train_LaengeNetMod

February 8, 2022

```python
[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
```

```python
[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
```

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

```python
    n_epochs = 10000
    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
```

```python
[100]: 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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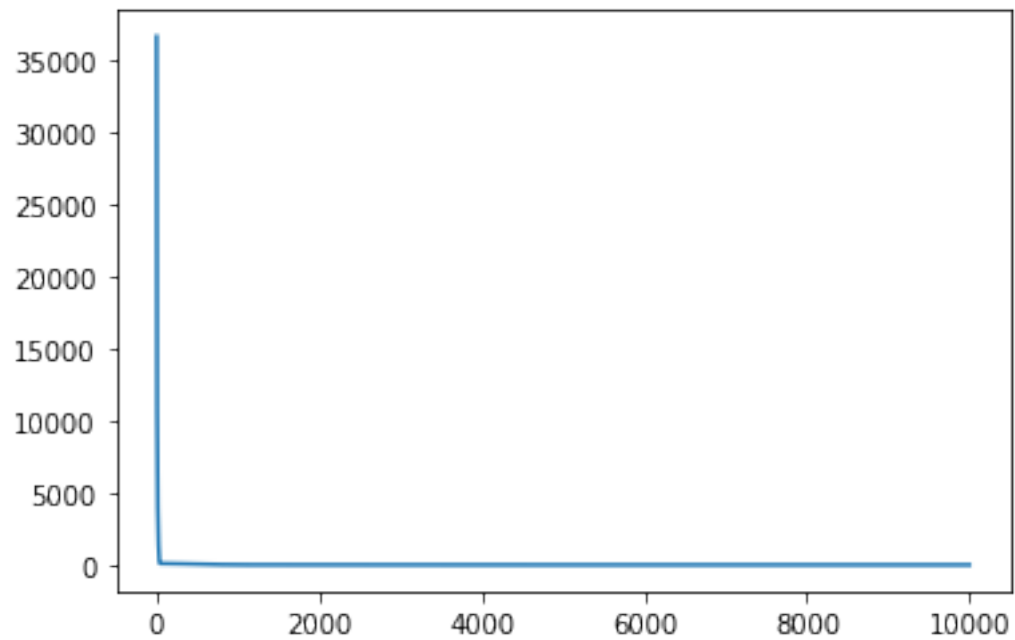4.369986515492201
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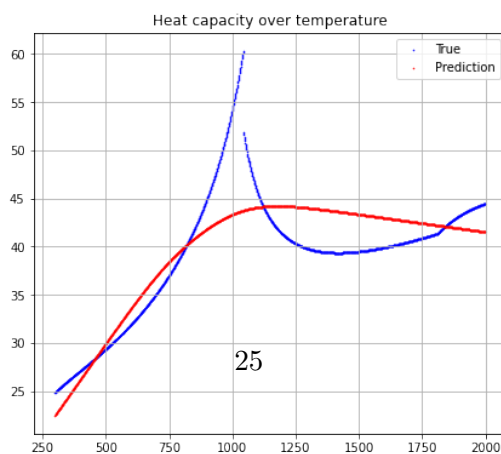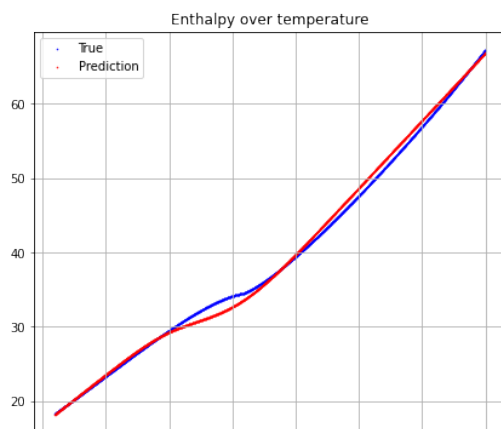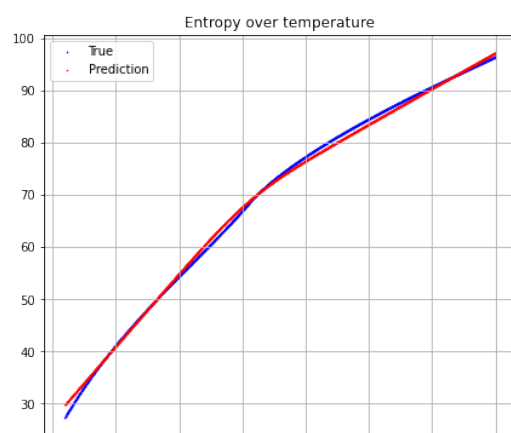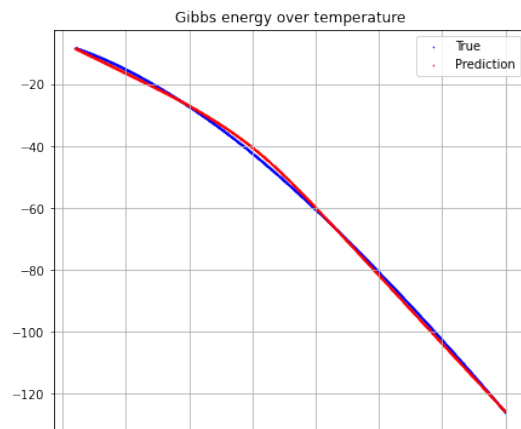
[101]:
```python
plt.plot(range(len(losses)), losses)
```

[101]: [<matplotlib.lines.Line2D at 0x1aa6215b8b0>]

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

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

Fe successfully selected!

Gibbs energy over temperature

Entropy over temperature

Enthalpy over temperature

Heat capacity over temperature

25

```
[77]: #torch.save(net, 'Neural_Nets/LaengeNetModified/Models/model_07_02_22_2122')
```

```
[ ]:
```

26