trainThermoNetNew

May 2, 2022

[1]:
```
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
```

[9]:
```
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]]

        # Remove NaN values from targets (can occur because not every phase is␣
↪defined in the same temperature range in the SGTE data)
        not_nas = torch.where(~torch.isnan(targets))
        targets = targets[not_nas]

        # Forward pass
        predictions = net(inp.float())
        predictions = predictions[not_nas]

        # 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
```

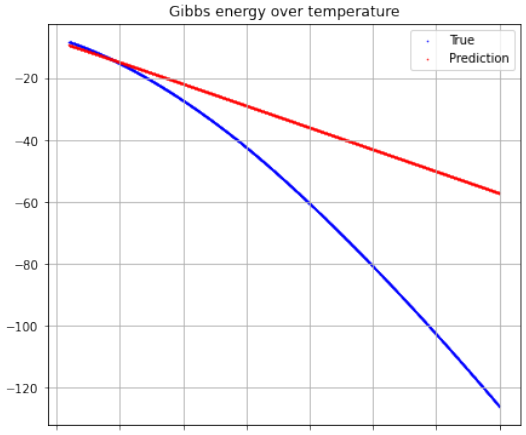
[10]:
```
# Hyperparameters
nr_epochs = 2500
lr = 0.005 # 0.000025
batch_size = 1024
hidden_size = 128
hidden_layers = 8
```

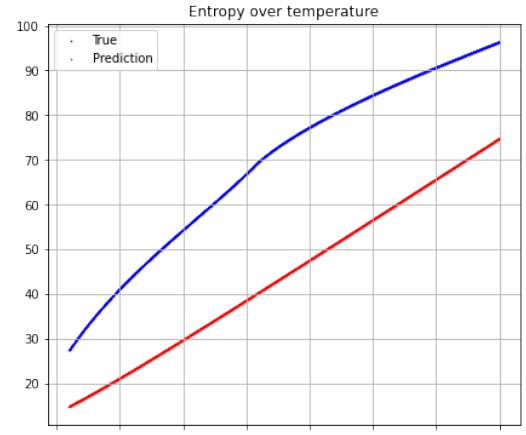
[11]:
```
# Network
net = ThermoNetNew(hidden_size_linear=hidden_size, hidden_layers=hidden_layers)

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

# Loss function
loss_func = MSELoss()
```

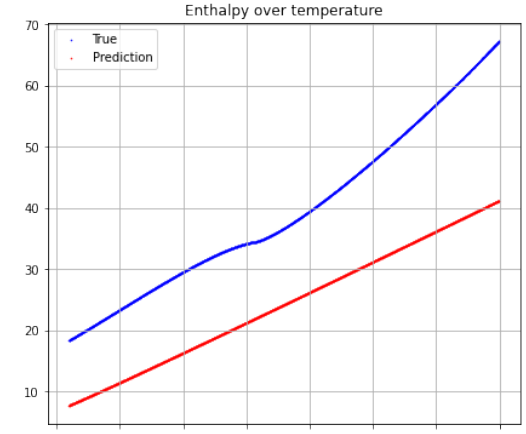
[12]:
```
# Dataset
start_temp, end_temp = 200, 2000
step = 1
dataset = ThermoDatasetNew(['Fe'], start_temp=start_temp, end_temp=end_temp,␣
 ↪step=step)
dataloader = DataLoader(dataset, batch_size=batch_size, shuffle=True)
```

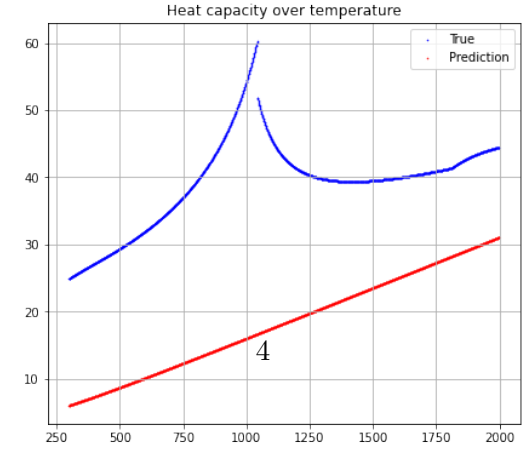
[13]:
```
losses, best_net = train(net, dataloader, optimizer=optimizer,␣
 ↪scheduler=scheduler, loss_func=loss_func, nr_epochs=nr_epochs)
```

```
0 :  1087.1859910753037
lr:  [0.0049501250000000005]
nan
nan 0.0 1087.1859910753037
```


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
20

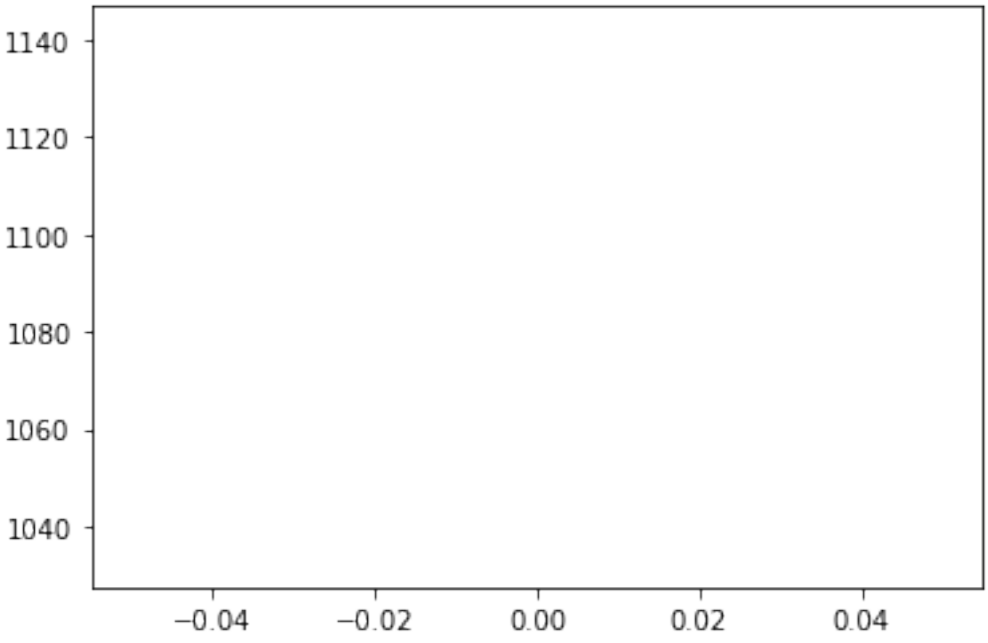

Enthalpy over temperature
True
Prediction
70
60
50
40
30
20
10

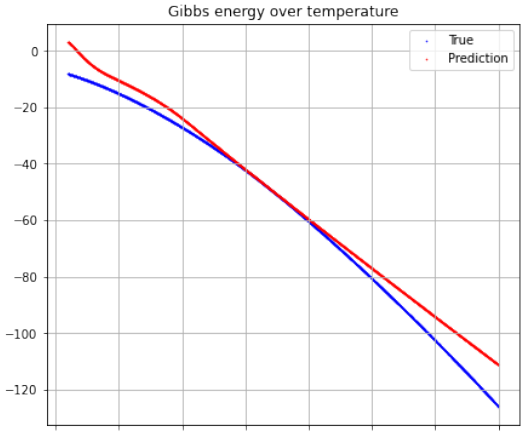

Heat capacity over temperature
True
Prediction
60
50
40
30
20
10
250
500
750
1000
1250
1500
1750
2000

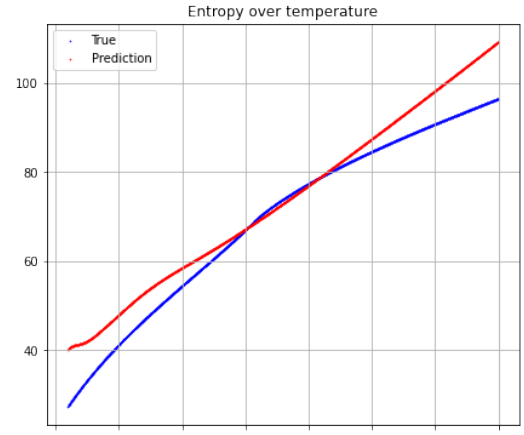
```
10 :  119.19605170355902
lr:  [0.0047081140345718794]
-96.79899393717452
-33.78080089604691 3269.9475411293442 1368.3354049836746

20 :  119.57812754313152
lr:  [0.004477934953669392]
-48.38039317660851
-50.58599293614865 2447.370227480012 773.8923208246784

30 :  114.86725362141927
lr:  [0.004259009298001735]
-32.41062458179611
-62.858835559651425 2037.2941209727178 563.4108108465816

40 :  110.21839480929904
lr:  [0.0040507868890773645]
-24.424189906650124
-72.95473820686279 1781.86038055436 454.48218991246006

50 :  199.74415334065756
lr:  [0.0038527444465594088]
-11.819062230808653
-136.70093553658245 1615.67686411663 377.6764973958333

60 :  116.89705657958984
lr:  [0.003664384273218397]
-0.08587935397954732
-279.0562444955668 23.965170001237883 126.6516138543023

70 :  112.67177327473958
lr:  [0.003485233004177472]
-0.043054835866629206
-12213.826484433133 525.8642945907574 201.47001346164282

80 :  97.27863396538629
lr:  [0.0033148404173068496]
-0.3384468441917795
-1555.059909009231 526.30511873333 198.65422485351561

90 :  584.2587780422634
lr:  [0.0031527783017779305]
9.925536313564612
4977.122499838336 49400.61010920488 7260.402719658746
```

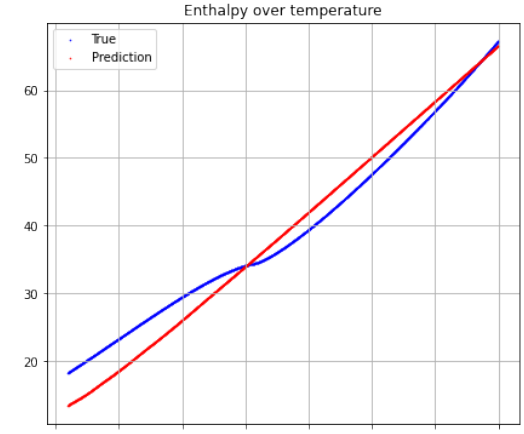
```
100 :  125.43880632188585
lr:  [0.0029986393819336618]
-0.43437495847894997
-113726.8355390577 49400.08946522056 7264.105533667669

110 :  76.75605095757379
lr:  [0.002852036293770727]
-77.59260619632782
-636.6706309535565 49400.93354434687 7258.263584645589

120 :  71.13478681776259
lr:  [0.0027126006114613927]
-0.8319498524918478
-59390.42364094377 49409.854187511526 7176.280132836235

130 :  179.77196078830295
lr:  [0.0025799819214685775]
1.799999349510755
27446.815613781477 49404.25025094829 7220.533275282116

140 :  105.29559580485027
lr:  [0.002453846941927312]
0.06576802779217039
4126.834191844576 271.4137458229131 157.5904717678494

150 :  113.8226081000434
lr:  [0.002333878685079522]
0.12551961193820002
2149.3633188414697 269.78724969518294 151.4228823852539

160 :  108.55856492784288
lr:  [0.0022197756606572683]
0.804703848702569
334.7344097586719 269.36206782598606 151.2318571811252

170 :  84.39203643798828
lr:  [0.0021112511182124795]
-1.6458904067404947
-163.25351457742147 268.6973935096475 153.76620005289715

180 :  70.72440507676866
lr:  [0.0020080323264890774]
-0.9916031679598921
-25.821876076426992 25.605054120052756 103.53225280761717

190 :  107.3471450805664
lr:  [0.0019098598880265135]
0.09118076246611868
```

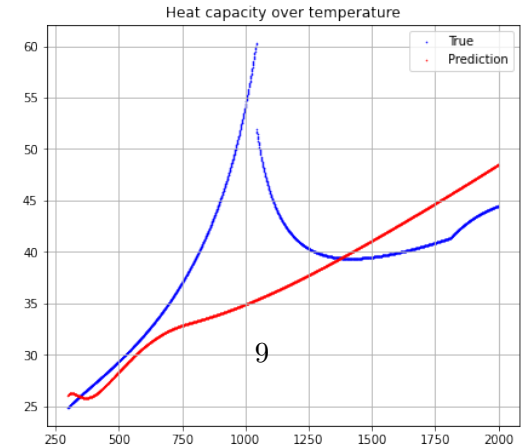
```
973.709143688998 88.78354214179436 111.00305672539605

200 :  81.58997090657552
lr:  [0.0018164870872722418]
-0.6353533824825464
-136.40695410224654 86.66661968300379 105.34079678005641

210 :  77.98310258653429
lr:  [0.0017276792705648916]
-0.6189116220625593
-141.07983837318596 87.31595160787224 100.57267913818359

220 :  66.05253982543945
lr:  [0.0016432132564299833]
-0.290456629123814
-305.9843523577506 88.87518355046558 96.00927873399523

230 :  52.04219775729709
lr:  [0.001562876774706207]
-0.410882158344289
-219.55298086406296 90.21040264834856 91.62040906270346

240 :  40.350442250569664
lr:  [0.001486467933092745]
-1.3562384797872595
-18.17418796426714 24.648533056025574 71.0624045138889

250 :  33.17459615071615
lr:  [0.0014137947097770268]
-0.9565872226983236
-25.47096806817952 24.365202603777533 59.92190298716227
```


1140
1120
1100
1080
1060
1040
−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
100
80
60
40


Enthalpy over temperature
True
Prediction
60
50
40
30
20


Heat capacity over temperature
True
Prediction
60
55
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45
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25
250
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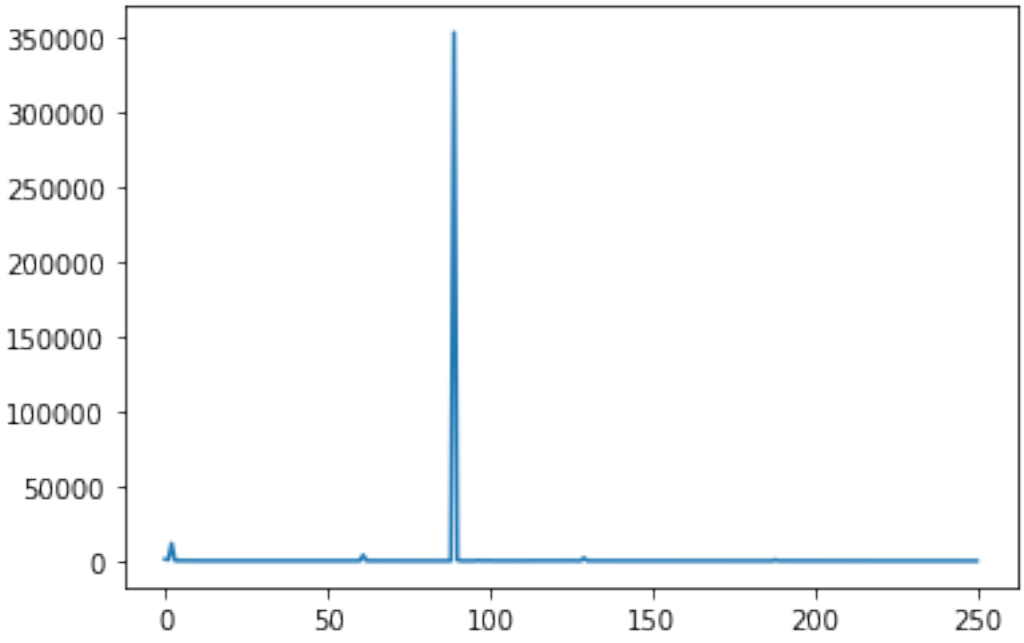
2000

```
260 :  30.470790439181858
lr:  [0.001344674470867846]
-0.8687017704624165
-22.957825244084933 19.94350343550334 48.91096458011202

270 :  28.01388168334961
lr:  [0.0012789335114211096]
-0.6887041295196464
-14.191171465553099 9.773518391047793 40.00776407877604

280 :  27.436061011420357
lr:  [0.001216406618904779]
-0.4911348425071526
-13.473072196267777 6.6170951912014715 34.8478533299764

290 :  24.189429812961155
lr:  [0.0011569366580059526]
-0.35823188833638925
-13.813519560518381 4.948443196736149 31.30786226908366

300 :  24.44517029656304
lr:  [0.0011003741757366753]
-0.21094044103644063
-20.01992258809361 4.223011300247866 29.117967851426865

310 :  24.707716200086807
lr:  [0.0010465770258460752]
-0.1017222069288327
-43.76888610136521 4.452267689047582 27.836478627522794

320 :  21.746562745836044
lr:  [0.00099541001159494]
-0.1497948618432562
-31.0801952437639 4.655653552601041 26.778323660956488

330 :  21.536892149183487
lr:  [0.0009467445459949988]
-0.10652772639614114
-39.014986525889114 4.156177809979049 25.55253210703532

340 :  20.219284269544815
lr:  [0.0009004583286590612]
-0.06837448241218684
-46.678037599020975 3.191586660849656 24.555038943820527
```

```
350 :  24.654058668348526
lr:  [0.0008564350384499106]
-0.06844113581304924
-229.5270526683109 15.709092184440772 27.00617500305176

360 :  21.059082878960503
lr:  [0.0008145640411555528]
-0.014603885122978284
-1078.762452976172 15.75412293824628 26.106345265706377

370 :  19.586260901557075
lr:  [0.000774740111456184]
-0.07573106121314106
-209.12248070118522 15.83706738702537 25.52590574476454

380 :  21.521821551852756
lr:  [0.0007368631684841578]
-0.03449225479783367
-462.22179643338234 15.943071975692629 25.139868151346846

390 :  21.507312350802952
lr:  [0.0007008380243123892]
-0.19573148091634104
-81.76354869760046 16.003700471556705 24.90329084184435

400 :  21.03825505574544
lr:  [0.0006665741447391304]
-0.034042773603582106
-60.84352653954703 2.071282399229339 21.415203904045953

410 :  21.65117284986708
lr:  [0.0006339854217679446]
0.011551461252225524
184.22020221355172 2.1280125277469932 21.425784975687666

420 :  21.490548875596787
lr:  [0.0006029899572111071]
0.006005739138510181
358.7982986791163 2.1548489852080346 21.431999638875322

430 :  21.322438557942707
lr:  [0.0005735098568726064]
-0.11463352558023539
-15.643720531719472 1.7932948377429176 21.325435456169977

440 :  21.98164219326443
lr:  [0.0005454710347935108]
-0.026840625166082033
```

```
-57.926261254400444 1.554777065601903 21.348640446133086

450 :  22.308352576361763
lr:  [0.0005188030270677557]
-0.029746793024664278
-55.994613906979325 1.665660190386902 21.519401329888236

460 :  26.570423126220703
lr:  [0.0004934388147604504]
0.11564006070160815
16.137247760040665 1.8661123105279926 21.806034181382923

470 :  21.65058920118544
lr:  [0.0004693146554836876 5]
0.009475906960277633
207.30270783357727 1.9643811720445954 22.2402725982666

480 :  27.45427237616645
lr:  [0.000446369923206589]
0.1243329902354822
20.11955111908195 2.501523952831101 22.98260365380181

490 :  28.963492923312717
lr:  [0.0004245469558970154 4]
0.15983572892861572
19.39207705596113 3.0995467716794316 23.934222742716475

500 :  30.623087565104168
lr:  [0.0004037909106120566]
0.1942026479984899
133.02472325327173 25.833753505051668 29.59532616085476
```


350000
300000
250000
200000
150000
100000
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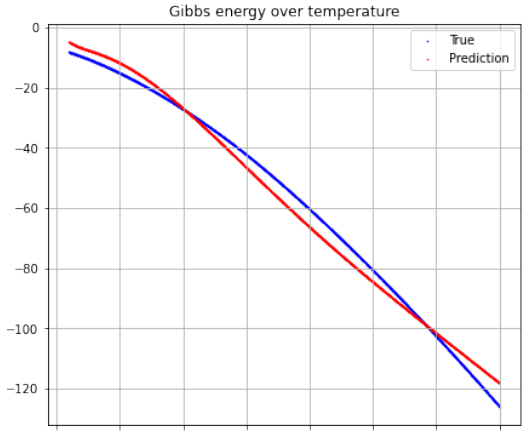
100
150
200
250


Gibbs energy over temperature
True
Prediction
0
−20
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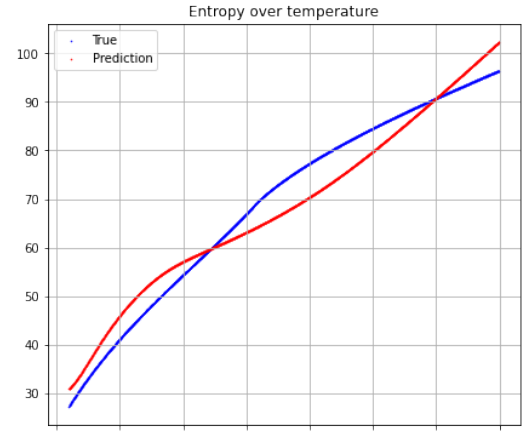
Entropy over temperature
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100
90
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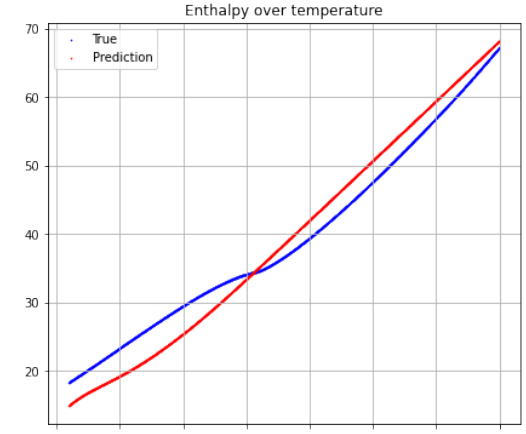
Enthalpy over temperature
True
Prediction
70
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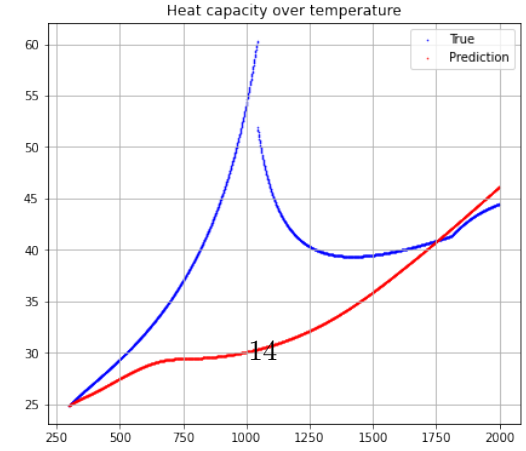
30
20


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

```
510 :  27.24840694003635
lr:  [0.00038404962567312596]
0.07285759940979962
352.1542340596892 25.65711211558565 30.435916328430174

520 :  33.00670305887858
lr:  [0.0003652734895792976]
0.1917685381138944
133.3118957140798 25.565027354281032 30.94522370232476

530 :  23.326289706759983
lr:  [0.00034741531632945347]
-0.020633576408265675
-1239.7051690656513 25.579551329638033 30.882201402452253

540 :  21.33294465806749
lr:  [0.0003304302268399139]
0.0030012887621672477
8538.458638113847 25.62637995680095 30.682925923665366

550 :  21.3612732357449
lr:  [0.00031427553615954513]
-0.16846084594726562
-21.564857789472814 3.632834185947071 25.493695890638563

560 :  21.831011454264324
lr:  [0.00029891064619890525]
-0.09343640333941192
-41.237056960204924 3.853042286664011 24.68143026987712

570 :  26.01112280951606
lr:  [0.000284296943703849]
0.07333492529905841
51.79676048259656 3.7985115607244397 24.051509251064722

580 :  26.20540894402398
lr:  [0.000270397703217188]
0.013166306510804159
292.27855934994585 3.8482290989376517 23.509311864640978

590 :  20.341689427693684
lr:  [0.0002571779947845447]
-0.05700025753099091
-60.49057044538577 3.4479780935835365 22.616823946634927
```

```
600 :  17.353055212232803
lr:  [0.0002446045961724539]
-0.11076110831193636
-25.870250089666204 2.8654175722383997 21.746691593594022

610 :  17.006089210510254
lr:  [0.00023264590937811005]
-0.16671725465597206
-16.68902705342733 2.7823487732266514 21.1596119456821

620 :  17.685036447313095
lr:  [0.0002212718812209424]
-0.09612990182543564
-26.53071034967845 2.550394581273659 20.365373651716446

630 :  19.194246292114258
lr:  [0.0002104539278164573]
-0.023892463199676046
-93.75443362573482 2.2400243552093397 19.71969888687134

640 :  15.39658292134603
lr:  [0.00020016486274254485]
-0.059656467567495736
-39.9715229562292 2.3845598628616984 19.088331960042318

650 :  15.631781578063965
lr:  [0.00019037882871772517]
-0.06852072761172345
-32.419410585423336 2.2214016020564165 18.50905662112766

660 :  19.059588856167263
lr:  [0.00018107123261963643]
0.020040317457549462
101.97617345952179 2.0436348892349465 17.880545368194582

670 :  18.76509443918864
lr:  [0.0001722186836804605]
0.05045013038479552
40.240633833111076 2.0301452236472675 17.329151145087348

680 :  15.369790818956163
lr:  [0.0001637989347039663]
-0.03894725894711728
-53.53778008235803 2.085149784321416 16.7657995944553

690 :  13.398290210300022
lr:  [0.00015579082615644384]
-0.06000905242366316
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-32.66569144142848 1.9602371901638866 16.187628192901613

700 :  12.852977964613173
lr:  [0.00014817423299102564]
-0.10983541492972514
-17.597822295447685 1.9328641136800646 15.578030272589793

710 :  12.21631579928928
lr:  [0.00014093001407176005]
-0.04609342605348618
-40.71011430696452 1.876468643437039 14.964829561445448

720 :  12.667315695020887
lr:  [0.00013403996407033 48]
-0.056767474496716014
-32.48350510891136 1.84400654783407 14.308331173790828

730 :  11.834468523661295
lr:  [0.00012748676771456 35]
-0.04777552805790286
-35.78293545947833 1.709548637038434 13.628686099582248

740 :  11.69593726264106
lr:  [0.00012125395627365804]
-0.0488263279402337
-37.29289901905331 1.8208753173463166 12.886584868960911

750 :  11.429923163519966
lr:  [0.00011532586617092 99]
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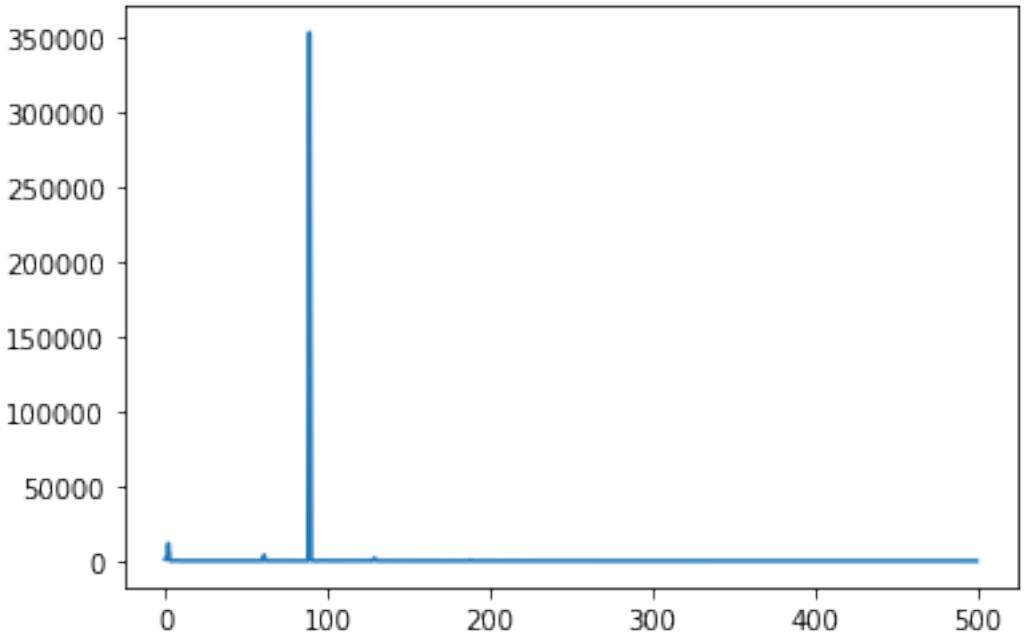
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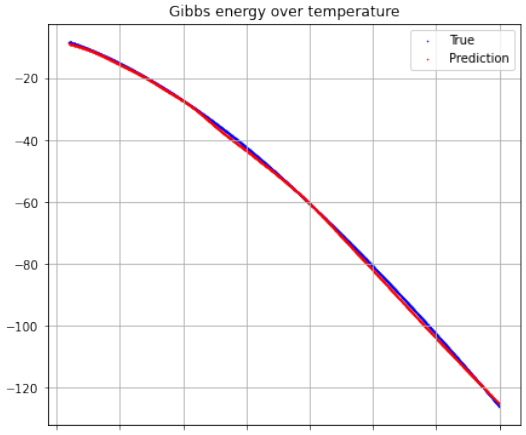
Gibbs energy over temperature
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Prediction
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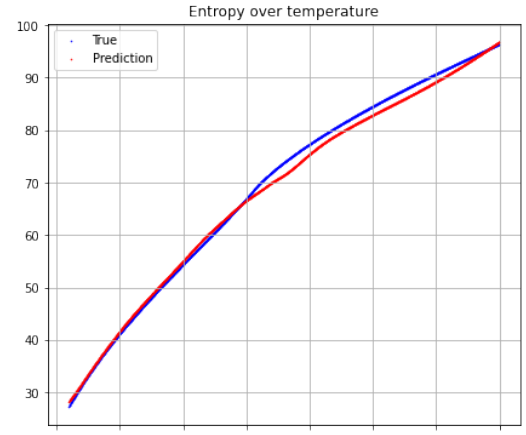
Entropy over temperature
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Prediction
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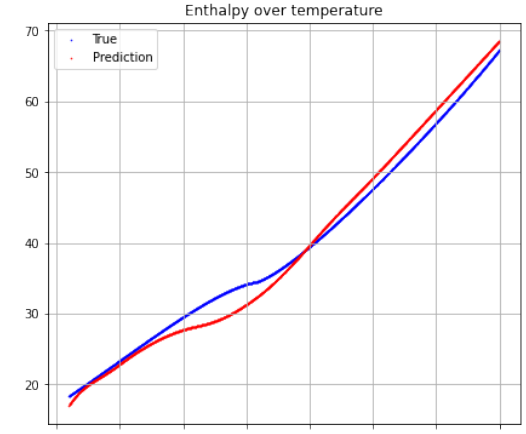
Enthalpy over temperature
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Prediction
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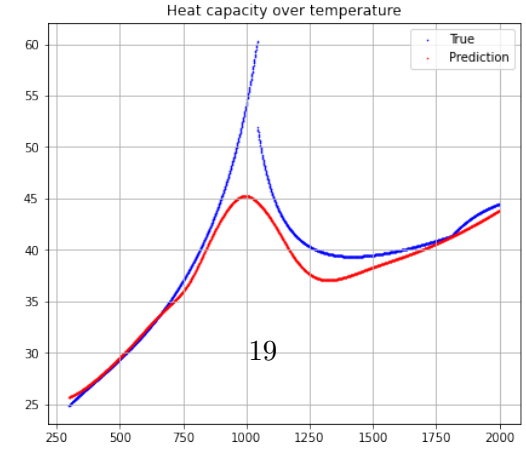
Heat capacity over temperature
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Prediction
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500
750
1000
1250
1500
1750
2000

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770 :  9.134431786007351
lr:  [0.00010432498718497115]
-0.07112474398277785
-24.329863714659073 1.730455327841003 10.712987075381808

780 :  9.419878005981445
lr:  [9.922455217233788e-05]
-0.002792888217502166
-555.1323423522863 1.5504225781100789 10.052075440088908

790 :  7.940833409627278
lr:  [9.437347676204006e-05]
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-51.28822297420187 1.5595848547029527 9.482177582846749

800 :  6.136090596516927
lr:  [8.975956979565241e-05]
-0.09983877367984136
-15.913282151743749 1.588762575251403 8.9171293258667

810 :  4.816716194152832
lr:  [8.537123613889452e-05]
-0.11738976113109631
-12.843690175613833 1.5077177217571163 8.312929304970634

820 :  3.56068754196167
lr:  [8.11974475420882e-05]
-0.07684765705445996
-20.98860988089248 1.612925494176675 7.7650764634874125

830 :  7.28488466474745
lr:  [7.722771492524318e-05]
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-68.03058836474885 1.5861665924797033 7.2364079655541325

840 :  3.1474686198764377
lr:  [7.345206201812147e-05]
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850 :  2.3097104761335583
lr:  [6.986100028903547e-05]
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-13.607233504497692 1.91697271493478 6.143749827808803

860 :  5.953944947984484
lr:  [6.644550509937384e-05]
-0.06712268539567112
-29.47872107767979 1.9786909207638397 5.718409251901838

870 :  2.4911328421698675
lr:  [6.319699302392957e-05]
-0.11975887951667075
-17.096419284954436 2.0474480173133447 5.170348459879557

880 :  1.6406447754965887
lr:  [6.0107300280034106e-05]
-0.055492292185759635
-41.36289936199007 2.2953220970457235 4.447116964790556

890 :  0.9412350787056817
lr:  [5.716866221128857e-05]
-0.12117605225569536
-23.763144486777012 2.8795240380893303 4.131870991388956

900 :  5.882651130358378
lr:  [5.437369377433232e-05]
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910 :  0.6116139954990811
lr:  [5.171537097961115e-05]
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930 :  0.4946247670385573
lr:  [4.678226657944606e-05]
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-161.79763561549203 3.4757598800779834 2.943865440818998

940 :  0.4009743266635471
lr:  [4.4495087669861456e-05]
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950 :  0.38020307819048565
lr:  [4.2319728638767885e-05]
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960 :  0.33502890997462803
lr:  [4.0250722626894584e-05]
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-569.708150374298 3.162511830161591 2.202353470193015

970 :  0.4669616719086965
lr:  [3.8282870049007304e-05]
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980 :  0.22349797023667228
lr:  [3.641122552691552e-05]
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990 :  0.3409184118111928
lr:  [3.463108546132327e-05]
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1000 :  0.19365973108344608
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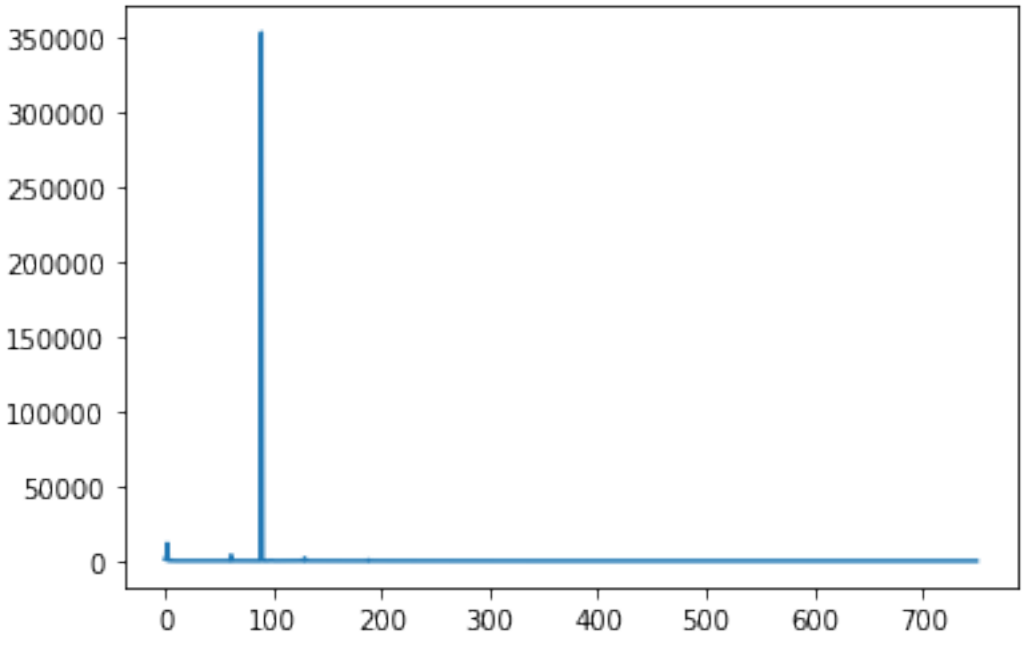
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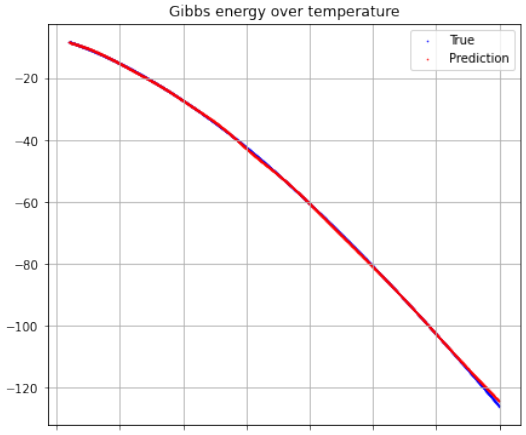
Gibbs energy over temperature
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Prediction
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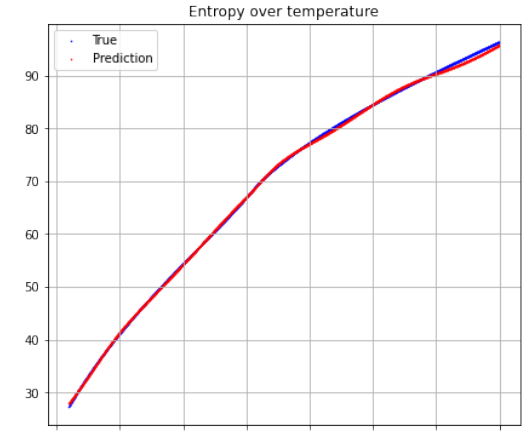
Entropy over temperature
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Prediction
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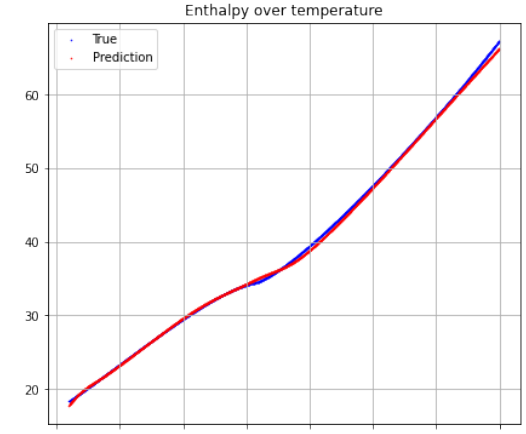
Enthalpy over temperature
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Prediction
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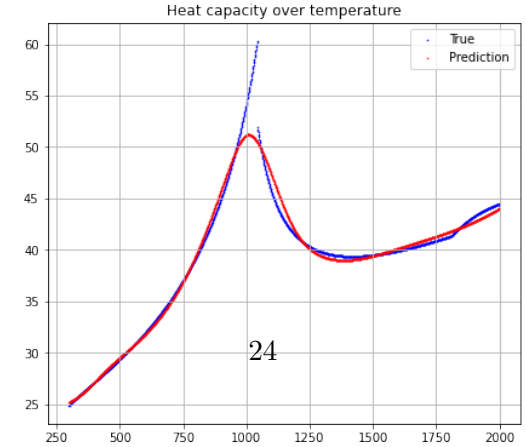
Heat capacity over temperature
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Prediction
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40
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25
250
500
750
1000
1250
1500
1750
2000

```
1010 :  0.2944855723116133
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lr:  [2.9796038479769403e-05]
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1030 :  0.32958900928497314
lr:  [2.8339314045856632e-05]
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1040 :  0.1416926226682133
lr:  [2.695380867946518e-05]
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lr:  [2.563604048967558e-05]
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1060 :  0.12092085265451008
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lr:  [2.319063089970496e-05]
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1080 :  0.10472624252239864
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lr:  [1.8977359884438732e-05]
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lr:  [1.8049559235584425e-05]
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lr:  [1.7167118639406374e-05]
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lr:  [1.5529555437324735e-05]
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lr:  [1.336138400573712e-05]
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1190 :  0.05876642010278172
lr:  [1.2708147684899912e-05]
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lr:  [1.0399332951481313e-05]
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lr:  [9.890910920240393e-06]
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1250 :  0.05532614141702652
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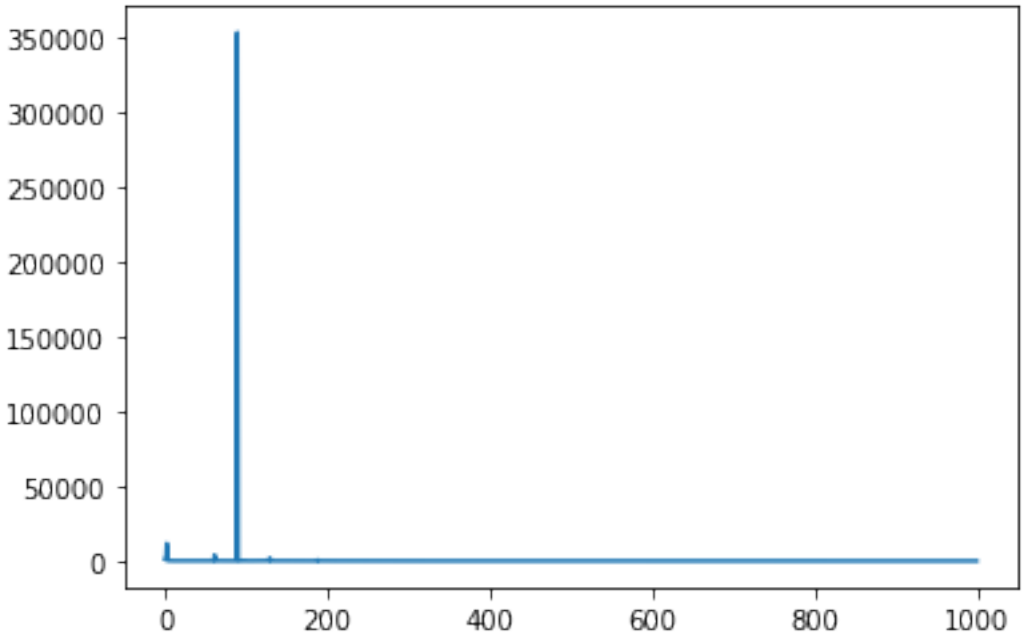
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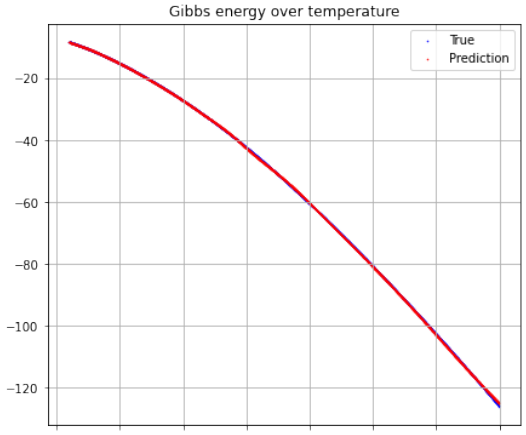
Gibbs energy over temperature
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Prediction
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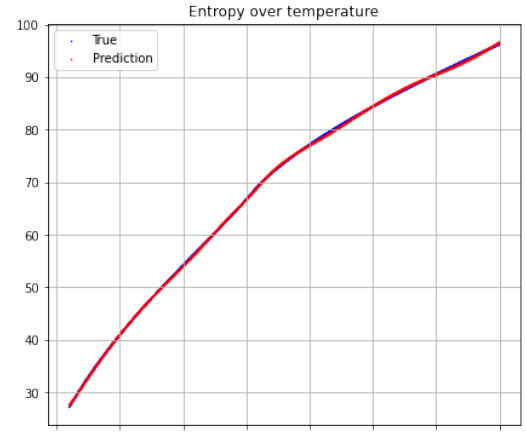
Entropy over temperature
True
Prediction
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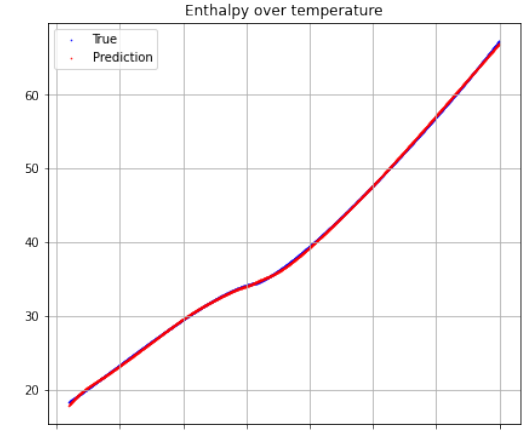
Enthalpy over temperature
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Prediction
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50
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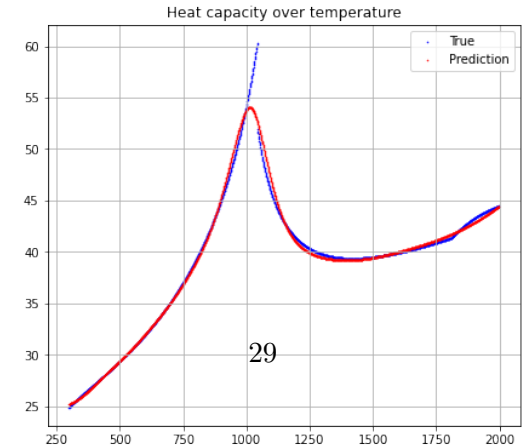
Heat capacity over temperature
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Prediction
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55
50
45
40
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25
250
500
750
1000
1250
1500
1750
2000

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lr:  [8.947421677912122e-06]
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lr:  [8.509983399411275e-06]
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lr:  [8.09393142127561e-06]
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1290 :  0.050913129415777
lr:  [7.698220170070455e-06]
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1300 :  0.060252781957387924
lr:  [7.3218551903099484e-06]
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1310 :  0.05286687157220311
lr:  [6.963890645307184e-06]
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1320 :  0.05714633771114879
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lr:  [5.698691835656445e-06]
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1360 :  0.050016223142544426
lr:  [5.42008353529543e-06]
-0.0001081945522437021
-71.56915810265497 0.007743393015375479 0.05842893857922818

1370 :  0.04568866019447645
lr:  [5.1550963583902185e-06]
-0.0004886184098904365
-18.114440776454753 0.008851049248245806 0.057954078697496

1380 :  0.05657410331898265
lr:  [4.903064369992145e-06]
-0.0002431158914047034
-38.81508024343297 0.0094365628333273 0.05755154152297311

1390 :  0.05240108403894636
lr:  [4.663354192625308e-06]
-1.9909066407859157e-05
-466.39586081294874 0.009285506165275632 0.05587504503627618

1400 :  0.07249778964453274
lr:  [4.435363414555961e-06]
0.0004413287301047318
18.988639917005813 0.008380232340988196 0.05432755230201614

1410 :  0.04207561372054948
lr:  [4.218519075881431e-06]
-0.00019725666396 2016
-43.02966044244278 0.008487887270294588 0.052864523596233795

1420 :  0.05269839386973116
lr:  [4.012276228633935e-06]
2.737583638994594e-05
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1430 :  0.058742374595668584
lr:  [3.8161165672807375e-06]
0.0001370539453700016
46.0009586192463 0.006304612869569886 0.05027461857431466

1440 :  0.043352539754576154
lr:  [3.6295471261789757e-06]
-0.00011906962917775523
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-53.61108051798401 0.006383451477095133 0.04947549982617299

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lr:  [3.4520990407117527e-06]
6.231683350744707e-05
86.9551992784762 0.0054187726760436825 0.048485510783890885

1460 :  0.04141967867811521
lr:  [3.283326368992121e-06]
-0.00013074611657871413
-35.52291138540649 0.004644482713211688 0.04784659654315975

1470 :  0.048803824103540845
lr:  [3.122804971173805e-06]
8.216313173035653e-05
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1480 :  0.04334503163894018
lr:  [2.9701314435522786e-06]
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-12.553832671528486 0.0031492190596962857 0.04611359831773573

1490 :  0.04653383853534857
lr:  [2.824922104777499e-06]
5.840831552368174e-05
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1500 :  0.0431697198914157
lr:  [2.68681203163057e-06]
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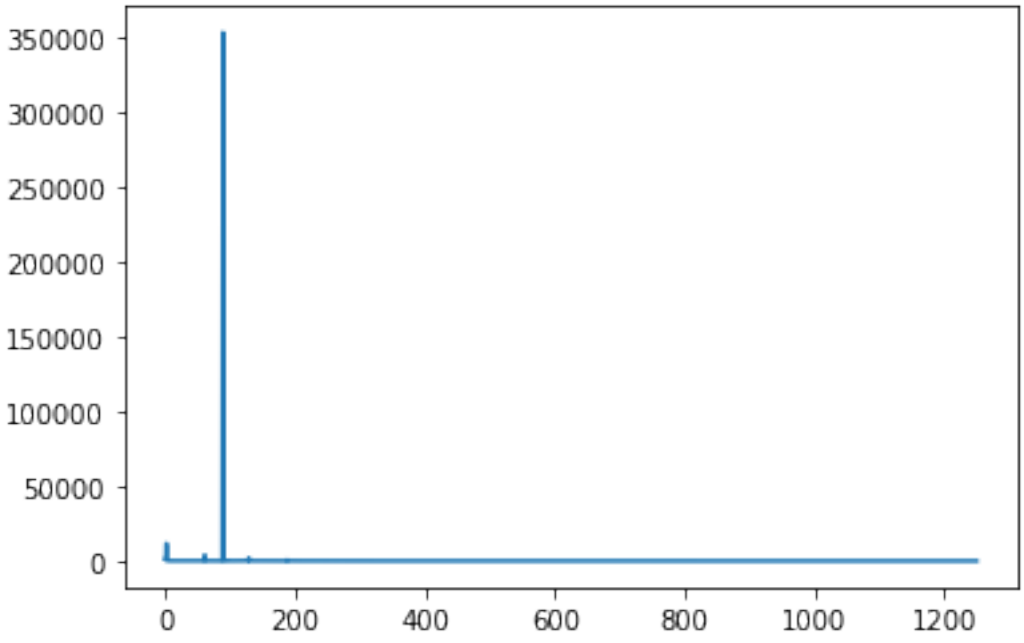
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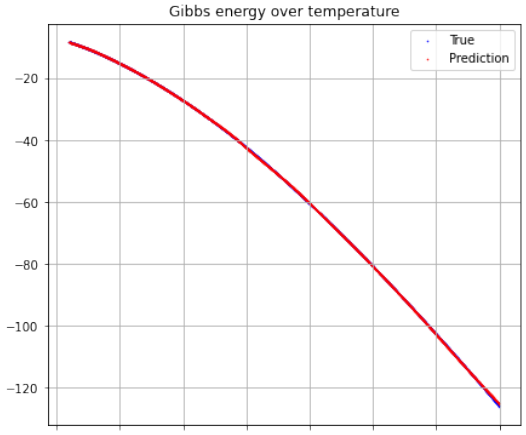
Gibbs energy over temperature
True
Prediction
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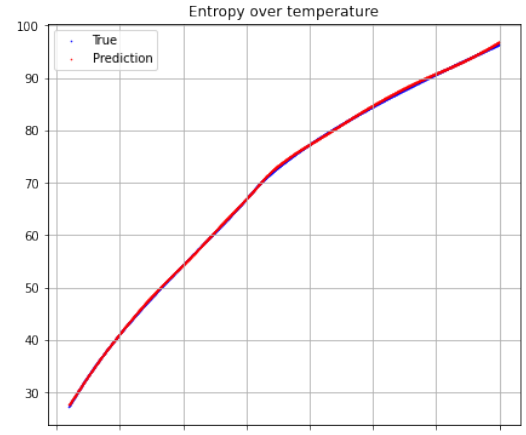
Entropy over temperature
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Prediction
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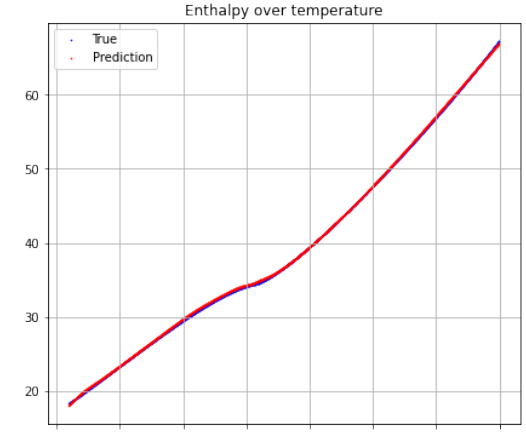
Enthalpy over temperature
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Prediction
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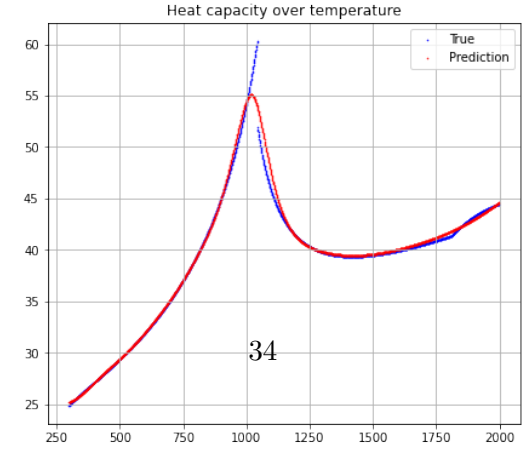
Heat capacity over temperature
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Prediction
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1250
1500
1750
2000

```
1510 :  0.04163643345236778
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1520 :  0.04086991730663511
lr:  [2.430518322340951e-06]
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1530 :  0.03946820812092887
lr:  [2.3116905986611514e-06]
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lr:  [2.1986723468891056e-06]
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1550 :  0.03985056198305554
lr:  [2.0911795427011816e-06]
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1560 :  0.03945813017586867
lr:  [1.9889420476858746e-06]
-3.8641756252637015e-05
-54.34167472932661 0.0020998577492507236 0.04172564030521445

1570 :  0.03910605340368218
lr:  [1.8917029304633716e-06]
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-11.7699367402607 0.001752274151295525 0.04116317487839195

1580 :  0.039430212436450854
lr:  [1.7992178209955004e-06]
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1590 :  0.039573984841505684
lr:  [1.7112542964633722e-06]
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1610 :  0.03852087300684717
lr:  [1.5480185709957339e-06]
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1620 :  0.037978278679980174
lr:  [1.4723361450231903e-06]
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1630 :  0.03710210157765283
lr:  [1.4003538229824783e-06]
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lr:  [1.3318907072751074e-06]
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1650 :  0.03981104348268774
lr:  [1.266774744362576e-06]
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1660 :  0.03651499168740378
lr:  [1.2048422923814346e-06]
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1680 :  0.03684020642605093
lr:  [1.089912964766341e-06]
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lr:  [1.0366272621152509e-06]
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lr:  [9.377438854478388e-07]
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1720 :  0.03649741618169679
lr:  [8.918977092317738e-07]
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lr:  [8.482929465895556e-07]
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1740 :  0.038325818669464856
lr:  [8.068200151039863e-07]
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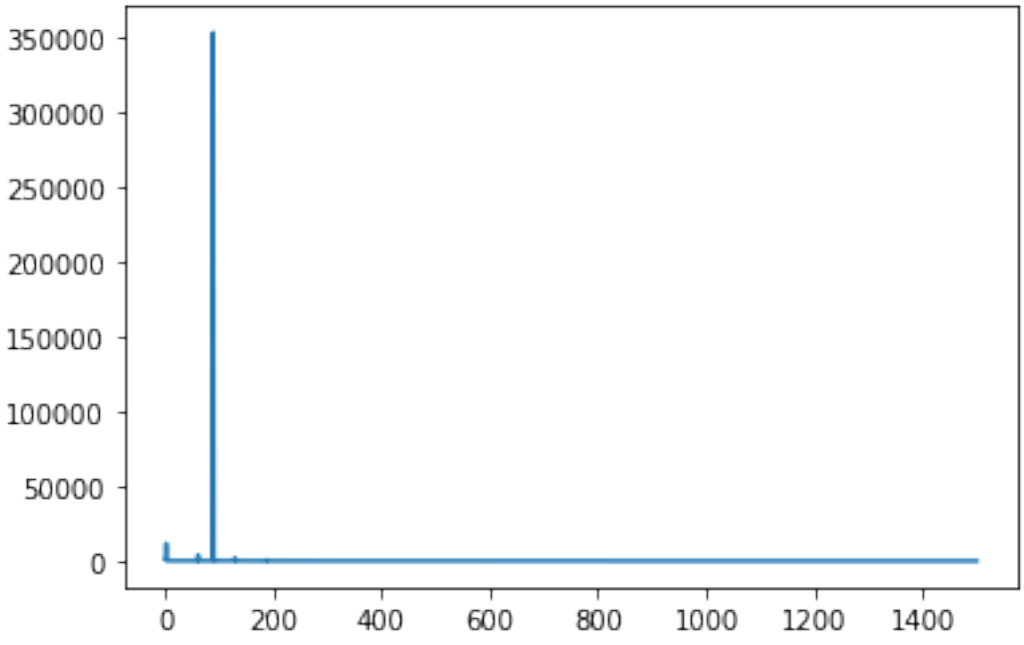
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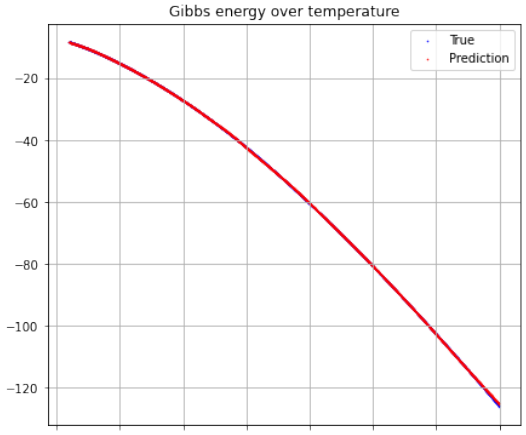
Gibbs energy over temperature
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Prediction
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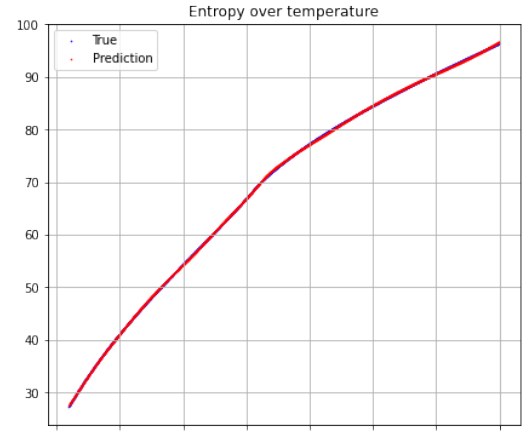
Entropy over temperature
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Prediction
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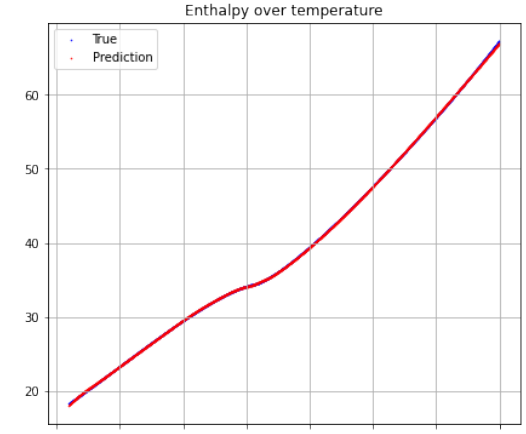
Enthalpy over temperature
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Prediction
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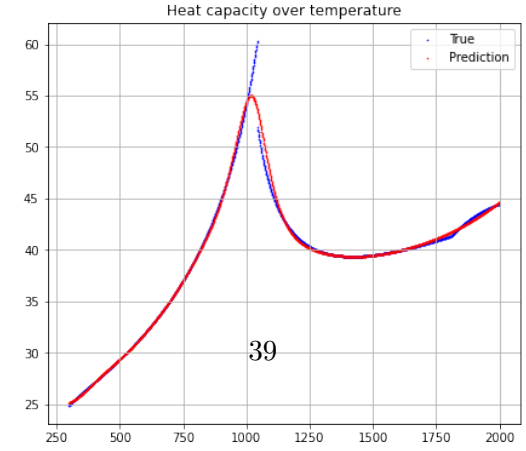
Heat capacity over temperature
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Prediction
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2000

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lr:  [6.941751867158463e-07]
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1780 :  0.035958574877844915
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lr:  [5.972573570697468e-07]
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1810 :  0.03510196879506111
lr:  [5.680575228042489e-07]
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lr:  [4.2051080585789107e-07]
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lr:  [3.618008498894394e-07]
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1910 :  0.0366269846757253
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lr:  [3.1128773186617547e-07]
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1940 :  0.03400281195839246
lr:  [2.9606891526763235e-07]
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lr:  [2.6782704363463796e-07]
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1970 :  0.03436077179180251
lr:  [2.5473301441360246e-07]
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1980 :  0.03405167017545965
lr:  [2.422791505728609e-07]
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1990 :  0.03345745657053259
lr:  [2.3043415451049007e-07]
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2000 :  0.03363995564480623
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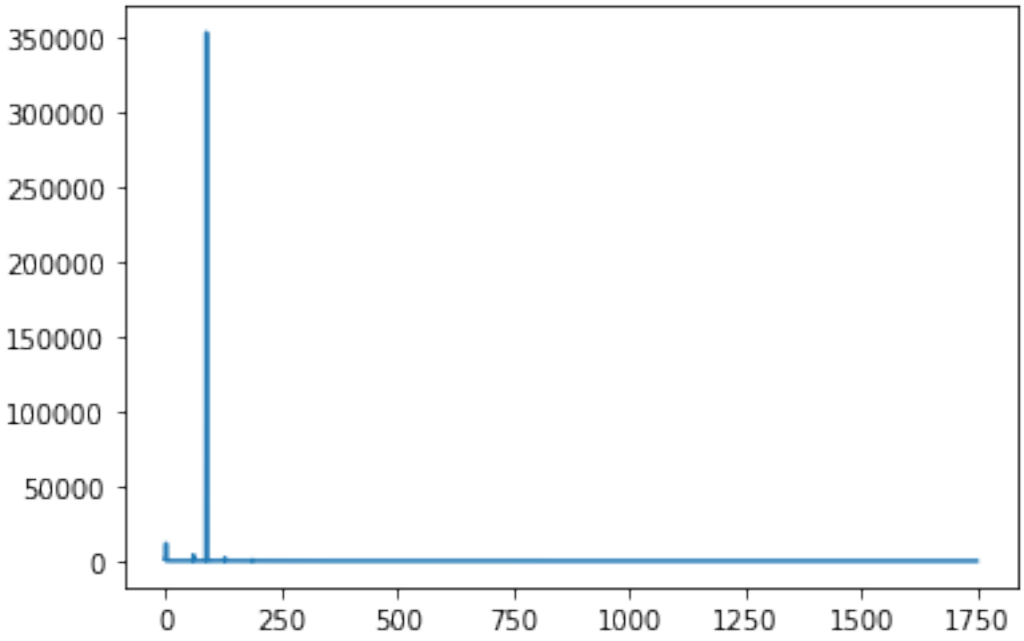
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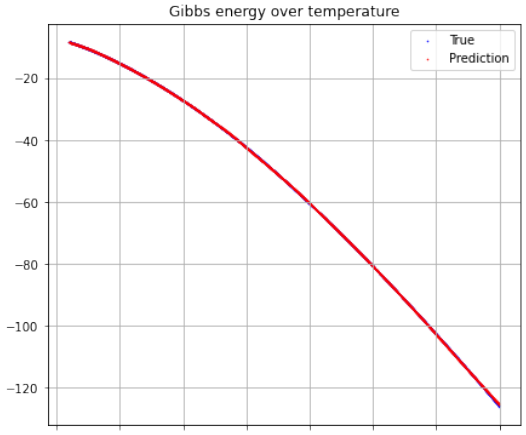
Gibbs energy over temperature
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Prediction
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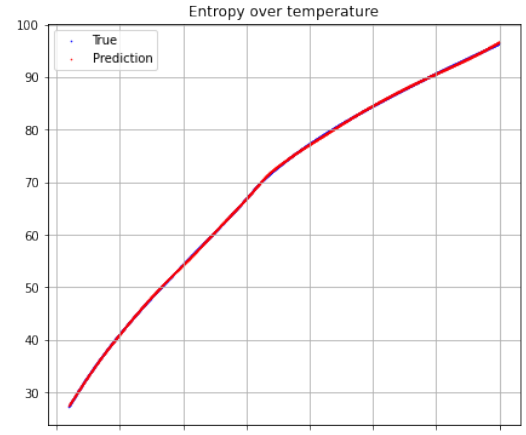
Entropy over temperature
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Prediction
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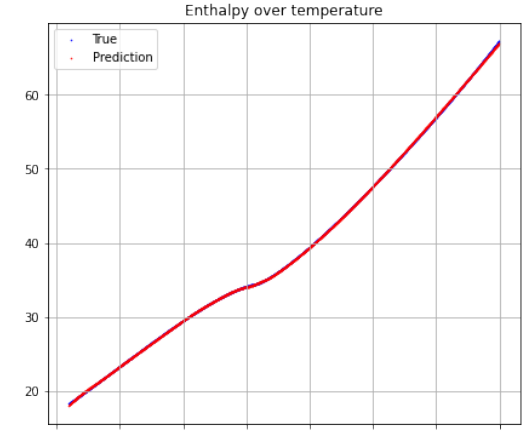
Enthalpy over temperature
True
Prediction
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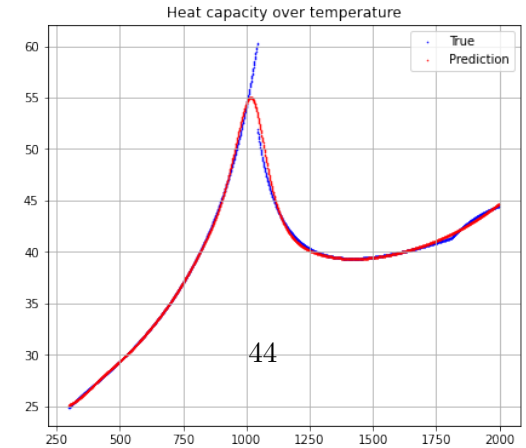
Heat capacity over temperature
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Prediction
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45
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25
250
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750
1000
1250
1500
1750
2000

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2020 :  0.035644401899642415
lr:  [1.9826190381805415e-07]
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-35.98440888164014 0.0016718405072042926 0.035023543327632876

2030 :  0.03330636355612013
lr:  [1.8856890520678178e-07]
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2040 :  0.03367367862827248
lr:  [1.7934979603301001e-07]
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-28.53762100763351 0.001549762301054004 0.03465824456885457

2050 :  0.03445611542297734
lr:  [1.7058140790396574e-07]
8.068484615306465e-06
194.26326497493758 0.001567410164769487 0.03460668935543962

2060 :  0.033951025249229536
lr:  [1.6224170512657589e-07]
-0.00011142336524803358
-12.753852561618563 0.001421077172292794 0.03450301250856784

2070 :  0.03661830578413275
lr:  [1.5430972932992683e-07]
7.054947586962428e-05
19.164719222698594 0.001352060896349899 0.03436032155735625

2080 :  0.034172672778367996
lr:  [1.4676554679512468e-07]
7.666934644824538e-06
169.8021604001311 0.0013018620663378185 0.034291270735363165

2090 :  0.03666887142592006
lr:  [1.395901983601914e-07]
7.397002939667021e-05
18.26770963038581 0.0013512630183694738 0.034365658859411875
```
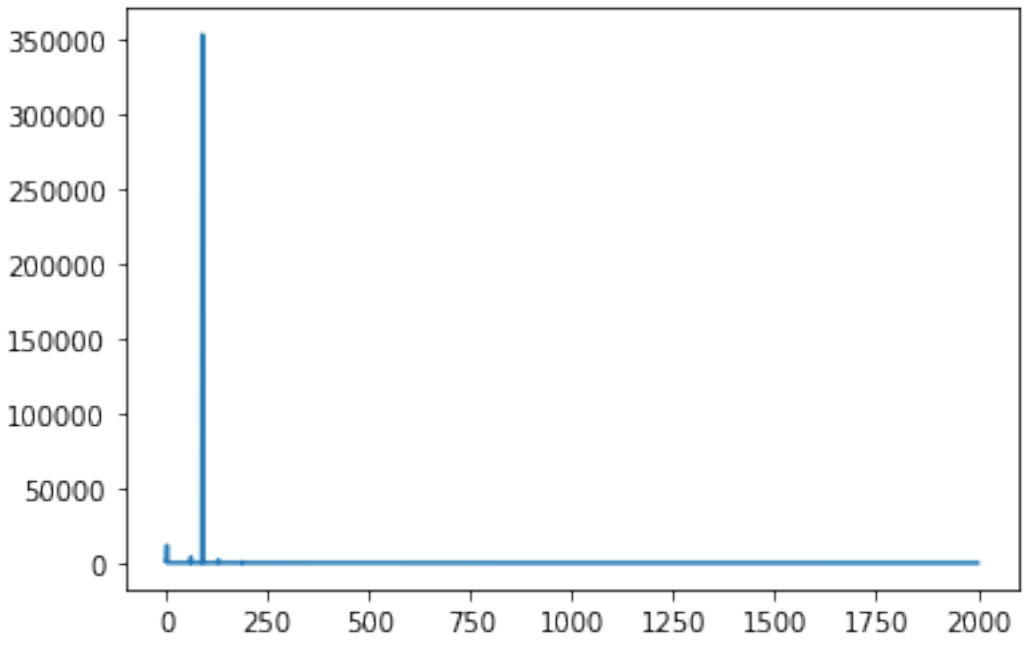
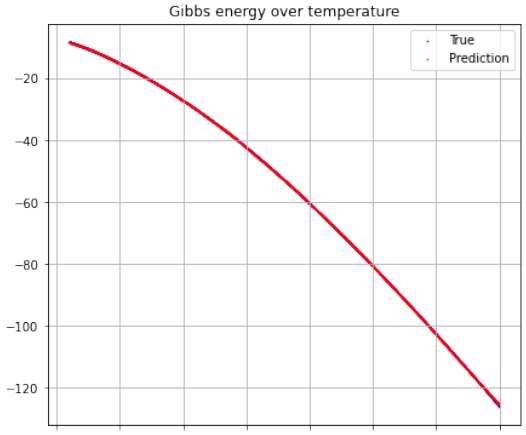
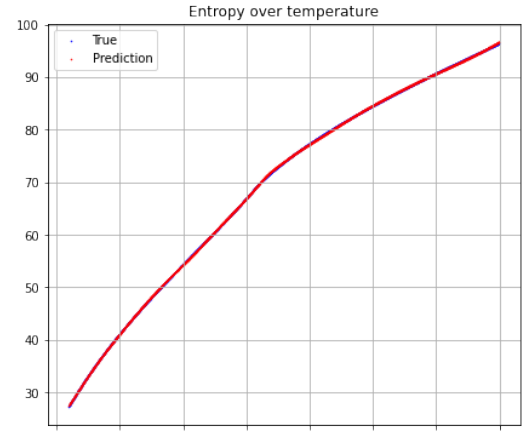
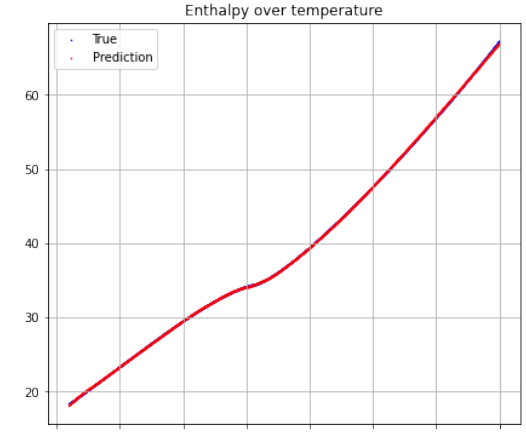

```
2100 :  0.03425726046164831
lr:  [1.3276565177410457e-07]
9.580677936947614e-06
146.73622908477037 0.0014058325525433501 0.03447824623021814

2110 :  0.037205507771836385
lr:  [1.2627475638024182e-07]
3.262037356424225e-05
40.67763759870013 0.0013269197341804644 0.03446699270357688

2120 :  0.03663178657492002
lr:  [1.2010120001534533e-07]
5.381349094060002e-05
24.85556976691585 0.0013375649784753778 0.034471035067819886

2130 :  0.03332607406708929
lr:  [1.1422946801569086e-07]
-1.5428049021026762e-05
-94.87147228038972 0.0014636817250388344 0.03461470414573947

2140 :  0.033976454494727984
lr:  [1.0864480422743945e-07]
-1.3971549211716165e-05
-101.1371404692505 0.0014130425351983839 0.03459791115381652

2150 :  0.035264979013138346
lr:  [1.0333317392318817e-07]
3.926320816654181e-06
351.6876565046761 0.001380838566694635 0.03462519479294618

2160 :  0.03555060923099518
lr:  [9.82812285315258e-08]
3.0157280887335543e-05
44.37989085333775 0.0013383768342134 0.03450018372800615

2170 :  0.03263507938633362
lr:  [9.347627209095586e-08]
-1.0993511177379862e-05
-113.00453693651107 0.00124231663990617 0.03432623620869385

2180 :  0.03460622951388359
lr:  [8.890622934388301e-08]
1.3001546128536823e-05
94.97145181795781 0.0012347757117052909 0.03429115250085791

2190 :  0.03287498839199543
lr:  [8.455961539048042e-08]
-7.19170797776744e-05
```

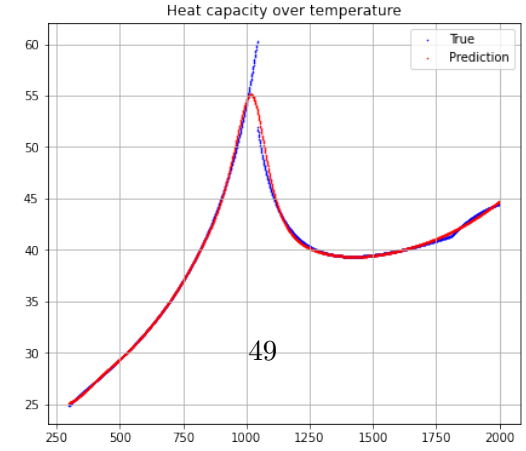
```
-18.198730875234673 0.0013087995802066783 0.0342143039426042

2200 :  0.03496292129986816
lr:  [8.042550682617533e-08]
3.045597990083588e-05
42.892226897899924 0.0013063248003045323 0.03407281000167131

2210 :  0.037073335920770965
lr:  [7.649351429021946e-08]
7.285814217023567e-05
19.540395789359323 0.0014236769344838159 0.034215642909208935

2220 :  0.03547645753456487
lr:  [7.275375635635602e-08]
-4.127175629544411e-05
-35.73142829156812 0.0014746988005377363 0.03427013147622347

2230 :  0.032989202067255974
lr:  [6.919683469996873e-08]
-6.744290476077811e-05
-19.68007515468336 0.0013272814343422655 0.0340854166696469

2240 :  0.03354591607219643
lr:  [6.581381047930572e-08]
-8.722526483795317e-06
-165.61327552318926 0.0014444566181819109 0.034095333984328645

2250 :  0.03487589293056064
lr:  [6.259618187142205e-08]
-9.556708523746043e-06
-148.42470768082975 0.0014184516690279006 0.034078175680090986
```


350000
300000
250000
200000
150000
100000
50000
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
100
90
80
70
60
50
40
30

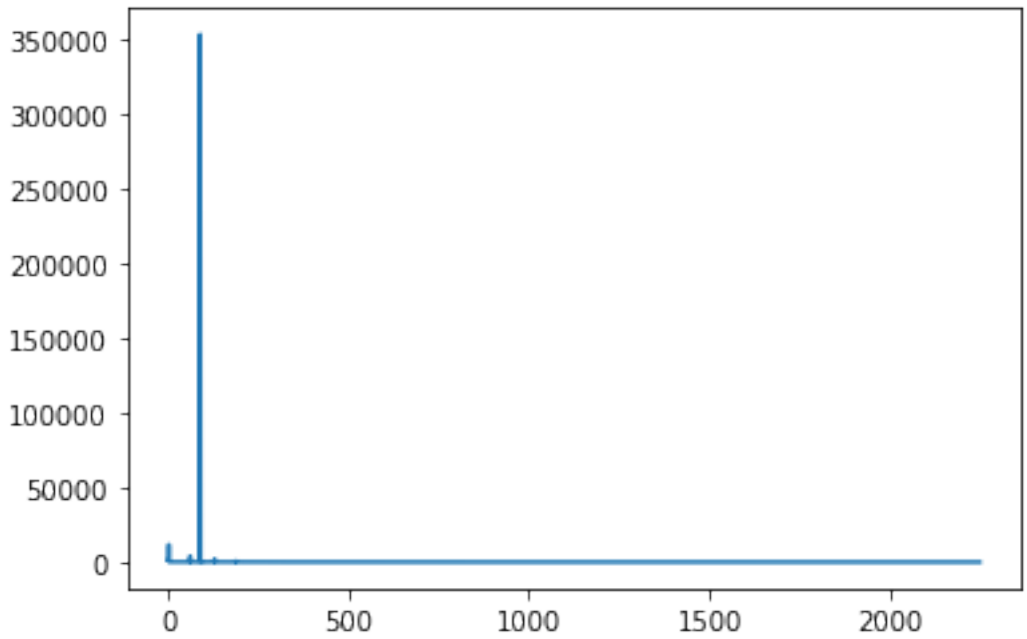

Enthalpy over temperature
True
Prediction
60
50
40
30
20


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

```
2260 :  0.03447117946214146
lr:  [5.9535862706387415e-08]
9.395498909106823e-06
143.90019668321952 0.0013520141409574464 0.03394539118847914

2270 :  0.03292264830734995
lr:  [5.662516214606441e-08]
-7.325732687703512e-06
-198.7239560364543 0.001455798580566009 0.03406272797534863

2280 :  0.035875834731592074
lr:  [5.3856765356388806e-08]
5.536346512586897e-05
26.93893007326192 0.0014914325156392592 0.03410385960506069

2290 :  0.03425675878922144
lr:  [5.122371512457942e-08]
-2.8383633007808608e-05
-46.451210861544254 0.0013184541218624053 0.03408016531624728

2300 :  0.033968064934015274
lr:  [4.871939437508027e-08]
1.6939169526640852e-05
85.38970382678448 0.0014464306689515555 0.03419233122012681

2310 :  0.03315624718864759
lr:  [4.633750954029599e-08]
8.954943206304944e-06
157.27231138887223 0.001408364616411657 0.034078741876615415

2320 :  0.03527825532688035
lr:  [4.407207474432987e-08]
4.40662224141379e-05
27.566552325320806 0.001214753825958557 0.03397016464008226

2330 :  0.03312532500260406
lr:  [4.1917396759976825e-08]
-1.6887378699384927e-05
-63.5625820868383 0.001073405394811179 0.03389703776273462

2340 :  0.033437100135617785
lr:  [3.986806070116709e-08]
-2.396044209430549e-05
-46.20416358115978 0.0011070721860021975 0.03390718461945653
```

```
2350 :  0.032982335736354194
lr:  [3.791891641490434e-08]
2.3868762784534816e-06
366.82126481558316 0.0008755569754206182 0.03378015836286876

2360 :  0.03324463218450546
lr:  [3.6065065538500366e-08]
-1.5567396841351933e-05
-59.93801514458052 0.0009330788676386471 0.03390495284563965

2370 :  0.03259392310347822
lr:  [3.4301849189579685e-08]
-2.1037951855161977e-05
-48.263178529079646 0.0010153584262718649 0.0337699484721654

2380 :  0.03276104749076896
lr:  [3.2624836257918366e-08]
-1.4439867196980487e-05
-82.54048454202233 0.001191873635161223 0.033968464696986805

2390 :  0.03366869708730115
lr:  [3.102981226969317e-08]
-1.1023847795938356e-05
-120.64934874333342 0.0013300200572255942 0.033950051050633194

2400 :  0.0328226869718896
lr:  [2.9512768796156287e-08]
-3.1807601384295445e-06
-416.8689869513664 0.0013259602566424123 0.03398511533728904

2410 :  0.033459179724256195
lr:  [2.806989338011837e-08]
2.282621790897816e-05
58.38783103620194 0.0013327733544649435 0.033984170624365415

2420 :  0.03267898162206014
lr:  [2.669755995492469e-08]
-5.175747281434585e-05
-24.950835785476862 0.0012913922048620261 0.034087187391188406

2430 :  0.037430850168069206
lr:  [2.539231973184619e-08]
8.038490115244641e-05
17.47249823586006 0.0014045250435759053 0.03406691186543968

2440 :  0.037038134410977364
lr:  [2.4150892532984822e-08]
7.157593272846026e-05
```

```
18.731959700531455 0.001340757487397468 0.03409456214557091

2450 :  0.037493379372689456
lr:  [2.2970158547912027e-08]
5.386053434575213e-05
27.113746467642706 0.0014603608728624854 0.034060503985318874

2460 :  0.03566230440305339
lr:  [2.184715049332407e-08]
1.9513176175472083e-05
73.34721797773518 0.0014312371863802998 0.033973590843379496

2470 :  0.033489089666141406
lr:  [2.0779046156010805e-08]
-4.567325013835409e-05
-30.759749452986707 0.0014048977309593623 0.03387682146703204

2480 :  0.03536535675326983
lr:  [1.9763161300397728e-08]
-2.3621212598147732e-06
-579.7914497452343 0.0013695377097020466 0.03383150364582738

2490 :  0.03292584874563747
lr:  [1.8796942922837378e-08]
-6.0357385718362976e-05
-21.688367269477595 0.0013090531488853781 0.0337545479565031
```

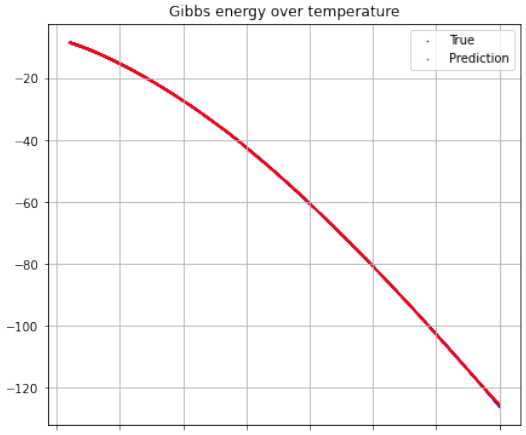


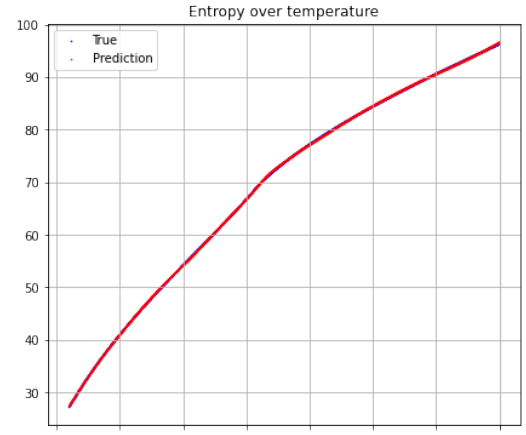
[ ]:
```
plt.plot(losses[1400:])
```

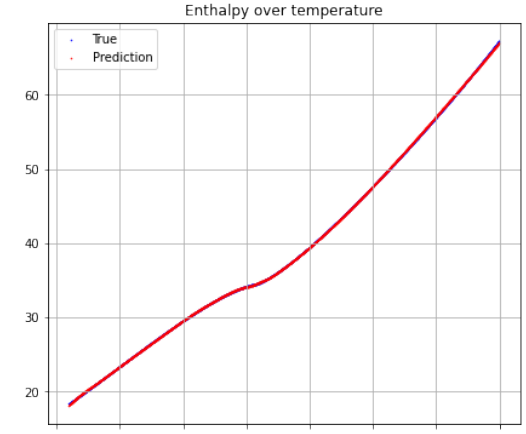
[14]:
```
torch.save(net, 'Fe_2.pth')
```

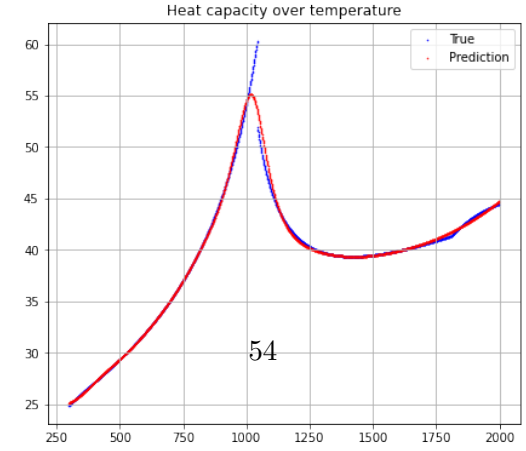
[3]:
```
net = torch.load(r"C:\Users\danie\Documents\Montanuni\Masterarbeit\5␣
↪Programmcodes\packages\thermonet\thermonet\models\Fe_2.pth")
```

[6]:
```
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
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

[ ]: