

a01-fnn

April 4, 2024

```
[1]: # Edited by: Kok Teng Ng (1936360), Minjeong Lee (1978925)
      # IE 678 Deep Learning, University of Mannheim
      # Author: Rainer Gemulla
```

```
[2]: %matplotlib ipyml

import math
import matplotlib.pyplot as plt
import torch
import torch.nn as nn
import torch.nn.functional as F

# import helper functions
import sys, os

sys.path.append(os.getcwd())
from a01helper import * # check out the helper functions there, if you like
```

Warning: Cannot change to a different GUI toolkit: notebook. Using ipyml instead.

1 Task 1: Implement an MLP

1.1 1a Logistic Regression

```
[3]: # nn.Module is the superclass of all PyTorch models.
      class LogisticRegression(nn.Module):
          """A logistic regression model.

          Parameters
          -----
          D number of inputs
          C number of classes
          """

          # the definition of all parameters the model uses happens here, i.e., during
          # initialization
          def __init__(self, D, C):
```

```

    super(LogisticRegression, self).__init__()

    # Create and initialize model parameters. For (multinomial) logistic
    ↪ regression,
    # we have a DxC-dimensional weight matrix W and a C-dimensional bias b.
    self.W = torch.randn(D, C) / math.sqrt(D)
    self.b = torch.randn(C) / math.sqrt(C)

    # Model parameters must be registered to PyTorch as follows. Here we
    ↪ provide
    # a useful name that helps to access/analyze the model later on.
    self.register_parameter("0_weight", nn.Parameter(self.W))
    self.register_parameter("0_bias", nn.Parameter(self.b))

    # the forward function computes the model output for the provided (for this
    # assignment: single) input
    def forward(self, x):
        eta = self.W.t() @ x + self.b
        logprob = F.log_softmax(eta, dim=-1)
        return logprob

```

```

[4]: # let's test it
logreg = LogisticRegression(3, 2)
x = torch.rand(3) # input
logreg(x) # output (log probabilities)
logreg(x).exp() # output (probabilities)

```

```

[4]: tensor([0.1429, 0.8571])

```

```

[5]: # you can access individual parameters as follows
logreg.get_parameter("0_bias")

```

```

[5]: Parameter containing:
tensor([0.0750, 0.1680], requires_grad=True)

```

```

[6]: # or all of them at once
list(logreg.named_parameters())

```

```

[6]: [('0_weight',
Parameter containing:
tensor([[ -1.1634,  0.1442],
        [ 0.9870, -0.0718],
        [-0.7443,  0.9194]], requires_grad=True)),
('0_bias',
Parameter containing:
tensor([0.0750, 0.1680], requires_grad=True))]

```

```
[7]: # or directly the tensors stored in the parameters
for par, value in logreg.state_dict().items():
    print(f"{par:<15}= {value}")
```

```
0_weight      = tensor([[ -1.1634,  0.1442],
                        [ 0.9870, -0.0718],
                        [-0.7443,  0.9194]])
0_bias        = tensor([0.0750, 0.1680])
```

1.2 1b MLP

```
[8]: class MLP(nn.Module):
    """A fully-connected MLP.

    Parameters
    -----

    sizes Contains the layer sizes. The first entry is the number of inputs,
    →the last
    entry the number of outputs. All entries in between correspond to the
    →number of
    units in the respective hidden layer. E.g., [2,5,7,1] means: 2 inputs → 5D
    →hidden
    layer → 7D hidden layer → 1 output.

    phi Activation function used in every hidden layer (the output layer is
    →linear).

    """
    def __init__(self, sizes: list[int], phi=F.sigmoid):
        super().__init__()

        # let's remember the specification in this model
        self.sizes = sizes
        self.phi = phi

        # Initialize and register the parameters. Follow the naming scheme used
        →for
        # logistic regression above, i.e., the layer-i weights should be named
        →"i_weight" and
        # "i_bias".

        for i in range(1, len(sizes)):
            self.register_parameter(f'{i - 1}_weight', torch.nn.Parameter(torch.
            →randn(sizes[i - 1], sizes[i]) / math.sqrt(sizes[i - 1])))
            self.register_parameter(f'{i - 1}_bias', torch.nn.Parameter(torch.
            →randn(sizes[i]) / math.sqrt(sizes[i])))
```

```

def num_layers(self):
    """Number of layers (excluding input layer)"""
    return len(self.sizes) - 1

def forward(self, x):
    for i in range(0, self.num_layers() - 1):
        weight = getattr(self, f"{i}_weight")
        bias = getattr(self, f"{i}_bias")
        x = weight.t() @ x + bias
        x = self.phi(x)
    weight = getattr(self, f"{self.num_layers() - 1}_weight")
    bias = getattr(self, f"{self.num_layers() - 1}_bias")
    x = weight.t() @ x + bias
    return x

```

[9]: *# here you should see the correct parameter sizes*

```

mlp = MLP([2, 3, 4, 2], torch.relu)
list(mlp.named_parameters())

```

```

[9]: [('0_weight',
      Parameter containing:
      tensor([[ -0.5704,  0.5691,  1.5064],
              [-0.9854, -0.7690, -0.2701]], requires_grad=True)),
      ('0_bias',
      Parameter containing:
      tensor([ 0.6671,  0.0168, -0.4676], requires_grad=True)),
      ('1_weight',
      Parameter containing:
      tensor([[ -0.8372, -0.3348, -0.9992,  0.2811],
              [ 0.1674,  0.1962, -0.2086,  0.0852],
              [ 0.1544, -0.7625,  0.0525, -0.5802]], requires_grad=True)),
      ('1_bias',
      Parameter containing:
      tensor([ 0.4051, -0.3382,  0.0240,  0.4486], requires_grad=True)),
      ('2_weight',
      Parameter containing:
      tensor([[ -1.0556,  0.0663],
              [-0.4395, -0.8077],
              [-0.0792,  0.0922],
              [ 0.2066,  1.0688]], requires_grad=True)),
      ('2_bias',
      Parameter containing:
      tensor([-0.2358, -0.5284], requires_grad=True))]

```

[10]: *# Test your code; we fix the parameters and check the result*
with torch.no_grad():

```

torch.manual_seed(0)
for l in range(mlp.num_layers()):
    W, b = mlp.get_parameter(f"{l}_weight"), mlp.get_parameter(f"{l}_bias")
    W[:] = torch.randn(W.shape)
    b[:] = torch.randn(b.shape)

mlp(torch.tensor([-1.0, 2.0])) # must give: [ 0.8315, -3.6792]

```

```
[10]: tensor([ 0.8315, -3.6792], grad_fn=<AddBackward0>)
```

```

[11]: # You can also evaluate your model on multiple inputs at once. Here "torch.func.
      ↪vmap"
      # produces a function that applies the provided function (mlp#forward) to each
      ↪row of
      # its argument (torch.tensor...).
      #
      # [[ 0.8315, -3.6792],
      # [ 4.8448, -6.8813]]
      torch.func.vmap(mlp)(torch.tensor([[-1.0, 2.0], [1.0, -2.0]]))

```

```
[11]: tensor([[ 0.8315, -3.6792],
              [ 4.8448, -6.8813]], grad_fn=<AddBackward0>)
```

1.3 1c Batching

```

[12]: class MLP(nn.Module):
      def __init__(self, sizes: list[int], phi=F.sigmoid):
          super().__init__()

          self.sizes = sizes
          self.phi = phi

          for i in range(1, len(sizes)):
              self.register_parameter(f'{i - 1}_weight', torch.nn.Parameter(torch.
              ↪randn(sizes[i - 1], sizes[i]) / math.sqrt(sizes[i - 1])))
              self.register_parameter(f'{i - 1}_bias', torch.nn.Parameter(torch.
              ↪randn(sizes[i]) / math.sqrt(sizes[i])))

          def num_layers(self):
              return len(self.sizes) - 1

          def forward(self, x):
              if x.dim == 1:
                  x = x.unsqueeze(0)
              for i in range(0, self.num_layers() - 1):
                  weight = getattr(self, f"{i}_weight")
                  bias = getattr(self, f"{i}_bias")

```

```

        x = x @ weight + bias.unsqueeze(0)
        x = self.phi(x)
        weight = getattr(self, f"{self.num_layers() - 1}_weight")
        bias = getattr(self, f"{self.num_layers() - 1}_bias")
        x = x @ weight + bias.unsqueeze(0)
        return x

```

```

[13]: # here you should see the correct parameter sizes
mlp = MLP([2, 3, 4, 2], torch.relu)

```

```

[14]: # Test your code; we fix the parameters and check the result
with torch.no_grad():
    torch.manual_seed(0)
    for l in range(mlp.num_layers()):
        W, b = mlp.get_parameter(f"{l}_weight"), mlp.get_parameter(f"{l}_bias")
        W[:] = torch.randn(W.shape)
        b[:] = torch.randn(b.shape)

```

```

[15]: # After you adapted the MLP class, you should get the same results as above.
mlp(torch.tensor([-1.0, 2.0])) # must give: [ 0.8315, -3.6792]

```

```

[15]: tensor([[ 0.8315, -3.6792]], grad_fn=<AddBackward0>)

```

```

[16]: # Now without vmap. Only proceed to task 2 once this works correctly.
#
# [[ 0.8315, -3.6792],
# [ 4.8448, -6.8813]]
mlp(torch.tensor([-1.0, 2.0], [1.0, -2.0]))

```

```

[16]: tensor([[ 0.8315, -3.6792],
            [ 4.8448, -6.8813]], grad_fn=<AddBackward0>)

```

2 2 Multi-Layer Feed-Forward Neural Networks

2.1 2a Conjecture how an FNN fit will look like

```

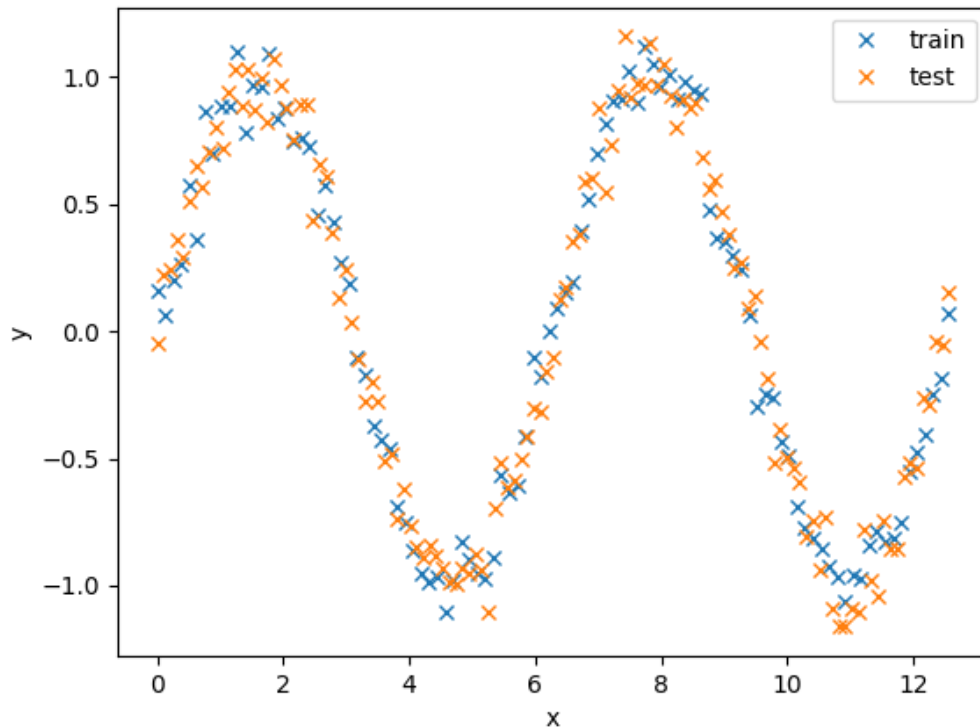
[17]: # here is the one-dimensional dataset that we will use
nextplot()
plot1(X1, y1, label="train")
plot1(X1test, y1test, label="test")
plt.legend()

```

```

[17]: <matplotlib.legend.Legend at 0x17ec1a2e0>

```



2.2 2b Train with 2 hidden units

```
[18]: # Training code. You do not need to modify this code.
train_bfgs = lambda model, **kwargs: train_scipy(X1, y1, model, **kwargs)

def train1(hidden_sizes, nreps=10, phi=F.sigmoid, train=train_bfgs, **kwargs):

    """Train an FNN.

    hidden_sizes is a (possibly empty) list containing the sizes of the hidden_
    ↪ layer(s).
    nreps refers to the number of repetitions.

    """

    best_model = None
    best_cost = math.inf
    for rep in range(nreps):
        model = MLP([1] + hidden_sizes + [1], phi) # that's your model!
        print(f"X1 shape: {X1.shape}")
```

```

    print(f"Repetition {rep: 2d}: ", end="")
    model = train(model, **kwargs)
    mse = F.mse_loss(y1, model(X1)).item()
    if mse < best_cost:
        best_model = model
        best_cost = mse
    print(f"best_cost={best_cost:.3f}")

    return best_model

```

```

[19]: # Let's fit the model with one hidden layer consisting of 2 units.
model = train1([2], nreps=1)
print("Training error:", F.mse_loss(y1, model(X1)).item())
print("Test error      :", F.mse_loss(y1test, model(X1test)).item())

```

```

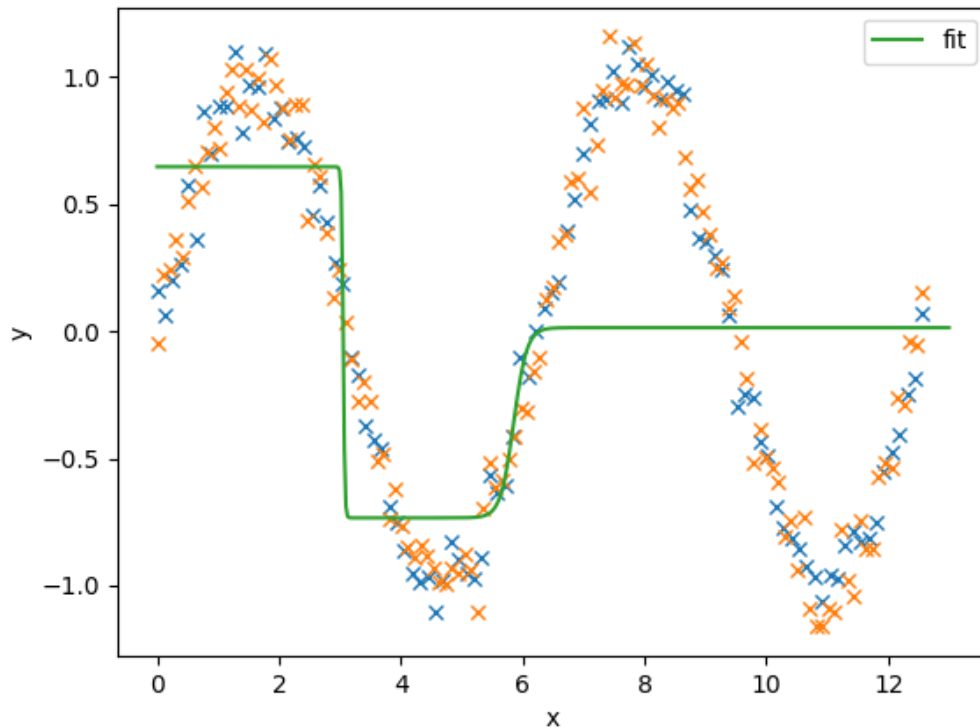
X1 shape: torch.Size([100, 1])
Repetition 0: Optimization terminated successfully.
    Current function value: 0.293673
    Iterations: 120
    Function evaluations: 240
    Gradient evaluations: 233
best_cost=0.294
Training error: 0.29367321729660034
Test error      : 0.30551230907440186

```

```

[20]: # plot the data and the fit
nextplot()
plot1(X1, y1, label="train")
plot1(X1test, y1test, label="test")
plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model)

```

```
[21]: # The weight matrices and bias vectors can be read out as follows. If you want,
      ↪ use
      # these parameters to compute the output of the network (on X1) directly and
      ↪ compare to
      # vmap(model)(X1).
      for par, value in model.state_dict().items():
          print(f"{par:<15}= {value}")
```

```
0_weight      = tensor([[75.7091,  9.2566]])
0_bias        = tensor([-231.3285, -54.1847])
1_weight      = tensor([[ -1.3810,
        [ 0.7480]])
1_bias        = tensor([0.6471])
```

```
[22]: # now repeat this multiple times
      for i in range(0, 5):
          model = train1([2], nreps=1)
          print("Training error:", F.mse_loss(y1, model(X1)).item())
          print("Test error      :", F.mse_loss(y1test, model(X1test)).item())
          nextplot()
          plot1(X1, y1, label="train")
```

```
plot1(X1test, y1test, label="test")
plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model)
```

```
X1 shape: torch.Size([100, 1])
Repetition 0:      Current function value: 0.079572
      Iterations: 387
      Function evaluations: 521
      Gradient evaluations: 511
best_cost=0.080
Training error: 0.07957355678081512
Test error      : 0.08671201020479202

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

X1 shape: torch.Size([100, 1])
Repetition 0: Optimization terminated successfully.
      Current function value: 0.303902
      Iterations: 143
      Function evaluations: 155
      Gradient evaluations: 155
best_cost=0.304
Training error: 0.30390220880508423
Test error      : 0.3037970960140228
X1 shape: torch.Size([100, 1])
Repetition 0:      Current function value: 0.079573
      Iterations: 400
      Function evaluations: 562
      Gradient evaluations: 551
best_cost=0.080
Training error: 0.07957581430673599
Test error      : 0.0867120772600174

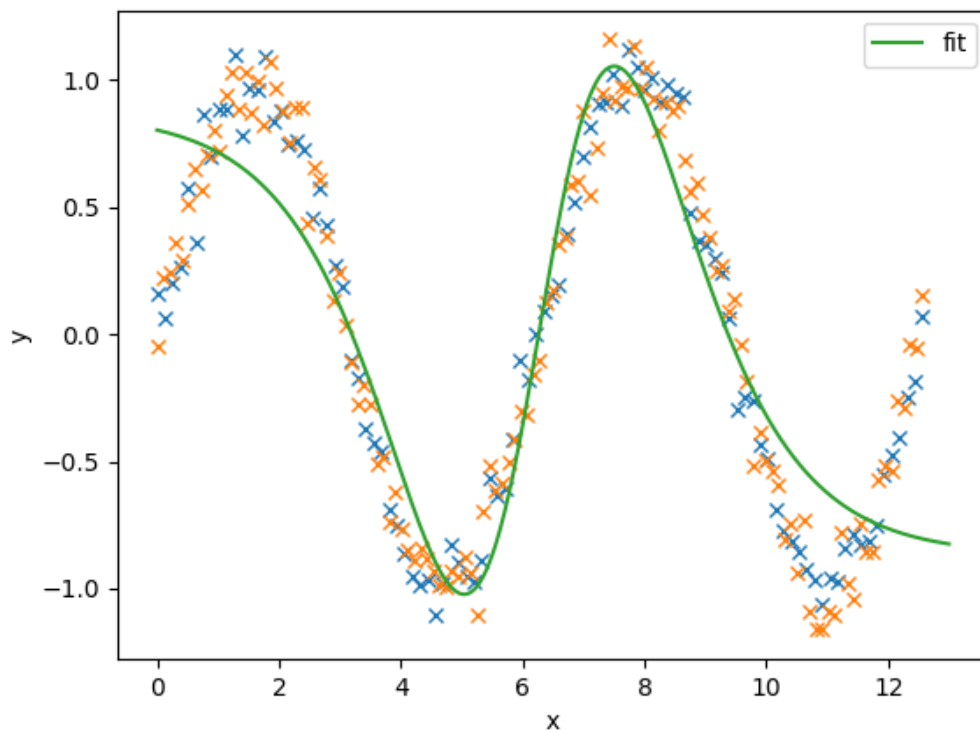
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

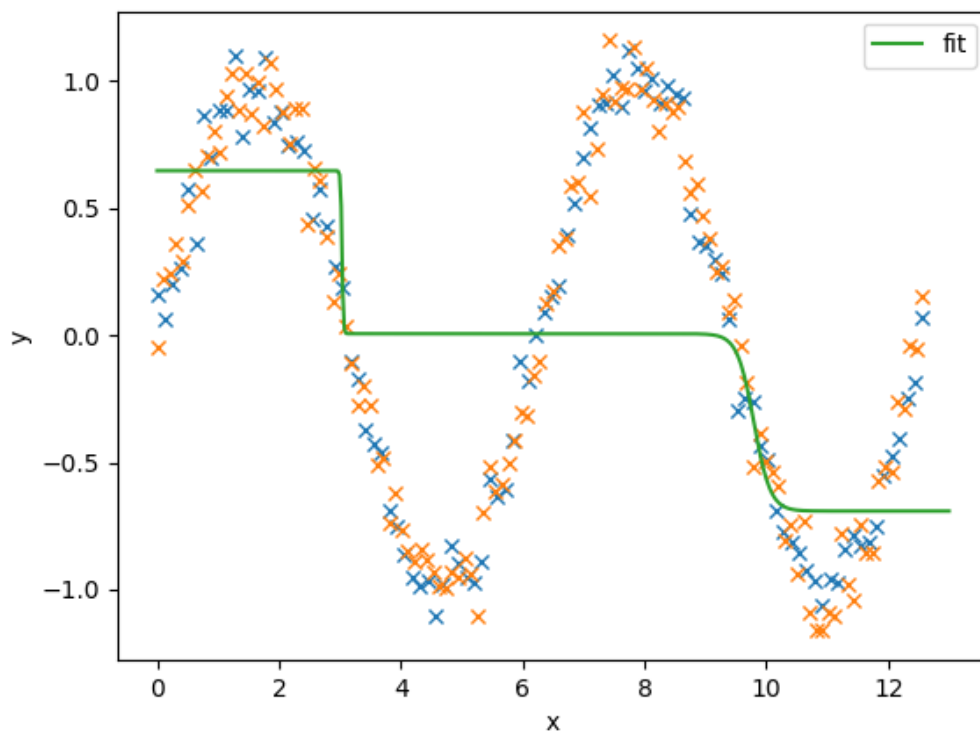
X1 shape: torch.Size([100, 1])
Repetition 0:      Current function value: 0.286909
      Iterations: 302
      Function evaluations: 458
      Gradient evaluations: 445
best_cost=0.287
```

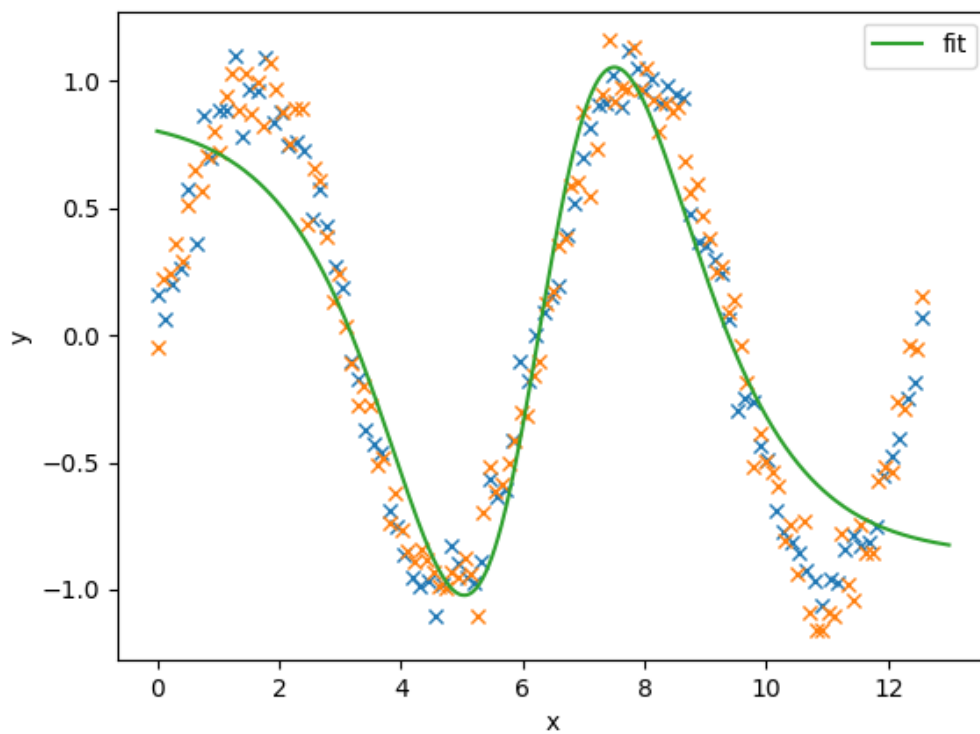
```
Training error: 0.28690817952156067
Test error    : 0.29484879970550537
X1 shape: torch.Size([100, 1])
Repetition  0:      Current function value: 0.079573
      Iterations: 336
      Function evaluations: 470
      Gradient evaluations: 458
best_cost=0.080
Training error: 0.07956987619400024
Test error    : 0.0867103710770607
```

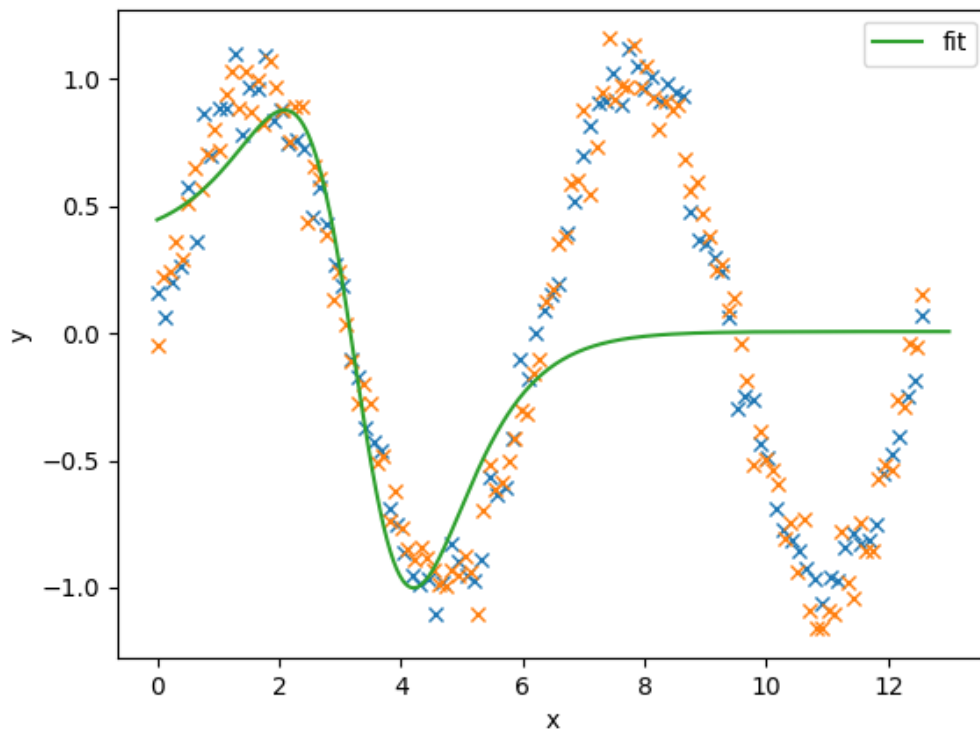
```
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
```

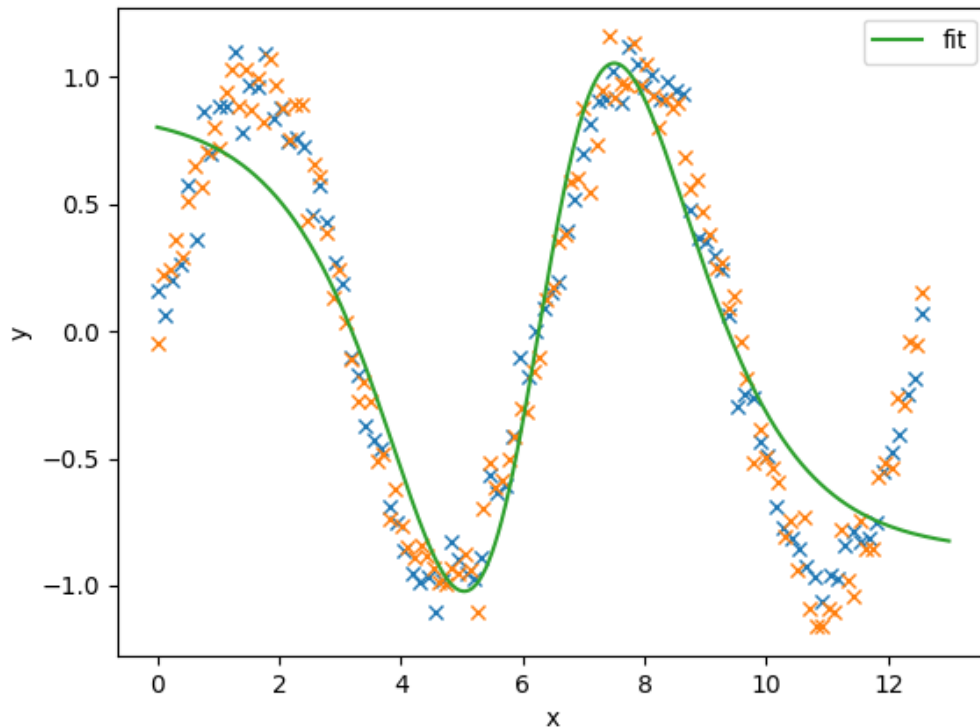
```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```











[23]: *# From now on, always train multiple times (nreps=10 by default) and report ↪ best model.*

```
model = train1([2], nreps=10)
```

```
print("Training error:", F.mse_loss(y1, model(X1)).item())
```

```
print("Test error      :", F.mse_loss(y1test, model(X1test)).item())
```

```
X1 shape: torch.Size([100, 1])
```

```
Repetition 0: Optimization terminated successfully.
```

```
    Current function value: 0.357250
```

```
    Iterations: 66
```

```
    Function evaluations: 76
```

```
    Gradient evaluations: 76
```

```
best_cost=0.357
```

```
X1 shape: torch.Size([100, 1])
```

```
Repetition 1:      Current function value: 0.438546
```

```
    Iterations: 278
```

```
    Function evaluations: 398
```

```
    Gradient evaluations: 386
```

```
best_cost=0.357
```

```
X1 shape: torch.Size([100, 1])
```

Repetition 2:

```
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not  
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not  
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
Current function value: 0.286909
```

```
Iterations: 448
```

```
Function evaluations: 577
```

```
Gradient evaluations: 565
```

```
best_cost=0.287
```

```
X1 shape: torch.Size([100, 1])
```

Repetition 3: Current function value: 0.079573

```
Iterations: 310
```

```
Function evaluations: 459
```

```
Gradient evaluations: 449
```

```
best_cost=0.080
```

```
X1 shape: torch.Size([100, 1])
```

Repetition 4:

```
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not  
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not  
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
Current function value: 0.286909
```

```
Iterations: 307
```

```
Function evaluations: 413
```

```
Gradient evaluations: 401
```

```
best_cost=0.080
```

```
X1 shape: torch.Size([100, 1])
```

Repetition 5: Current function value: 0.286909

```
Iterations: 534
```

```
Function evaluations: 690
```

```
Gradient evaluations: 681
```

```
best_cost=0.080
```

```
X1 shape: torch.Size([100, 1])
```

Repetition 6:

```
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
```



```

necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.079573
        Iterations: 330
        Function evaluations: 470
        Gradient evaluations: 458
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition  7:          Current function value: 0.079573
        Iterations: 381
        Function evaluations: 537
        Gradient evaluations: 524
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition  8: Optimization terminated successfully.
        Current function value: 0.357250
        Iterations: 78
        Function evaluations: 80
        Gradient evaluations: 80
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition  9:          Current function value: 0.286909
        Iterations: 324
        Function evaluations: 546
        Gradient evaluations: 533
best_cost=0.080
Training error: 0.07957330346107483
Test error      : 0.0867152065038681

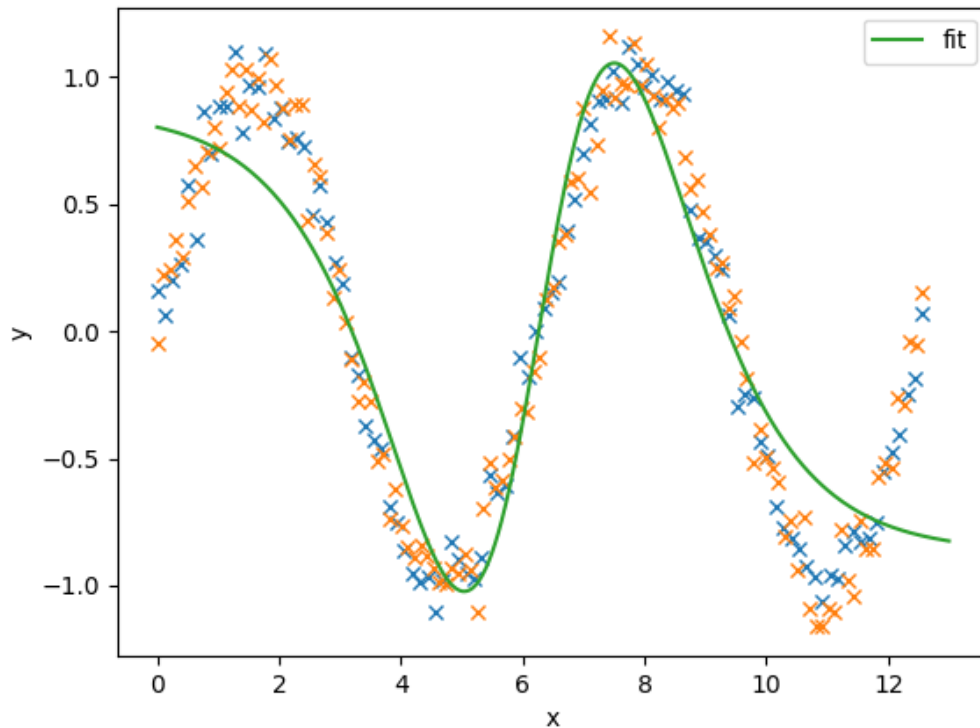
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

```

```

[24]: # plot the data and the fit
nextplot()
plot1(X1, y1, label="train")
plot1(X1test, y1test, label="test")
plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model)

```



2.3 2c Width

[25]: *# Experiment with different hidden layer sizes. To avoid recomputing
models, you may want to save your models using torch.save(model, filename) and
load them again using torch.load(filename).*

```
for i in [1, 2, 3, 10, 50, 100]:
    model = train1([i], nreps = 1)
    print("Training error:", F.mse_loss(y1, model(X1)).item())
    print("Test error      :", F.mse_loss(y1test, model(X1test)).item())
    torch.save(model, f"model_{i}.pth")
```

X1 shape: torch.Size([100, 1])

Repetition 0: Optimization terminated successfully.

Current function value: 0.372919

Iterations: 42

Function evaluations: 47

Gradient evaluations: 47

best_cost=0.373

Training error: 0.3729189336299896

Test error : 0.3743167221546173

```

X1 shape: torch.Size([100, 1])
Repetition 0:          Current function value: 0.079573
                    Iterations: 390
                    Function evaluations: 593
                    Gradient evaluations: 583
best_cost=0.080
Training error: 0.07957376539707184
Test error      : 0.08670931309461594
X1 shape: torch.Size([100, 1])
Repetition 0:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

                    Current function value: 0.049892
                    Iterations: 289
                    Function evaluations: 469
                    Gradient evaluations: 456
best_cost=0.050
Training error: 0.04989229515194893
Test error      : 0.0598050132393837
X1 shape: torch.Size([100, 1])
Repetition 0:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

                    Current function value: 0.005721
                    Iterations: 1026
                    Function evaluations: 1250
                    Gradient evaluations: 1234
best_cost=0.006
Training error: 0.0057213036343455315
Test error      : 0.0150537034496665
X1 shape: torch.Size([100, 1])
Repetition 0:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

                    Current function value: 0.003007

```

```

        Iterations: 5655
        Function evaluations: 6282
        Gradient evaluations: 6268
best_cost=0.003
Training error: 0.0030068017076700926
Test error      : 2.0873610973358154
X1 shape: torch.Size([100, 1])
Repetition  0:      Current function value: 0.001826
        Iterations: 8126
        Function evaluations: 8804
        Gradient evaluations: 8792
best_cost=0.002
Training error: 0.001825749408453703
Test error      : 4.303783893585205

/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

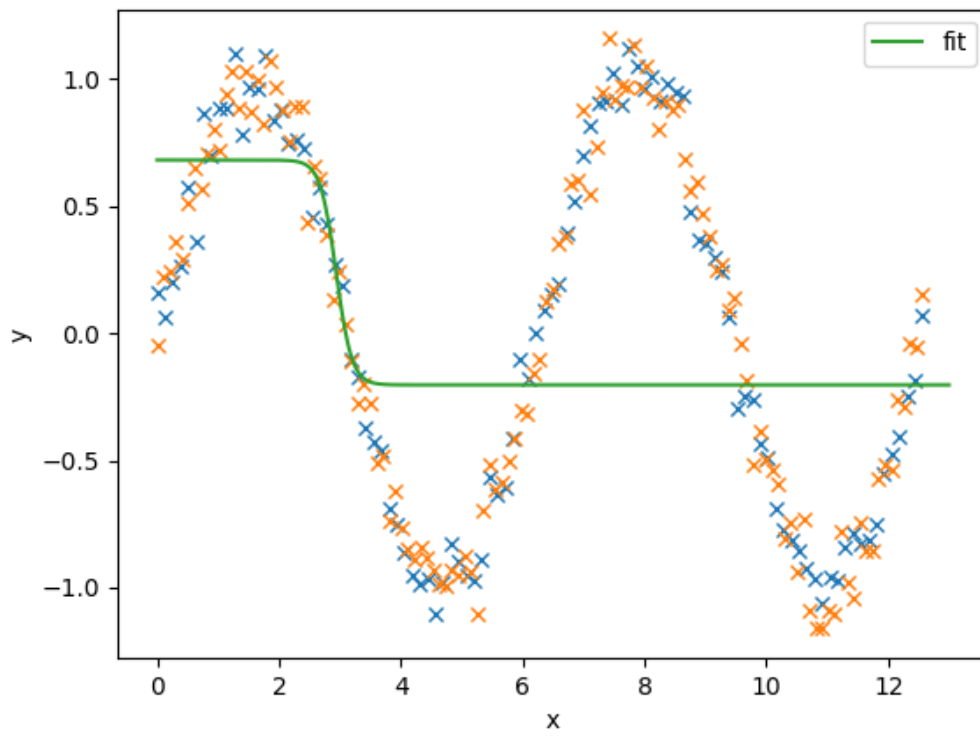
```

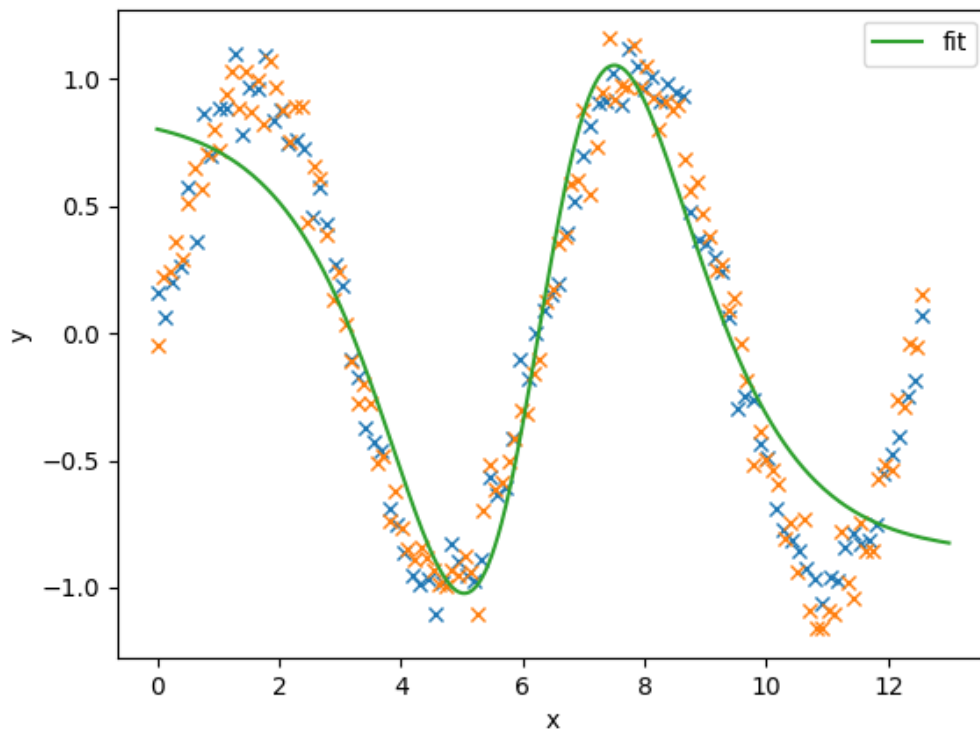
```

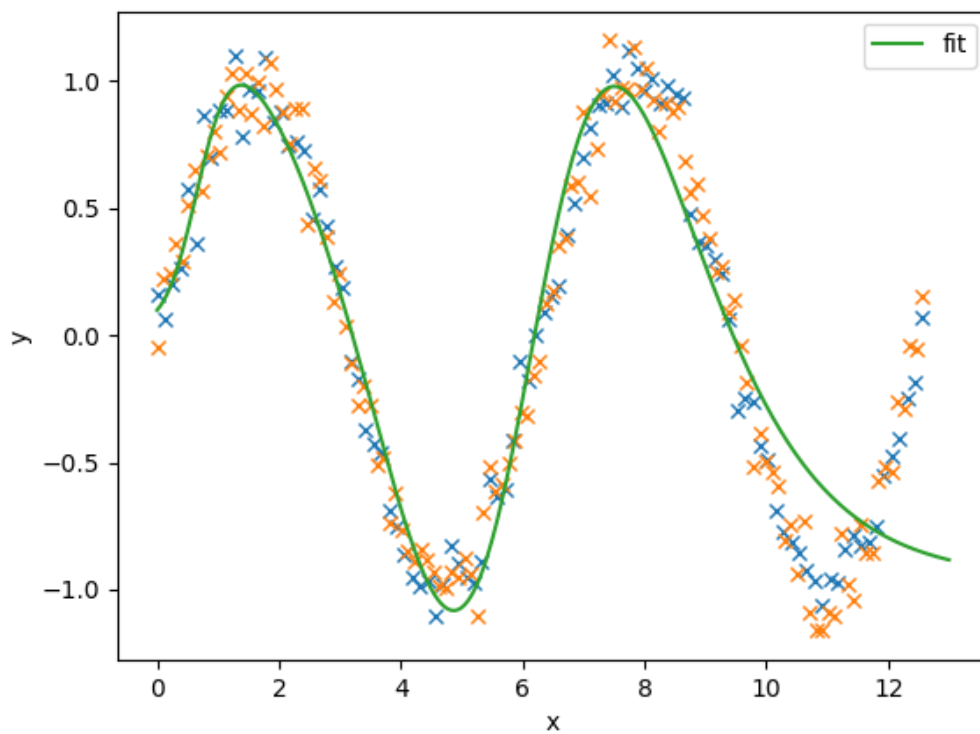
[26]: # torch.load(filename)

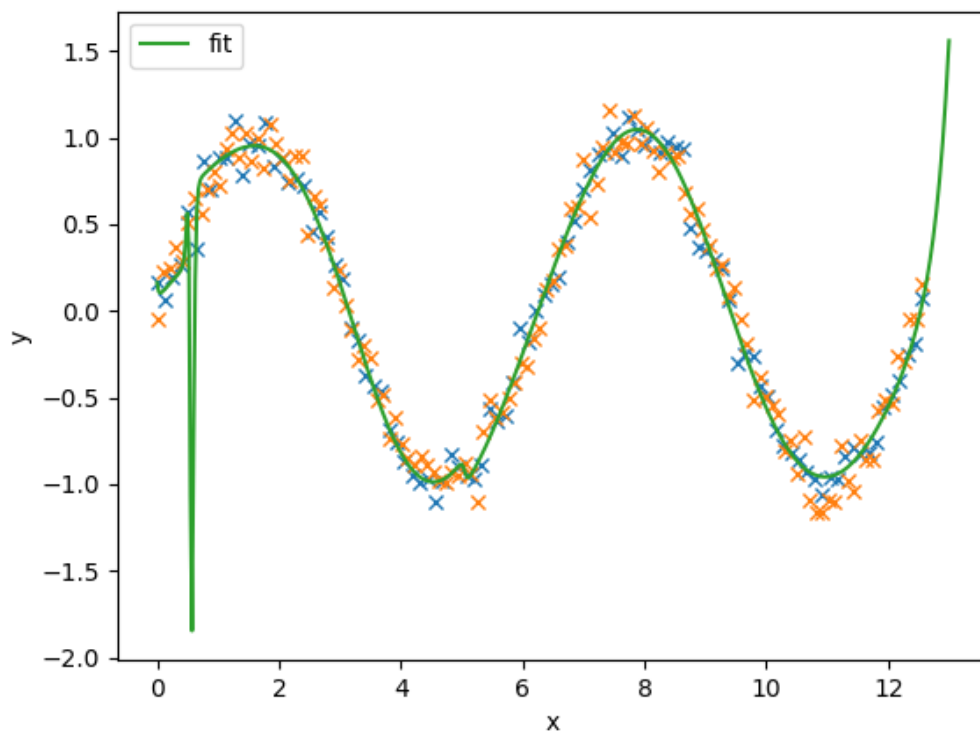
for i in [1, 2, 3, 10, 50, 100]:
    model = torch.load(f"model_{i}.pth")
    nextplot()
    plot1(X1, y1, label="train")
    plot1(X1test, y1test, label="test")
    plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model)

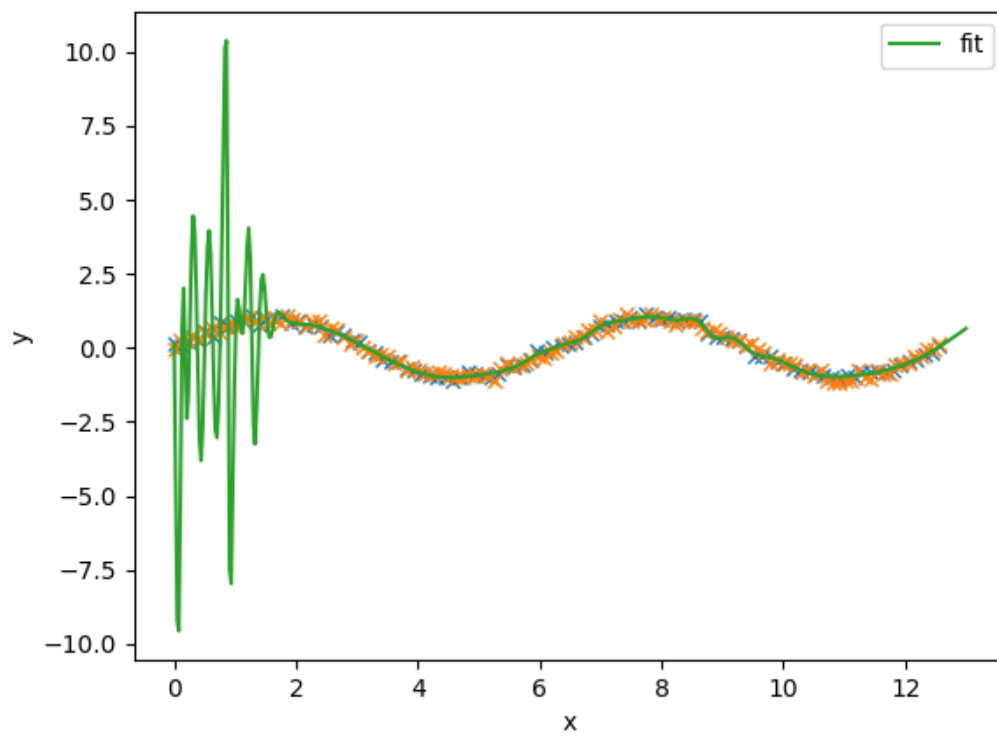
```

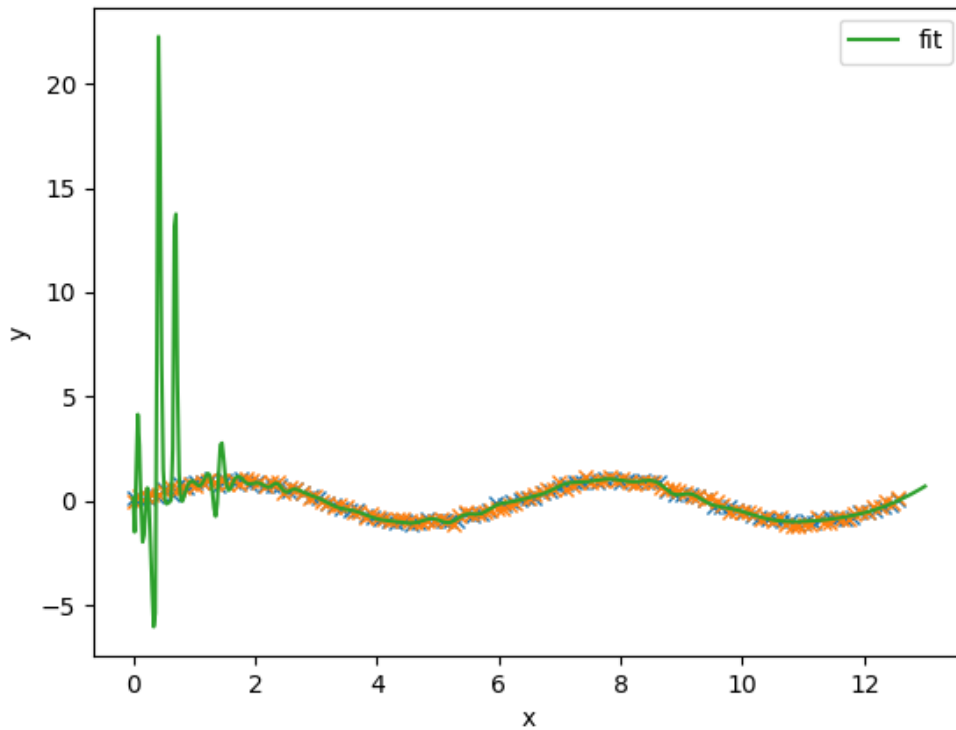












2.4 2d Distributed representations

```
[27]: # train a model to analyze
      model = train1([2])
```

```
X1 shape: torch.Size([100, 1])
Repetition 0:      Current function value: 0.079573
      Iterations: 399
      Function evaluations: 542
      Gradient evaluations: 533
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 1: Optimization terminated successfully.
      Current function value: 0.301865
      Iterations: 131
      Function evaluations: 161
      Gradient evaluations: 161
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 2:
```

```

/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.079573
        Iterations: 384
        Function evaluations: 538
        Gradient evaluations: 526
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 3:          Current function value: 0.079573
        Iterations: 379
        Function evaluations: 534
        Gradient evaluations: 523
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 4: Optimization terminated successfully.
        Current function value: 0.372457
        Iterations: 131
        Function evaluations: 137
        Gradient evaluations: 137
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 5:

/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.079573
        Iterations: 402
        Function evaluations: 536
        Gradient evaluations: 525
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 6: Optimization terminated successfully.
        Current function value: 0.277769
        Iterations: 86
        Function evaluations: 97

```

```

        Gradient evaluations: 97
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 7: Optimization terminated successfully.
    Current function value: 0.357250
    Iterations: 85
    Function evaluations: 90
    Gradient evaluations: 90
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 8:      Current function value: 0.079572
    Iterations: 392
    Function evaluations: 619
    Gradient evaluations: 605
best_cost=0.080
X1 shape: torch.Size([100, 1])
Repetition 9:      Current function value: 0.079573
    Iterations: 403
    Function evaluations: 646
    Gradient evaluations: 633
best_cost=0.080

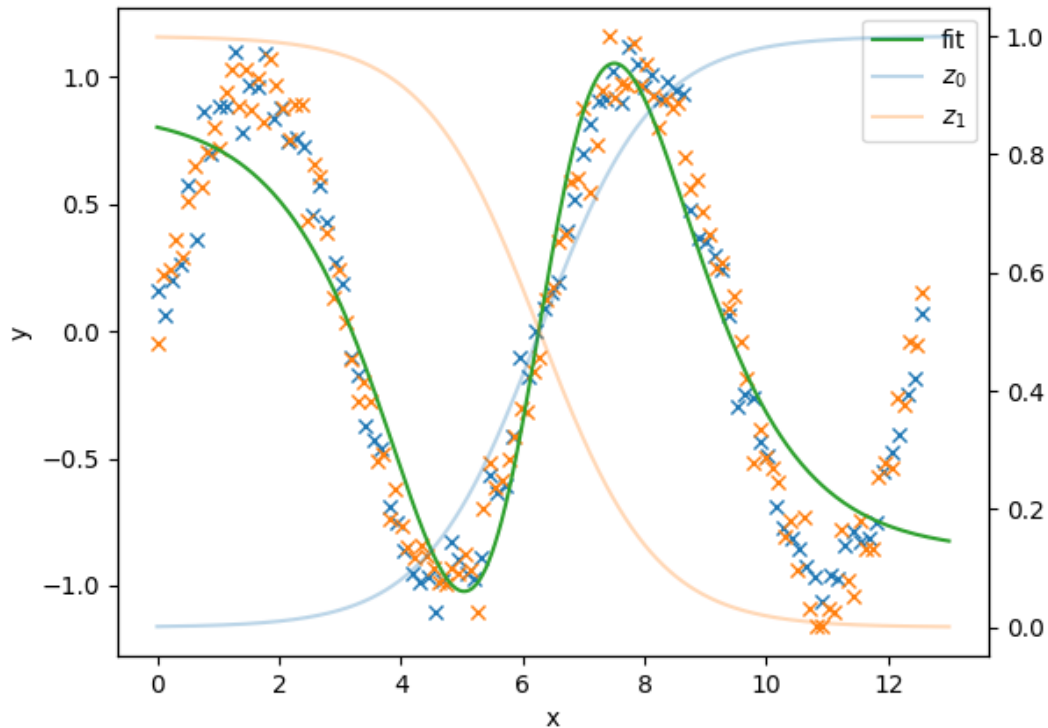
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

```

```

[28]: # plot the fit as well as the outputs of each neuron in the hidden
      # layer (scale for the latter is shown on right y-axis)
      nextplot()
      plot1(X1, y1, label="train")
      plot1(X1test, y1test, label="test")
      plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model, hidden=True,
        ↪scale=False)

```



```
[29]: # train a model to analyze
model = train1([3])
```

X1 shape: torch.Size([100, 1])

Repetition 0: Current function value: 0.007324

Iterations: 422

Function evaluations: 535

Gradient evaluations: 523

best_cost=0.007

X1 shape: torch.Size([100, 1])

Repetition 1:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not necessarily achieved due to precision loss.

res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not necessarily achieved due to precision loss.

res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

Current function value: 0.079572

```

        Iterations: 397
        Function evaluations: 577
        Gradient evaluations: 565
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 2:          Current function value: 0.007324
        Iterations: 543
        Function evaluations: 689
        Gradient evaluations: 677
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 3:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.049886
        Iterations: 317
        Function evaluations: 514
        Gradient evaluations: 503
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 4: Optimization terminated successfully.
        Current function value: 0.042560
        Iterations: 155
        Function evaluations: 172
        Gradient evaluations: 172
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 5:          Current function value: 0.079573
        Iterations: 364
        Function evaluations: 561
        Gradient evaluations: 548
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 6:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not

```

```

necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.079573
        Iterations: 343
        Function evaluations: 561
        Gradient evaluations: 548
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 7:          Current function value: 0.049901
        Iterations: 221
        Function evaluations: 320
        Gradient evaluations: 308
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 8:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.049877
        Iterations: 563
        Function evaluations: 811
        Gradient evaluations: 799
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 9:          Current function value: 0.053823
        Iterations: 540
        Function evaluations: 743
        Gradient evaluations: 728
best_cost=0.007

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

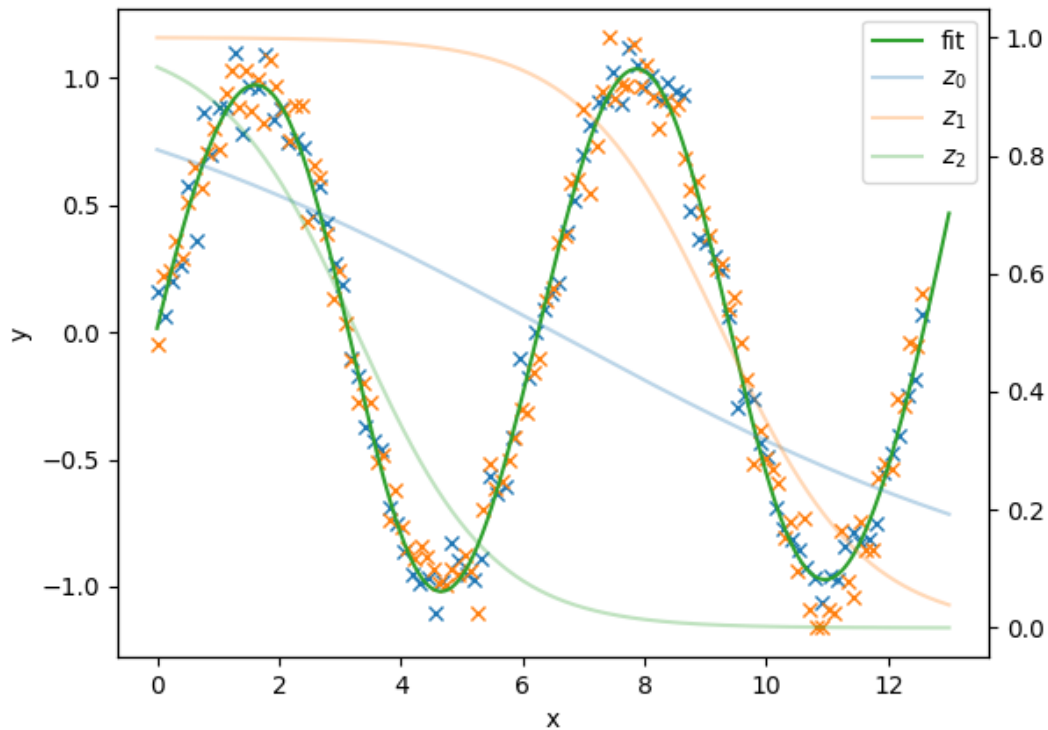
```

```

[30]: # plot the fit as well as the outputs of each neuron in the hidden
      # layer (scale for the latter is shown on right y-axis)
      nextplot()
      plot1(X1, y1, label="train")
      plot1(X1test, y1test, label="test")

```

```
plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model, hidden=True,
↪scale=False)
```



```
[31]: # train a model to analyze
model = train1([10])
```

```
X1 shape: torch.Size([100, 1])
```

```
Repetition 0:
```

```
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
Current function value: 0.006069
```

```
Iterations: 2361
```

```
Function evaluations: 2702
```

```
Gradient evaluations: 2683
```

```
best_cost=0.006
```

```
X1 shape: torch.Size([100, 1])
```

```
Repetition 1:
```



```

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.006260
        Iterations: 2624
        Function evaluations: 3005
        Gradient evaluations: 2995
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition  2:          Current function value: 0.006688
        Iterations: 587
        Function evaluations: 696
        Gradient evaluations: 686
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition  3:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.006667
        Iterations: 1257
        Function evaluations: 1487
        Gradient evaluations: 1475
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition  4:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.006232
        Iterations: 1648
        Function evaluations: 1908
        Gradient evaluations: 1897
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition  5:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not

```

```

necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.006114
        Iterations: 1489
        Function evaluations: 1719
        Gradient evaluations: 1707
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 6:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.006576
        Iterations: 2629
        Function evaluations: 2955
        Gradient evaluations: 2945
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 7:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.006076
        Iterations: 1852
        Function evaluations: 2128
        Gradient evaluations: 2116
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 8:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.006614
        Iterations: 2289
        Function evaluations: 2825
        Gradient evaluations: 2807
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 9:          Current function value: 0.006805
        Iterations: 1034
        Function evaluations: 1288

```

```

        Gradient evaluations: 1275
best_cost=0.006

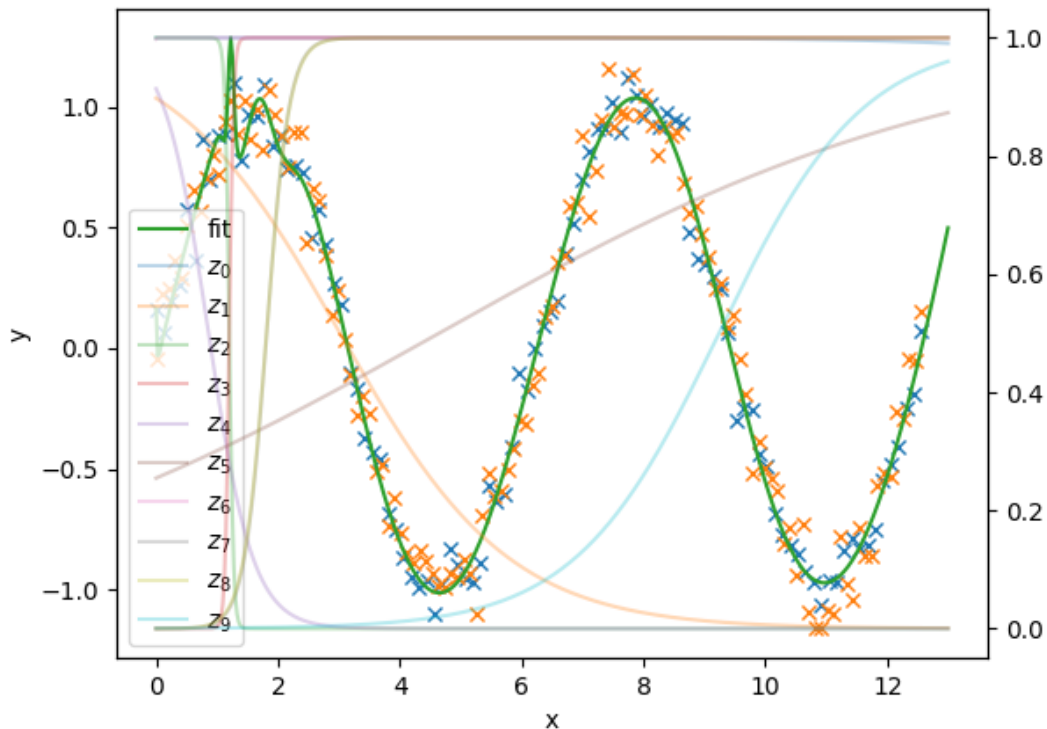
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

```

```

[32]: # plot the fit as well as the outputs of each neuron in the hidden
# layer (scale for the latter is shown on right y-axis)
nextplot()
plot1(X1, y1, label="train")
plot1(X1test, y1test, label="test")
plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model, hidden=True,
↪scale=False)

```



```

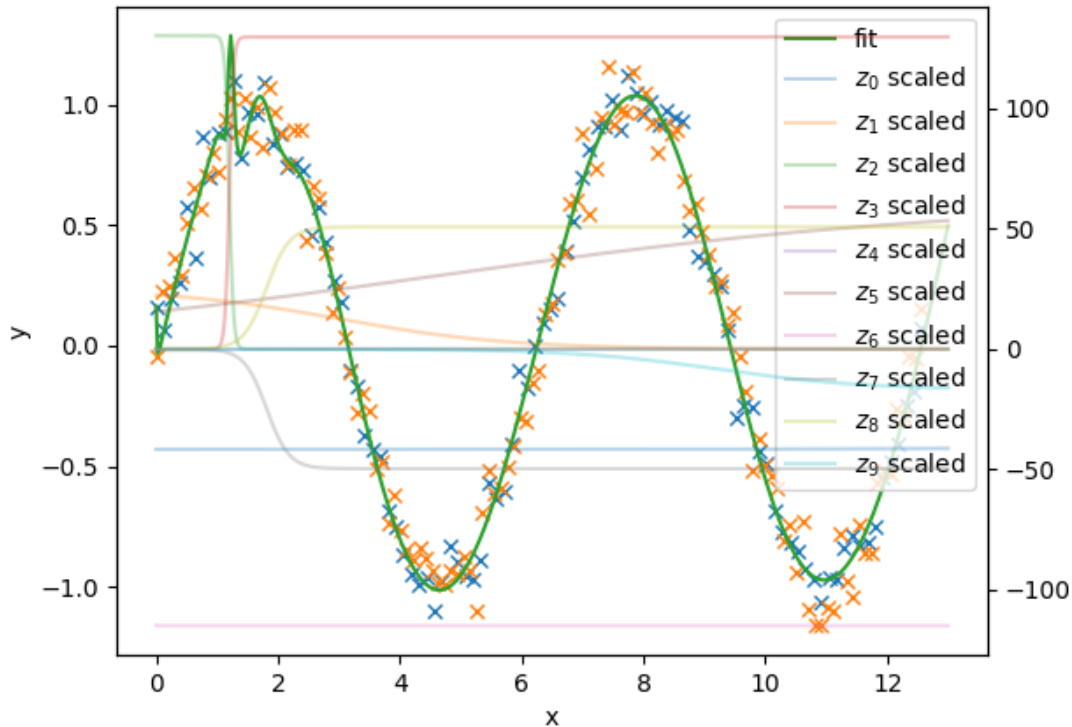
[33]: # plot the fit as well as the outputs of each neuron in the hidden layer, scaled
# by its weight for the output neuron (scale for the latter is shown on right
# y-axis)
nextplot()

```

```

plot1(X1, y1, label="train")
plot1(X1test, y1test, label="test")
plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model, hidden=True,
↪scale=True)

```



2.5 2e Experiment with different optimizers (optional)

```

[34]: # PyTorch provides many gradient-based optimizers; see
# https://pytorch.org/docs/stable/optim.html. You can use a PyTorch optimizer
# as follows.
train_adam = lambda model, **kwargs: fnn_train(
    X1, y1, model, optimizer=torch.optim.Adam(model.parameters()), lr=0.01,
↪**kwargs
)
model = train1([50], nreps=1, train=train_adam, max_epochs=5000, tol=1e-8,
↪verbose=True)

```

```

X1 shape: torch.Size([100, 1])
Repetition 0: Epoch    0: cost=    0.561
Epoch      1: cost=    0.547
Epoch      2: cost=    0.508

```

Epoch	3:	cost=	0.491
Epoch	4:	cost=	0.482
Epoch	5:	cost=	0.464
Epoch	6:	cost=	0.450
Epoch	7:	cost=	0.447
Epoch	8:	cost=	0.445
Epoch	9:	cost=	0.439
Epoch	10:	cost=	0.437
Epoch	11:	cost=	0.440
Epoch	12:	cost=	0.443
Epoch	13:	cost=	0.443
Epoch	14:	cost=	0.443
Epoch	15:	cost=	0.445
Epoch	16:	cost=	0.446
Epoch	17:	cost=	0.445
Epoch	18:	cost=	0.443
Epoch	19:	cost=	0.441
Epoch	20:	cost=	0.441
Epoch	21:	cost=	0.438
Epoch	22:	cost=	0.436
Epoch	23:	cost=	0.434
Epoch	24:	cost=	0.433
Epoch	25:	cost=	0.431
Epoch	26:	cost=	0.430
Epoch	27:	cost=	0.429
Epoch	28:	cost=	0.428
Epoch	29:	cost=	0.428
Epoch	30:	cost=	0.428
Epoch	31:	cost=	0.427
Epoch	32:	cost=	0.427
Epoch	33:	cost=	0.427
Epoch	34:	cost=	0.426
Epoch	35:	cost=	0.426
Epoch	36:	cost=	0.425
Epoch	37:	cost=	0.425
Epoch	38:	cost=	0.424
Epoch	39:	cost=	0.423
Epoch	40:	cost=	0.422
Epoch	41:	cost=	0.421
Epoch	42:	cost=	0.421
Epoch	43:	cost=	0.420
Epoch	44:	cost=	0.419
Epoch	45:	cost=	0.419
Epoch	46:	cost=	0.418
Epoch	47:	cost=	0.418
Epoch	48:	cost=	0.417
Epoch	49:	cost=	0.417
Epoch	50:	cost=	0.416

Epoch	51:	cost=	0.416
Epoch	52:	cost=	0.415
Epoch	53:	cost=	0.415
Epoch	54:	cost=	0.414
Epoch	55:	cost=	0.414
Epoch	56:	cost=	0.413
Epoch	57:	cost=	0.412
Epoch	58:	cost=	0.412
Epoch	59:	cost=	0.411
Epoch	60:	cost=	0.411
Epoch	61:	cost=	0.410
Epoch	62:	cost=	0.410
Epoch	63:	cost=	0.409
Epoch	64:	cost=	0.409
Epoch	65:	cost=	0.408
Epoch	66:	cost=	0.408
Epoch	67:	cost=	0.407
Epoch	68:	cost=	0.407
Epoch	69:	cost=	0.406
Epoch	70:	cost=	0.406
Epoch	71:	cost=	0.405
Epoch	72:	cost=	0.405
Epoch	73:	cost=	0.404
Epoch	74:	cost=	0.403
Epoch	75:	cost=	0.403
Epoch	76:	cost=	0.402
Epoch	77:	cost=	0.402
Epoch	78:	cost=	0.401
Epoch	79:	cost=	0.401
Epoch	80:	cost=	0.400
Epoch	81:	cost=	0.400
Epoch	82:	cost=	0.399
Epoch	83:	cost=	0.399
Epoch	84:	cost=	0.398
Epoch	85:	cost=	0.398
Epoch	86:	cost=	0.397
Epoch	87:	cost=	0.397
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Epoch 3363: cost= 0.007
Epoch 3364: cost= 0.007
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best_cost=0.007

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```

[35]: # Experiment with different number of layers and activation functions. Here is
      # an example with three hidden layers (of sizes 4, 5, and 6) and ReLU
      ↪activations.
      #
      # You can also plot the outputs of the hidden neurons in the first layer (using
      # the same code above).
      model = train1([4, 5, 6], nreps=50, phi=F.relu)

```

```

nextplot()
plot1(X1, y1, label="train")
plot1(X1test, y1test, label="test")
plot1fit(torch.linspace(0, 13, 500).unsqueeze(1), model)
print("Training error:", F.mse_loss(y1, model(X1)).item())
print("Test error      :", F.mse_loss(y1test, model(X1test)).item())

```

X1 shape: torch.Size([100, 1])

Repetition 0:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not necessarily achieved due to precision loss.

res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not necessarily achieved due to precision loss.

res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not necessarily achieved due to precision loss.

res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

Current function value: 0.027642

Iterations: 106

Function evaluations: 226

Gradient evaluations: 221

best_cost=0.028

X1 shape: torch.Size([100, 1])

Repetition 1: Current function value: 0.372736

Iterations: 20

Function evaluations: 93

Gradient evaluations: 89

best_cost=0.028

X1 shape: torch.Size([100, 1])

Repetition 2: Current function value: 0.082316

Iterations: 77

Function evaluations: 175

Gradient evaluations: 169

best_cost=0.028

X1 shape: torch.Size([100, 1])

Repetition 3:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not necessarily achieved due to precision loss.

res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not

```

necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.372829
        Iterations: 54
        Function evaluations: 224
        Gradient evaluations: 219
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition  4:          Current function value: 0.356289
        Iterations: 62
        Function evaluations: 159
        Gradient evaluations: 151
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition  5:          Current function value: 0.436769
        Iterations: 19
        Function evaluations: 107
        Gradient evaluations: 98
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition  6:

/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.082545
        Iterations: 87
        Function evaluations: 201
        Gradient evaluations: 196
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition  7:          Current function value: 0.355800
        Iterations: 47
        Function evaluations: 226
        Gradient evaluations: 220
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition  8:

```

```

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.098439
        Iterations: 131
        Function evaluations: 239
        Gradient evaluations: 227
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition  9:          Current function value: 0.355687
        Iterations: 139
        Function evaluations: 261
        Gradient evaluations: 257
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition 10: Optimization terminated successfully.
        Current function value: 0.101445
        Iterations: 53
        Function evaluations: 66
        Gradient evaluations: 66
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition 11:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.356116
        Iterations: 52
        Function evaluations: 161
        Gradient evaluations: 155
best_cost=0.028
X1 shape: torch.Size([100, 1])

```

```

Repetition 12:          Current function value: 0.435001
    Iterations: 46
    Function evaluations: 123
    Gradient evaluations: 119
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition 13:          Current function value: 0.435068
    Iterations: 41
    Function evaluations: 131
    Gradient evaluations: 125
best_cost=0.028
X1 shape: torch.Size([100, 1])
Repetition 14:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

    Current function value: 0.007341
    Iterations: 212
    Function evaluations: 447
    Gradient evaluations: 433
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 15:          Current function value: 0.355830
    Iterations: 46
    Function evaluations: 140
    Gradient evaluations: 135
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 16:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

    Current function value: 0.353423
    Iterations: 154
    Function evaluations: 435
    Gradient evaluations: 415

```

```

best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 17:          Current function value: 0.405736
    Iterations: 15
    Function evaluations: 95
    Gradient evaluations: 90
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 18:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

    Current function value: 0.085500
    Iterations: 113
    Function evaluations: 241
    Gradient evaluations: 234
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 19:          Current function value: 0.082287
    Iterations: 96
    Function evaluations: 187
    Gradient evaluations: 183
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 20:          Current function value: 0.434775
    Iterations: 18
    Function evaluations: 113
    Gradient evaluations: 102
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 21:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not

```



```

necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.356477
        Iterations: 34
        Function evaluations: 122
        Gradient evaluations: 118
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 22:          Current function value: 0.355919
        Iterations: 54
        Function evaluations: 154
        Gradient evaluations: 149
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 23:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.008464
        Iterations: 251
        Function evaluations: 460
        Gradient evaluations: 451
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 24:          Current function value: 0.008703
        Iterations: 185
        Function evaluations: 276
        Gradient evaluations: 270
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 25:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not

```

```

necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.355581
        Iterations: 138
        Function evaluations: 261
        Gradient evaluations: 255
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 26:          Current function value: 0.085421
        Iterations: 55
        Function evaluations: 161
        Gradient evaluations: 155
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 27:          Current function value: 0.357612
        Iterations: 46
        Function evaluations: 123
        Gradient evaluations: 116
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 28:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.434378
        Iterations: 34
        Function evaluations: 122
        Gradient evaluations: 116
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 29:          Current function value: 0.083644
        Iterations: 205
        Function evaluations: 328
        Gradient evaluations: 323
best_cost=0.007
X1 shape: torch.Size([100, 1])
Repetition 30:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

```

```
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not  
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
    Current function value: 0.434433
```

```
    Iterations: 28
```

```
    Function evaluations: 111
```

```
    Gradient evaluations: 107
```

```
best_cost=0.007
```

```
X1 shape: torch.Size([100, 1])
```

```
Repetition 31:          Current function value: 0.356297
```

```
    Iterations: 72
```

```
    Function evaluations: 166
```

```
    Gradient evaluations: 161
```

```
best_cost=0.007
```

```
X1 shape: torch.Size([100, 1])
```

```
Repetition 32:
```

```
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not  
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not  
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-  
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not  
necessarily achieved due to precision loss.
```

```
res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
    Current function value: 0.005862
```

```
    Iterations: 382
```

```
    Function evaluations: 528
```

```
    Gradient evaluations: 523
```

```
best_cost=0.006
```

```
X1 shape: torch.Size([100, 1])
```

```
Repetition 33:          Current function value: 0.308671
```

```
    Iterations: 68
```

```
    Function evaluations: 180
```

```
    Gradient evaluations: 175
```

```
best_cost=0.006
```

```
X1 shape: torch.Size([100, 1])
```

```
Repetition 34:          Current function value: 0.436922
```

```
    Iterations: 60
```

```
    Function evaluations: 163
```

```
    Gradient evaluations: 155
```

```
best_cost=0.006
```

```

X1 shape: torch.Size([100, 1])
Repetition 35:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.435347
        Iterations: 37
        Function evaluations: 109
        Gradient evaluations: 101
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 36:          Current function value: 0.371726
        Iterations: 35
        Function evaluations: 118
        Gradient evaluations: 113
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 37:          Current function value: 0.008174
        Iterations: 108
        Function evaluations: 221
        Gradient evaluations: 217
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 38:

/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkochteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.355790

```

```

        Iterations: 129
        Function evaluations: 232
        Gradient evaluations: 227
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 39: Optimization terminated successfully.
    Current function value: 0.435275
    Iterations: 35
    Function evaluations: 52
    Gradient evaluations: 52
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 40:      Current function value: 0.435287
    Iterations: 18
    Function evaluations: 99
    Gradient evaluations: 94
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 41:      Current function value: 0.372387
    Iterations: 57
    Function evaluations: 177
    Gradient evaluations: 173
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 42:

/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

    Current function value: 0.356134
    Iterations: 110
    Function evaluations: 214
    Gradient evaluations: 209
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 43: Optimization terminated successfully.
    Current function value: 0.098100
    Iterations: 147
    Function evaluations: 169
    Gradient evaluations: 169
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 44:

/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.

```

```

    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.356624
        Iterations: 28
        Function evaluations: 115
        Gradient evaluations: 103
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 45: Optimization terminated successfully.
        Current function value: 0.506238
        Iterations: 14
        Function evaluations: 16
        Gradient evaluations: 16
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 46:          Current function value: 0.092225
        Iterations: 89
        Function evaluations: 209
        Gradient evaluations: 204
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 47:

/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

        Current function value: 0.355652
        Iterations: 168
        Function evaluations: 310
        Gradient evaluations: 306
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 48:          Current function value: 0.008766
        Iterations: 145
        Function evaluations: 251
        Gradient evaluations: 243
best_cost=0.006
X1 shape: torch.Size([100, 1])
Repetition 49:          Current function value: 0.007130

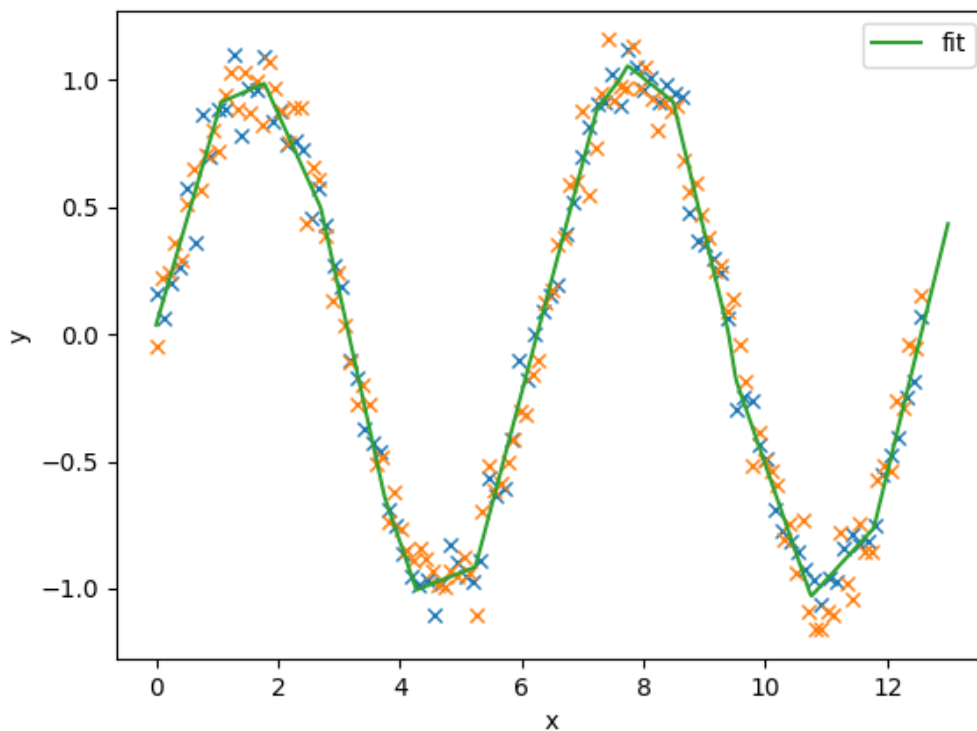
```

```

        Iterations: 196
        Function evaluations: 295
        Gradient evaluations: 288
best_cost=0.006
Training error: 0.005861788988113403
Test error      : 0.010837704874575138

/Users/ngkokteng/PycharmProjects/Deep Learning/.venv/lib/python3.9/site-
packages/scipy/optimize/_minimize.py:708: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
    res = _minimize_bfgs(fun, x0, args, jac, callback, **options)

```



3 3 Backpropagation

```

[ ]: # Let's fit the model with one hidden layer consisting of 50 units.
model = train1([50], nreps=1)
print("Training error:", F.mse_loss(y1, model(X1)).item())
print("Test error      :", F.mse_loss(y1test, model(X1test)).item())

# Extract parameters

```

```

pars = dict(model.named_parameters())
W1 = pars["0_weight"].data # 1x50
b1 = pars["0_bias"].data # 50
W2 = pars["1_weight"].data # 50x1
b2 = pars["1_bias"].data # 1

```

X1 shape: torch.Size([100, 1])
Repetition 0:

3.1 3a Forward pass

```

[ ]: # Compute results of forward pass on an example x (i.e., z1, z2, z3, z4, yhat, l) using Pytorch
x = X1test[1, :]
y = y1test[1, :]
print(f"x={x}, y={y}, yhat={model(x).detach()}, l={torch.nn.
    ↳MSELoss()(y,model(x))}")

```

```

[ ]: # Now do this by hand (including all intermediate values). You should get the
    ↳same
# results as above.
z1 = W1.t() * x
z2 = z1 + b1.unsqueeze(1)
z3 = 1/ (1 + torch.exp(-1 * z2))
z4 = torch.zeros(1, 1)
for i in range(W2.shape[0]):
    z4 += W2[i] * z3[i]
y_hat = z4 + b2
l = (y - y_hat)**2
print(f"x={x}, y={y}, yhat={y_hat}, l={l}")

```

3.2 3b Backward pass

```

[ ]: # Compute results of backward pass on example output (i.e., delta_x, delta_W1,
    ↳delta_z1,
# delta_b1, delta_z2, delta_z3, delta_W2, delta_z4, delta_b2, delta_yhat,
    ↳delta_l, delta_y)

delta_l = 1
delta_y = (2 * (y - y_hat)).squeeze(1)
delta_yhat = -2 * (y - y_hat)
delta_b2 = (delta_yhat * 1).squeeze(1)
delta_z4 = delta_yhat * 1
delta_W2 = delta_z4 * z3
delta_z3 = delta_z4 * W2
delta_z2 = delta_z3 * z3 * (1 - z3)
delta_b1 = delta_z2.squeeze(1)

```



```

delta_z1 = delta_z2

delta_x = torch.zeros(1, 1)
for i in range(W1.shape[0]):
    delta_x += delta_z1[i] * W1[0][i]
delta_x = delta_x.squeeze(1)

delta_W1 = (delta_z1 * x).t()

```

```

[ ]: # Use PyTorch's backprop
x.requires_grad = True
y.requires_grad = True
if x.grad is not None:
    x.grad.zero_()
if y.grad is not None:
    y.grad.zero_()
model.zero_grad()
t_yhat = model(x)
t_yhat.retain_grad()
t_l = torch.nn.MSELoss()(t_yhat, y)
t_l.backward()
t_delta_l = 1
t_delta_y = y.grad
t_delta_yhat = t_yhat.grad
t_delta_b2 = model.get_parameter("1_bias").grad
t_delta_W2 = model.get_parameter("1_weight").grad
t_delta_b1 = model.get_parameter("0_bias").grad
t_delta_W1 = model.get_parameter("0_weight").grad
t_delta_x = x.grad

```

```

[ ]: # Check if equal (show squared error)
for v in ["y", "yhat", "b2", "W2", "b1", "W1", "x"]:
    print(f'{v}, squared error={torch.
    ↪sum((eval("t_delta_"+v)-eval("delta_"+v))**2)}')

```

```

[ ]: # Check if equal (show actual values)
for v in ["l", "y", "yhat", "b2", "W2", "b1", "W1", "x"]:
    print(f'{v}, pytorch={eval("t_delta_"+v)}, you={eval("delta_"+v)}')

```