CHBE 552 Problem Set 4

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For Question 1

$$\mathbf{k} = [kH, kR, KA]^T$$
$$\mathbf{x} = [pA]$$

Note this input vector contains information for two different temperatures and will be treated separately in the code.

$$\mathbf{f}_{modelA} = R - \sqrt{R^2 - kH^2}$$
$$\text{with} R = kH + \frac{kH^2}{2kR}\frac{(1 + KAp_A)^2}{KAp_A}$$
$$\mathbf{f}_{modelB} = (kH^{\lambda} + (\frac{kRKAp_A}{(1 + KAp_A)^2})^2)^{\frac{1}{\lambda}}$$
$$\mathbf{y} = [rA]$$

The same separate treatment will also be applied to the output vector.

For Question 2

$$\mathbf{k} = [ko, kp]^T$$
$$\mathbf{x} = [Cp, Co, n]^T$$
$$\mathbf{f} = \frac{kokpCo^{0.5}Cp}{koCo^{0.5} + nkpCp}$$
$$\mathbf{y} = [rp]$$

The sensitivity matrix of those vector valued functions are equivalent to their Jacobian matrix which is computed and embeded in the code. Thus, it could not be presented here explicitly, but I shall provide the computation procedure here:

For a parameter vector $\boldsymbol{\theta}$ of length n, and m residuals, the Jacobian matrix $\mathbf{J}$ is an $m \times n$ matrix. The approximation of the j-th column of $\mathbf{J}$ (the derivative of the residuals with respect to the j-th parameter) can be calculated as follows:

1. **Slightly Perturb the j-th Parameter**: For a small value ε, create a new parameter vector $\boldsymbol{\theta}_\varepsilon$ where only the j-th parameter is increased by ε, i.e.,

$$\theta_{\varepsilon,j} = \theta_j + \varepsilon.$$

2. **Calculate the Difference in Predictions**: Use the model function to calculate predictions using $\boldsymbol{\theta}$ and $\boldsymbol{\theta}_\varepsilon$, and compute the difference in the resulting predictions. This difference approximates the change in the residuals caused by the perturbation in the j-th parameter.

3. **Divide by ε**: The approximation of the derivative is the difference in the residuals divided by ε.

From now on, result tables for each model and equestions are presented. In table 1, the final results for those parameters with their corresponding 95% confidence intervals in each case are listed.

Table 1: GN-M Method Results

Q1	kH & CI	kR & CI	KA & CI
Model A 600	0.094 [0.069 0.118]	0.607 [0.400 0.812]	0.517 [0.390 0.642]
Model A 575	0.832 [0.779 0.934]	0.119 [0.112 0.124]	0.397 [0.352 0.442]
Model B 600	0.084 [0.064 0.103]	0.732 [0.515 0.948]	0.516 [0.346 0.451]
Model B 575	0.922 [0.834 1.012]	0.126 [0.118 0.133]	0.399 [0.352 0.442]
Q2	ko & CI	kp & CI	
	1330.8 [1209.5 1407.7]	0.612 [0.411 0.803]	

Note that "CI" refers to 95% confidence interval.

Table 2: Results for Model A at T = 600 degree Parameter Estimation of Q1 using modified G-N method

Iteration Number	Objective Function Value	kH	kR	KA
1	0.000260	0.085	0.683	0.520
2	0.000066	0.088	0.668	0.522
3	0.000064	0.089	0.656	0.522
4	0.000064	0.090	0.646	0.521
5	0.000064	0.091	0.638	0.520
6	0.000064	0.092	0.631	0.519
7	0.000063	0.092	0.626	0.519
8	0.000063	0.092	0.621	0.518
9	0.000063	0.093	0.618	0.518
10	0.000063	0.093	0.616	0.518
11	0.000063	0.093	0.613	0.517
12	0.000063	0.093	0.612	0.517
13	0.000063	0.094	0.611	0.517
14	0.000063	0.094	0.610	0.517
15	0.000063	0.094	0.609	0.517
16	0.000063	0.094	0.608	0.517
17	0.000063	0.094	0.608	0.517
18	0.000063	0.094	0.608	0.517
19	0.000063	0.094	0.607	0.517
20	0.000063	0.094	0.607	0.517
21	0.000063	0.094	0.607	0.517
22	0.000063	0.094	0.607	0.517
23	0.000063	0.094	0.607	0.517

Table 3: Results for Model A at T = 575 degree Parameter Estimation of Q1 using modified G-N method

Iteration Number	Objective Function Value	kH	kR	KA
1	0.000889	0.109	0.177	0.472
2	0.000013	0.127	0.172	0.447
3	0.000006	0.142	0.163	0.431
4	0.000005	0.157	0.157	0.421
5	0.000004	0.171	0.152	0.415
6	0.000003	0.183	0.149	0.412
7	0.000003	0.194	0.146	0.410
8	0.000003	0.203	0.145	0.408
9	0.000003	0.212	0.143	0.407
10	0.000003	0.219	0.142	0.407
11	0.000002	0.226	0.141	0.406
12	0.000002	0.233	0.140	0.406
13	0.000002	0.239	0.139	0.405
14	0.000002	0.245	0.138	0.405
15	0.000002	0.250	0.137	0.405
16	0.000002	0.256	0.137	0.405
17	0.000002	0.260	0.136	0.404
18	0.000002	0.265	0.136	0.404
19	0.000002	0.270	0.135	0.404
20	0.000002	0.274	0.135	0.404
21	0.000002	0.278	0.135	0.404
22	0.000002	0.282	0.134	0.403
23	0.000002	0.286	0.134	0.403
24	0.000002	0.290	0.134	0.403
25	0.000002	0.293	0.133	0.403
26	0.000002	0.297	0.133	0.403
27	0.000002	0.300	0.133	0.403
28	0.000002	0.303	0.132	0.403
29	0.000002	0.306	0.132	0.403
30	0.000002	0.310	0.132	0.403
...	...	...	...	...
996	0.000001	0.831	0.119	0.397
997	0.000001	0.831	0.119	0.397
998	0.000001	0.832	0.119	0.397
999	0.000001	0.832	0.119	0.397
1000	0.000001	0.832	0.119	0.397

Table 4: Results for Model B at T = 600 degree Parameter Estimation of Q1 using modified G-N method

Iteration Number	Objective Function Value	kH	kR	KA
1	0.000092	0.094	0.628	0.504
2	0.000066	0.091	0.649	0.506
3	0.000065	0.090	0.665	0.508
4	0.000064	0.088	0.678	0.510
5	0.000064	0.087	0.688	0.511
6	0.000064	0.087	0.696	0.512
7	0.000064	0.086	0.702	0.512
8	0.000064	0.086	0.707	0.513
9	0.000064	0.085	0.712	0.513
10	0.000064	0.085	0.715	0.514
11	0.000064	0.085	0.718	0.514
12	0.000064	0.085	0.721	0.514
13	0.000063	0.084	0.723	0.515
14	0.000063	0.084	0.724	0.515
15	0.000063	0.084	0.726	0.515
16	0.000063	0.084	0.727	0.515
17	0.000063	0.084	0.728	0.515
18	0.000063	0.084	0.728	0.515
19	0.000063	0.084	0.729	0.515
20	0.000063	0.084	0.730	0.515
21	0.000063	0.084	0.730	0.515
22	0.000063	0.084	0.731	0.515
23	0.000063	0.084	0.731	0.515
24	0.000063	0.084	0.731	0.515
25	0.000063	0.084	0.731	0.515
26	0.000063	0.084	0.732	0.515
27	0.000063	0.084	0.732	0.516
28	0.000063	0.084	0.732	0.516
29	0.000063	0.084	0.732	0.516
30	0.000063	0.084	0.732	0.516

Table 5: Results for Model B at T = 575 degree Parameter Estimation of Q1 using modified G-N method

Iteration Number	Objective Function Value	kH	kR	KA
1	0.001072	0.033	0.564	0.512
2	0.000095	0.042	0.555	0.515
3	0.000021	0.043	0.542	0.517
4	0.000020	0.044	0.529	0.518
5	0.000019	0.045	0.516	0.518
6	0.000019	0.045	0.502	0.517
7	0.000019	0.046	0.489	0.515
8	0.000018	0.047	0.475	0.513
9	0.000018	0.048	0.460	0.511
10	0.000018	0.049	0.445	0.507
11	0.000017	0.050	0.430	0.504
12	0.000017	0.051	0.414	0.500
13	0.000016	0.052	0.397	0.495
14	0.000016	0.054	0.380	0.490
15	0.000015	0.056	0.361	0.485
16	0.000014	0.059	0.342	0.479
17	0.000014	0.062	0.322	0.472
18	0.000013	0.066	0.300	0.466
19	0.000012	0.071	0.278	0.458
20	0.000011	0.079	0.255	0.450
21	0.000009	0.089	0.232	0.442
22	0.000008	0.103	0.212	0.434
23	0.000007	0.120	0.195	0.427
24	0.000006	0.137	0.184	0.421
25	0.000005	0.153	0.177	0.417
26	0.000004	0.166	0.172	0.414
27	0.000004	0.178	0.168	0.412
28	0.000003	0.189	0.165	0.411
29	0.000003	0.199	0.163	0.410
30	0.000003	0.207	0.161	0.409
...	...	...	...	...
996	0.000001	0.922	0.126	0.399
997	0.000001	0.923	0.126	0.399
998	0.000001	0.923	0.126	0.399
999	0.000001	0.923	0.126	0.399
1000	0.000001	0.923	0.126	0.399

We can see here, that for the situation of 600 degrees, those three parameters converge but not for the 575 degrees situation. The reason for that might be the lack of data points in the later case. For converged cases, the values of the parameters generally agree with the values shown on the reference but some error appears. The reason for those errors is unclear up to this stage. I tried tuning the modified GN method with various ranges of involved parameters but still could not get closer to the reference value. There might be some limitations in the code since I implemented the code in a straightforward and efficient way which might lead to uncertainties. I also compared the estimated data from the determined parameters with the experimental data and the results for each case are presented below from figure 1 to 3. We can see here the models for question 1 with estimated parameters actually predict the output well enough with some error, whereas the values of those parameters seem a little bit further from the reference values. Nevertheless, the situation looks different for question 2, though the comparison between the estimated data and experimental data looks quite off, the values of estimated parameters are very close to the reference values. The reason is still unclear and requires further investigation in future. Regarding the uncertainties related to those parameters, one can conclude that their 95% confidence intervals are good enough. In fact, almost all the reference values for those parameters stay in the estimated 95% confidence intervals, which verifies the implemented method to some extent.

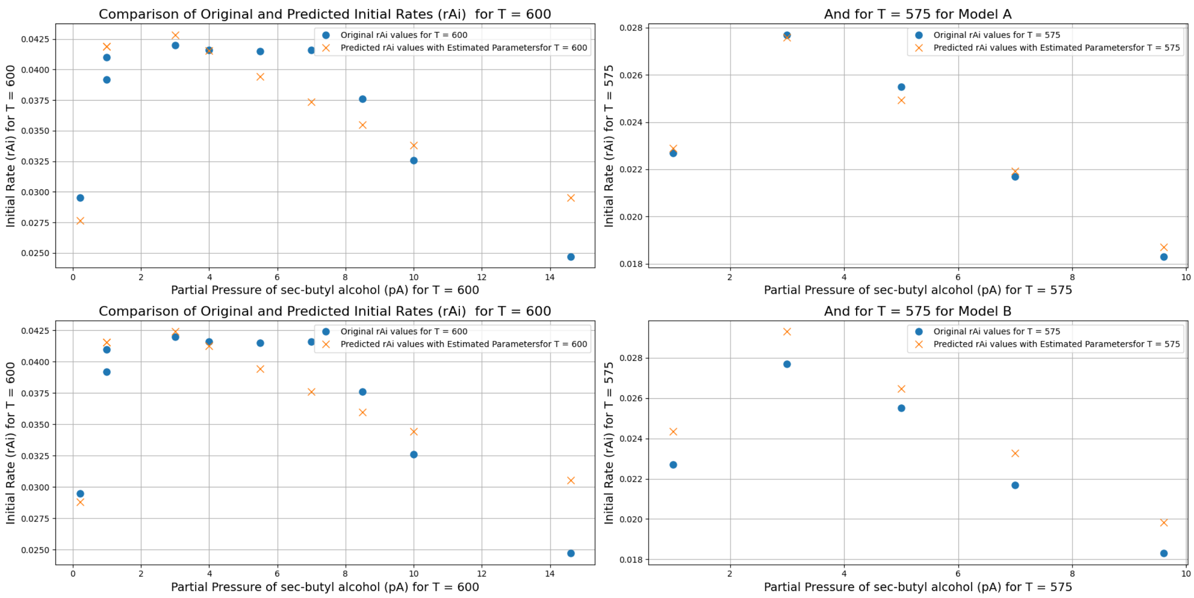

Figure 1: GNM Q1 Data Comparison

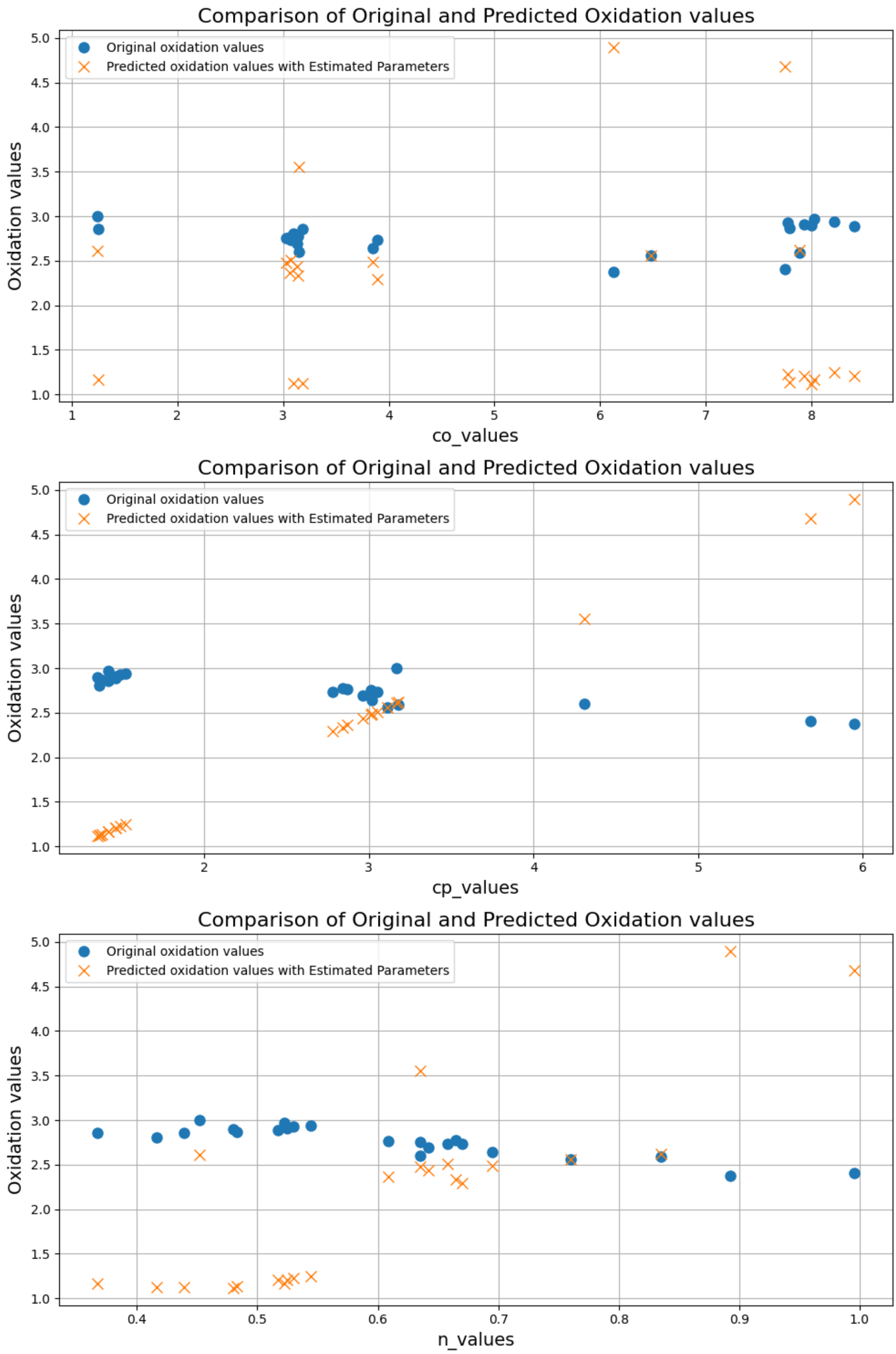

Figure 2: GNM Q2 Data Comparison

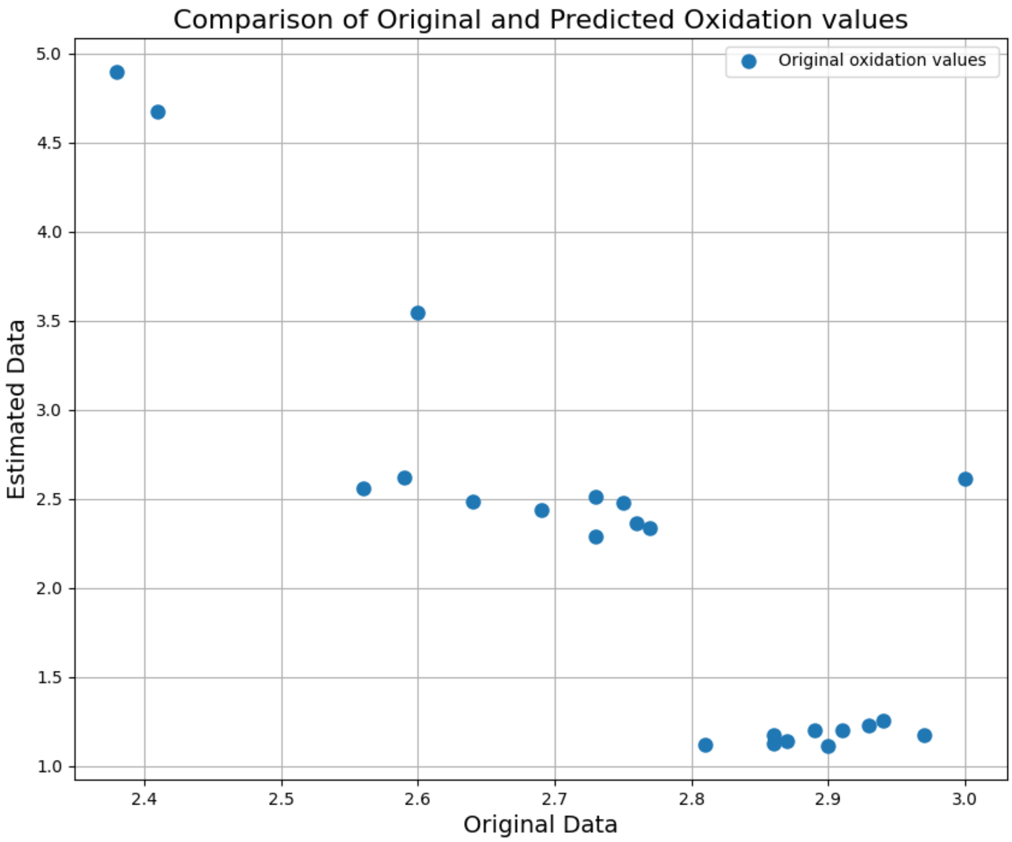

Figure 3: GNM Q2 Estimated Data vs. Original Data

In table 6, the results of those parameters estimated by the Luus-Jaakola Method are presented. As we can see, they are all quite different than the reference values. Since the Luus-Jaakola Method is actually a random process of seeking global minimum, the result highly relies on the initial condition/guess of the parameters as well as the number of iterations, given in limited performance/executing time of the code, in this case, the Luus-Jaakola Method did not reach the real solution that we are looking for. By the experience with tuning parameters in the last assignment, one could definitely make the LJ method converge to the real solution but it requires too much effort and the time limitation does not allow it. Thus, with further work, the LJ method could also return useful information.

Table 6: LJ Method Results

Q1	kH	kR	KA
Model A 600	0.0876	0.6444	0.4261
Model A 575	0.1259	0.0773	0.3467
Model B 600	0.1896	0.2715	0.5857
Model B 575	0.1610	0.9212	0.0468
Q2	ko	kp	
	1325	0.692	