# Problem 1: Newton Raphson

### **Problem Statement**

a

Using Newton-Raphson, solve the following system of equations in  $\mathbb{R}^2$ :

$$f_1(x) := 4x_2^2 + 4x_2 + 52x_1 - 19 = 0$$

$$f_2(x) := 169x_1^2 + 3x_2^2 + 111x_1 - 10x_2 - 10 = 0$$

starting from  $x^0 = (5,0)$ .

Report  $x^1$  and  $x^2$ . Terminate your iteration when the 2-norm of f is less than  $10^{-10}$ . Report if it does not converge in 100 iterations. If it converges, report  $x^*$  and the iteration count.

Plot the error magnitudes  $||x^k - x^*||$  as a function of k on a semilog plot.

b

Repeat (a), but with forward-difference approximation, using h = 0.5.

b

Repeat (a), but with center-difference approximation, using h = 0.5.

 $\mathbf{d}$ 

Repeat (a), but using Jacobian surrogates defined by Broyden's method. Clearly state how you start the sequence of Jacobian surrogates and how you choose  $x^1$ .

 $\mathbf{e}$ 

Vary the starting point appropriately and discuss qualitatively how the iterative process in parts a-d behave. If you have to choose between methods b-d, which one would you choose? Will this change if evaluation of f is much more computationally expensive?

#### Solution

#### a-e

See code at end of document for implementation, or my repo here:

Values requested  $(x^1, x^2)$ , iteration count) are reported in the subplot titles. Broyden's method used the center-difference approximation to initialize the Jacobian surrogate; scaled identity matrices tended to fail to converge, at least for these constraints. As such,  $x_1$  is chosen in the exact same fashion as the center-difference method. Specific to part (e), in general it appears that the symbolic and center difference approximation methods tend to behave *very* similarly, and typically converge in far fewer iterations than the forward-difference or Broyden's method; however, these methods also appear to fail in cases where the forward-difference and Broyden's method do not. This may simply be an artifact of the relatively low limit on iterations, but it is worth noting.

From this, for an arbitrary function, I'd probably pick Broyden's method (or some other quasi-Newton method), especially as the computational cost of each function evaluation increases. It requires only one evaluation of f per iterate (which can quickly become the most significant cost), and empirically demonstrates good convergence properties in this limited set of experiments.

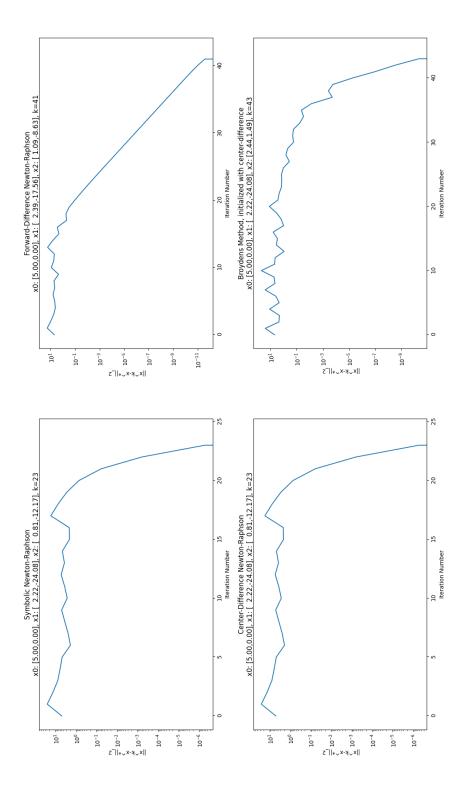


Figure 1: The four methods, started from (5,0)

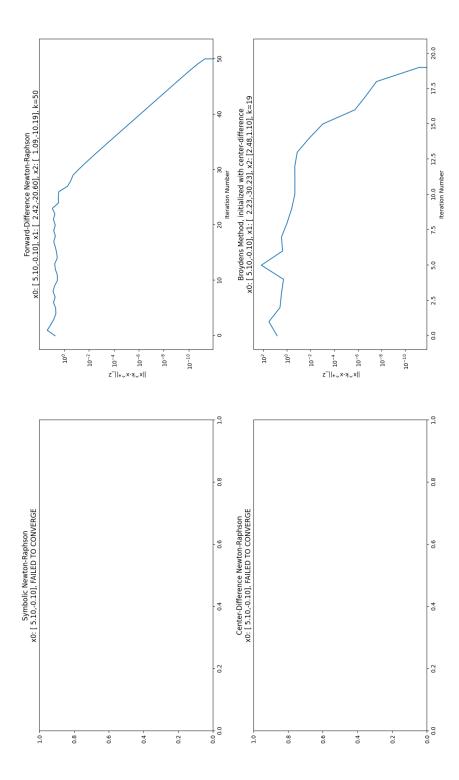


Figure 2: The four methods, started from (5.1, -0.1)

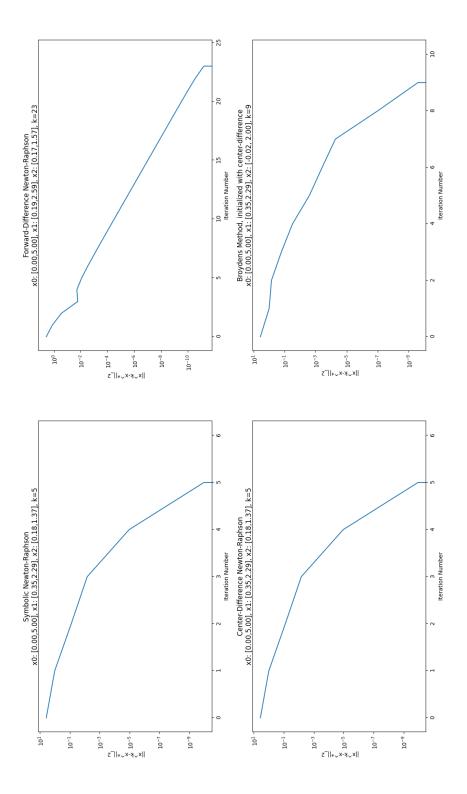


Figure 3: The four methods, started from (0,5)

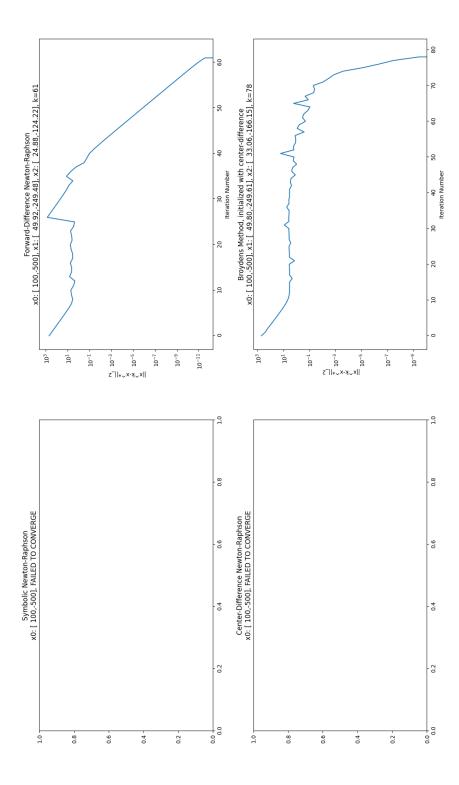


Figure 4: The four methods, started from (100, -500)

# Problem 2: Understanding Numerical Differentiation

## **Problem Statement**

We have empirically seen in class that the approximation quality of center difference approximation is far superior to that of forward and backward difference ones, when performing numerical differentiation. In this problem, we gain analytical insight into this behavior.

Suppose  $f: \mathbb{R} \to \mathbb{R}$  is at least  $C^3$  over [a, b]. The following Taylor's series expansion of f might be useful:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(\zeta)$$

 $\forall x, x + h \in (a, b)$  where  $\zeta$  lies on the line segment joining x and x + h.

a

Show that

$$\left| \frac{f(x+h) - f(x)}{h} - f'(x) \right| \le M|h| \forall x \in (a,b), M > 0$$

b

Show that

$$\left| \frac{f(x+h) - f(x-h)}{2h} - f'(x) \right| \le N|h|^2 \forall x \in (a,b), N > 0$$

 $\mathbf{c}$ 

Qualitatively discuss what the results in (a) and (b) mean.

#### Solution

 $\mathbf{a}$ 

Re-arrange the provided Taylor series expansion and take the absolute value of both sides:

$$\left| \frac{f(x+h) - f(x)}{h} - f'(x) \right| = \left| h(\frac{1}{2}f''(x) + \frac{1}{6}hf'''(\zeta)) \right| = |h| \left| \frac{1}{2}f''(x) + \frac{1}{6}hf'''(\zeta) \right|$$

Now we just need to bound the rightmost absolute value. From the class notes ("Solving nonlinear equations"), note that because  $\zeta$  lies on the line segment connecting a and b,  $\zeta \in [a, b]$ . Because the function is  $C^3$  over [a, b], there exists a scalar  $M_1$  and  $M_2$  that bounds f'' and f''' (repsectively) from above. So:

$$\left| \frac{1}{2}f''(x) + \frac{1}{6}hf'''(\zeta) \right| \le \left| \frac{1}{2}M_1 + \frac{1}{6}hM_2 \right|$$

Finally, because h is some fixed value, the whole quantity is bounded, and we can say:

$$\left| \frac{1}{2} M_1 + \frac{1}{6} h M_2 \right| \le M$$

$$\therefore \left| \frac{f(x+h) - f(x)}{h} - f'(x) \right| \le M|h|$$

b

We can modify the expansion to consider a negative h, or equivalently the subtraction of a positive h:

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(\zeta)$$

Then, subtract the two series to find: <sup>1</sup>

$$f(x+h) - f(x-h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(\zeta_1) - f(x) + hf'(x) - \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(\zeta_2)$$
$$= 2hf'(x) + \frac{h^3}{6}f'''(\zeta_1) + \frac{h^3}{6}f'''(\zeta_2)$$

Rearranging:

$$\frac{f(x+h) - f(x-h)}{2h} - f'(x) = \frac{h^2}{12}f'''(\zeta_1) + \frac{h^2}{12}f'''(\zeta_2)$$

$$\left| \frac{f(x+h) - f(x-h)}{2h} - f'(x) \right| = \left| \frac{h^2}{12}f'''(\zeta_1) + \frac{h^2}{12}f'''(\zeta_2) \right| = \left| h^2 \right| \left| \frac{1}{12}f'''(\zeta_1) + \frac{1}{12}f'''(\zeta_2) \right|$$

By the same logic as in (2.a), we know that  $f'''(\zeta_1)$  and  $f'''(\zeta_2)$  are upper bounded, so we can say:

$$\left| \frac{1}{12} f'''(\zeta_1) + \frac{1}{12} f'''(\zeta_2) \right| \le N$$

Thus:

$$\left| \frac{f(x+h) - f(x-h)}{2h} - f'(x) \right| \le |h^2| N$$

 $\mathbf{c}$ 

As the proofs show, there's a cancellation effect that occurs for some of the more significant error terms, resulting in the far better approximation (at least for "small" h). There's an "averaging" effect that reduces the error. Alternatively, for h < 1,  $|h^2|$  will be smaller than |h|.

Expanding on the numerical example provided in class, it's worth looking at it as a form of a statistical filter<sup>2</sup>. Some "signal" (the error of the approximation) is oversampled at a 2x rate and then is passed through an averaging filter. Assume that:

- 1. The samples are uncorrelated
- 2. The distribution of each sample is normal

which seems justified based on the numerical results presented in class. Then, letting  $X_i$  denote the distribution of the samples (where i = 1, 2), and  $\overline{X}$  denote the average (i.e. the output of the filter), we can say:

$$\operatorname{Var}(\overline{X}) = \operatorname{Var}\left(\frac{1}{N}\sum_{i=1}^{N}X_{i}\right) = \operatorname{Var}\left(\frac{1}{N}\sum_{i=1}^{N}X_{i}\right) = \frac{1}{N^{2}}\operatorname{Var}\left(\sum_{i=1}^{N}X_{i}\right) = \frac{1}{N^{2}}\sum_{i=1}^{N}\operatorname{Var}\left(X_{i}\right)$$

<sup>&</sup>lt;sup>1</sup>Credit to Bryan Wolhaupter for pointing out the  $\zeta_1 \neq \zeta_2$  and can't be called just  $\zeta$ .

<sup>&</sup>lt;sup>2</sup>Note: I'm not exactly a wizard at stats, take this with a grain of salt...i.e. this probably isn't correct:)

If the variances are the same  $(X_1 = X_2 = X)$ , then we get:

$$\operatorname{Var}(\overline{X}) = \frac{1}{2} \operatorname{Var}(X)$$

Now, this doesn't seem to imply quite the aggressive reduction in variance as demonstrated by the numerical example given in class, but it's at least a way to start thinking about how this works.

# **Code Listing**

```
import time
     import numpy as np
     import matplotlib.pyplot as plt
     14
15
            \begin{array}{ll} \textbf{return} & \texttt{np.array} \; (\, [\, \texttt{fx1} \; , \; \; \texttt{fx2} \, ] \, ) \end{array}
     17
18
19
20
21
            return ret
22
23
     def symbolic_newton(x):
25
26
              \begin{array}{lll} \textbf{def} & forward\_difference\_newton(x): \\ J = np.zeros((2, 2)) \\ J[:, 0] = (f(x + np.array([h, 0])) - f(x)) / h \\ J[:, 1] = (f(x + np.array([0, h])) - f(x)) / h \\ \end{array} 
28
29
30
31
33
             \begin{array}{lll} \textbf{return} & \textbf{x} - (\texttt{np.linalg.pinv}(\textbf{J}) & \textbf{@} & \textbf{f}(\textbf{x})) \end{array}
\frac{34}{35}
36
     {\color{red} \textbf{def} \hspace{0.1cm}} \texttt{center\_difference\_newton} \hspace{0.1cm} (x):
            \begin{array}{l} J = np.zeros\left((2\;,\;2)\right) \\ J[:,\;0] = \left(f(x+np.array([h,\;0])) - f(x-np.array([h,\;0]))\right) \;/\; (2\;*\;h) \\ J[:,\;1] = \left(f(x+np.array([0\;,\;h])) - f(x-np.array([0\;,\;h]))\right) \;/\; (2\;*\;h) \end{array} 
37
38
39
40
            \frac{\text{return } x - (\text{np.linalg.pinv}(J) @ f(x))}{}
42
43
     class BroydensMethod:
           def __init__(self, J0):
    self.J = J0
45
46
            def __call__(self, x):
    fx = f(x)
    dx = -np.linalg.solve(self.J, fx)
48
49
50
51
52
                   x.i = x + dx

dfx = f(x.i) - fx

self.J += np.outer((dfx - (self.J @ dx)), dx.T) / (
53
54
55
                  np.linalg.norm(dx, ord=2) ** 2
56
57
58
                   return x_i
59
60
     def solve_and_plot (
61
62
             iterator,
            x0: np.ndarray,
fig: plt.Figure,
ax: plt.Axes,
epsilon: float = 1e-10,
iter: int = 100,
63
64
65
66
67
68
        —> None:
            _ = fig
x = x0
xs = []
70
71
72
73
74
75
76
77
78
79
80
             xs.append(x0)
            t0 = time.time()
tf = np.inf
             converged = False
            k = 0 for i in range(iter):
                   try:
x = iterator(x)
                           eps = np.linalg.norm(f(x), ord=2)
                           if eps = hp.:naig.indim(f(x), bid=2)
xs.append(x)
if eps < epsilon:
    tf = time.time() - t0
    print(f"Converged at iteration {i+1}")
    converged = True</pre>
81
82
84
85
87
                                   break
              except Exception as e:
```

```
print(f"Exception occurred at iterate {i}")
   90
   92
   93
                                            print(f"Failed to converge in {iter} iterations!")
   94
   95
                            xs = np.array(xs)
                            errors = np.array(xs)
errors = np.array([np.linalg.norm(i, ord=2) for i in errors])
   96
   97
                            convert = lambda x: np.array2string(
    x, precision=2, separator=",", floatmode="fixed"
   98
   99
 100
                             if converged:
 102
                                          ax.semilogy(errors)
                                          ax.set_xlabel("Iteration Number")
ax.set_ylabel("||x^k-x^*||_2")
104
                                                         f"\{desc\}\nx0: \{convert(x0)\}, x1: \{convert(xs[1])\}, x2: \{convert(xs[2])\}, k=\{k\}", x2: \{convert(xs[2])\}, k=\{k\}", x3: \{convert(
106
                                                         pad=-20,
107
                            else
110
                                          ax.set_title(f"{desc}\nx0: {convert(x0)}, FAILED TO CONVERGE")
111
113
             if -name = "-main = ":
114
                                         = [
np.array([5.0, 0.0]),
np.array([5.1, -0.1]),
np.array([0.0, 5.0]),
np.array([100, -500]),
115
117
118
119
120
121
                           for x0 in x0s:
122
                                            fig , axes = plt.subplots(2, 2)
                                          fig.tight_layout() solve_and_plot("Symbolic Newton-Raphson", symbolic_newton, x0, fig, axes[0, 0])
123
124
 125
                                          solve_and_plot(
    "Forward-Difference Newton-Raphson",
126
127
 128
                                                          forward\_difference\_newton\ ,
                                                         x0,
                                                         fig,
131
                                                         axes[0, 1],
                                          )
133
                                          solve_and_plot(
    "Center-Difference Newton-Raphson",
134
135
136
                                                          center_difference_newton ,
                                                         x0,
137
                                                         fig,
                                                         axes[1, 0],
139
140
                                           \begin{array}{l} J0 = np.zeros\left((2\,,\,2)\right) \\ J0\,[:\,,\,\,0] = \left(f\left(x0\,+\,np.array\left(\left[h\,,\,\,0\right]\right)\right)\,-\,f\left(x0\,-\,np.array\left(\left[h\,,\,\,0\right]\right)\right)\right)\,/\,\left(2\,*\,h\right) \\ J0\,[:\,,\,\,1] = \left(f\left(x0\,+\,np.array\left(\left[0\,,\,h\right]\right)\right)\,-\,f\left(x0\,-\,np.array\left(\left[0\,,\,h\right]\right)\right)\right)\,/\,\left(2\,*\,h\right) \\ print \left(f^{"}Broyden's \;Method\;\,J0:\\ \backslash n\{J0\}"\right) \\ \endalign{\column}
142
143
145
146
                                            solve_and_plot (
                                                                                              Method
                                                                                                                           initialized with center-difference",
                                                         BroydensMethod (J0),
148
149
                                                         x0,
 150
                                                         axes[1, 1],
151
152
                            plt.show()
154
```