predict

May 6, 2022

[1]:
```
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import torch
import torch.nn as nn
from torch.optim import Adam
from torch.utils.data import DataLoader
from scipy.optimize import least_squares
import time

from binarypredictor import BinaryPredictor
from binarypredictor.dataset import FunctionPairDataset
from binarypredictor.net import DerivativeNet, TangentNet
from binarypredictor.cm import base_function, first_derivative,␣
↪second_derivative
```

[2]:
```
bp = BinaryPredictor(net_1='net_1.pth', net_2='net_2.pth')
```

1 AuAg

net_1.pth
net_2.pth

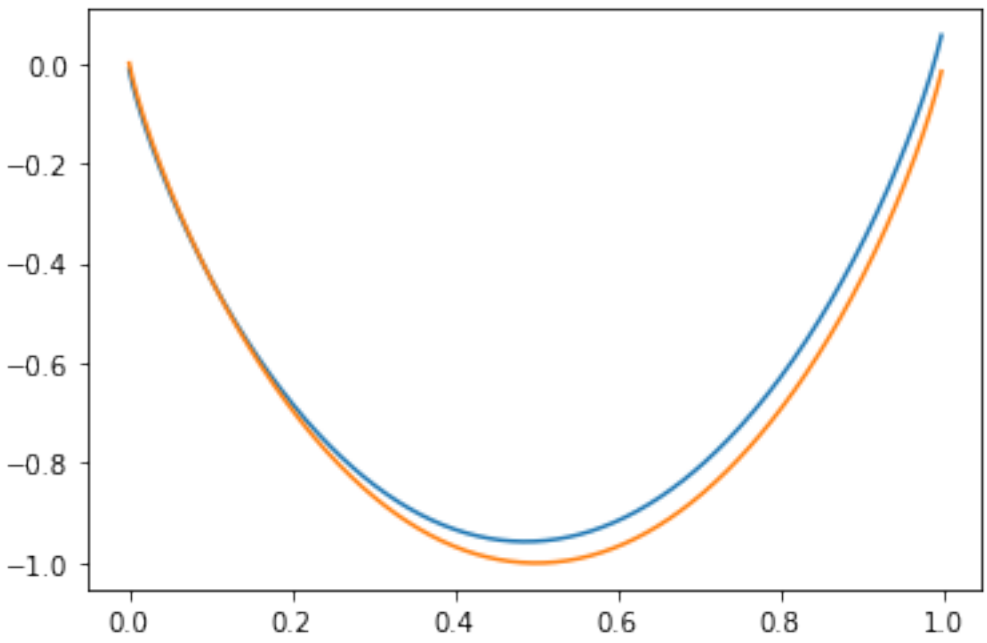
[46]:
```
%%timeit -n 20
R = 8.3143

gf = lambda t: 3815.93 + 109.3029 * t - 1.044523e-20 * t ** 7 - (-7209.5 + 118.
↪2007 * t)
gg = lambda t: -3352 + 215.88 * t - 3.5899325e-21 * t ** 7 - (-15745 + 225.14 *␣
↪t)

real_data = pd.read_csv('auag.txt', delimiter='\t')
t_range = real_data['LIQUID + FCC_A1']

f = lambda x, t: (1 - x) * gf(t) + x * gg(t) + R * t * ((1 - x) * torch.log(1 -␣
↪x) + x * torch.log(x)) + (1 - x) * x * (-16402 + 1.14 * t)
```

```
g = lambda x, t: R * t * ((1 - x) * torch.log(1 - x) + x * torch.log(x)) + (1 -␣
↪x) * x * (-15599)

df = lambda x, t: -16402 - gf(t) + gg(t) + 1.14 * t + 32804 * x - 2.28 * t * x␣
↪- R * t * torch.log(1 - x) + R * t * torch.log(x)
dg = lambda x, t: 15599 * (-1 + 2 * x) - R * t * torch.log(1 - x) + R * t *␣
↪torch.log(x)

xf_eq, xg_eq, ts = bp.get_phase_diagram(t_range, f, g, df, dg, plot=False,␣
↪threshold=0.1, max_threshold=0.3)
```

```
2.36 s ± 71.3 ms per loop (mean ± std. dev. of 7 runs, 20 loops each)
```

[4]:
```
x = torch.arange(1e-10, 1., step=1/500)

t = 1250

scale = torch.max(torch.max(abs(f(x, t))), torch.max(abs(g(x, t))))

plt.plot(x, f(x, t)/scale)
plt.plot(x, g(x, t)/scale)
```

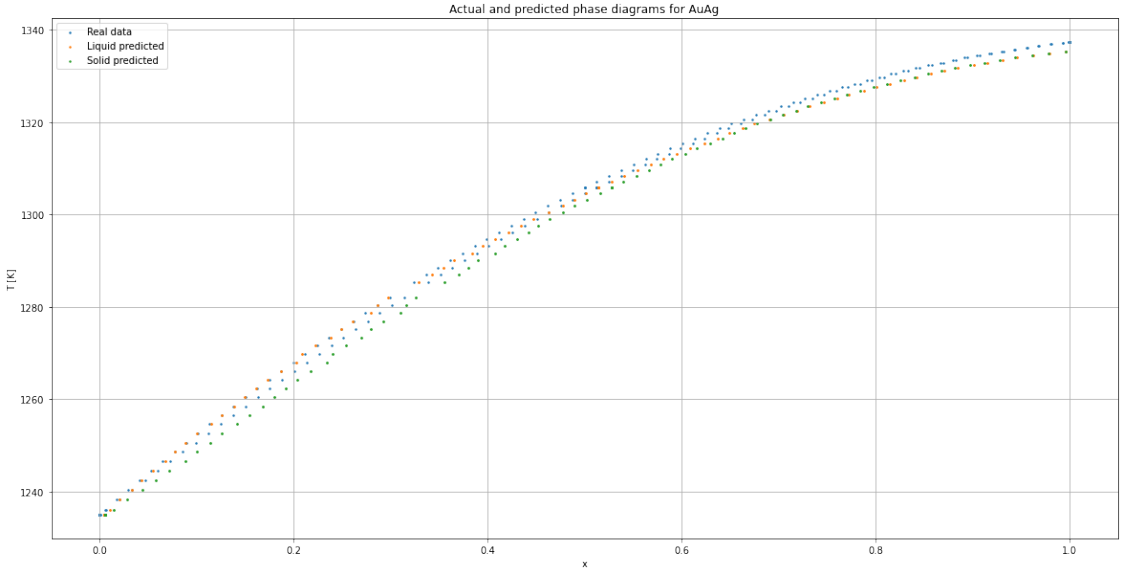
[4]:
```
[<matplotlib.lines.Line2D at 0x180afcaa400>]
```



[6]:
```
x_fs_ = []
for x_ in xf_eq:
```

```
    x_fs_.append(x_[0])

x_gs_ = []
for x_ in xg_eq:
    x_gs_.append(x_[0])

fig, ax = plt.subplots(1, 1, figsize=(20, 10))
s = 2
ax.scatter(real_data['Mole fraction Au'], real_data['LIQUID + FCC_A1'], s=s,␣
↪label='Real data')
ax.scatter(x_fs_, ts, s=s, label='Liquid predicted')
ax.scatter(x_gs_, ts, s=s, label='Solid predicted')
ax.grid()
plt.xlabel('x')
plt.ylabel('T [K]')
plt.title('Actual and predicted phase diagrams for AuAg')
ax.legend()
```

[6]: <matplotlib.legend.Legend at 0x2677ae45a90>



[7]:
```
r_x = []

for x_, r_t in zip(real_data['Mole fraction Au'], real_data['LIQUID + FCC_A1']):
    if r_t in ts:
        r_x.append(x_)

x_fs_t = torch.tensor(x_fs_)
r_x_t = torch.tensor(r_x)
```

```
print('Mean error: ', nn.L1Loss()(x_fs_t, r_x_t).item())
print('Mean squared error: ', nn.MSELoss()(x_fs_t, r_x_t).item())
print('Max deviation: ' , torch.max(abs(x_fs_t - r_x_t)).item())
print('Min deviation: ' , torch.min(abs(x_fs_t - r_x_t)).item())
```

```
Mean error:  0.01565570756793022
Mean squared error:  0.0004928208072669804
Max deviation:  0.06612342596054077
Min deviation:  9.797513484954834e-06
```

[48]:
```
%%timeit -n 20

f_eq = []
g_eq = []
funcs = []

x_ = np.arange(1e-10, 1., step=1/(len(t_range)))

for x_t, t in zip(x_, t_range):
    gf = lambda t: 3815.93 + 109.3029 * t - 1.044523e-20 * t ** 7 - (-7209.5 +␣
 ↪118.2007 * t)
    gg = lambda t: -3352 + 215.88 * t - 3.5899325e-21 * t ** 7 - (-15745 + 225.
 ↪14 * t)

    f = lambda x: (1 - x) * gf(t) + x * gg(t) + R * t * ((1 - x) * np.log(1 -␣
 ↪x) + x * np.log(x)) + (1 - x) * x * (-16402 + 1.14 * t)
    g = lambda x: R * t * ((1 - x) * np.log(1 - x) + x * np.log(x)) + (1 - x) *␣
 ↪x * (-15599)

    df = lambda x: -16402 - gf(t) + gg(t) + 1.14 * t + 32804 * x - 2.28 * t * x␣
 ↪- R * t * np.log(1 - x) + R * t * np.log(x)
    dg = lambda x: 15599 * (-1 + 2 * x) - R * t * np.log(1 - x) + R * t * np.
 ↪log(x)

    scale = max(torch.max(abs(f(x))), torch.max(abs(g(x))))

    def eqns(x):
        x1, x2 = x[0], x[1]
        eq1 = (df(x1) - dg(x2))/scale
        eq2 = (f(x1) - g(x2) - x1 * df(x1) + x2 * dg(x2))/scale
        return [eq1, eq2]

    x0 = [1e-10, 1.]
    lb = (0, 0)   # lower bounds on x1, x2
    ub = (1, 1)    # upper bounds
```

```
    res = least_squares(eqns, x0, bounds=(lb, ub))

    if res.success:
        f_eq.append((res.x[0], t))
        g_eq.append((res.x[1], t))
        funcs.append(res.fun)
```

```
6.65 s ± 629 ms per loop (mean ± std. dev. of 7 runs, 20 loops each)
```

2 Lukas-Petzow-Mager functions

[95]:
```
def a(a_sum, a_diff, TM):
    r = 8.314

    a_sum *= TM * r
    a_diff *= TM * r

    a_1 = (a_sum - a_diff) / 2
    a_2 = (a_sum + a_diff) / 2

    return a_1, a_2
```

[96]:
```
x = torch.arange(1e-10, 1., step=1/500)

tm_1, tm_2 = 900, 1100
tm = (tm_1 + tm_2)/2

a_diff = -1
a_sum = 0
a_1, a_2 = a(a_sum, a_diff, tm)
print(a_1, a_2)

k = dict()
k['step'] = 1/500
k['tm1'] = tm_1
k['tm2'] = tm_2
k['tm'] = tm
k['s1'] = 10
k['s2'] = 10
k['a'] = a_1

c = dict()
c['step'] = 1/500
c['tm1'] = tm_1
c['tm2'] = tm_2
c['tm'] = tm
c['s1'] = 0
```

```
c['s2'] = 0
c['a'] = a_2
```

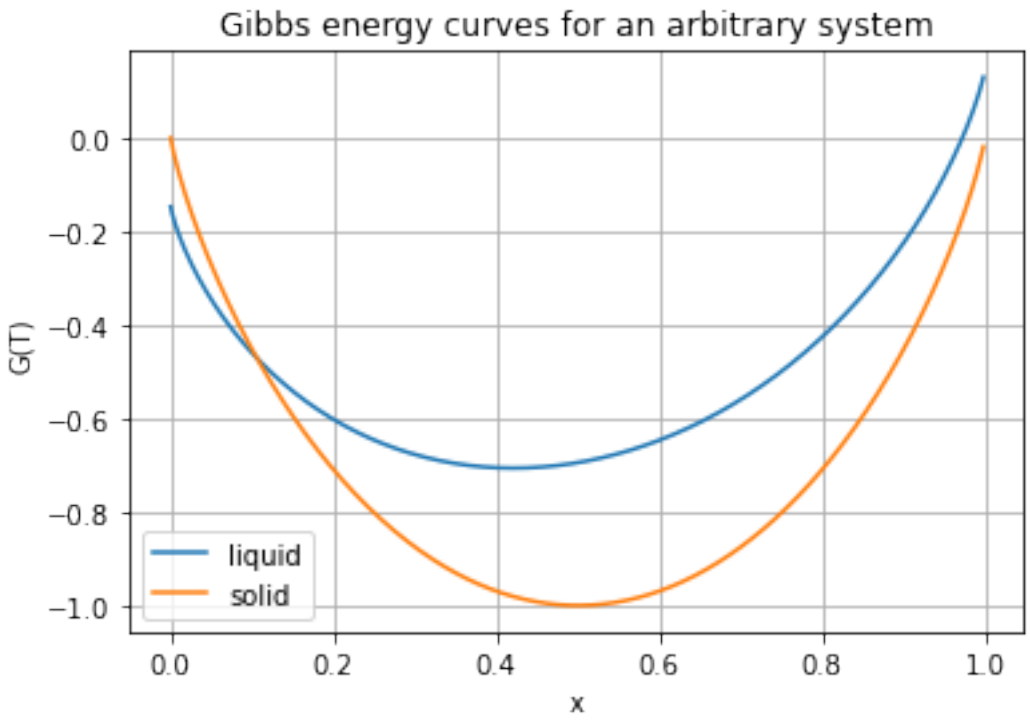
```
4157.0 -4157.0
```

[5]:
```
x = torch.arange(1e-10, 1., step=1/500)
t_range = range(0, 1500)
```

[6]:
```
t_range = range(1000, 1001)

f = lambda x, t: base_function(**k, x=x, t=t)
g = lambda x, t: base_function(**c, x=x, t=t)

df = lambda x, t: first_derivative(**k, x=x, t=t)
dg = lambda x, t: first_derivative(**c, x=x, t=t)
```

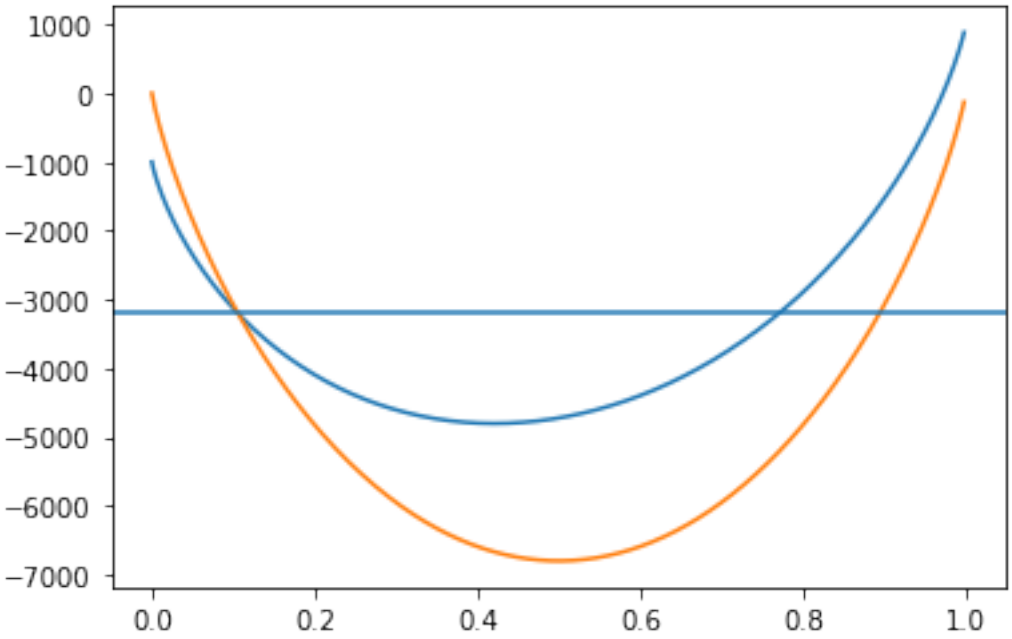
[7]:
```
t = 1000

scale = max(torch.max(abs(f(x, t))), torch.max(abs(g(x, t))))


plt.rcParams['text.usetex'] = False
plt.plot(x, f(x, t)/scale, label='liquid')
plt.plot(x, g(x, t)/scale, label='solid')
plt.xlabel('x')
plt.ylabel('G(T)')
plt.grid()
plt.legend()
plt.title('Gibbs energy curves for an arbitrary system')
```

[7]:
```
Text(0.5, 1.0, 'Gibbs energy curves for an arbitrary system')
```

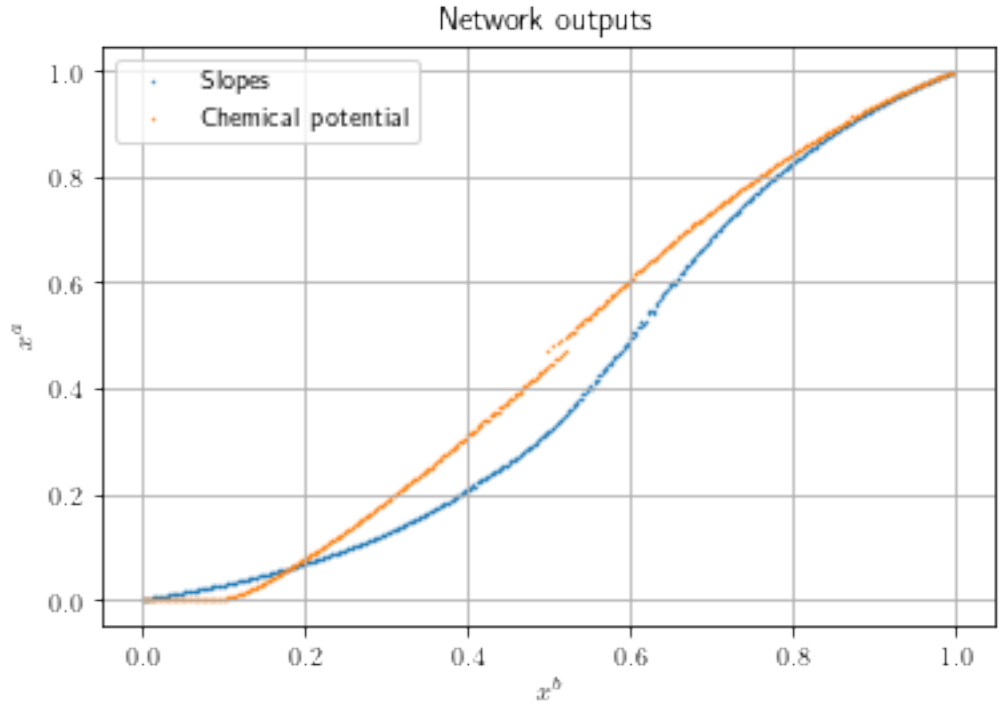


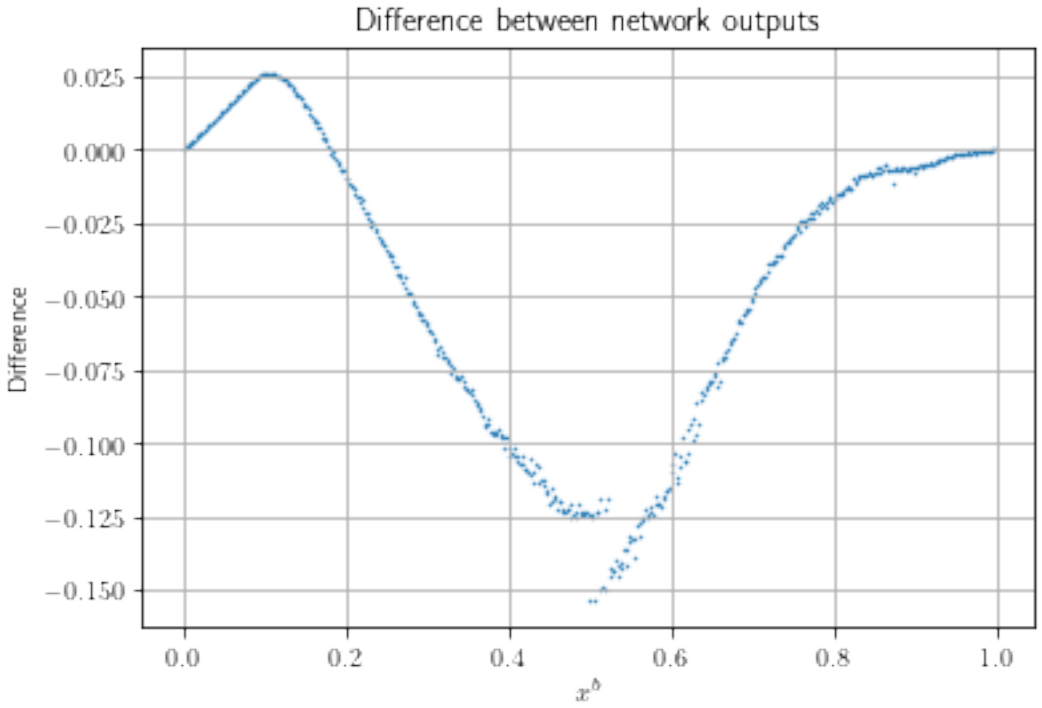
[13]:
```
diff = f(x, t) - g(x, t)
sig = torch.sign(diff)
t0 = torch.where(torch.diff(sig) != 0)[0]
print(t0)

x0 = x[t0]
y0 = f(x0, t)

plt.plot(x, f(x, t))
plt.plot(x, g(x, t))
print(y0)
for yy in y0:
    plt.axhline(yy)
```

```
tensor([53])
tensor([-3204.7783])
```

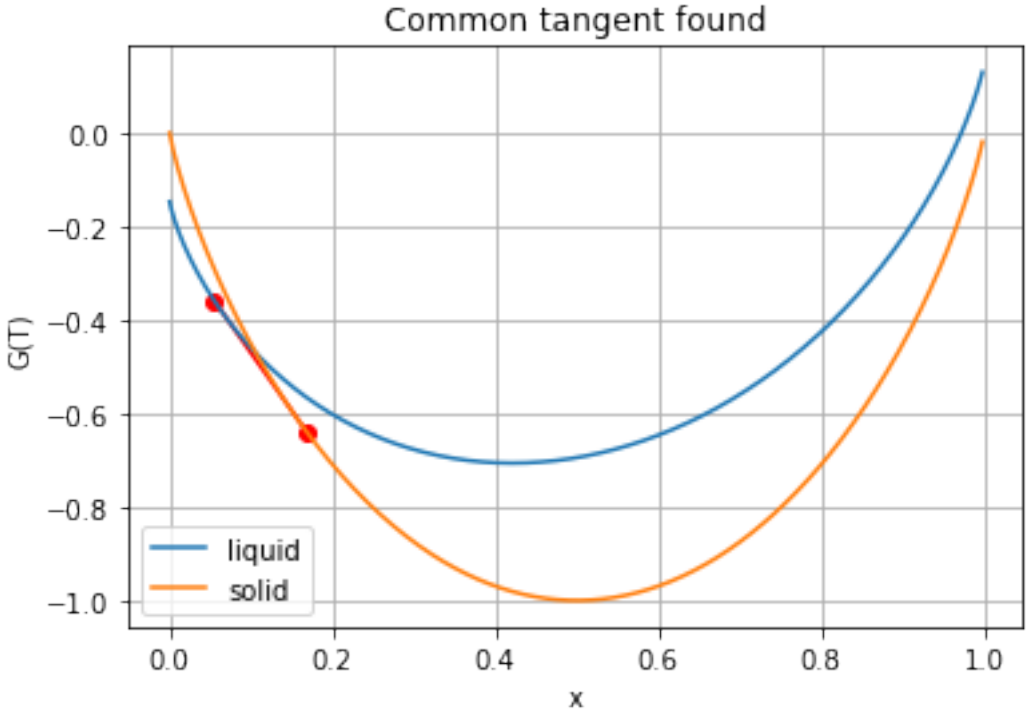


[8]:
```
xf_eq, xg_eq, ts = bp.get_phase_diagram(t_range, f, g, df, dg, plot=True,␣
↪threshold=.3, max_threshold=2.)
```






```
x'_eq:  [0.0543]
x''_eq:  [0.168]
```



[ ]:
```
x_fs_ = []
x_gs_ = []
ts_ = []
for i, xs in enumerate(zip(xf_eq, xg_eq)):
    for xf_, xg_ in zip(xs[0], xs[1]):
        x_fs_.append(xf_)
        x_gs_.append(xg_)
        ts_.append(ts[i])

fig, ax = plt.subplots(1, 1, figsize=(20, 10))
s = 2
ax.scatter(x_fs_, ts_, s=s, label='Liquid predicted')
ax.scatter(x_gs_, ts_, s=s, label='Solid predicted')
plt.xlabel('x')
plt.ylabel('T [K]')
plt.title('Lukas-Petzow-Mager function with A_diff=4 & A_sum=0')
plt.grid()
ax.legend()
```

[ ]:
```
x_fs_ = []
x_gs_ = []
ts_ = []
for i, xs in enumerate(zip(xf_eq, xg_eq)):
    for xf_, xg_ in zip(xs[0], xs[1]):
        x_fs_.append(xf_)
        x_gs_.append(xg_)
        ts_.append(ts[i])

fig, ax = plt.subplots(1, 1, figsize=(20, 10))
s = 2
ax.scatter(x_fs_, ts_, s=s, label='Liquid predicted')
ax.scatter(x_gs_, ts_, s=s, label='Solid predicted')
plt.xlabel('x')
plt.ylabel('T [K]')
plt.title('Lukas-Petzow-Mager function with A_diff=0 & A_sum=0')
plt.grid()
ax.legend()
```

[ ]:
```

```