Assignment 2: Results/Description

Problem 1

Let $\{f_i(\boldsymbol{x})\}$ be the system of nonlinear equations for which we wish to find a root. Then we may introduce $\boldsymbol{f}(\boldsymbol{x})$ comprised of components f_i that satisfies

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}.$$

Let $\boldsymbol{\xi}$ be the root of $\boldsymbol{f}(\boldsymbol{x})$. Then one may Taylor expand around $\boldsymbol{\xi}$ so that

$$\begin{aligned} 0 &= f_i(\boldsymbol{\xi}) \\ &= f_i(\boldsymbol{x}) + \sum_j (\xi_j - x_j)\partial_j f_i(\boldsymbol{x}) + \mathcal{O}(|\boldsymbol{\xi} - \boldsymbol{x}|^2) \\ \Rightarrow \boldsymbol{0} &\approx \boldsymbol{f}(\boldsymbol{x}) + \boldsymbol{J}(\boldsymbol{x})(\boldsymbol{\xi} - \boldsymbol{x}) \end{aligned}$$

for $J_{ij} = \partial_j f_i(\boldsymbol{x})$. Here we assume we may neglect the quadratic and higher order terms, assuming $|\boldsymbol{\xi} - \boldsymbol{x}|$ is small. Therefore, rearranging this gives

$$\boldsymbol{\xi} \approx \boldsymbol{x} - \boldsymbol{J}^{-1}(\boldsymbol{x})\boldsymbol{f}(\boldsymbol{x}),$$

assuming $\boldsymbol{J}$ is invertible. Using iteration to make this approximation converge to the true value of $\boldsymbol{\xi}$, this means

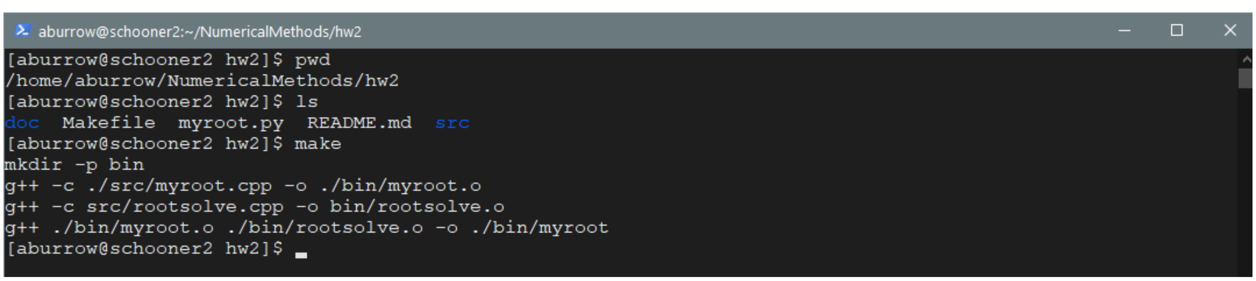
$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \boldsymbol{J}^{-1}(\boldsymbol{x}_k)\boldsymbol{f}(\boldsymbol{x}_k).$$

for iteration index k.

Problem 2

(a)

I've written this program to solve the system of equations, which is the attached "./bin/myroot". This should compile with `make` as shown below.



```
aburrow@schooner2:~/NumericalMethods/hw2
[aburrow@schooner2 hw2]$ pwd
/home/aburrow/NumericalMethods/hw2
[aburrow@schooner2 hw2]$ ls
doc  Makefile  myroot.py  README.md  src
[aburrow@schooner2 hw2]$ make
mkdir -p bin
g++ -c ./src/myroot.cpp -o ./bin/myroot.o
g++ -c src/rootsolve.cpp -o bin/rootsolve.o
g++ ./bin/myroot.o ./bin/rootsolve.o -o ./bin/myroot
[aburrow@schooner2 hw2]$
```

This program makes use of the Newton-Raphson method derived in Problem 1. Here I have analytically found $\boldsymbol{J}(\boldsymbol{x})$ with $\boldsymbol{x} = (x, y)^\mathsf{T}$ to be

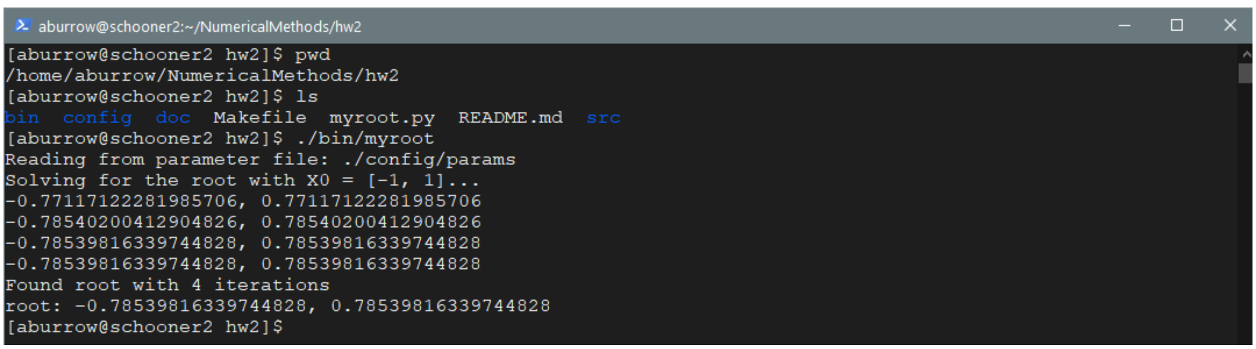
$$\boldsymbol{J}(\boldsymbol{x}) = \begin{pmatrix} \cos(x+y) & \cos(x+y) \\ -\sin(x-y) & \sin(x-y) \end{pmatrix}$$

and for the sake of computation speed in the program I use the inverse,

$$\boldsymbol{J}^{-1}(\boldsymbol{x}) = \frac{1}{2\cos(x+y)\sin(x-y)} \begin{pmatrix} \sin(x-y) & -\cos(x+y) \\ \sin(x-y) & \cos(x+y) \end{pmatrix}.$$

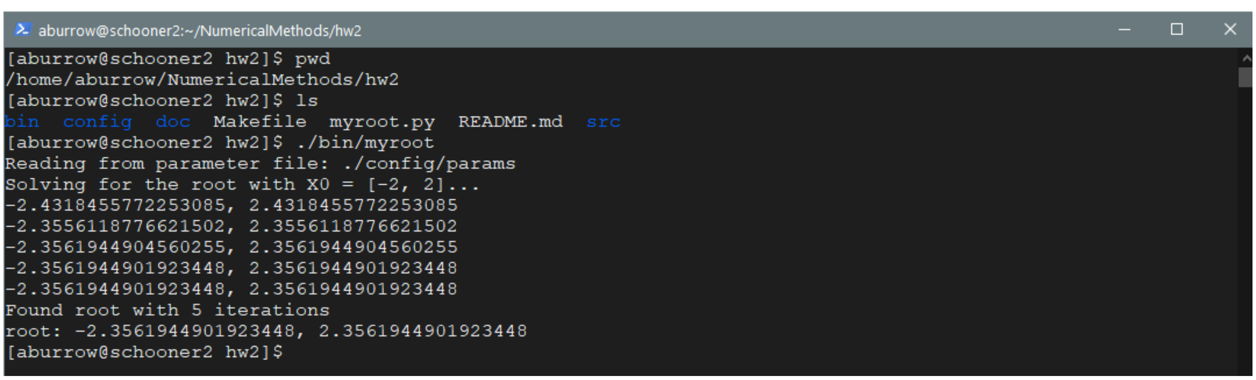
The main problem here is determining the initial approximation $\boldsymbol{x}_0$. x and y need to be such that one is between 0 and π, while the other is between $-\pi$ and 0, at least I have found through basic testing. This is because in the iteration step, if $\boldsymbol{x}_0$ is not on the same scale as outputs to the periodic sin and cos functions, it attempts to overcorrect and fails to converge to a single result.

In addition, there are 4 roots that this program finds with initial conditions within these bounds. With $\boldsymbol{x}_0 = (-1, 1)^\mathsf{T}$ for example, where $|x|, |y| < \pi/2$, the program yields two roots which are effectively $x = \pi/4$ and $y = -\pi/4$:



```
aburrow@schooner2:~/NumericalMethods/hw2
[aburrow@schooner2 hw2]$ pwd
/home/aburrow/NumericalMethods/hw2
[aburrow@schooner2 hw2]$ ls
bin  config  doc  Makefile  myroot.py  README.md  src
[aburrow@schooner2 hw2]$ ./bin/myroot
Reading from parameter file: ./config/params
Solving for the root with X0 = [-1, 1]...
-0.77117122281985706, 0.77117122281985706
-0.78540200412904826, 0.78540200412904826
-0.78539816339744828, 0.78539816339744828
-0.78539816339744828, 0.78539816339744828
Found root with 4 iterations
root: -0.78539816339744828, 0.78539816339744828
[aburrow@schooner2 hw2]$
```

When $\pi/2 < |x|, |y| < \pi$, where in this case $\boldsymbol{x}_0 = (-2, 2)^\mathsf{T}$, the other two roots ($x = 3\pi/4$ and $y = -3\pi/4$) are found:



```
aburrow@schooner2:~/NumericalMethods/hw2
[aburrow@schooner2 hw2]$ pwd
/home/aburrow/NumericalMethods/hw2
[aburrow@schooner2 hw2]$ ls
bin  config  doc  Makefile  myroot.py  README.md  src
[aburrow@schooner2 hw2]$ ./bin/myroot
Reading from parameter file: ./config/params
Solving for the root with X0 = [-2, 2]...
-2.4318455772253085, 2.4318455772253085
-2.3556118776621502, 2.3556118776621502
-2.3561944904560255, 2.3561944904560255
-2.3561944901923448, 2.3561944901923448
-2.3561944901923448, 2.3561944901923448
Found root with 5 iterations
root: -2.3561944901923448, 2.3561944901923448
[aburrow@schooner2 hw2]$
```

Numerically, we find these roots to be

$$\begin{pmatrix} -0.78539816339744828 \\ 0.78539816339744828 \end{pmatrix}$$

and

$$\begin{pmatrix} -2.3561944901923448 \\ 2.3561944901923448 \end{pmatrix}.$$

Each estimate of the root is shown, and a final value is reached when the difference between the new and old estimates are machine zero.

(b)

I solved this problem in Python as well ("./myroot.py"), using SciPy's `scipy.optimize.fsolve` function. Using the same two sets of initial conditions, it was able to solve the same roots to the same (double) precision:

```
Python roots:
-0.78539816339744828, 0.78539816339744828
-2.3561944901923448, 2.3561944901923448
[Finished in 0.5s]
```

Typically Python can be used to perform the same calculations for these simple problems (as we saw, it only takes 5 iterations to find a decent result). This is true especially when you are able to vectorize the problem so that one may take advantage of Numpy's C-based functionality. However its flexibility makes it quite burdensome to perform heavy calculations with more complicated problems.