train_LaengeNetMod

February 7, 2022

[26]:
```
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
```

[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
```

[73]:
```
def train(net, dataset):
    # Hyperparameters
```

```
    n_epochs = 5000
    lr = 0.001
    batch_size = 64

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

    # Optimizer
    #optimizer = RMSprop(net.parameters(), lr=lr)
    optimizer = AdamW(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
```

[74]:
```
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)
```

```
Fe successfully selected!

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106.42783655439105
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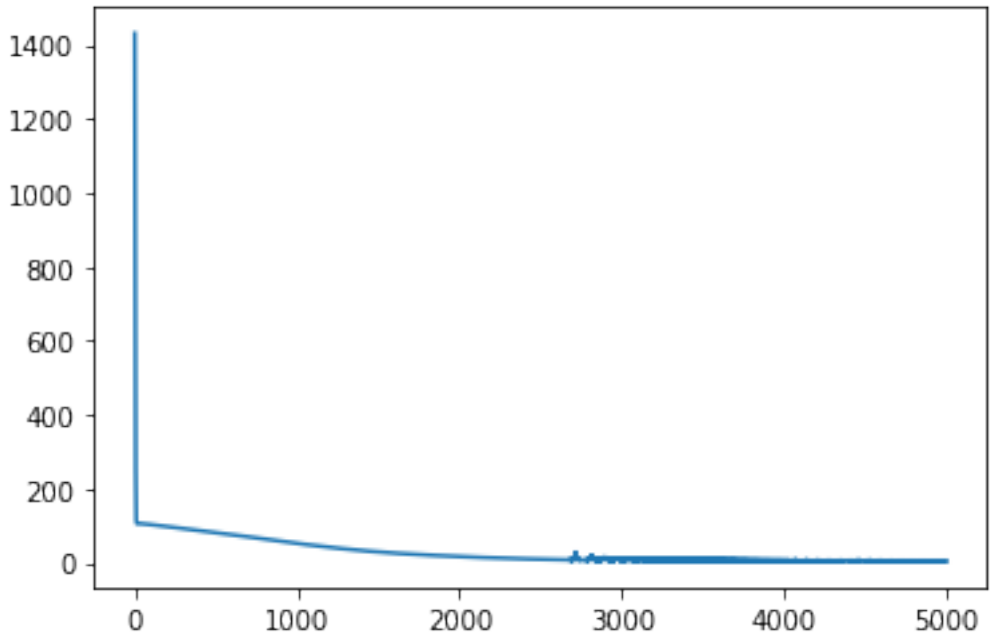
```

[75]:
```
plt.plot(range(len(losses)), losses)
```

[75]:
```
[<matplotlib.lines.Line2D at 0x1aa6249b5b0>]
```



[76]:
```
ph = PlotHandler('Laenge')

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

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Fe successfully selected!
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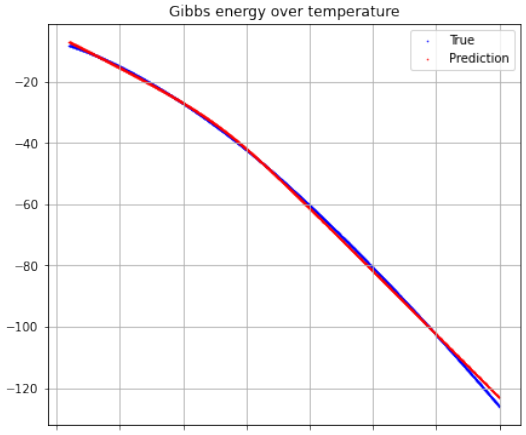
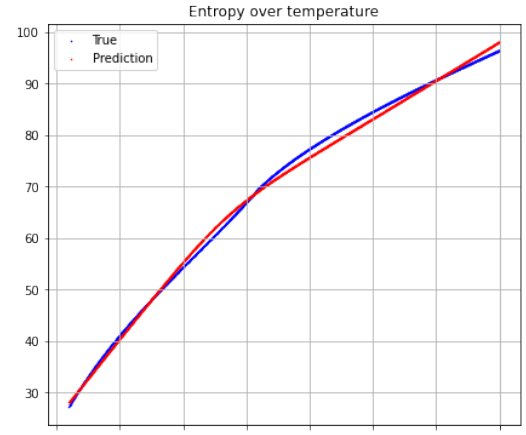
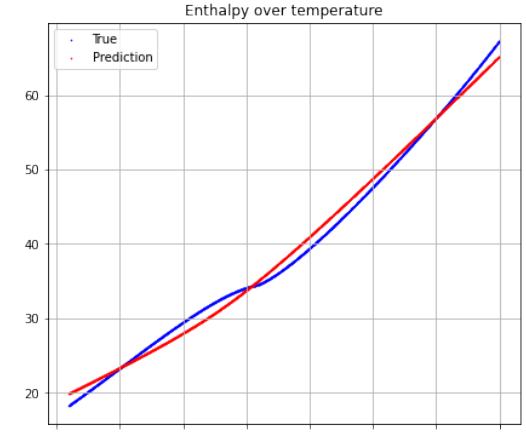
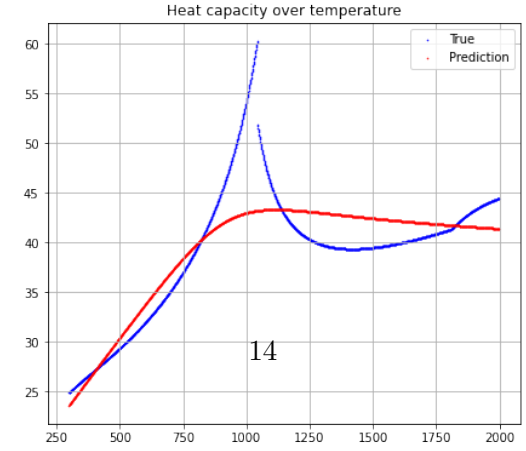

Gibbs energy over temperature
True
Prediction
−20
−40
−60
−80
−100
−120


Entropy over temperature
True
Prediction
100
90
80
70
60
50
40
30


Enthalpy over temperature
True
Prediction
60
50
40
30
20


Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

[39]:
```
torch.save(net, 'Neural_Nets/LaengeNetModified/Models/model_07_02_22_1937')
```

[ ]:
```

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