

train_LaengeNetMod

February 8, 2022

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[1]: from Neural_Nets.LaengeNetModified.Development.LaengeNetModified import   
      ↪ LaengeNetModified, LaengeNetModifiedLossFunc  
from Neural_Nets.ThermoDatasetModified.Development.ThermoDatasetModified import   
      ↪ ThermoDatasetModified  
from Utils.PlotHandler.Development.PlotHandler import PlotHandler  
import torch  
from torch.utils.data import DataLoader, Dataset  
import torch.nn as nn  
from torch.optim import *  
from Data_Handling.SGTEHandler.Development.SGTEHandler import SGTEHandler  
import numpy as np  
import matplotlib.pyplot as plt
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[2]: def epoch(net: LaengeNetModified, dataloader, loss_func, optimizer):  
    epoch_losses = np.zeros([len(dataloader), ])  
  
    for i, (temp, target) in enumerate(dataloader):  
        temp = temp.unsqueeze(-1)  
  
        # Forward pass  
        prediction = net(temp.float())  
  
        # Get the loss  
        loss = loss_func(prediction, target)  
  
        # Backward pass  
        net.zero_grad()  
        loss.backward()  
        optimizer.step()  
        epoch_losses[i] = loss  
  
    mean_epoch_loss = epoch_losses.mean(axis=0)  
    #print('Mean epoch loss: ', mean_epoch_loss)  
    return mean_epoch_loss
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[7]: def train(net, dataset):  
    # Hyperparameters
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n_epochs = 100000
lr = 0.001
batch_size = 64

# Data
dataloader = DataLoader(dataset, batch_size=batch_size, shuffle=False)

# Optimizer
#optimizer = RMSprop(net.parameters(), lr=lr)
optimizer = RMSprop(net.parameters(), lr=lr)
loss_func = LaengeNetModifiedLossFunc()

losses = []

best_loss = epoch(net, dataloader, loss_func, optimizer)
best_net = net

for i in range(n_epochs):
    #print('-----\nEpoch %i:\n' % i)
    loss = epoch(net, dataloader, loss_func, optimizer)
    losses.append(loss)

    if loss < best_loss:
        best_net = net

    if i % 10 == 0:
        print(loss)

return losses, net

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[8]: net = LaengeNetModified(hidden_dim=4)

element = 'Fe'
phase = ['BCC_A2']
start_temp, end_temp = 200, 2000

dataset = ThermoDatasetModified(element, phase, step=2, start_temp=start_temp,
↪end_temp=end_temp)

losses, best_net = train(net, dataset)

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Fe successfully selected!

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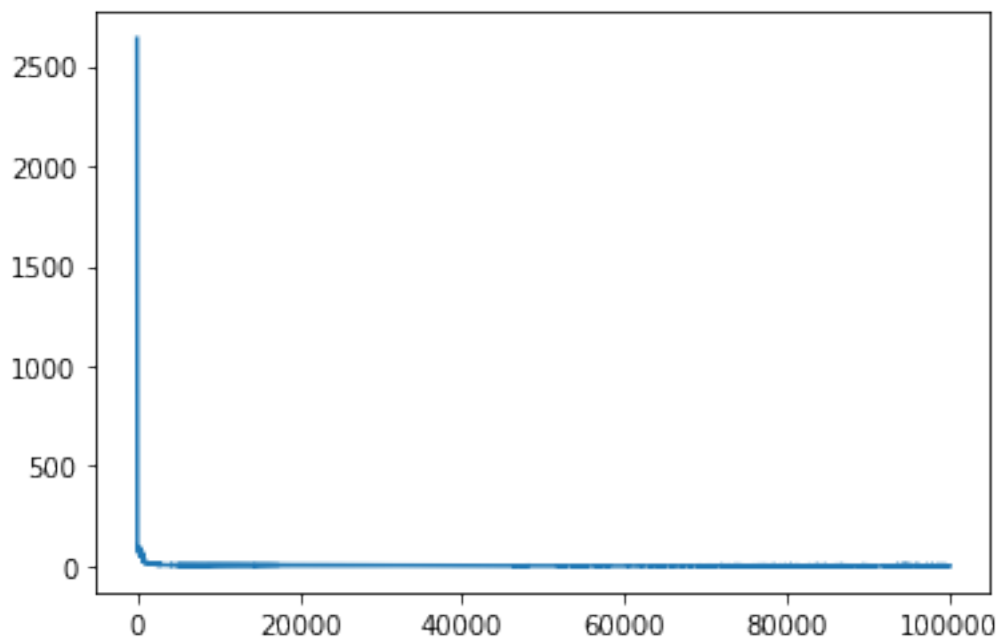
```

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0.5167135162545102
0.5401634499430656
0.5284973199346236
0.5206817186304501

```

```
[9]: plt.plot(range(len(losses)), losses)
```

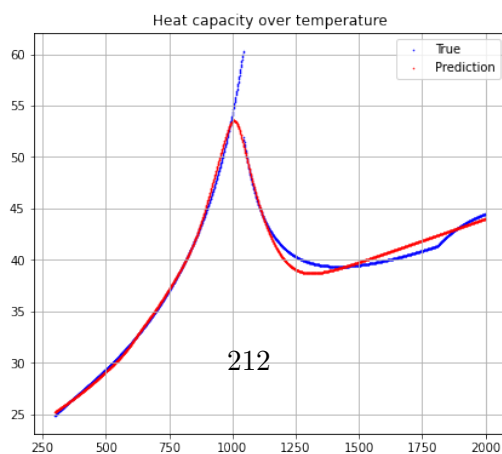
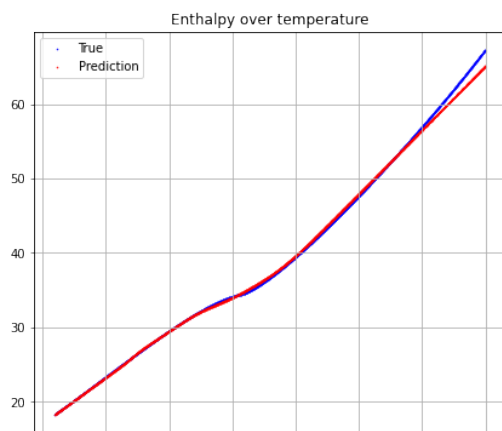
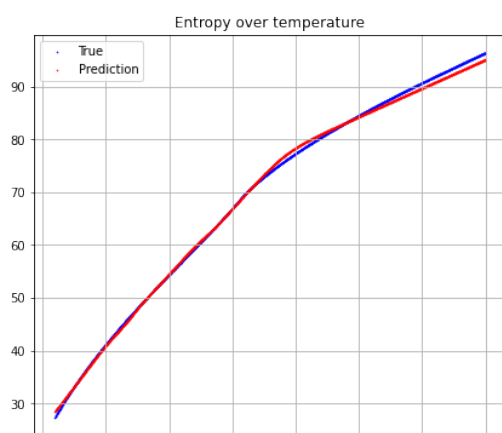
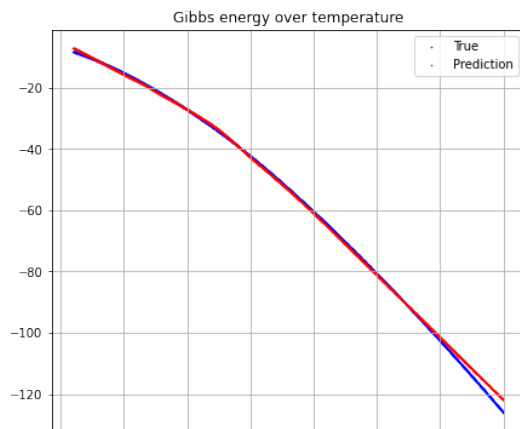
```
[9]: [<matplotlib.lines.Line2D at 0x1d3d2e8e490>]
```



```
[10]: ph = PlotHandler('Laenge')

ph.properties_temp_modified(best_net, element, phase, start_temp=start_temp,
                             ↪end_temp=end_temp)
```

Fe successfully selected!



```
[11]: torch.save(net, 'Neural_Nets/LaengeNetModified/Models/model_08_02_22_1156')
```

```
[ ]:
```