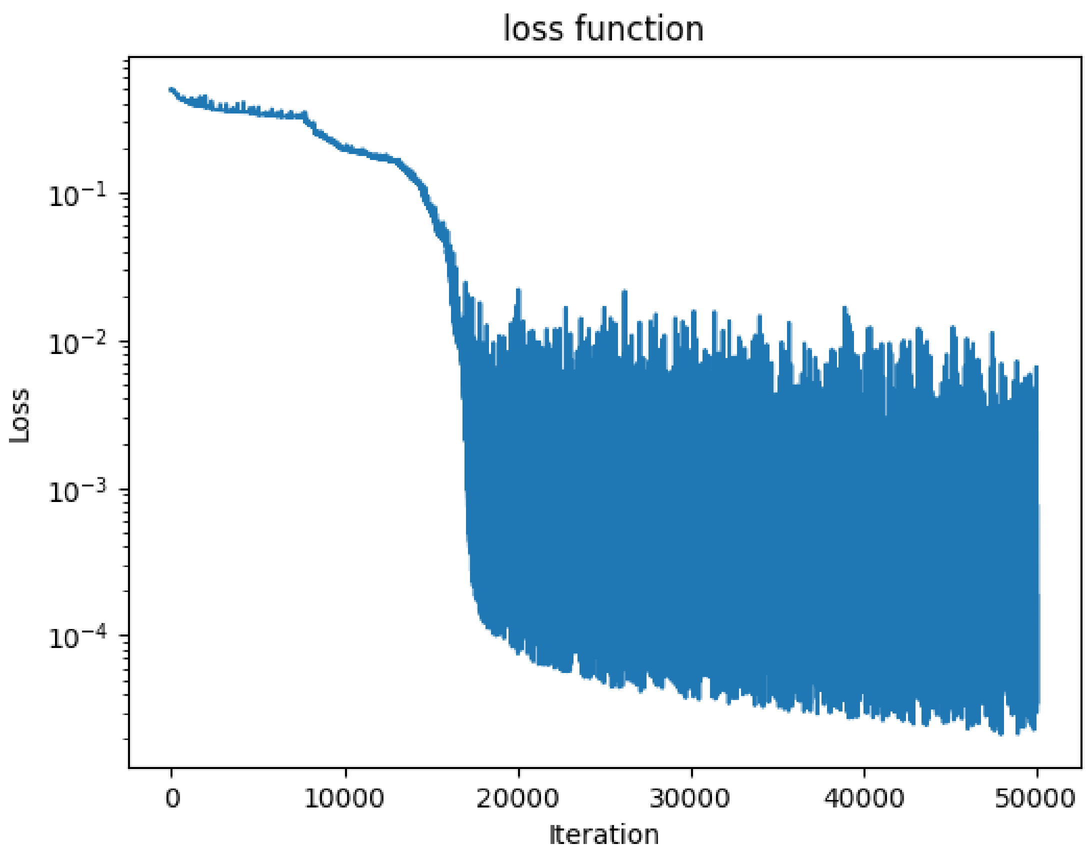



Training step 20000
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6
Exact solution
PINN solution


Training step 30000
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6
Exact solution
PINN solution


Training step 40000
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6
Exact solution
PINN solution

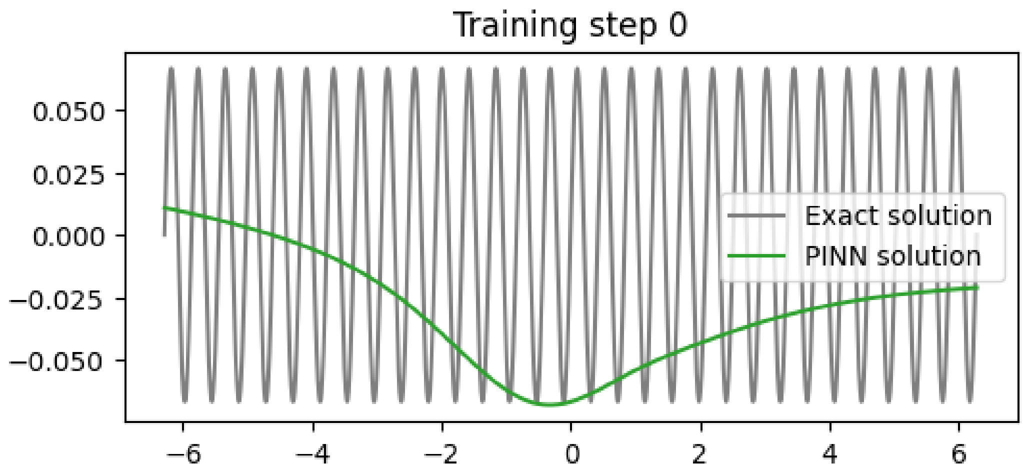


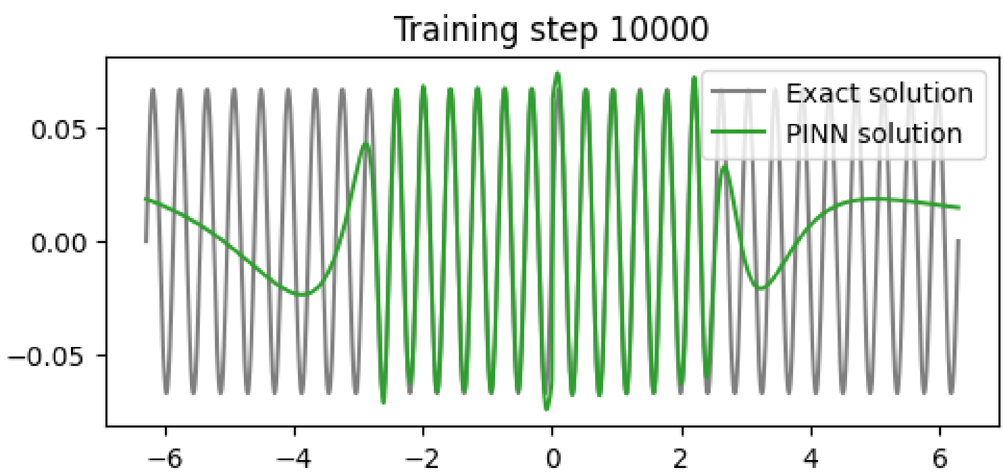


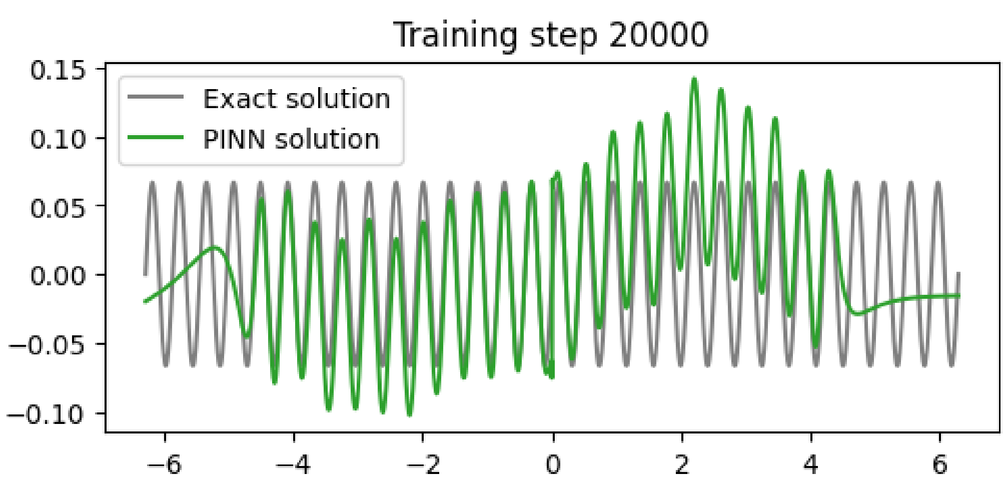
Po 50000 iteracjach można zauważyć, że sieć osiągneła zbieżność dla \$ x 0\$ natomiast nie dla \$

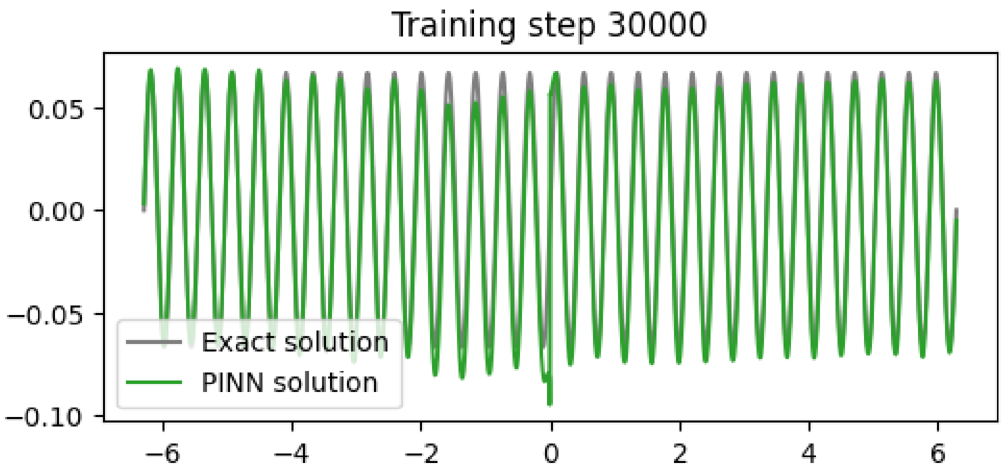
x <0$, gdyż tanh jest ujemny dla takich x, w celu naprawieniu tego problemu ustalmy $\hat{u}(x) = |tanh(\omega x)| \cdot NN(x)$

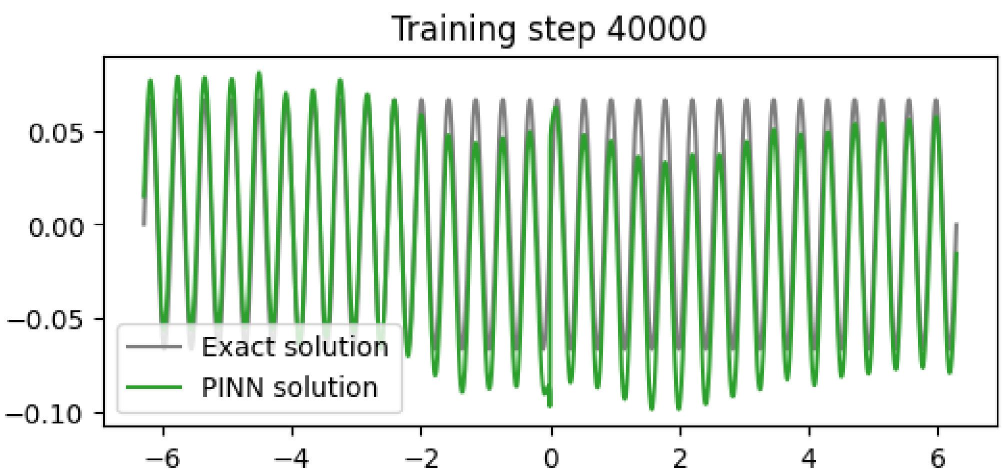
[ ]:
```
# zadanie 1 podpunkt c
# zastoswoanie u = |tanh(w0, x)| * NN(x;0)
def train_using_absolute_tanh_in_output(pinn, w0, test_points,␣
↪train_steps=50001,train_points=3000):
  x_boundary = torch.tensor(0.,device=device).view(-1,1).requires_grad_(True)#
  x_physics = torch.linspace(-2*np.pi,2*np.pi,train_points,device=device).
↪view(-1,1).requires_grad_(True)#
  x_test = torch.linspace(-2*np.pi,2*np.pi,test_points,device=device).view(-1,1)
  u_exact = exact_solution(x_test.cpu(),w0)
  optimiser = torch.optim.Adam(pinn.to(device).parameters(),lr=0.001)
  losses = []
  for i in range(train_steps):
      optimiser.zero_grad()
      # compute physics loss
      u = abs(torch.tanh(x_physics*w0)) * pinn(x_physics)#
      dudx = torch.autograd.grad(u, x_physics, torch.ones_like(u),␣
↪create_graph=True)[0]#
      loss2 = torch.mean((dudx - torch.cos(x_physics*w0))**2)
      loss =loss2
      losses.append(loss.cpu().detach().numpy())
      # backpropagate joint loss, take optimiser step
      loss.backward()
      optimiser.step()

      #plot the result as training progresses
      if i % 10000 == 0:
          u = pinn(x_test).detach()
          plt.figure(figsize=(6,2.5))
          plt.plot(x_test.cpu()[:,0], u_exact[:,0], label="Exact solution",␣
↪color="tab:grey")
          plt.plot(x_test.cpu()[:,0], u.cpu()[:,0], label="PINN solution",␣
↪color="tab:green")
          plt.title(f"Training step {i}")
          plt.legend()
          plt.show()
  plt.title("loss function")
  plt.yscale("log")
  plt.xlabel('Iteration')
  plt.ylabel('Loss')
  plt.plot(losses)
  plt.show()

pinn = FCN(1,1,64,4)
train_using_absolute_tanh_in_output(pinn=pinn,w0=15,test_points=5000,train_points=3000)
```

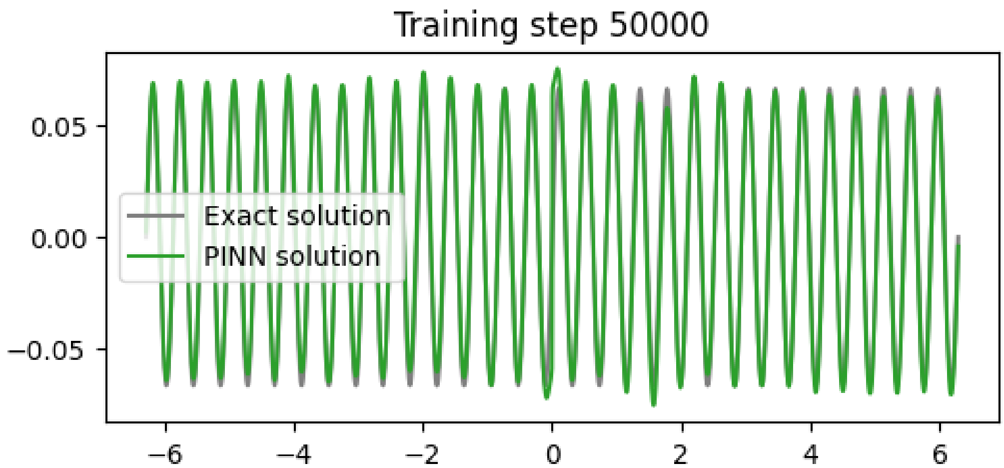

Training step 0
Exact solution
PINN solution
0.050
0.025
0.000
−0.025
−0.050
−6
−4
−2
0
2
4
6

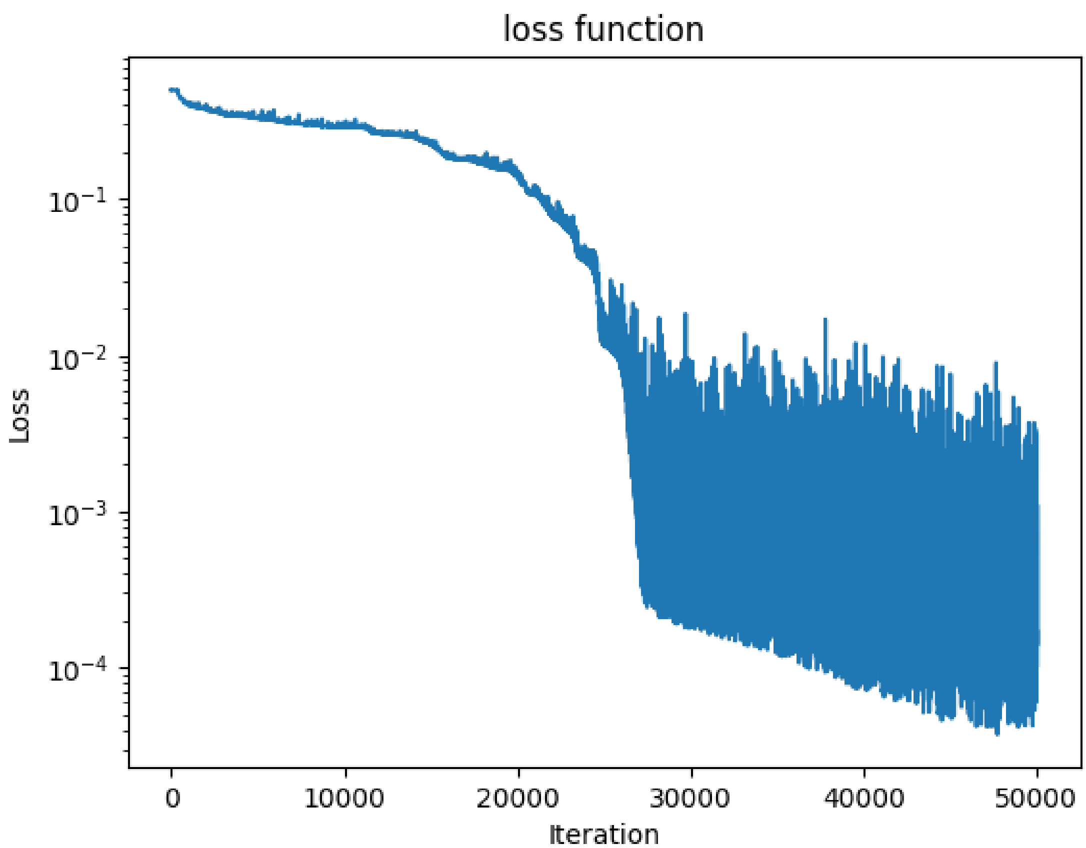

Training step 10000
Exact solution
PINN solution
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6


Training step 20000
Exact solution
PINN solution
0.15
0.10
0.05
0.00
−0.05
−0.10
−6
−4
−2
0
2
4
6


Training step 30000
0.05
0.00
−0.05
−0.10
−6
−4
−2
0
2
4
6
Exact solution
PINN solution


Training step 40000
0.05
0.00
−0.05
−0.10
−6
−4
−2
0
2
4
6
Exact solution
PINN solution





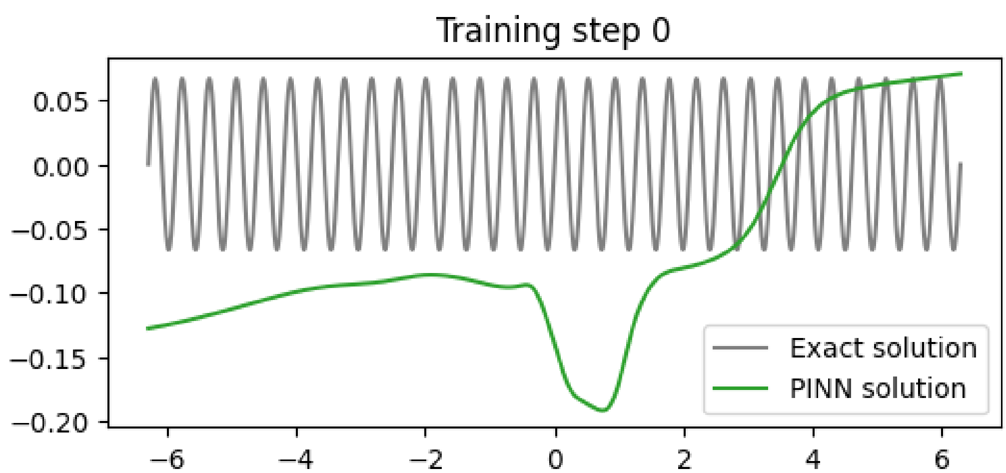
Tym razem sieć daje poprawną odpowiedz dla całej dziedziny.

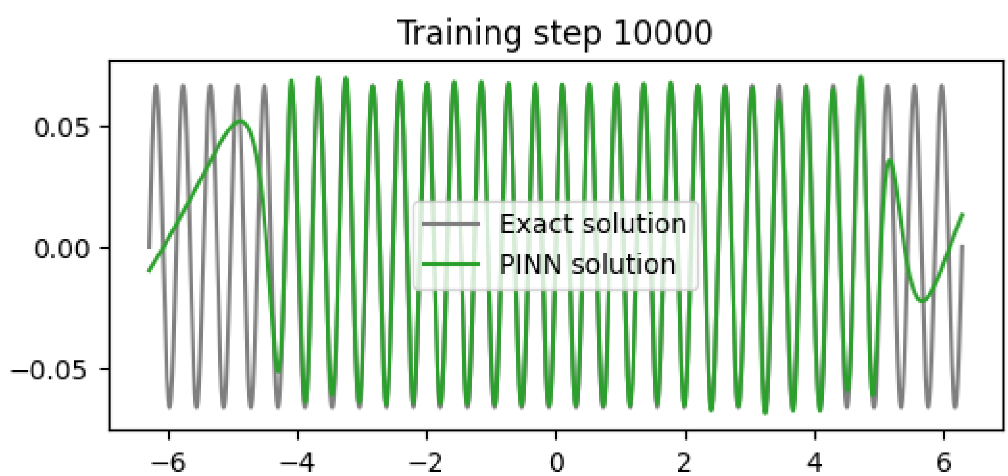
(d) 4 warstwy ukryte, 64 neuronów w każdej warstwie
liczba punktów treningowych: 3000

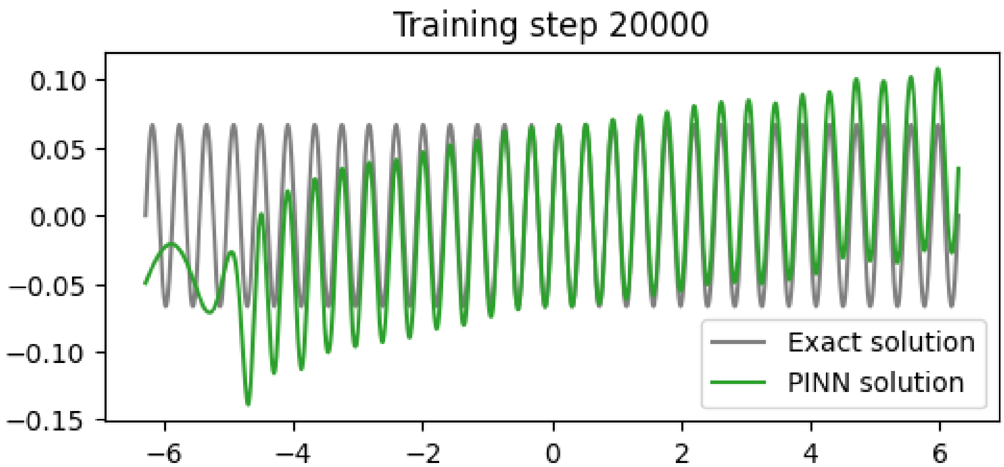
liczba punktów testowych: 5000
Wagi pierwszej warstwy ukrytej zostały zainicjalizowane cechami Fouriera

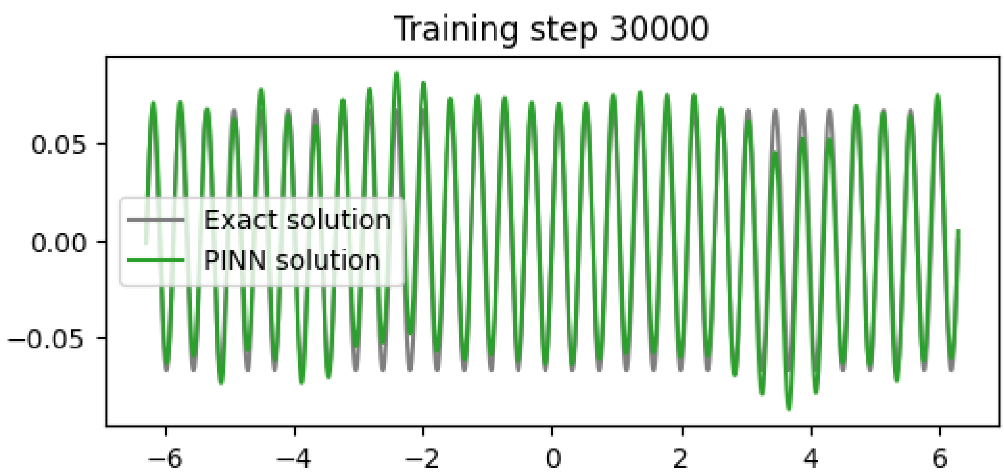
[ ]:
```
# podpunkt d
from torch.nn import functional as F
class FourierLayer(nn.Linear):
    def __init__(self, N_INPUT, N_HIDDEN):
        super().__init__( N_INPUT, N_HIDDEN)
        self.N_INPUT = N_INPUT
        self.N_HIDDEN = N_HIDDEN
        self.weight = torch.nn.Parameter(self._initialize_weights())

    def _initialize_weights(self):
        weights = np.zeros((self.N_HIDDEN, self.N_INPUT))
        for i in range(self.N_HIDDEN):
            for j in range(self.N_INPUT):
                if j % 2 == 0:
                    weights[i, j] = np.sin(2 ** (j+i) * np.pi)
                else:
                    weights[i, j] = np.cos(2 ** (j+i) * np.pi)
        weights = torch.tensor(weights, dtype=torch.float32)
        return weights

class FCN_fourier_variant(nn.Module):
    "Defines a fully-connected network in PyTorch with Fourier-initialized␣
 ↪first layer"
    def __init__(self, N_INPUT, N_OUTPUT, N_HIDDEN, N_LAYERS):
        super().__init__()
        activation = nn.Tanh


        self.fcs = nn.Sequential(*[
                        nn.Linear(N_INPUT, N_HIDDEN),
                        activation()])

        # Pierwsza warstwa ukryta
        self.ffch = nn.Sequential(
            FourierLayer(N_HIDDEN, N_HIDDEN),
            activation()

        )



        # Warstwy ukryte dalesze
        self.fch = nn.Sequential(*[
            nn.Sequential(
                nn.Linear(N_HIDDEN, N_HIDDEN),
```

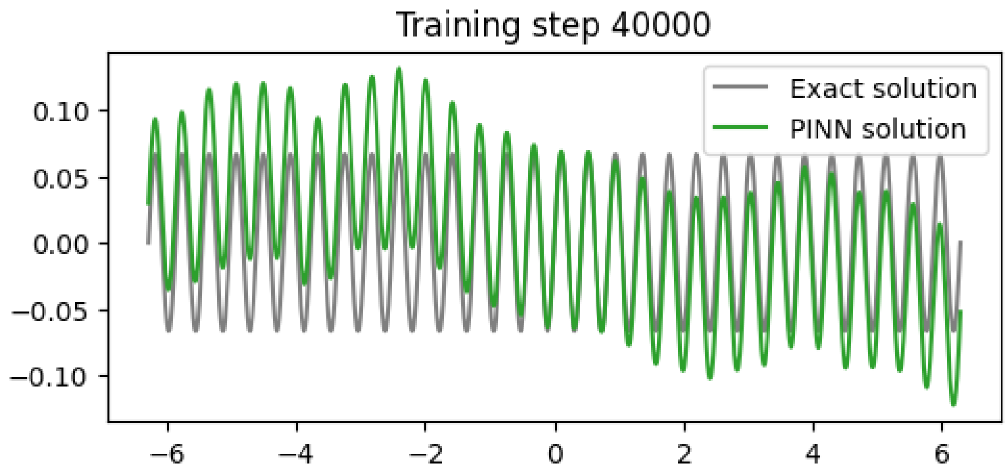
```
                activation()
            ) for _ in range(N_LAYERS-2)
        ])

        # Warstwa końcowa
        self.fce = nn.Linear(N_HIDDEN, N_OUTPUT)

    def forward(self, x):
        x = self.fcs(x)
        x = self.ffch(x)
        x = self.fch(x)
        x = self.fce(x)
        return x
pinn = FCN_fourier_variant(1,1,64,4)
train(pinn=pinn,w0=15,test_points=5000,train_points=3000,train_steps=100001)
```

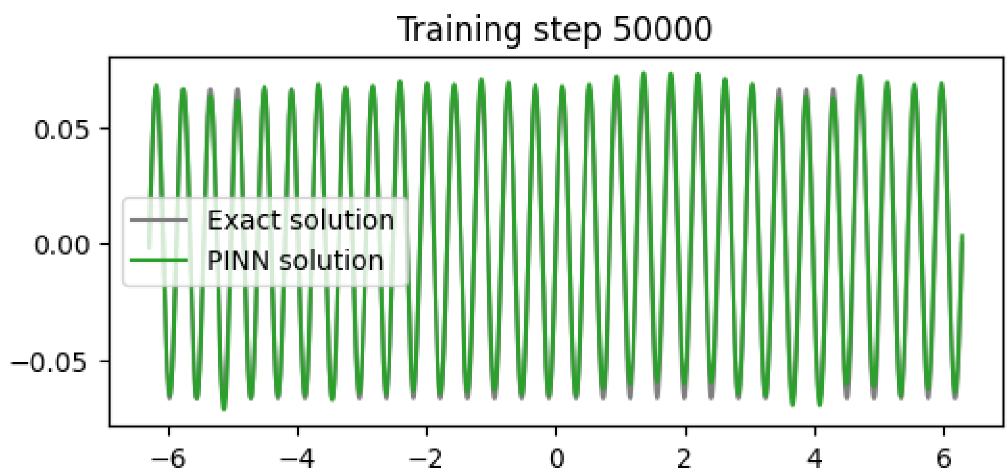


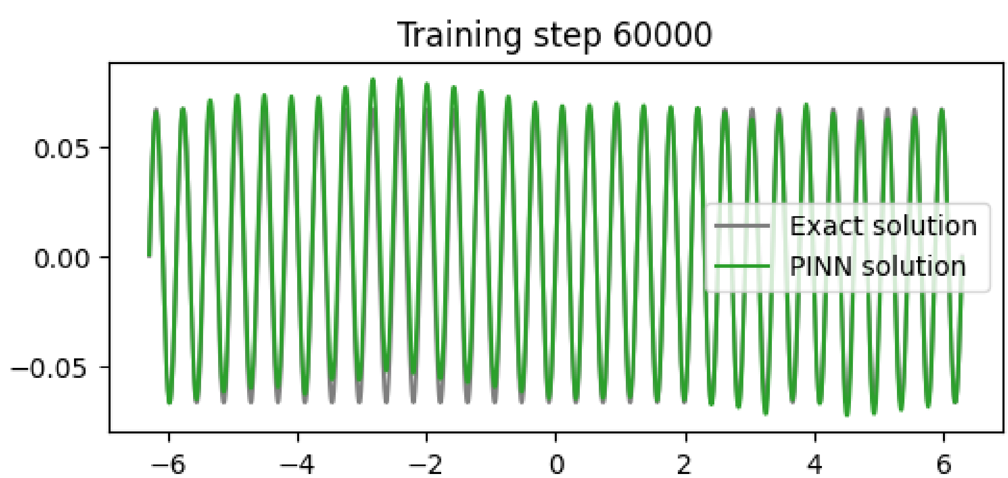


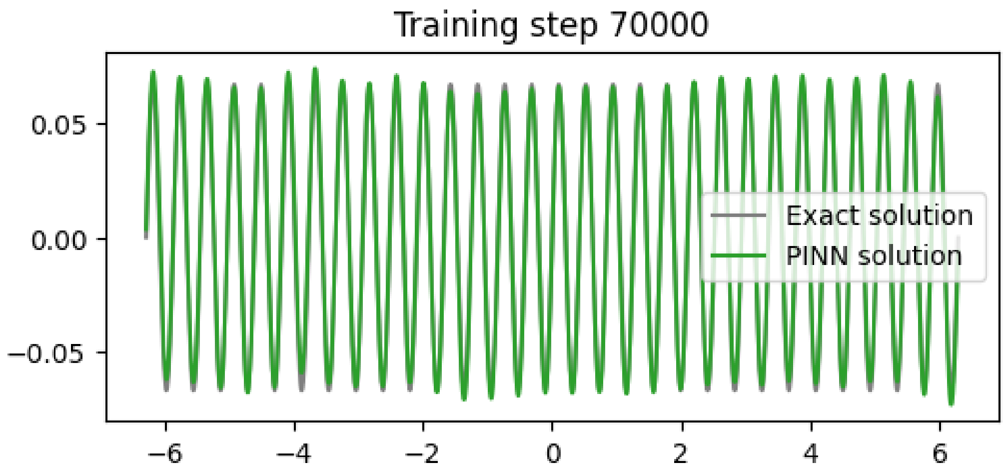

Training step 20000
0.10
0.05
0.00
−0.05
−0.10
−0.15
−6
−4
−2
0
2
4
6
Exact solution
PINN solution

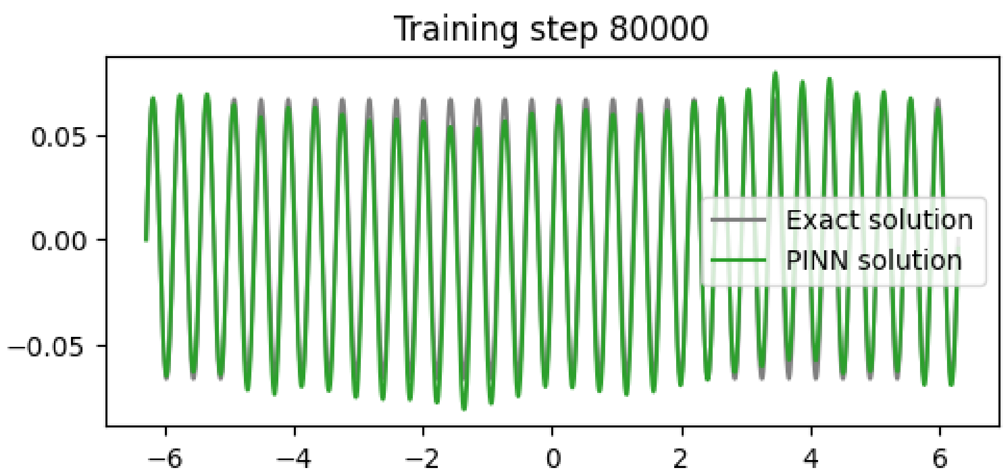

Training step 30000
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6
Exact solution
PINN solution

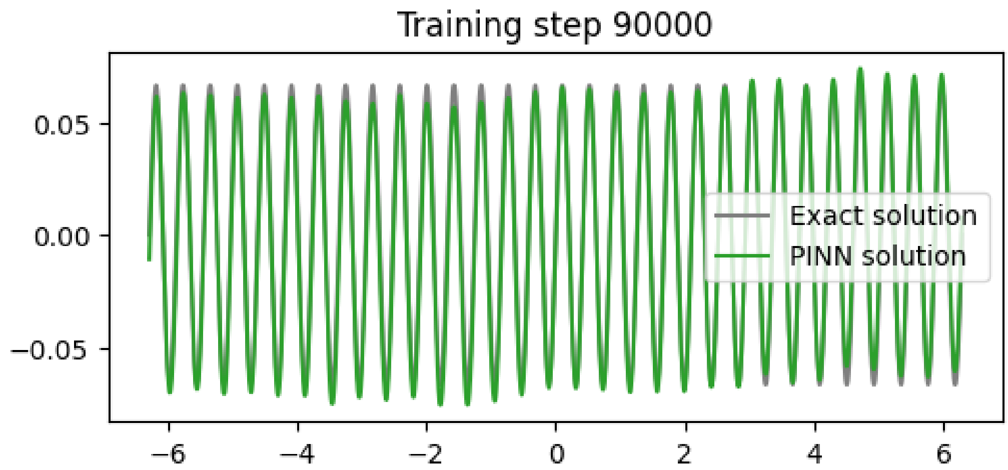

Training step 40000
Exact solution
PINN solution
0.10
0.05
0.00
−0.05
−0.10
−6
−4
−2
0
2
4
6


Training step 50000
Exact solution
PINN solution
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6

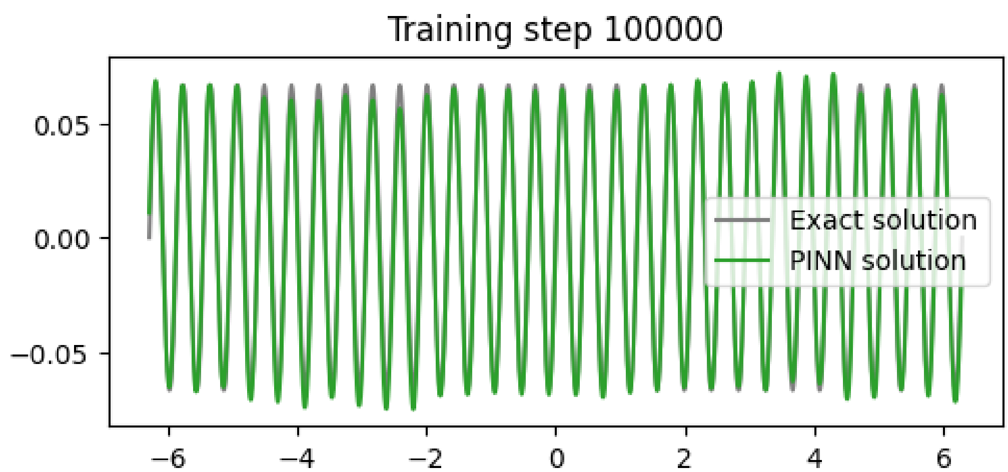

Training step 60000
Exact solution
PINN solution
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6


Training step 70000
Exact solution
PINN solution
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6

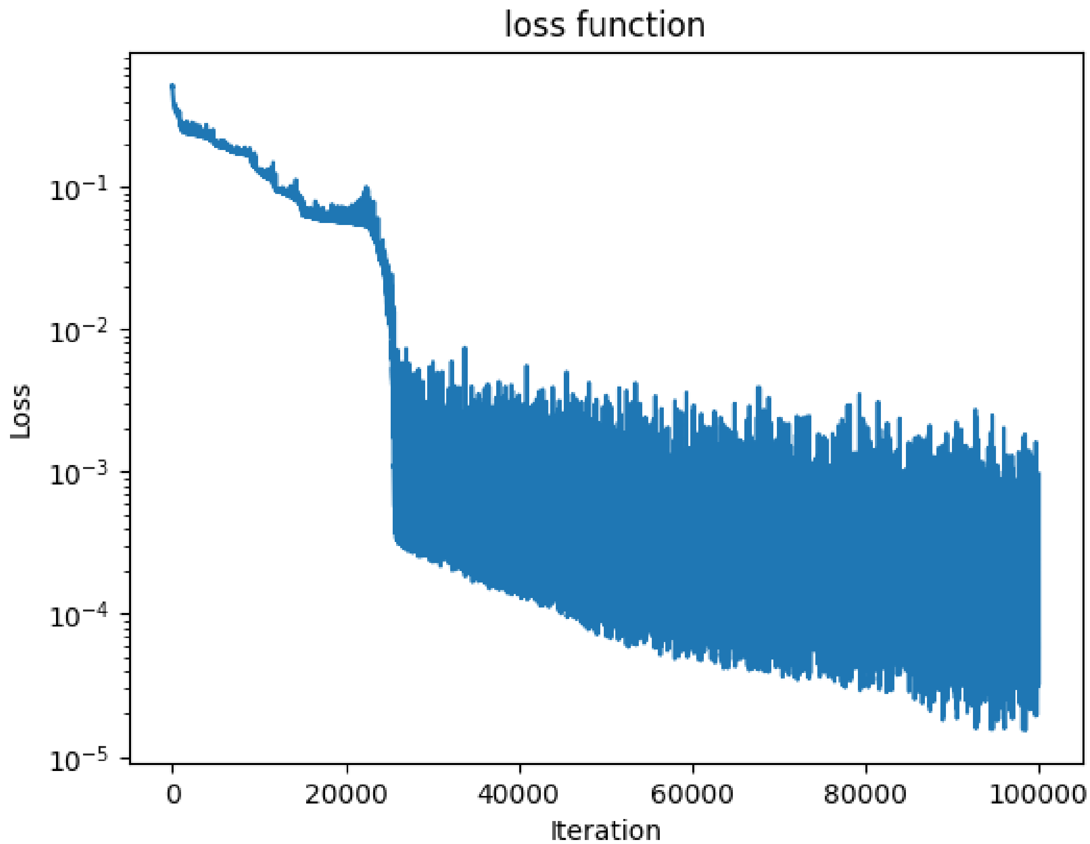

Training step 80000
Exact solution
PINN solution
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6



Training step 90000
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6
Exact solution
PINN solution



Training step 100000
0.05
0.00
−0.05
−6
−4
−2
0
2
4
6
Exact solution
PINN solution



Sieć osiąga zadowalające wyniki już po 30000 iteeracji.

Wnioski Bardzo małe sieci dają poprawne wyniki dla niskich wartości ω, dla wyższych częstotliwości, nie udaje im się to.

Najlepszy stosunek wielkości do jakości wyników oferują sieci o 4 warstwach ukrytych i 64 neuronach na warstwe.