trainThermoNetNew

March 16, 2022

[219]:
```
import numpy as np
import torch
from torch.utils.data import DataLoader
from torch.optim import RMSprop, SGD
from torch.optim.lr_scheduler import ExponentialLR
from torch.nn import MSELoss
import matplotlib.pyplot as plt

from thermonet.net import ThermoNetNew
from thermonet.dataset import ThermoDatasetNew
from utils.plot import PlotHandler
```

[224]:
```
def epoch(net, dataloader, loss_func, optimizer, scheduler):
    epoch_losses = np.zeros([len(dataloader), ])

    for i, d in enumerate(dataloader):
        inp = d[:, [0, -2, -1]]
        targets = d[:, [1, 2, 3, 4]]

        # Forward pass
        predictions = net(inp.float())

        # Get the loss
        loss = loss_func(predictions, targets.float())

        # Backward pass
        net.zero_grad()
        loss.backward()
        optimizer.step()
        epoch_losses[i] = loss
    scheduler.step()

    mean_epoch_loss = epoch_losses.mean(axis=0)
    #print('Mean epoch loss: ', mean_epoch_loss)
    return mean_epoch_loss

def train(net, dataloader, optimizer, scheduler, loss_func, nr_epochs=500):
    losses = []
```

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

    ph = PlotHandler()

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

        if loss < best_loss:
            best_net = net

        if i % 10 == 0:
            print(i, ': ', loss)
            print('lr: ', scheduler.get_last_lr())
            last_losses = np.array(losses[-50:])
            last_losses_std, last_losses_mean = last_losses.std(), last_losses.
↪mean()
            last_loss_diffs = np.diff(last_losses)
            print(np.mean(last_loss_diffs))
            print(last_losses_std/np.mean(last_loss_diffs), last_losses_std,␣
↪last_losses_mean)
            print()

        if i % 250 == 0:
            ph.properties_temp_modified_new(best_net, ['Fe'], 'BCC_A2',␣
↪start_temp=200, end_temp=2000)
            plt.plot(losses)

    return losses, net
```

[253]:
```
# Hyperparameters
nr_epochs = 2500
lr = 0.005 # 0.000025
batch_size = 2048
hidden_size = 128
hidden_layers = 8
```

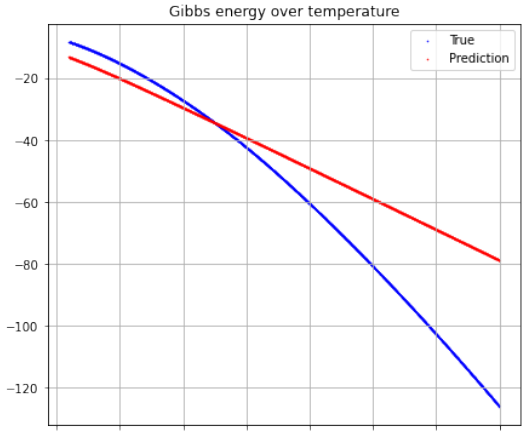
[254]:
```
# Network
net = ThermoNetNew(hidden_size_linear=hidden_size, hidden_layers=hidden_layers)

# Optimizer
optimizer = RMSprop(net.parameters(), lr=lr)
scheduler = ExponentialLR(optimizer, gamma=0.995)
```

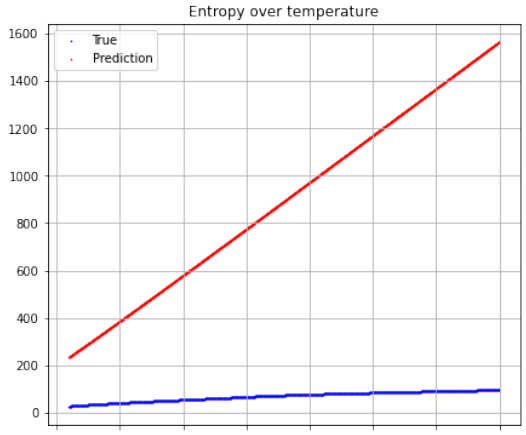
```
# Loss function
loss_func = MSELoss()
```

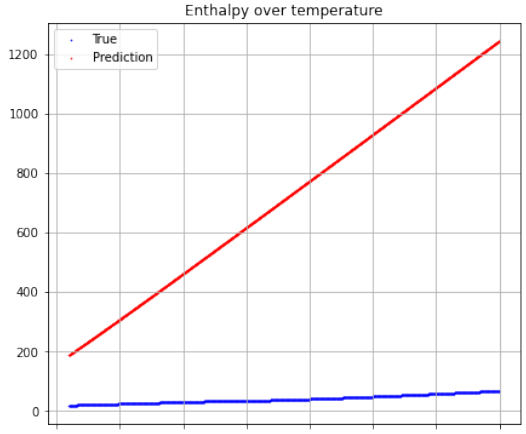
[255]:
```
# Dataset
start_temp, end_temp = 200, 2000
step = 1
dataset = ThermoDatasetNew(['Fe', 'C'], start_temp=start_temp,␣
 ↪end_temp=end_temp, step=step)
dataloader = DataLoader(dataset, batch_size=batch_size, shuffle=True)
```

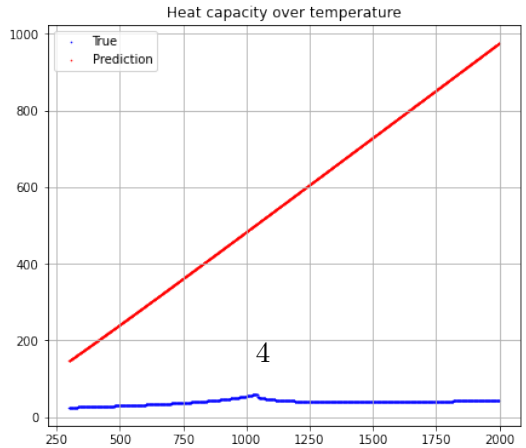
[256]:
```
losses, best_net = train(net, dataloader, optimizer=optimizer,␣
 ↪scheduler=scheduler, loss_func=loss_func, nr_epochs=nr_epochs)
```

```
0 :  28376.793980189734
lr:  [0.0049501250000000005]
nan
nan 0.0 28376.793980189734
```


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


Entropy over temperature
True
Prediction
1600
1400
1200
1000
800
600
400
200
0

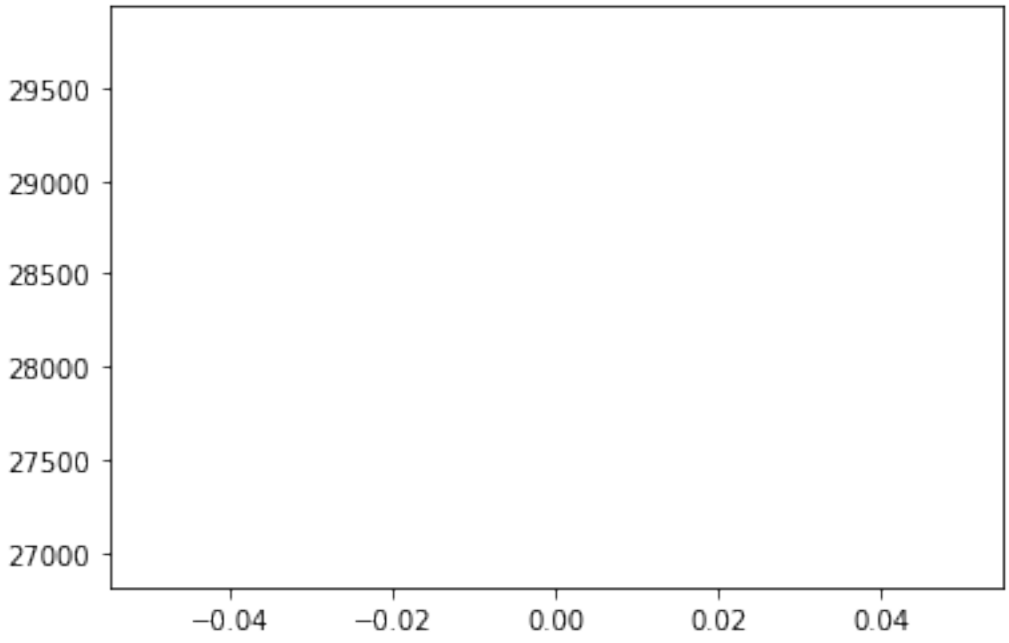

Enthalpy over temperature
True
Prediction
1200
1000
800
600
400
200
0

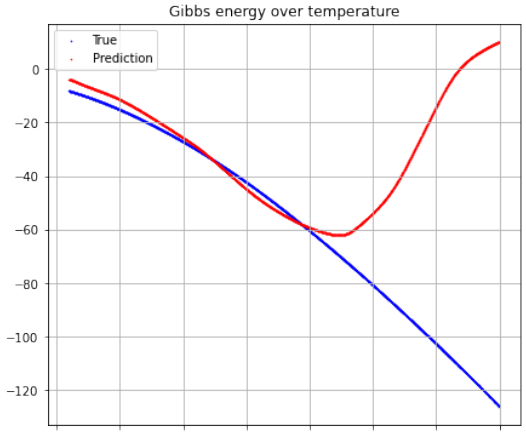

Heat capacity over temperature
True
Prediction
1000
800
600
400
200
0
250
500
750
1000
1250
1500
1750
2000

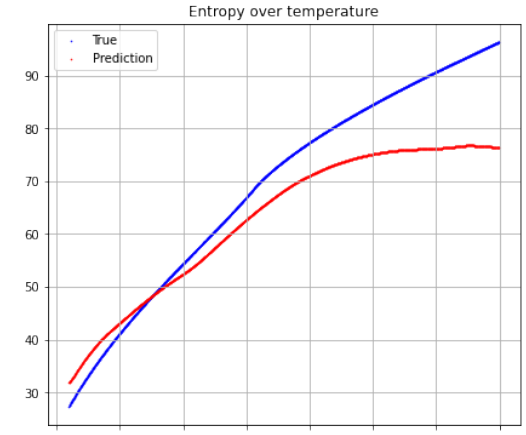
```
10 :  947.7408447265625
lr:  [0.0047081140345718794]
-2742.9053135463173
-6.19217860076289 16984.55958646033 8752.397343623175

20 :  943.9701363699777
lr:  [0.004477934953669392]
-1371.6411921909876
-9.400365009088341 12893.927868096376 5041.57926058607

30 :  978.9525495256696
lr:  [0.004259009298001735]
-913.2613810221354
-11.8065313355484 10782.449112584049 3725.406026954475

40 :  922.2151140485491
lr:  [0.0040507868890773645]
-686.3644716535296
-13.770964082075997 9451.900486353825 3045.3771951389645

50 :  937.1407034737723
lr:  [0.0038527444465594088]
-1134.0292151982164
-6.853104756338983 7771.621008502261 2147.8356691196987

60 :  954.6657976422991
lr:  [0.003664384273218397]
-0.11688926407616551
-1180.8229759006242 138.0255286572517 980.1129893275669

70 :  944.2010062081473
lr:  [0.003485233004177472]
0.21115050023915816
653.8309952288932 138.05674171444744 981.5427641950333

80 :  900.5455932617188
lr:  [0.0033148404173068496]
-1.228676131445881
-113.55339440511871 139.5203453502296 976.8313180106026

90 :  997.6508701869419
lr:  [0.0031527783017779305]
1.1172634825414285
1144.4584745863076 1278.6616609403488 1278.1131668526787
```

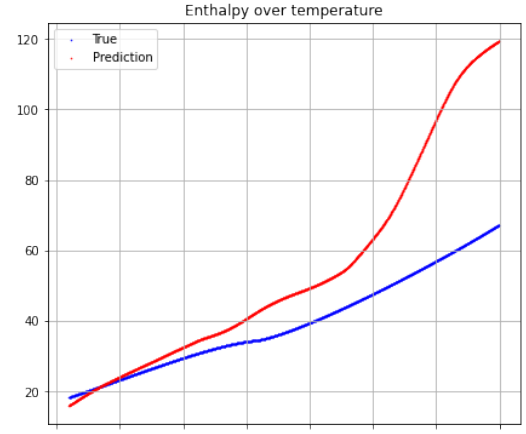
```
100 :  1019.0528826032366
lr:  [0.0029986393819336618]
1.052726367472216
1212.4009186721714 1276.3264150337327 1257.0039451381137

110 :  982.4007306780134
lr:  [0.002852036293770727]
0.8101936540520326
1577.1953163434205 1277.8336365020273 1280.4160939243861

120 :  964.483642578125
lr:  [0.0027126006114613927]
0.16681103942693082
7659.661039277738 1277.7160196198847 1280.7800275530133

130 :  967.0377371651786
lr:  [0.0025799819214685775]
-121.09119310740475
-10.54178646856962 1276.5175009625902 1285.468688267299

140 :  897.0123378208706
lr:  [0.002453846941927312]
-2.0561920254988144
-66.20539733925305 136.13101005395256 983.5089362444197

150 :  897.9445364815848
lr:  [0.002333878685079522]
-1.4438435635135753
-97.53934753943787 140.83155913413106 965.9234877232142

160 :  857.2617100306919
lr:  [0.0022197756606572683]
-2.416132534905705
-20.448788751025 49.40698380076529 922.7284605189732

170 :  841.3477085658482
lr:  [0.0021112511182124795]
-2.8218691634019684
-20.14751286057111 56.8536452604902 893.6117858886718

180 :  773.5940900530134
lr:  [0.0020080323264890774]
-3.6319389676908713
-15.293950305354784 55.54669408394574 859.1057875279018

190 :  803.9661254882812
lr:  [0.0019098598880265135]
-1.478533597451258
```

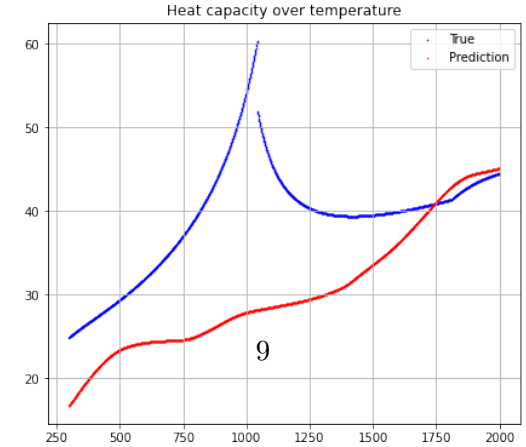
```
-34.573397038651315 51.1179290996678 827.4565924944196

200 :  685.1053118024554
lr:  [0.0018164870872722418]
-3.683927041101038
-11.710278349769823 43.13981107153709 800.7988208007813

210 :  775.3699515206473
lr:  [0.0017276792705648916]
-1.3619123186383928
-39.339654286577804 53.577159783865966 771.9798866489956

220 :  640.2145124162946
lr:  [0.0016432132564299833]
-3.2568950152605693
-18.530947434284826 60.35335032677789 743.7711010742188

230 :  755.8372017996652
lr:  [0.001562876774706207]
0.40956529444925227
193.40837440937585 79.21335781392725 742.6099711390904

240 :  693.0492640904018
lr:  [0.001486467933092745]
-1.486345029780885
-52.12115255772957 77.47001605063261 731.4090182931084

250 :  692.4485560825893
lr:  [0.0014137947097770268]
-0.4909609246879552
-196.89260412939538 96.66657498758747 724.1095663888115
```


29500
29000
28500
28000
27500
27000
−0.04
−0.02
0.00
0.02
0.04


Gibbs energy over temperature
True
Prediction
0
−20
−40
−60
−80
−100
−120


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

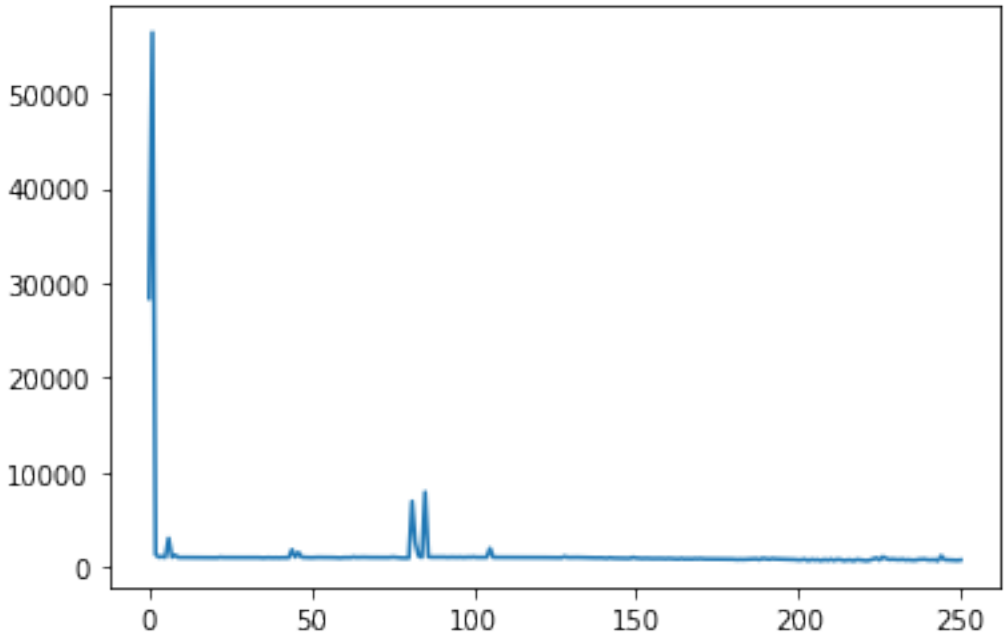

Enthalpy over temperature
True
Prediction
120
100
80
60
40
20

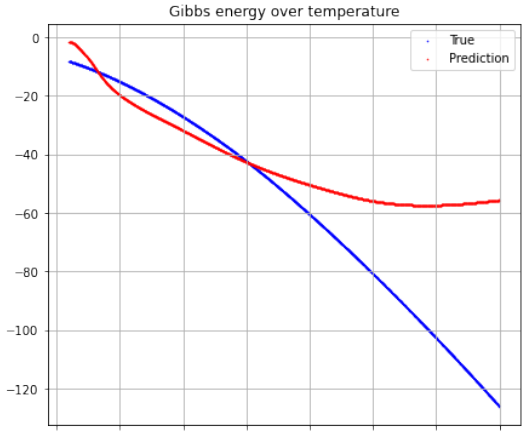

Heat capacity over temperature
True
Prediction
60
50
40
30
20
250
500
750
1000
1250
1500
1750
2000

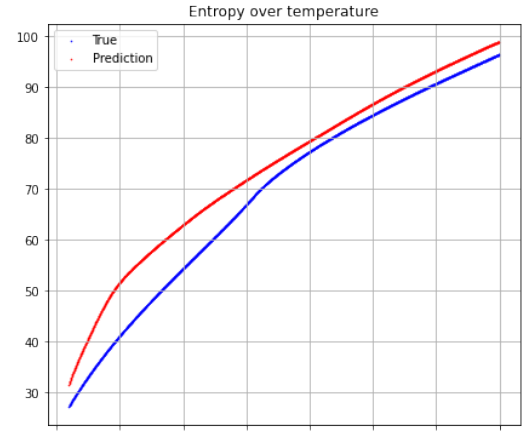
```
260 :  590.8630632672991
lr:  [0.0013446744708678 46]
-0.9768029037786989
-101.00796245240726 98.6648710282812 712.5036046491351

270 :  556.5204031808036
lr:  [0.0012789335114211096]
-1.1210791585049196
-94.59436819785576 106.04777469855665 697.9345649065291

280 :  528.7793448311942
lr:  [0.001216406618904779]
-3.7648528074036527
-25.993845331312027 97.86300157080642 654.2995750209263

290 :  724.4887172154018
lr:  [0.0011569366580059526]
0.601699695642767
182.1072298390167 109.57386476848377 615.5572521972656

300 :  567.8849400111607
lr:  [0.0011003741757366753]
-2.505934645761208
-39.80890699431823 99.75851924694773 578.1307560511997

310 :  364.0140577043806
lr:  [0.0010465770258460752]
-4.85552493615331
-41.47727872804885 201.39396114782247 571.0430811854771

320 :  292.1096954345703
lr:  [0.00099541001159494]
-4.934578631431652
-44.617794742778266 220.17001651931713 522.1828436279297

330 :  130.01788984026228
lr:  [0.0009467445459949988]
-7.2353439553486005
-33.106007931259064 239.53335437115808 471.3367738124302

340 :  467.7225995744978
lr:  [0.0009004583286590612]
0.5461988087645817
500.93893238493735 273.6122481324541 469.2913716452463
```

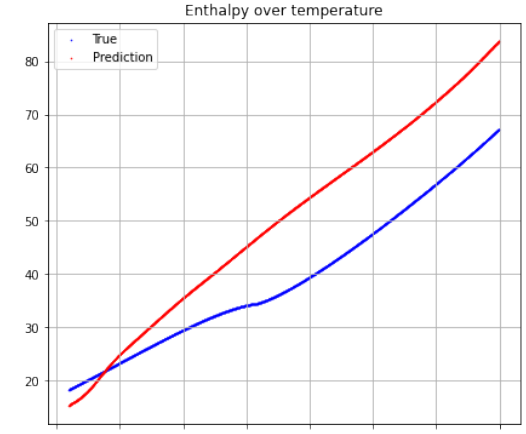
```
350 :  189.18915557861328
lr:  [0.0008564350384499106]
-8.621439430525983
-31.915978237744536 275.1616732426999 420.3566877419608

360 :  836.9031720842634
lr:  [0.0008145640411555528]
9.934075402796443
34.81580259159211 345.86280815375187 438.1737268611364

370 :  671.4925711495536
lr:  [0.000774740111456184]
9.85064559358202
35.559446210979246 350.28350212839956 497.08312867300845

380 :  407.9427185058594
lr:  [0.0007368631684841578]
2.785555113856371
119.87092517440037 333.90706862224533 549.0783276040214

390 :  338.57029506138394
lr:  [0.0007008380243123892]
-4.502435267145365
-69.30504538161279 312.0414805172834 552.1508384050642

400 :  70.40796443394252
lr:  [0.0006665741447391304]
-3.6174484786764824
-88.4091360981807 319.81549487946586 547.5863597215925

410 :  954.3008676256452
lr:  [0.0006339854217679446]
4.660943996106919
56.29251176505378 262.37624473710554 430.35273058210106

420 :  692.6166556222098
lr:  [0.0006029899572111071]
1.2424482784882915
222.7731099464895 276.7840669464988 445.1625033569336

430 :  620.365984235491
lr:  [0.0005735098568726064]
3.0238907260727963
97.7962469499079 295.7251641965515 469.0768678065709

440 :  869.0652640206473
lr:  [0.0005454710347935108]
11.12474269144042
```

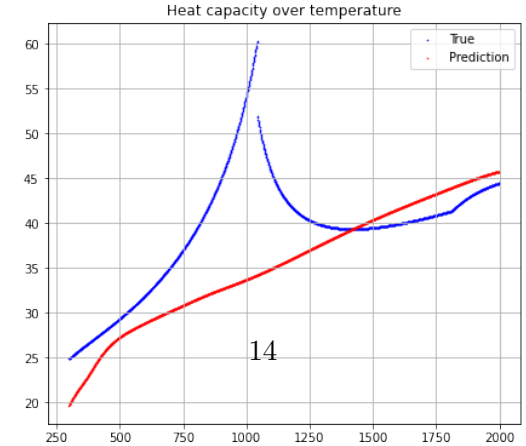
```
56.02166258869401 623.2265814459149 551.6091755894251

450 :  514.1361345563616
lr:  [0.00051880302706775 57]
9.605940276610262
62.86696108843664 603.8962735875036 617.8696994345528

460 :  441.2024710518973
lr:  [0.0004934388147604504]
-8.48843143563228
-64.02055257657958 543.4340710175873 703.1083984374999

470 :  436.17557852608815
lr:  [0.00046931465548368765]
-4.701050383008947
-116.40321598541561 547.2173830917112 672.8582449776785

480 :  533.1555306570871
lr:  [0.000446369923206589]
-0.8185747774974999
-666.399796569284 545.4980652010809 664.3245780726843

490 :  738.7096710205078
lr:  [0.00042454695589701544]
0.5887078821832853
176.4145388227939 103.85662953670796 585.3553296334403

500 :  662.4752546037946
lr:  [0.0004037909106120566]
1.366456234767901
451.69364242628126 617.2195938984149 672.2993965802873
```


50000
40000
30000
20000
10000
0
0
50
100
150
200
250


Gibbs energy over temperature
True
Prediction
0
−20
−40
−60
−80
−100
−120


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

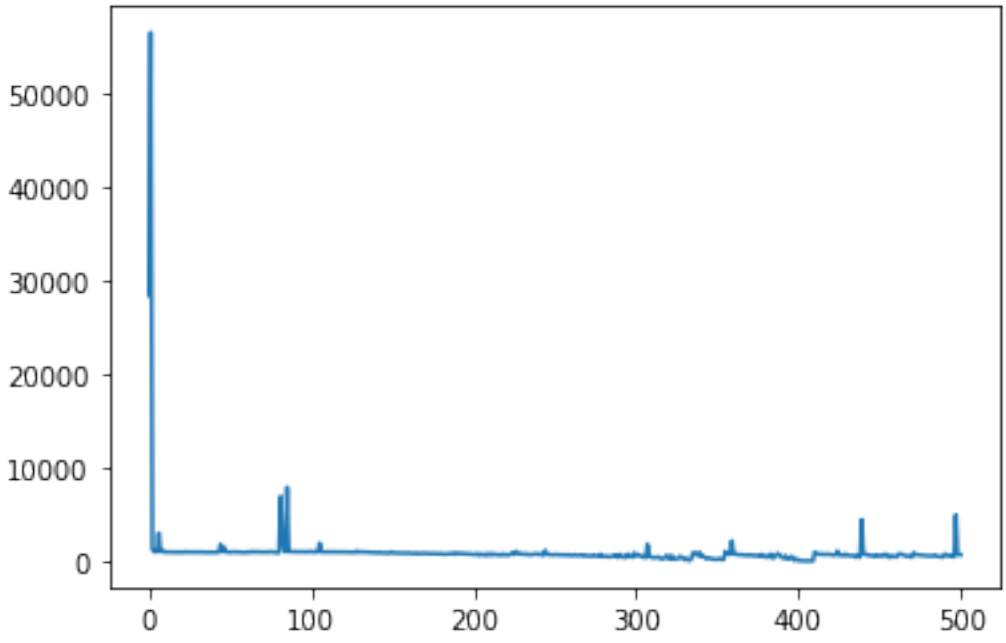

Enthalpy over temperature
True
Prediction
80
70
60
50
40
30
20

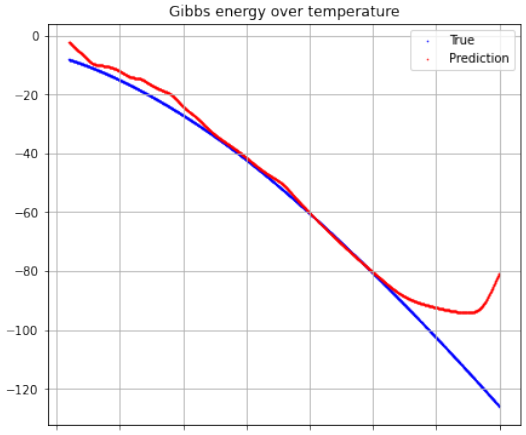

Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
20
250
500
750
1000
1250
1500
1750
2000

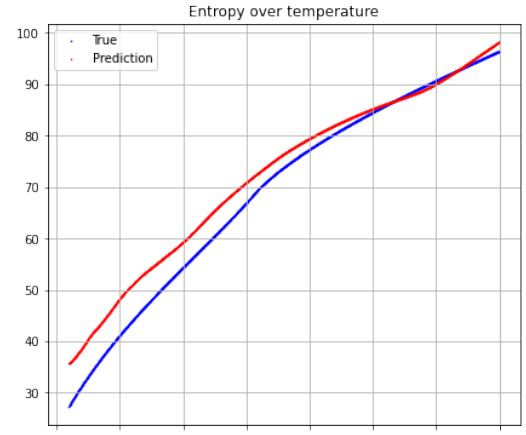
```
510 :  538.5108729771206
lr:  [0.00038404962567312596]
0.8121498486043354
756.6109865084718 614.4814981452322 677.3561566598074

520 :  505.02710396902904
lr:  [0.0003652734895792976]
-8.092030783783944
-76.14877041171097 616.198194318861 659.6629490879604

530 :  408.79323032924106
lr:  [0.00034741531632945347]
-3.1729366202396143
-196.2492546139607 622.6864466593639 613.372359401158

540 :  323.46675763811385
lr:  [0.0003304302268399139]
-7.462292996509413
-84.62100479685655 631.4667314531721 571.7887418910435

550 :  281.77364240373885
lr:  [0.00031427553615954513]
-7.087217547803161
-14.779440655712074 104.74511116187807 422.3324493844168

560 :  308.52832467215404
lr:  [0.00029891064619890525]
-4.50477800285851
-22.730049478381964 102.39382689410061 352.21582981654586

570 :  30.32943562098912
lr:  [0.000284296943703849]
-8.279509285796141
-12.918402879067703 106.95803659489665 284.2997708674839

580 :  32.162212644304546
lr:  [0.000270397703217188]
-6.2011271496208344
-18.162935422087926 112.63067196271939 216.84684841700965

590 :  21.043131147112167
lr:  [0.0002571779947845447]
-6.108828864361733
-18.200834547178488 111.18578343727617 156.99587843213763
```

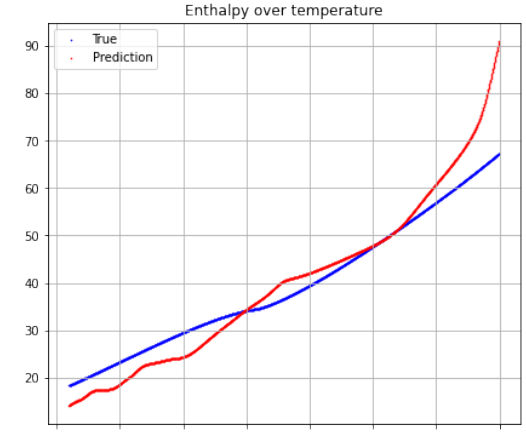
```
600 :  505.7765110560826
lr:  [0.0002446045961724539]
5.043739385577058
50.49738394979064 254.69564429616582 168.13477414267402

610 :  104.7096437726702
lr:  [0.00023264590937811005]
0.2954318433044212
944.4054104720905 279.0074312424382 193.64240120479042

620 :  31.14563533238002
lr:  [0.0002212718812209424]
-0.011236413227230893
-25157.97989634378 282.6854580776861 170.77168870653426

630 :  13.76330075945173
lr:  [0.0002104539278164573]
-0.29517323908236237
-967.7677836331934 285.6591513745685 159.17912246704103

640 :  291.22191946847096
lr:  [0.00020016486274254485]
5.339769719293443
58.19909929497381 310.76978810545353 236.54012696674894

650 :  31.893524714878627
lr:  [0.00019037882871772517]
-15.084630482398385
-14.430442133879538 217.67788728720527 206.67048941748487

660 :  453.28397478376115
lr:  [0.00018107123261963643]
8.002853882903608
24.570290822651312 196.63244731412593 153.95527512959072

670 :  21.47301537649972
lr:  [0.0001722186836804605]
0.02428944534879961
8068.061182963433 195.96873117436184 159.43339094161988

680 :  333.9910583496094
lr:  [0.0001637989347039663]
6.384347556978898
34.63687820080205 221.13386872266622 183.49710664204187

690 :  19.430758340018137
lr:  [0.00015579082615644384]
-7.401430079957838
```

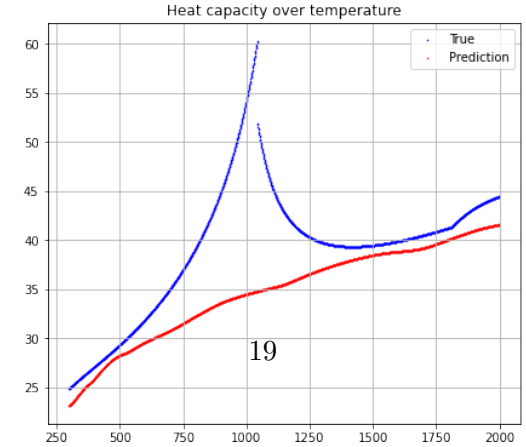
```
-21.80024435851997 161.35298434558086 111.14724401746476

700 :  13.954300335475377
lr:  [0.00014817423299102564]
-2.8015619200103177
-52.870833925646565 148.12091500528103 74.89596669878277

710 :  21.17025920322963
lr:  [0.00014093001407176005]
-3.9542441076161956
-46.15965833348851 182.52655697477374 104.12949668884278

720 :  14.234899384634835
lr:  [0.00013403996407033 48]
-0.12122267953856532
-1510.9518589061518 183.16163299037999 93.9010201508658

730 :  12.517101424080986
lr:  [0.00012748676771456 35]
-5.041332709198444
-27.253712757489676 137.3950335714316 68.36946516036987

740 :  13.447968346732003
lr:  [0.00012125395627365804]
-0.064342796281202
-2093.0480720470946 134.67256570648883 57.91259687696184

750 :  14.239328248160225
lr:  [0.00011532586617092 99]
-0.035170844275472624
-5120.5578502092985 180.09434275326012 90.22003511701313
```


50000
40000
30000
20000
10000
0
0
100
200
300
400
500


Gibbs energy over temperature
True
Prediction
0
−20
−40
−60
−80
−100
−120


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

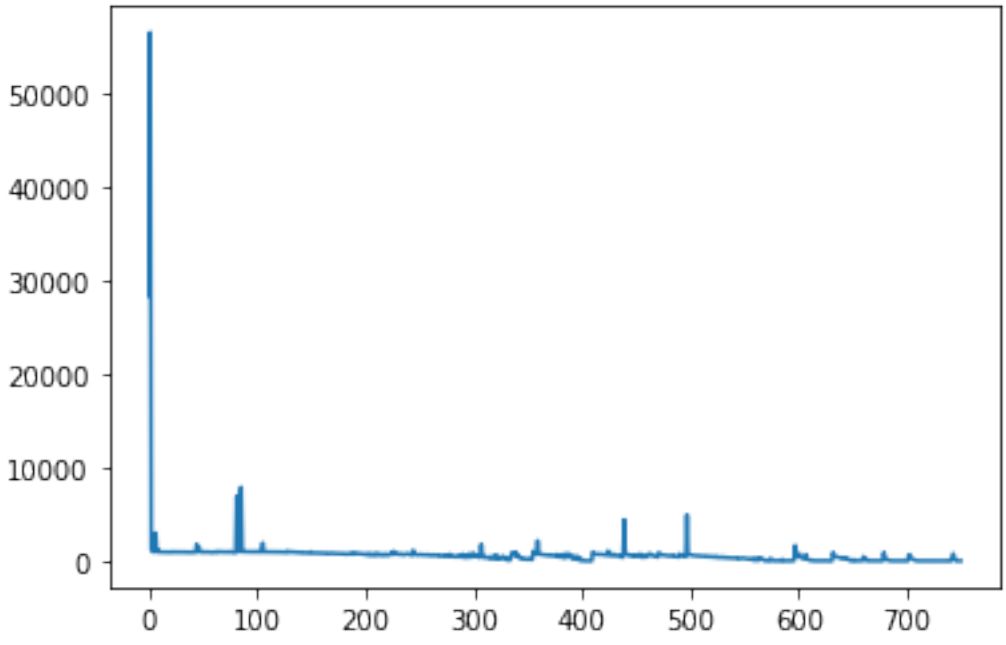

Enthalpy over temperature
True
Prediction
90
80
70
60
50
40
30
20

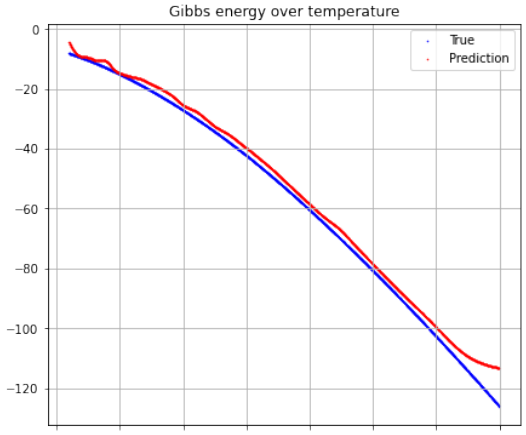

Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

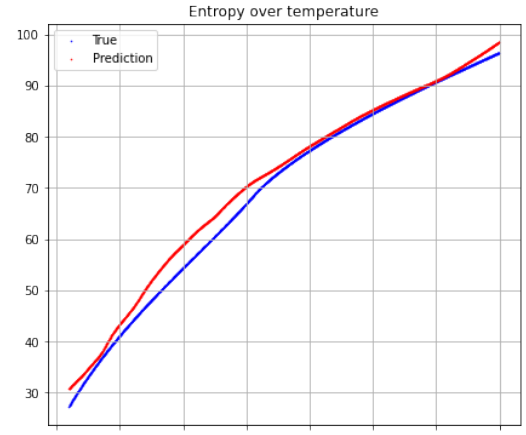
```
760 :  11.815307889665876
lr:  [0.00010968759961991128]
-0.11798657342226725
-1108.2250011614285 130.75567046792509 46.96421908242362

770 :  15.063761983598981
lr:  [0.00010432498718497115]
0.04164719929152751
3144.1379848087336 130.94454125339104 46.19473139081683

780 :  11.844791412353516
lr:  [9.922455217233788e-05]
-0.17935905234111774
-730.2874484387216 130.983664688582 46.04392733710152

790 :  104.64356463296073
lr:  [9.437347676204006e-05]
1.7197524701888642
76.39038140585005 131.3725471213801 49.50269288471766

800 :  10.241463797433036
lr:  [8.975956979565241e-05]
-0.07296653669707583
-251.71632393880563 18.366868387933888 15.955565411703928

810 :  11.388531412397112
lr:  [8.537123613889452e-05]
-0.02101984385498722
-876.6775117742012 18.42762440867243 15.672971616472516

820 :  12.097984858921595
lr:  [8.11974475420882e-05]
0.019428002938584477
947.8053837307882 18.413965780327942 15.745802432468958

830 :  12.581634657723564
lr:  [7.722771492524318e-05]
-0.03672587836796613
-501.527746831801 18.419047028304835 15.722048952920098

840 :  254.44489397321428
lr:  [7.345206201812147e-05]
4.961881209392936
7.534893564689569 37.38724679340893 19.049218384878973
```

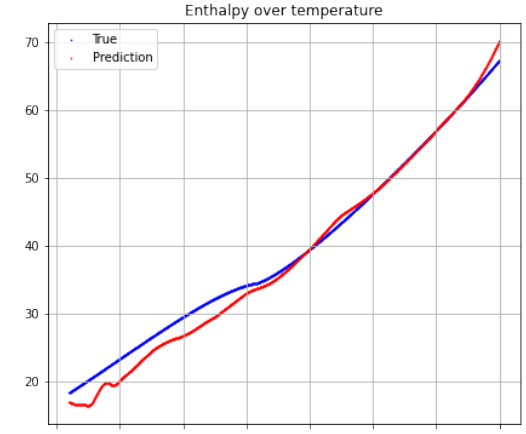
```
850 :  10.494285038539342
lr:  [6.986100028903547e-05]
0.001589722258009091
23494.34578513738 37.349484431994966 19.421493674686978

860 :  10.291887419564384
lr:  [6.644550509937384e-05]
-0.06991121442255326
-534.7283006937438 37.383504887607856 19.271296651022777

870 :  10.595173699515206
lr:  [6.319699302392957e-05]
0.0037983040767932776
9866.458829513496 37.47581079565414 18.80560280391148

880 :  10.515848568507604
lr:  [6.0107300280034106e-05]
-0.07234286983923689
-519.1661336105259 37.557968028726144 18.34779935019357

890 :  11.905280930655342
lr:  [5.716866221128857e-05]
-0.24122767267699838
-7.980329479916904 1.9250763076359956 10.797098364148821

900 :  9.982581411089216
lr:  [5.437369377433232e-05]
-0.009010748682494756
-54.54180206592934 0.4914624711064625 10.397419801439558

910 :  11.513540404183525
lr:  [5.171537097961115e-05]
0.027035968991827353
26.308726410742135 0.7112819114552937 10.486051712036135

920 :  9.972545351300921
lr:  [4.9187013239503754e-05]
-0.01265629248438352
-58.45645882928525 0.7398420405447577 10.489941122872489

930 :  9.638491358075823
lr:  [4.678226657944606e-05]
-0.020556839144959742
-49.13392936321934 1.0100382824795142 10.60500386101859

940 :  13.01615537915911
lr:  [4.4495087669861456e-05]
0.06579165277953748
```

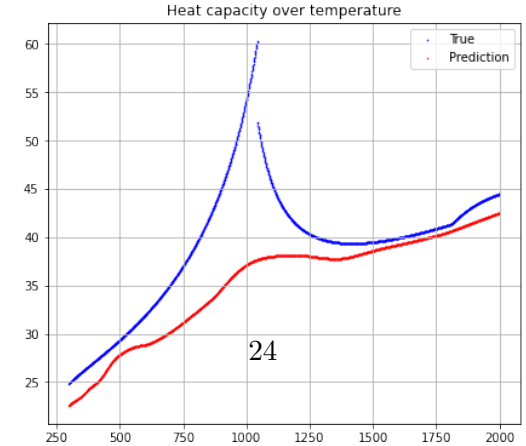
```
16.834096495421903 1.1075430314840267 10.558926617758615

950 :  9.60471589224679
lr:  [4.2319728638767885e-05]
-0.01456301552908761
-74.68498513049765 1.0876385982451147 10.452209153856547

960 :  8.745985371725899
lr:  [4.0250722626894584e-05]
-0.021034486787312248
-51.67161065803756 1.0868858116656337 10.25127279962812

970 :  8.832188742501396
lr:  [3.8282870049007304e-05]
-0.03589522803837633
-102.40102314999749 3.6757080773322137 10.799260538646152

980 :  8.708169528416224
lr:  [3.641122552691552e-05]
-0.015658545424569827
-236.62466084418358 3.7051980004020777 10.368255543027606

990 :  8.674844196864537
lr:  [3.463108546132327e-05]
-0.022064272933381635
-168.64275558174444 3.7209797873931785 10.052764885766164

1000 :  8.768666812351771
lr:  [3.293797621129047e-05]
-0.009691883454169981
-386.8097249663387 3.7489147733132993 9.846557809284755
```


50000
40000
30000
20000
10000
0
0
100
200
300
400
500
600
700


Gibbs energy over temperature
True
Prediction
0
−20
−40
−60
−80
−100
−120


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

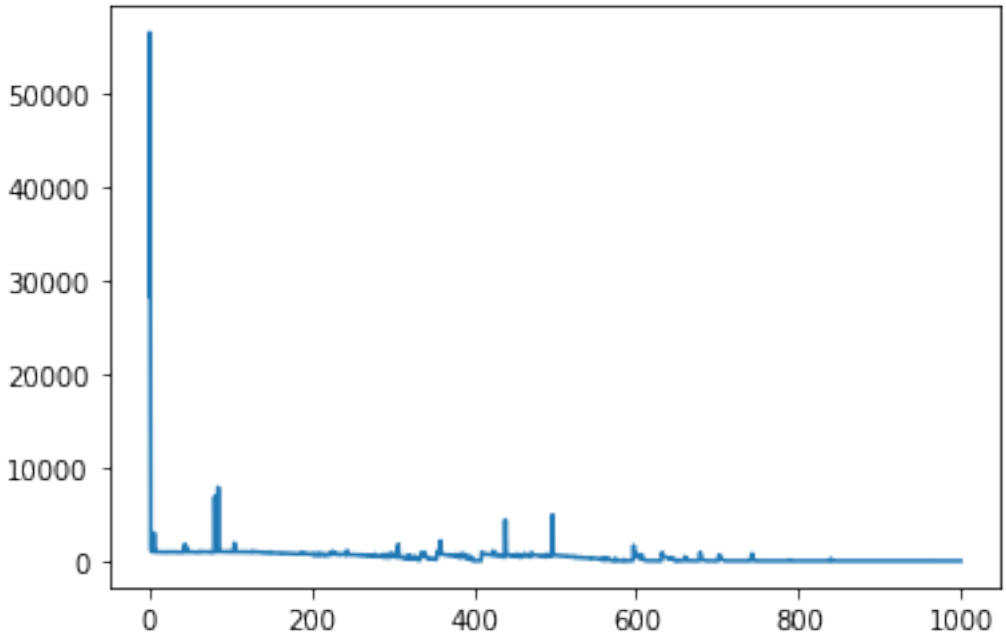

Enthalpy over temperature
True
Prediction
70
60
50
40
30
20

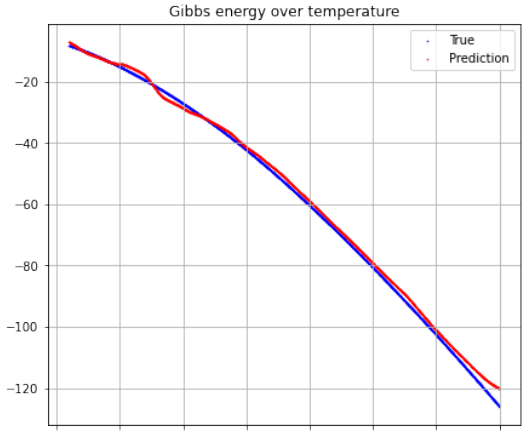

Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

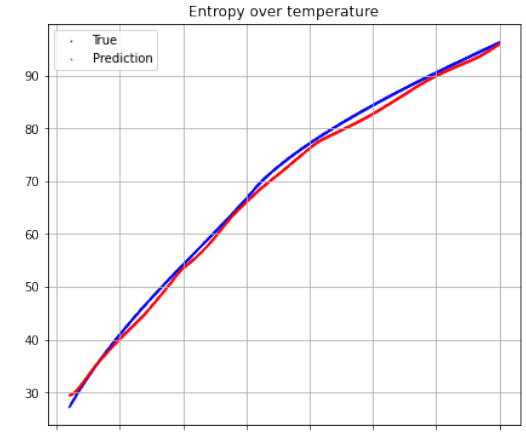
```
1010 :  9.163391930716378
lr:  [3.132764285159898e-05]
-0.005081874636102369
-736.4662673953771 3.742629244621552 9.66644721031189

1020 :  9.082205636160714
lr:  [2.9796038479769403e-05]
0.0070894563858432446
42.487294599359515 0.30121182201463254 8.837570610046386

1030 :  8.184466906956263
lr:  [2.8339314045856632e-05]
-0.01003625163531514
-33.65359404849907 0.3377559383034807 8.803204142706736

1040 :  8.35679258619036
lr:  [2.695380867946518e-05]
-0.008687158367724162
-41.694987892251426 0.3622109629603296 8.732334235055106

1050 :  7.885438305991037
lr:  [2.563604048967558e-05]
-0.02624133446473769
-15.695422984286678 0.4118688440961981 8.606826497486658

1060 :  8.049849578312465
lr:  [2.438269781476115e-05]
-0.02951039934297346
-13.216765705681475 0.39003203399717673 8.456488419941493

1070 :  7.7076583589826315
lr:  [2.319063089970496e-05]
-0.015685392885791995
-21.498731297568884 0.3372160469484407 8.274347260338919

1080 :  7.770505905151367
lr:  [2.2056843980601938e-05]
-0.00476369635356758
-78.25284961323932 0.3727728143588604 8.105793995176041

1090 :  8.065032345908028
lr:  [2.0978487756053488e-05]
-0.0036400261147724504
-96.14859515934407 0.34998339727869643 7.937425003051758
```

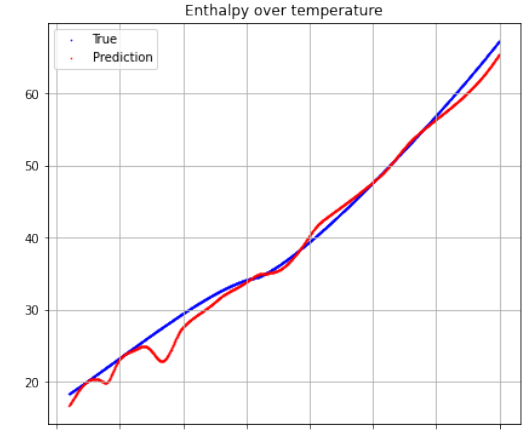
```
1100 :  7.484244210379464
lr:  [1.995285222663463e-05]
-0.011323190639039873
-32.08714640315436 0.36332887578569933 7.767422985349383

1110 :  7.2707343101501465
lr:  [1.8977359884438732e-05]
-0.022807625917929612
-15.493995715753028 0.35338125825889916 7.589957079206194

1120 :  7.1650824546813965
lr:  [1.8049559235584425e-05]
-0.010932449696710441
-28.12510238841125 0.3074762670761367 7.4252621364593505

1130 :  6.692244052886963
lr:  [1.7167118639406374e-05]
-0.01924445399737567
-16.123930104999566 0.3102962311625648 7.292760358537946

1140 :  6.749267441885812
lr:  [1.6327820448847178e-05]
-0.017738278336149615
-15.205728163184078 0.2697234384623882 7.137120573861259

1150 :  6.5319196837288995
lr:  [1.5529555437324735e-05]
-0.027967860330298057
-10.602492412361034 0.2965290269419583 6.983800854001728

1160 :  6.442825998578753
lr:  [1.4770317498069367e-05]
-0.021201791290639087
-14.217347830763531 0.30143324141426875 6.8400377096448635

1170 :  6.14471789768764
lr:  [1.404819860260963e-05]
-0.021355816643717683
-14.444548211497832 0.3084751231060879 6.694562537329538

1180 :  6.184471470969064
lr:  [1.336138400573712e-05]
-0.012445434536947806
-22.23810240559834 0.2767628477148157 6.545546421323504

1190 :  6.048768315996442
lr:  [1.2708147684899912e-05]
-0.011922492925349202
```

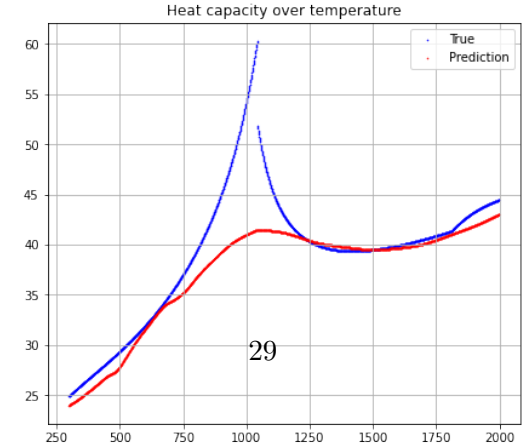
```
-20.835478073863715 0.24841083993190854 6.395533578055245

1200 :  5.822454384395054
lr:  [1.2086848002563453e-05]
-0.02010310426050303
-13.095510580337441 0.2632604145410441 6.273797822679792

1210 :  5.946149076734271
lr:  [1.1495923580638079e-05]
-0.01780531635784894
-14.07461677647441 0.25060300432061494 6.139756671360561

1220 :  5.654295853206089
lr:  [1.0933889376605226e-05]
-0.013193526698966071
-17.831666266080276 0.23526256496858278 6.007134895324708

1230 :  5.465341908591134
lr:  [1.0399332951481313e-05]
-0.014899034194279001
-15.300563958965634 0.22796362561638187 5.869941646030972

1240 :  5.376826763153076
lr:  [9.890910920240393e-06]
-0.013035770060369637
-17.36759591483493 0.2263999868472032 5.741233305249895

1250 :  5.413293770381382
lr:  [9.40734557577517e-06]
-0.008761732640836411
-25.113820609488616 0.22004058177026659 5.618285800388881
```


50000
40000
30000
20000
10000
0
0
200
400
600
800
1000


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


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

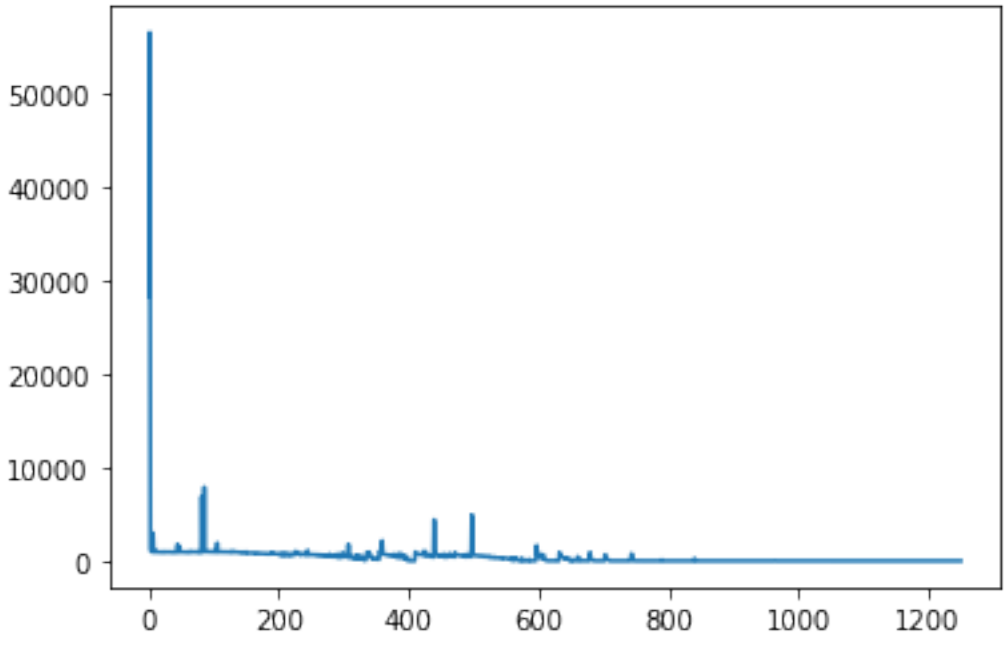

Enthalpy over temperature
True
Prediction
60
50
40
30
20

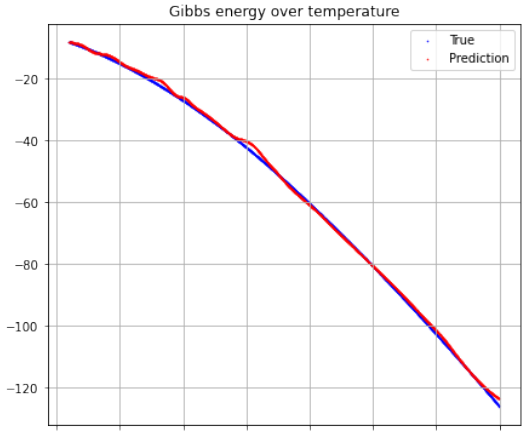

Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

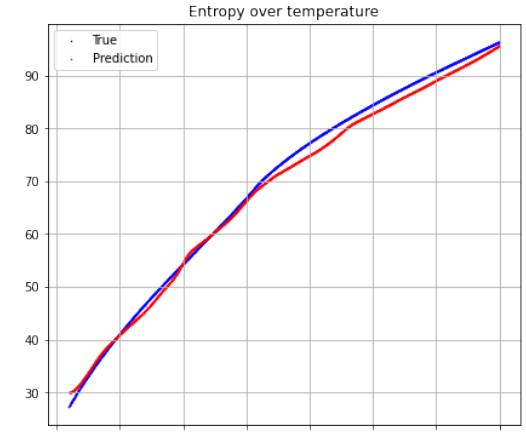
```
1260 :  5.223289557865688
lr:  [8.947421677912122e-06]
-0.015401313325754052
-14.237369559672812 0.21927418952307398 5.4821875953674315

1270 :  4.973927770342145
lr:  [8.509983399411275e-06]
-0.015160000359004168
-14.055833502497249 0.21308644094396112 5.353500483376639

1280 :  4.906327451978411
lr:  [8.09393142127561e-06]
-0.011661925746817634
-18.31311316841059 0.21356616596307254 5.229922325951712

1290 :  4.8199310302734375
lr:  [7.698220170070455e-06]
-0.017355497654951004
-11.863481407698544 0.2058966237508669 5.104512292998177

1300 :  4.61935635975429
lr:  [7.3218551903099484e-06]
-0.012843294671951163
-14.954651442331263 0.1920669951901799 4.97150368622371

1310 :  4.553582872663226
lr:  [6.963890645307184e-06]
-0.014753765684522618
-13.61069006391469 0.2008089320076575 4.853081192970276

1320 :  4.425436156136649
lr:  [6.6234269402074865e-06]
-0.014191471800512197
-14.89264239942199 0.21134851464650947 4.716029914447239

1330 :  4.1412307875497
lr:  [6.29960846123125e-06]
-0.013224325791739851
-16.57574327120638 0.21920302925867283 4.577282658985683

1340 :  4.12332204410008
lr:  [5.991621425444934e-06]
-0.013953219349808331
-14.924697090216947 0.2082475722292432 4.446676331928798
```

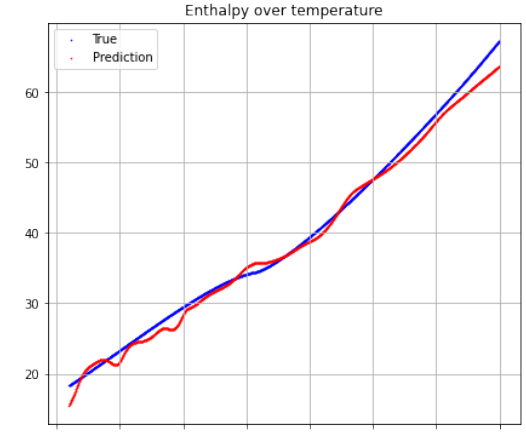
```
1350 :  4.044460160391671
lr:  [5.698691835656445e-06]
-0.012639390483889571
-15.676459368734907 0.1981408913662695 4.3156397342681885

1360 :  4.042197261537824
lr:  [5.42008353529543e-06]
-0.010213311837643993
-16.289391759664873 0.16636863768700577 4.1929628910337176

1370 :  3.828765392303467
lr:  [5.1550963583902185e-06]
-0.011281659929814914
-14.184904079733364 0.160029263964596 4.084498385701861

1380 :  3.720388412475586
lr:  [4.903064369992145e-06]
-0.008596715704692687
-18.73622283611622 0.16106998110186208 3.9818354899542676

1390 :  3.683795690536499
lr:  [4.663354192625308e-06]
-0.007457297327914672
-18.743817154227468 0.1397782175791417 3.88527872630528

1400 :  3.59218008177621
lr:  [4.435363414555961e-06]
-0.008981389137468258
-14.611245550475868 0.13122928207192538 3.801854784829276

1410 :  3.59686541557312
lr:  [4.218519075881431e-06]
-0.007193857309769611
-16.97863712194136 0.12214189276960352 3.7148238815580097

1420 :  3.44633902822222
lr:  [4.012276228633935e-06]
-0.007480155622298793
-16.129035533709914 0.12064769582973721 3.6376935345785957

1430 :  3.3361524173191617
lr:  [3.8161165672807375e-06]
-0.008281399140205047
-15.440076521183496 0.12786543642722914 3.5645631136213027

1440 :  3.4159979479653493
lr:  [3.6295471261789757e-06]
-0.005880594253540039
```

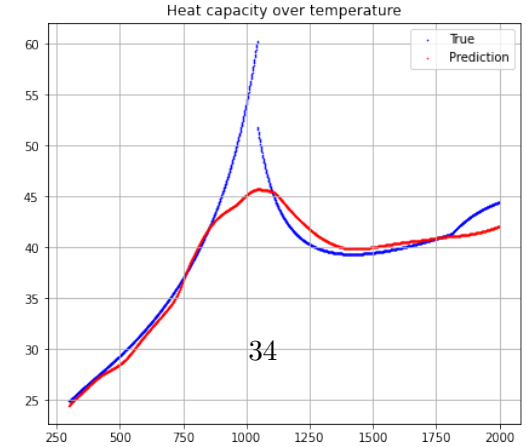
```
-20.31655655305914 0.1194734257176408 3.49080942426409

1450 :  3.2887145451136996
lr:  [3.4520990407117527e-06]
-0.006985619186312396
-15.796757415403187 0.11035013168256312 3.4166363089425227

1460 :  3.1305679253169467
lr:  [3.283326368992121e-06]
-0.008539940108363208
-13.360481061242014 0.11409770808192772 3.345605268478393

1470 :  3.1170264312199185
lr:  [3.122804971173805e-06]
-0.007099444247543285
-15.337076711806283 0.1088847210357632 3.274705634798322

1480 :  3.0261954239436557
lr:  [2.9701314435522786e-06]
-0.005994363011841182
-18.562182258768743 0.11126845875101796 3.205928062711443

1490 :  3.0370966366359164
lr:  [2.824922104777499e-06]
-0.006012774069872265
-16.889735195945157 0.10155416183318801 3.1404504735129217

1500 :  2.917233977999006
lr:  [2.68681203163057e-06]
-0.00639117563431186
-15.205178021027011 0.09717896328336206 3.073830980573382
```


50000
40000
30000
20000
10000
0
0
200
400
600
800
1000
1200


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


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

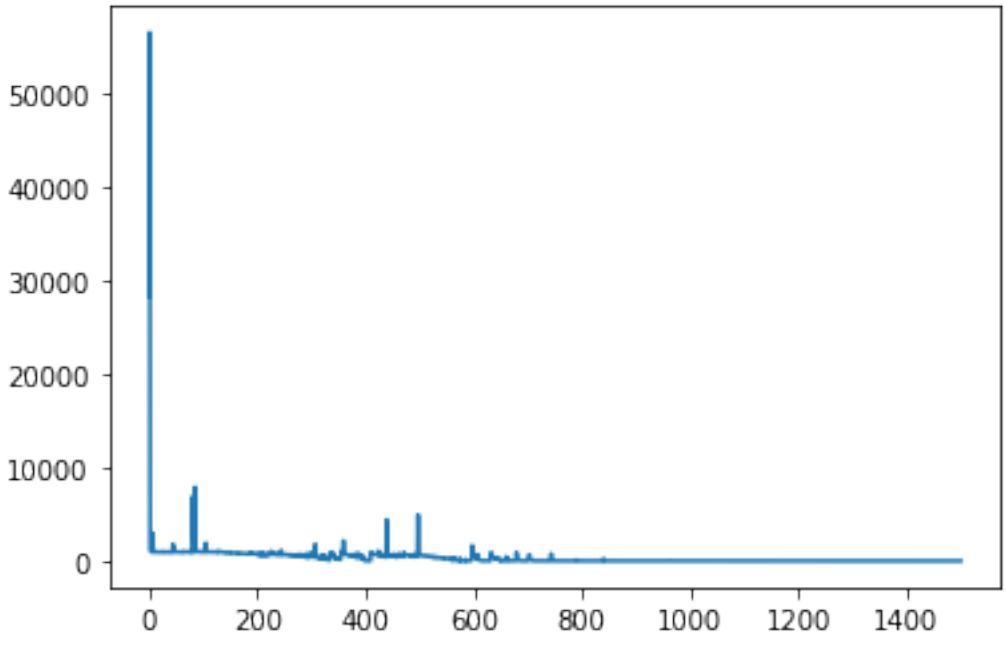

Enthalpy over temperature
True
Prediction
60
50
40
30
20

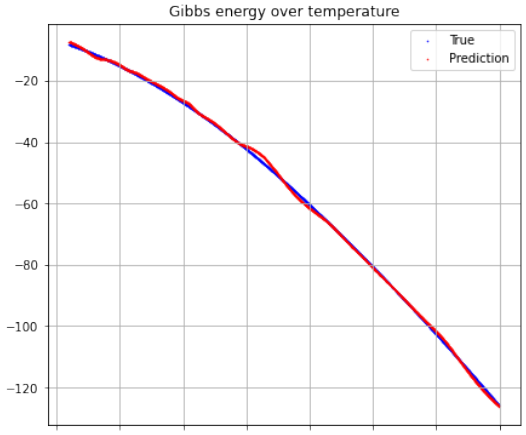

Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

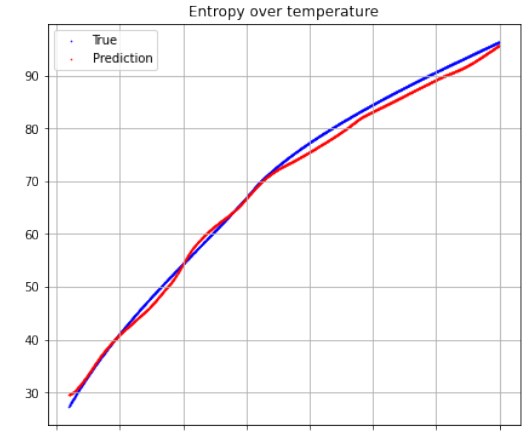
```
1510 :  2.865323237010411
lr:  [2.5554541419411577e-06]
-0.005354113898541419
-16.912664336788907 0.09055233118696727 3.0156569365092682

1520 :  2.7930764130183627
lr:  [2.430518322340951e-06]
-0.006811383166744138
-12.730708124520303 0.08671373102009043 2.960317618506295

1530 :  2.8342514719281877
lr:  [2.3116905986611514e-06]
-0.0051105147548041584
-15.697193069492096 0.08022073679064894 2.913158768245152

1540 :  2.757479872022356
lr:  [2.1986723468891056e-06]
-0.0037874584642860754
-19.641215139127965 0.07439028652755401 2.8589043399265823

1550 :  2.651231527328491
lr:  [2.0911795427011816e-06]
-0.005762700784310658
-14.509261434459788 0.0836125322481298 2.808489642824445

1560 :  2.6600117342812672
lr:  [1.9889420476858746e-06]
-0.005754246308574181
-13.600565112568434 0.0782610015935197 2.7624122565133233

1570 :  2.5789644036974226
lr:  [1.8917029304633716e-06]
-0.0051459369436992475
-14.543929774097965 0.07484214553109816 2.7162105240140644

1580 :  2.6314735412597656
lr:  [1.7992178209955004e-06]
-0.002185011744151655
-28.545014241644985 0.06237119135497054 2.6696107700892857

1590 :  2.457333513668605
lr:  [1.7112542964633722e-06]
-0.0049373620453103265
-13.638471438927013 0.06733807123860715 2.6244109422819957
```

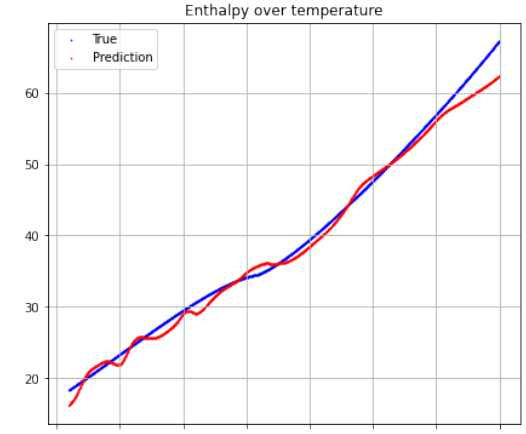
```
1600 :  2.475304331098284
lr:  [1.6275912971693907e-06]
-0.003982350012998891
-17.191747198448482 0.06846355467921496 2.5894771419252667

1610 :  2.4246757711683
lr:  [1.5480185709957339e-06]
-0.005288846291188946
-13.809939874474383 0.07303864928665618 2.5428118102891104

1620 :  2.425685610089983
lr:  [1.4723361450231903e-06]
-0.0035732814243861605
-19.396956877188256 0.06931078569887618 2.503518809250423

1630 :  2.3683218274797713
lr:  [1.4003538229824783e-06]
-0.0031410028218527937
-19.758448062817532 0.062061341120741735 2.466463554246085

1640 :  2.3301189626966203
lr:  [1.3318907072751074e-06]
-0.004973031341508253
-12.522393477774662 0.06227425523567193 2.4337400351251874

1650 :  2.3088009698050365
lr:  [1.266774744362576e-06]
-0.0035150871332463264
-14.445376352434364 0.05077675655134278 2.3994184844834465

1660 :  2.2644111088344028
lr:  [1.2048422923814346e-06]
-0.0034153433652382922
-17.290133397702274 0.05905174238392748 2.369105252879007

1670 :  2.215277007647923
lr:  [1.145937709897586e-06]
-0.004209215022384594
-14.191687691748099 0.05973586502509664 2.3375550413131716

1680 :  2.230468954358782
lr:  [1.089912964766341e-06]
-0.003909097120991257
-13.834937439988515 0.05408211411575326 2.3047367627280098

1690 :  2.1588514362062727
lr:  [1.0366272621152509e-06]
-0.00432731493568976
```

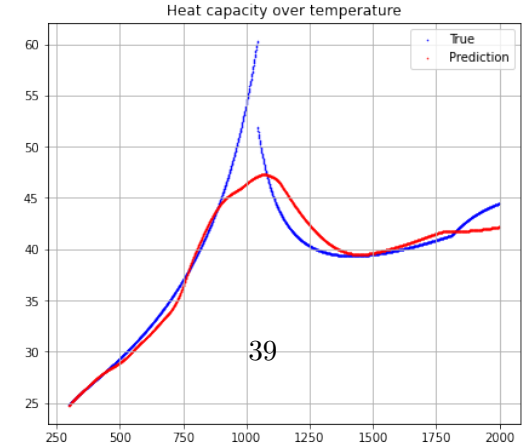
```
-13.335975002000485 0.05770896380814197 2.2710111641883852

1700 :  2.2063569681985036
lr:  [9.859466905148121e-07]
-0.0015241863428677523
-31.058392306784036 0.04733877738542909 2.242008919034685

1710 :  2.1442171164921353
lr:  [9.377438854478388e-07]
-0.0034640266318362897
-13.092133723285162 0.0453514998850218 2.21879846061979

1720 :  2.137293645313808
lr:  [8.918977092317738e-07]
-0.002801372427982072
-15.757087710375853 0.04414147105714207 2.193091034548623

1730 :  2.1798949922834123
lr:  [8.482929465895556e-07]
-3.550664328973248e-05
-1096.7061402098936 0.038940353714092026 2.1713633441925047

1740 :  2.055477806500026
lr:  [8.068200151039863e-07]
-0.003488781500835808
-12.5457767242948 0.04376947374933616 2.153422944545746

1750 :  2.0748809235436574
lr:  [7.673746898279486e-07]
-0.0030793132309315865
-13.586037177493882 0.04183566403658534 2.13025559425354
```


50000
40000
30000
20000
10000
0
0
200
400
600
800
1000
1200
1400


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


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

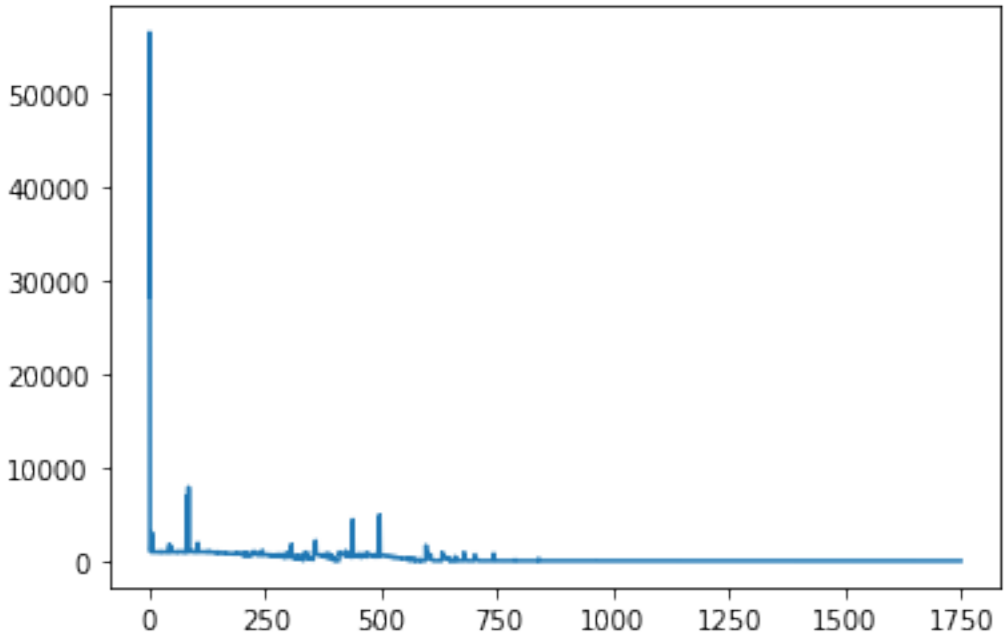

Enthalpy over temperature
True
Prediction
60
50
40
30
20

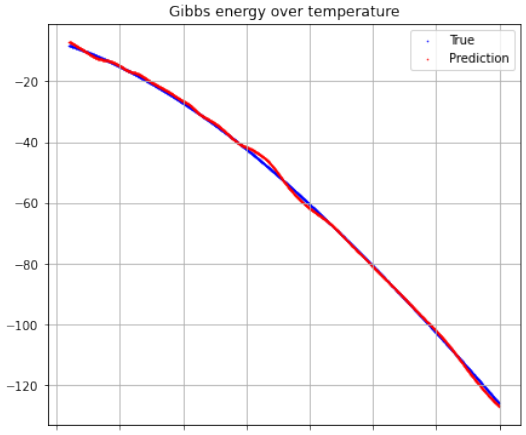

Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

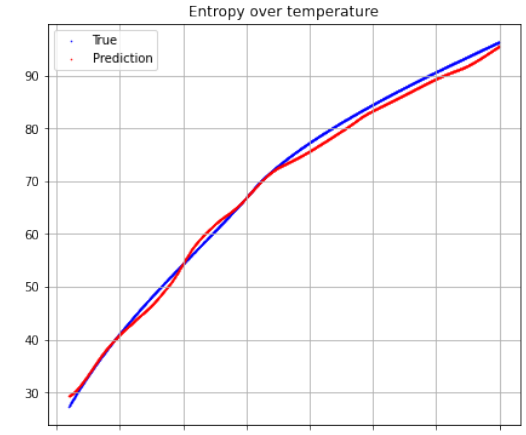
```
1760 :  2.0487573657717024
lr:  [7.298578413583913e-07]
-0.0018056735352941521
-23.34964983716859 0.04216184476936073 2.1065902335303175

1770 :  2.029332331248692
lr:  [6.941751867158463e-07]
-0.002526329835719337
-16.277069317111756 0.0411212458538912 2.086959598405021

1780 :  2.017325588635036
lr:  [6.602370524034101e-07]
-0.0013634088088055045
-29.90963952935331 0.04077906600251763 2.062358178070613

1790 :  1.9941481692450387
lr:  [6.279581490497442e-07]
-0.0005840243820546288
-66.88729391699346 0.039063810497178435 2.0414245254652843

1800 :  2.021459698677063
lr:  [5.972573570697468e-07]
-0.0014833601153626734
-22.194955873267556 0.03292311230463961 2.0227879394803727

1810 :  1.9678088767187936
lr:  [5.680575228042489e-07]
-0.0024103499710038554
-13.366456886329107 0.032217838968387646 2.0049939046587264

1820 :  1.9543409177235194
lr:  [5.402852646264125e-07]
-0.0015330248601930128
-19.576953239524617 0.030011956003027373 1.9876130396979195

1830 :  1.963925565992083
lr:  [5.138707885275612e-07]
-0.0017209963617797464
-18.679105812296402 0.03214667314426102 1.9744859879357473

1840 :  1.8623576164245605
lr:  [4.887477127189977e-07]
-0.0027494301948881015
-11.877270953773861 0.03265572739317325 1.9609029442923411
```

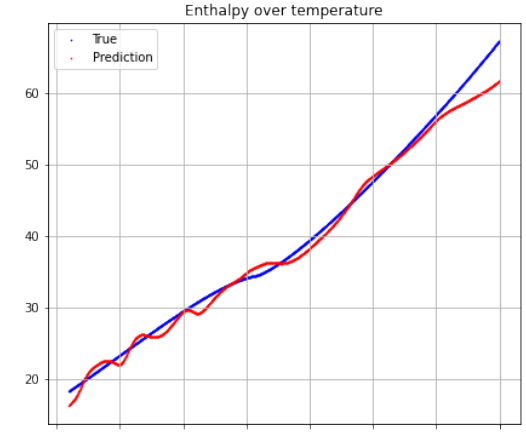
```
1850 :  1.8975661993026733
lr:  [4.648529008090135e-07]
-0.002028162208312456
-15.763667321959856 0.031971274326809 1.9453402069636754

1860 :  1.9121699673788888
lr:  [4.4212630313585343e-07]
-0.0007555710678545442
-43.99402328802886 0.03324061115495365 1.9334917756489345

1870 :  1.8985175234930856
lr:  [4.2051080585789107e-07]
-0.0010226301132068695
-31.585118187295507 0.032299892987526356 1.9203491047450472

1880 :  1.8733386312212263
lr:  [3.9995208742176574e-07]
-0.0013508522128224728
-21.109242674361397 0.028515467177667668 1.909777107579368

1890 :  1.847044484955924
lr:  [3.8039848204777344e-07]
-0.0016420961468977388
-14.33991586685541 0.023547520591801017 1.9008667458806718

1900 :  1.8676926919392176
lr:  [3.618008498894394e-07]
8.136468448023993e-06
2928.3044043085965 0.02382605639186659 1.8937086244991845

1910 :  1.8351948090962
lr:  [3.441124535409718e-07]
-0.0013161265120214345
-21.43181561892388 0.028206980736820788 1.8809391127313884

1920 :  1.834635887827192
lr:  [3.2728884058225054e-07]
-0.0013145569809671768
-23.683704167580164 0.03113357864865392 1.8708147409984042

1930 :  1.8564071144376482
lr:  [3.1128773186617547e-07]
-0.0006403099343658556
-46.08419924895173 0.02950817059639929 1.859769949913025

1940 :  1.7643428530011858
lr:  [2.9606891526763235e-07]
-0.003074941760249461
```

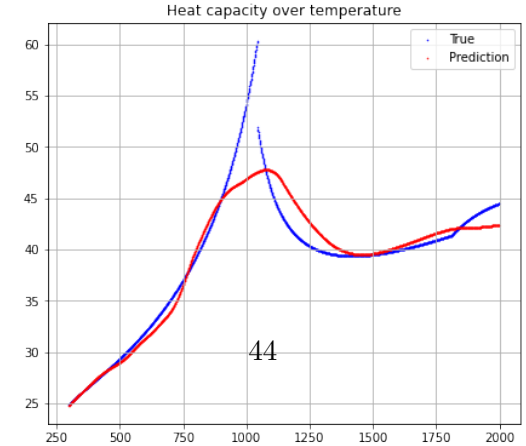
```
-9.519486088432737 0.029271865309435617 1.8470283130237033

1950 :  1.8121688195637293
lr:  [2.8159414462705735e-07]
0.00016350231782340382
158.24012773793646 0.025872627657824106 1.8372107073238917

1960 :  1.8536759785243444
lr:  [2.6782704363463796e-07]
0.000421431252282148
67.48482647084884 0.02844021492965328 1.8313665533065795

1970 :  1.819168073790414
lr:  [2.5473301441360246e-07]
-0.0006850092473600083
-45.66507179046555 0.03128099645782755 1.8248653479984827

1980 :  1.7571138824735368
lr:  [2.422791505728609e-07]
-0.0016706681460055262
-20.231728352346224 0.033800504096901704 1.8162279820442198

1990 :  1.8412674495152064
lr:  [2.3043415451049007e-07]
0.0006009350712723325
54.117074578706514 0.03252084806900513 1.812729728562491

2000 :  1.7779651369367326
lr:  [2.1916825876024198e-07]
-2.516636695528299e-05
-1208.3084155494946 0.030408732980875146 1.8062886187008447
```


50000
40000
30000
20000
10000
0
0
250
500
750
1000
1250
1500
1750


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


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

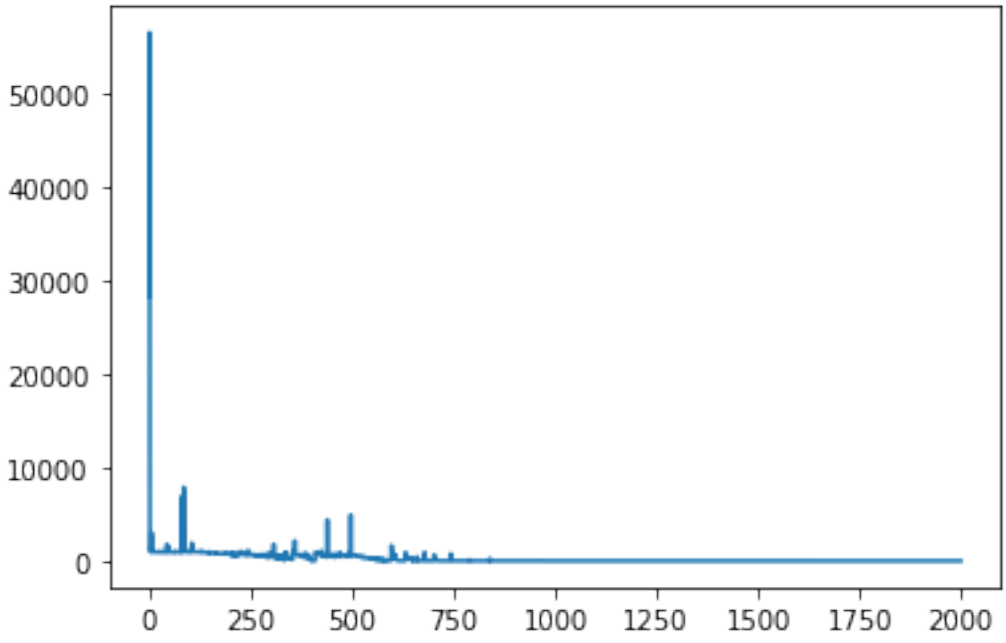

Enthalpy over temperature
True
Prediction
60
50
40
30
20

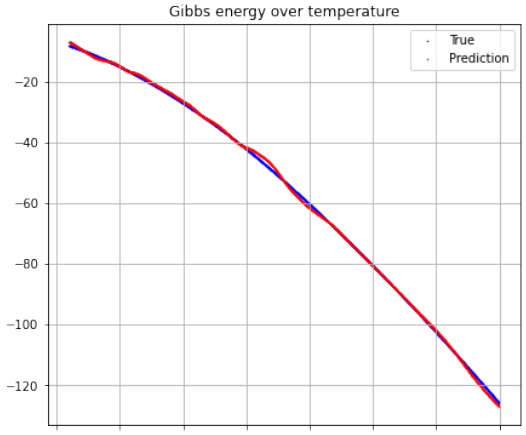

Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

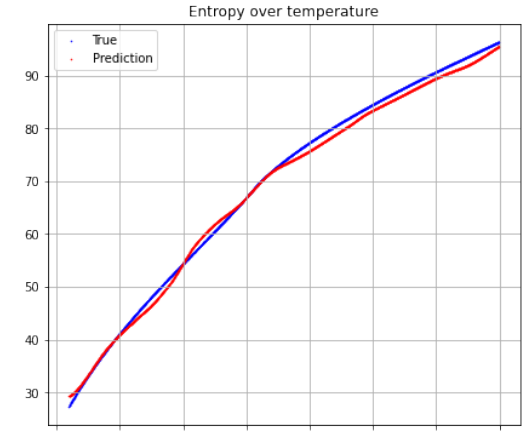
```
2010 :  1.803044319152832
lr:  [2.0845315118340978e-07]
-8.125381636550123e-05
-359.09779922821804 0.029178066635745258 1.7998754940714157

2020 :  1.813429628099714
lr:  [1.9826190381805415e-07]
-0.0004800773570558446
-54.92309545240174 0.026367334506114906 1.7937853397641865

2030 :  1.801389251436506
lr:  [1.8856890520678178e-07]
0.00013724708001050523
200.1069633599382 0.027464096410920676 1.7884562253952025

2040 :  1.7637672424316406
lr:  [1.7934979603301001e-07]
-0.0009928034623927354
-25.66799334958191 0.025483272670138626 1.7805193022319248

2050 :  1.7623042038508825
lr:  [1.7058140790396574e-07]
-0.0014106132546249702
-17.86796448029847 0.025204787529077188 1.7715164807864598

2060 :  1.7052623885018485
lr:  [1.6224170512657589e-07]
-0.0017032664996889527
-14.236994365625142 0.024249395559229676 1.765579240662711

2070 :  1.7486212934766496
lr:  [1.5430972932992683e-07]
-0.0009660143893939755
-23.866147932187737 0.023055042321898627 1.761919677257538

2080 :  1.7648798057011195
lr:  [1.4676554679512468e-07]
0.00015918993046262482
136.145178317324 0.02167294146915646 1.7566667430741445

2090 :  1.7233596869877406
lr:  [1.395901983601914e-07]
-0.0008207371909138799
-23.751520851492323 0.019493756503586254 1.7512766677992684
```

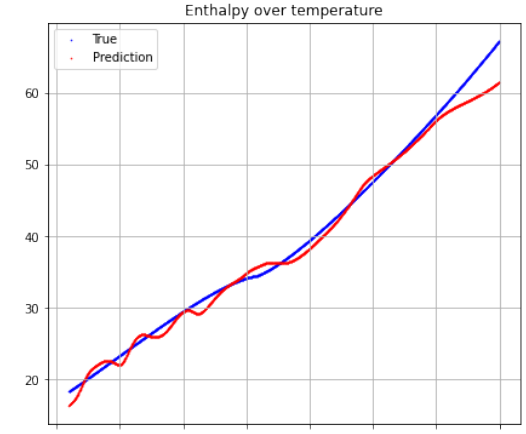
```
2100 :  1.7182759727750505
lr:  [1.3276565177410457e-07]
-0.0012394526957075407
-17.39776634406215 0.021563708394437754 1.746548409802573

2110 :  1.7745831523622786
lr:  [1.2627475638024182e-07]
0.0005256976747651844
40.00683845951186 0.021031501952871737 1.7455683946609495

2120 :  1.7205524614879064
lr:  [1.2010120001534533e-07]
-0.0004415307031080939
-44.39770564598705 0.019602950190258855 1.7402412360055106

2130 :  1.7671712466648646
lr:  [1.1422946801569086e-07]
0.0005167684471641931
41.305303211737574 0.021345277400375784 1.7426521338735304

2140 :  1.6964761699948991
lr:  [1.0864480422743945e-07]
-0.0016307417227297413
-14.178890306949347 0.023122108005550607 1.7399180051258631

2150 :  1.7278892483030046
lr:  [1.0333317392318817e-07]
-0.000279227081610232
-83.39992729517056 0.023287518305136003 1.7394262014116557

2160 :  1.714963504246303
lr:  [9.82812285315258e-08]
-0.0005417905813055933
-42.094796448507374 0.022806564237777435 1.7345697103227886

2170 :  1.731930136680603
lr:  [9.347627209095586e-08]
8.504418520468729e-05
264.14521019841754 0.022464014177045275 1.734001136166709

2180 :  1.7054253646305628
lr:  [8.890622934388301e-08]
-0.0004884136661496189
-46.202995383124765 0.022566174362165882 1.7266738455636161

2190 :  1.7098193509238107
lr:  [8.455961539048042e-08]
-0.0003887213353860489
```

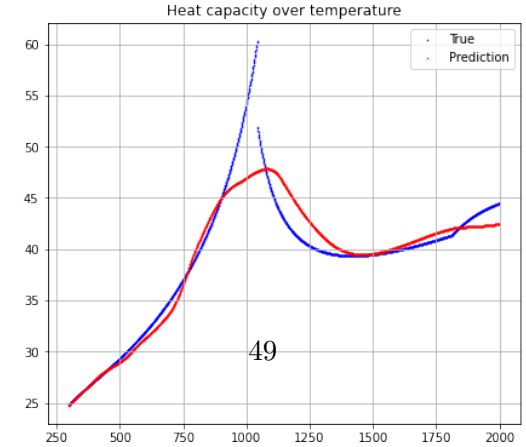
```
-56.10718535591328 0.02181006001630318 1.722699693271092

2200 :  1.7176100356238229
lr:  [8.042550682617533e-08]
0.0006941282366872188
30.577705586169536 0.02122484886046878 1.7193490695953366

2210 :  1.714778287070138
lr:  [7.649351429021946e-08]
-0.0004917720316450407
-42.62046332815237 0.02095955184053844 1.7175423247473578

2220 :  1.712317705154419
lr:  [7.275375635635602e-08]
-0.0007935505219173166
-26.61923924332369 0.02112371119458143 1.715989007609231

2230 :  1.716602052961077
lr:  [6.919683469996873e-08]
0.0002959980561503851
59.68377535997503 0.01766628149026886 1.7169160212789263

2240 :  1.6756117003304618
lr:  [6.581381047930572e-08]
-0.0009741974294011844
-22.60814257862514 0.022024794383632078 1.7145076813016618

2250 :  1.7324403524398804
lr:  [6.259618187142205e-08]
0.0003990880254406256
59.087945393020206 0.023581291454243945 1.711954073905945
```


50000
40000
30000
20000
10000
0
0
250
500
750
1000
1250
1500
1750
2000


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


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

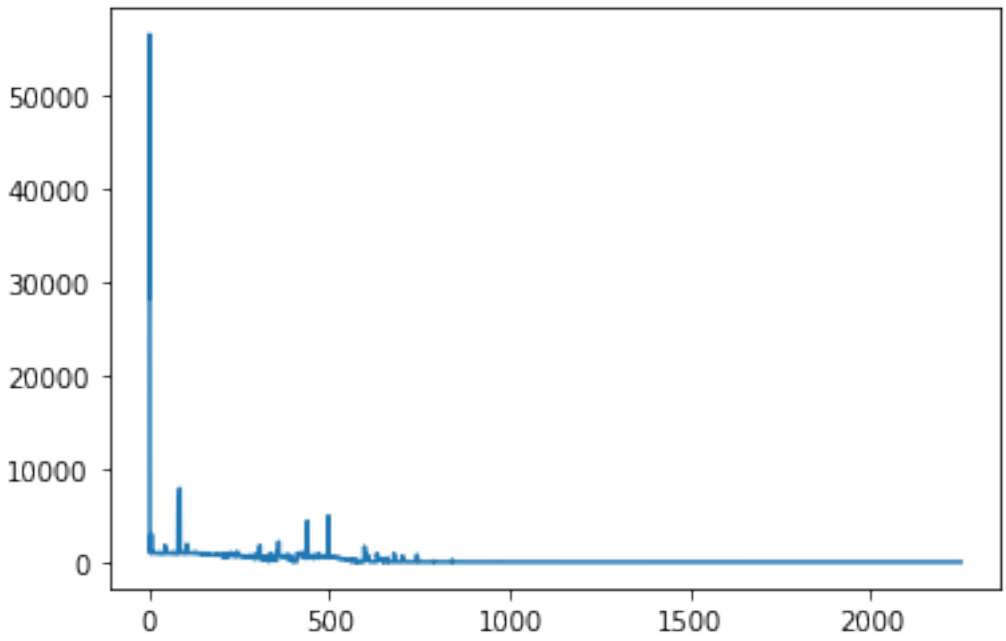

Enthalpy over temperature
True
Prediction
60
50
40
30
20


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

```
2260 :  1.7098056418555123
lr:  [5.9535862706387415e-08]
8.85207173427975e-06
2803.6151876243475 0.024817802756166903 1.7096516527448384

2270 :  1.6987624849591936
lr:  [5.662516214606441e-08]
-0.00048167364937918525
-47.55450297032812 0.02290575099013125 1.7057981075559343

2280 :  1.7289004836763655
lr:  [5.3856765356388806e-08]
0.0012058242069388984
18.474562753208986 0.022277074980431136 1.7017662804467337

2290 :  1.714113984789167
lr:  [5.122371512457942e-08]
0.00011295723150492151
201.84808941688362 0.02280020136508902 1.7032353898457118

2300 :  1.7368429899215698
lr:  [4.871939437508027e-08]
0.0009432464577366249
23.974381866205498 0.02261375077172351 1.704698040485382

2310 :  1.71597535269601
lr:  [4.633750954029599e-08]
0.0009268953223270167
24.359631038688374 0.02257882806337226 1.7042573179517473

2320 :  1.6957642861774989
lr:  [4.407207474432987e-08]
0.0001892862792612847
117.14045376785852 0.022173080644696475 1.7029838170324052

2330 :  1.7112743854522705
lr:  [4.1917396759976825e-08]
0.00036775648767676996
57.23831733454129 0.021049762543479282 1.7034137088911874

2340 :  1.7114385877336775
lr:  [3.986806070116709e-08]
0.00042509059516751037
49.06774207995948 0.02085823568429587 1.7013445660046167
```

```
2350 :  1.6507302522659302
lr:  [3.791891641490434e-08]
-0.0018831088313555938
-11.960747182686411 0.02252338864932832 1.7004157035691398

2360 :  1.651319912501744
lr:  [3.6065065538500366e-08]
-0.000861692011530125
-28.204006778513392 0.024303167334186485 1.6994891701425825

2370 :  1.6941571916852678
lr:  [3.4301849189579685e-08]
0.00019695112378534442
122.89857223291918 0.024205011912887757 1.6987766415732246

2380 :  1.7113850627626692
lr:  [3.2624836257918366e-08]
-3.918683911203667e-05
-669.416809185716 0.026232328800453605 1.6957200496537346

2390 :  1.7117235660552979
lr:  [3.102981226969317e-08]
0.0004425521494695827
56.82598078961354 0.025148459944160685 1.6933905914851595

2400 :  1.6719006981168474
lr:  [2.9512768796156287e-08]
-0.00014156433305657204
-163.60512014756915 0.023160649718330963 1.6900468965939115

2410 :  1.68451612336295
lr:  [2.806989338011837e-08]
0.00019585321665505537
100.5981146631464 0.019702464346211316 1.6874349434035167

2420 :  1.6762679644993372
lr:  [2.669755995492469e-08]
-0.0002581294702023876
-78.08634903270074 0.020156387905849765 1.6852226124491012

2430 :  1.7483529363359724
lr:  [2.539231973184619e-08]
0.00159278729219131
13.001277515503835 0.020708269608947116 1.6838587539536614

2440 :  1.6481270619801112
lr:  [2.4150892532984822e-08]
-0.00029811706209322084
```

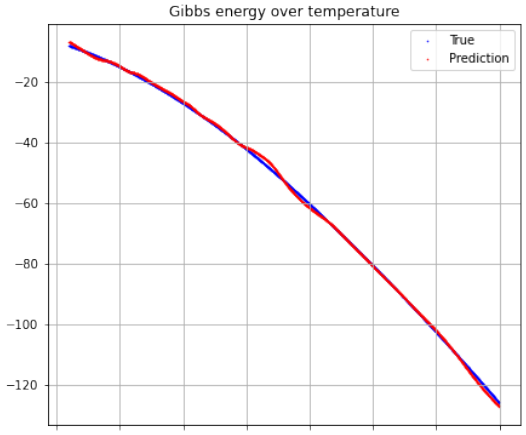
```
-72.95661008066737 0.02174961025752922 1.6836890336445398

2450 :  1.6480133533477783
lr:  [2.2970158547912027e-08]
-0.0010904084141678447
-23.02353319563443 0.025105054320392468 1.6818683123588558

2460 :  1.691212228366307
lr:  [2.184715049332407e-08]
0.0003825936998639788
66.54856033610427 0.025461059919611364 1.6829272093091692

2470 :  1.668925745146615
lr:  [2.0779046156010805e-08]
-8.023619304245613e-05
-314.8974759737791 0.02526617467081433 1.6835419038363864

2480 :  1.6694672448294503
lr:  [1.9763161300397728e-08]
-0.0002797855927714788
-84.60776435720643 0.023672033503750602 1.6826186425345282

2490 :  1.7244282790592738
lr:  [1.8796942922837378e-08]
0.0005678741299376196
43.19462664939012 0.024529111026502733 1.6862339881488253
```

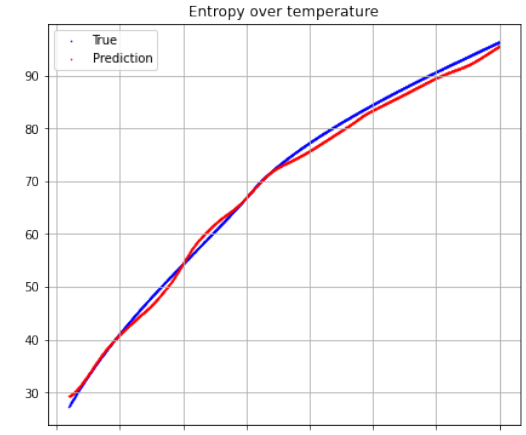


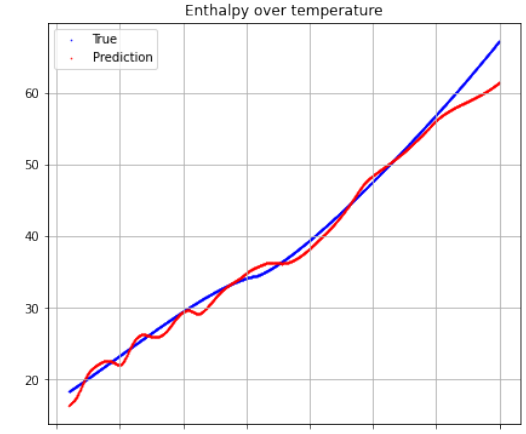
[ ]:
```
plt.plot(losses[1400:])
```

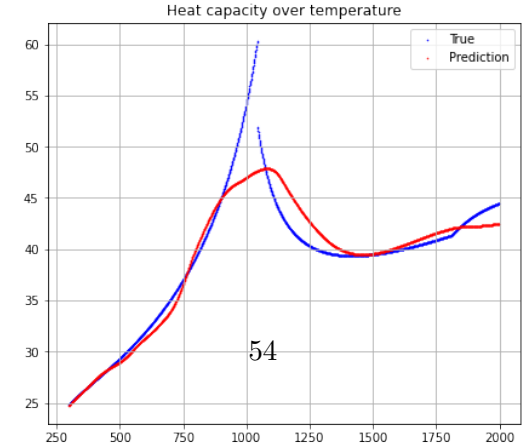
[259]:
```
torch.save(net, 'Fe_C.pth')
```

[258]:
```
ph = PlotHandler()

ph.properties_temp_modified_new(net, ['Fe'], 'BCC_A2', start_temp=200,␣
↪end_temp=2000)
```


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


Entropy over temperature
True
Prediction
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

[ ]: