Homework No.2, 553.481, Due February 19, 2021.

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Problem 1. (a) Compute $\sqrt{3}$ by using the bisection method to solve the equation $x^2 = 3$ on $[1, 2]$ with tolerance set to $tol = 10^{-15}$. State the total number of iterations required and also the wall clock time (obtained in Matlab with `tic` and `toc` commands). Rewrite the Matlab script `bisect.m` to save the sequence of iterates and use these to estimate the constants c and p in the asymptotic error relation

$$e_{n+1} \sim c\, e_n^p$$

where $e_n = |\sqrt{3} - x_n|$ is the error of the nth iterate. You can obtain these constants by plotting $\ln e_{n+1}$ versus $\ln e_n$ and using `polyfit` in Matlab to fit a straight line. Compare your numerical results to the theoretical estimates for both c and p.

Solution: I listed the data. Note that the $\hat{p}, \hat{c}$ corresponds to the empirical values, and the non-hatted ones refers to the theoretical values.
Elapsed time is 0.000280 seconds.
max iteration = 50
$\hat{p} = 0.9871883, \hat{c} = 0.3995903$
$p = 1, c = 0.5.$

(b) Repeat part (a) for the Newton method with initial guess $x_0 = 1$.

Solution:
Elapsed time is 0.004642 seconds.
max iteration = 6
$\hat{p} = 2.031644, \hat{c} = 0.3586279$
$p = 2, c = M \leq \frac{\max_{x\in[1,2]} |2|}{2 \min_{x\in[1,2]} |2x|} = 0.5.$

(c) Repeat part (a) for the secant method with initial guess $a = 1$ and generate b with the Newton method (counting this as the first iteration for secant).

Solution:
Elapsed time is 0.002940 seconds.
max iteration = 8
$\hat{p} = 1.619750, \hat{c} = 0.4791629$
$p = \phi \approx 1.618, c = M^{\phi-1} = 0.359^{0.618} = 0.5305.$

(d) Repeat part (a) for the IQI method with initial guess $a = 1$ and generate b with the Newton method and c with the secant method (counting these as the first and second iterations for IQI).

Solution:
Elapsed time is 0.005338 seconds.
max iteration = 7
$\hat{p} = 1.589099, \hat{c} = 0.1696900$
$p = 1.84, c = 0.5$

Problem 2. (a) Find a condition on the initial guess x_0 so that Newton's method for solving $f(x) := \frac{x^2}{1+x^2} = 0$ diverges. Verify numerically that the method diverges when this condition is satisfied.

Solution: Through trial an error, I was able to find that Newton's method will diverge for $|x_0| \geq \sqrt{3}$.

(b) Consider now an initial guess x_0 for which Newton's method does converge and use your numerical results to estimate the asymptotic rate of convergence. Explain how your results are consistent with theoretical estimates for convergence rates of Newton's method.

Solution: I used the method from problem 1 to estimate a convergence rate with constants $p = 0.9561527, c = 0.4111649$, which means there is linear convergence. This is because the root has multiplicity of 2. Newton's method only converges quadratically for roots with multiplicity of 1.

Problem 3. Given below is a table of iterates from a linearly convergent iteration $x_{n+1} = g(x_n)$. Estimate from this data (a) the rate of linear convergence, (b) the error $x_7 - x_*$ and (c) the fixed point x_*.

n	x_n
0	4.0000000
1	0.2893402
2	0.7303450
3	0.5920853
4	0.6253791
5	0.6168039
6	0.6189751
7	0.6184230

Given that the true fixed point is $x_* = 0.618534836105584$ to 16 decimals, compare your best estimates for x_* and the error $x_7 - x_*$ with the true values.

Solution: I estimate the linear rate of convergence at $\lambda_* \approx \lambda_7 = -0.2542$, the error to be $err \approx \frac{x_7 - x_6}{1-\lambda_7} = -4.4017e-04$, and $x_* \approx x_7 - err = 0.61886$. Since the true values are $x_* = 0.618534836105584$ and $err_* = x_7 - x_* = -1.1183e-04$, the estimates deviate from the true values on the order of $10e-4$.

Problem 4. Show that the iterative method to solve $f(x) = 0$ given by:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} - \frac{f''(x_n)}{2f'(x_n)} \left[\frac{f(x_n)}{f'(x_n)}\right]^2,$$

for $n = 1, 2, \cdots$, will generally yield cubic convergence.

Solution: Suppose we have a function with sufficient differentiability over some interval, $f \in C^3(I)$, and we want to find some simple root in that interval, i.e. $f(x_*) \in I, f'(x_*) \neq 0$. Then there exists some $\epsilon > 0$, and $x_0 \in (x_* - \epsilon, x_* + \epsilon)$ for which $x_n \to x_*$ as $n \to \infty$. More over, this will converge with a cubic rate. For some constant M:

$$\lim_{n\to\infty} \frac{x_{n+1} - x_*}{(x_n - x_*)^3} = M$$

First, we can derive through Taylor's theorem an approximation for a root. Using Taylor's theorem we get the approximation and remainder:

$$f(x_*) = 0 \approx f(x_n) + f'(x_n)(x_* - x_n) + \frac{f''(x_n)}{2!}(x_* - x_n)^2$$
$$R = \frac{f'''(\xi)}{3!}(x_* - x_n)^3$$

However, we use the x_* term in the second order term of the approximation, which we obviously do not have. By substituting the first order approximation to the series we get:

$$0 = f(x_n) + f'(x_n)(x_{n+1} - x_n) + \frac{f''(x_n)}{2!}\left[\frac{f(x_n)}{f'(x_n)}\right]^2$$
$$R = \frac{f'''(\xi)}{3!}(x_* - x_n)^3 + \left[\frac{f''(\zeta)}{2!}(x_* - x_n)^2\right]^2$$

We must add a term to the remainder to account for the substitution we made. Now we must solve for the next term:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} + \frac{f''(x_n)}{2f'(x_n)}\left[\frac{f(x_n)}{f'(x_n)}\right]^2$$
$$R = \frac{f'''(\xi)}{6f'(x_n)}(x_* - x_n)^3 + \left[\frac{f''(\zeta)}{2f'(x_n)}\right]^2 (x_* - x_n)^4$$

We want to show that the remainder stays finite after may iterations. It can only become infinite if $f'(x_n) \to 0$. But we know from the assumptions that $f'(x_*) \neq 0$, so there exists some interval $J = [x_* - \delta, x_* + \delta]$ for which $f'(x) \neq 0$. We also want to ensure stability. Since we already know the remainder must stay finite in this interval, let us approximate the remainder as a cubic error and ignore the fourth power, we can do this because the asymptotic bound of a fourth power will be lower than the asymptotic bound of a third power. So now we want to ensure for some arbitrary M, we can guarantee that at each subsequent approximation the remainder grows smaller. We can express this as:

$$R_{n+1} = |M[x_{n+1} - x_*]|^3 \leq |M[x_n - x_*]| = R_n$$

We see that for any M, we can see that if $|x_* - x_n| < \frac{1}{M}$, the statement is true. So we will have stability if we pick some x_n such that $|x_* - x_n| < min\delta, \frac{1}{M}$. Hence we have shown stability. Now we show convergence. We have already shown that $|Me_{n+1}|^3 \leq |Me_n|$, if we pick x_n some interval. Assume we pick x_0 in this interval as well. Then the base case will be true and the induction will follow. Hence the series converges.

Problem 5. (a) Verify that the Sherman-Morrison formula is correct by checking that

$$\left[\mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{x}\mathbf{y}^\top\mathbf{A}^{-1}}{1 + \langle \mathbf{y}, \mathbf{A}^{-1}\mathbf{x}\rangle}\right](\mathbf{A} + \mathbf{x}\mathbf{y}^\top) = \mathbf{I}.$$

Solution: We can verify this below:

$$\begin{aligned}
&\left[\mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{x}\mathbf{y}^\top\mathbf{A}^{-1}}{1+\langle \mathbf{y}, \mathbf{A}^{-1}\mathbf{x}\rangle}\right](\mathbf{A}+\mathbf{x}\mathbf{y}^\top) \\
&= \mathbf{A}^{-1}(\mathbf{A}+\mathbf{x}\mathbf{y}^\top) - \frac{\mathbf{A}^{-1}\mathbf{x}\mathbf{y}^\top\mathbf{A}^{-1}}{1+\langle \mathbf{y}, \mathbf{A}^{-1}\mathbf{x}\rangle}(\mathbf{A}+\mathbf{x}\mathbf{y}^\top) \\
&= \mathbf{I} + \langle \mathbf{y}, \mathbf{A}^{-1}\mathbf{x}\rangle - \frac{\langle \mathbf{y}, \mathbf{A}^{-1}\mathbf{x}\rangle + \langle \mathbf{y}, \mathbf{A}^{-1}\mathbf{x}\rangle^2}{1+\langle \mathbf{y}, \mathbf{A}^{-1}\mathbf{x}\rangle} \\
&= \mathbf{I}
\end{aligned}$$

(b) Use the Sherman-Morrison formula to verify that the approximation $D\mathbf{f}(\mathbf{x}_n) \doteq \mathbf{A}_n$ used in Broyden's method has an inverse $\mathbf{A}_n^{-1}$ that can be iterated with the formulas

$$\Delta\mathbf{p}_{n-1} = \mathbf{A}_{n-1}^{-1}\Delta\mathbf{f}_{n-1}, \quad \mathbf{A}_n^{-1} = \mathbf{A}_{n-1}^{-1} + \frac{(\Delta\mathbf{x}_{n-1} - \Delta\mathbf{p}_{n-1})\,\Delta\mathbf{x}_{n-1}^\top\mathbf{A}_{n-1}^{-1}}{\langle \Delta\mathbf{x}_{n-1}, \Delta\mathbf{p}_{n-1}\rangle}$$

where $\Delta\mathbf{x}_{n-1} = \mathbf{x}_n - \mathbf{x}_{n-1}$ and $\Delta\mathbf{f}_{n-1} = \mathbf{f}(\mathbf{x}_n) - \mathbf{f}(\mathbf{x}_{n-1})$.

Solution: First, we write down the method for iteratively approximating the Jacobean of a systems of equations:

$$\begin{aligned}
\mathbf{A}_n &= \mathbf{A}_{n-1} + \frac{[\mathbf{f}(\mathbf{x}_n) - \mathbf{f}(\mathbf{x}_{n-1}) - \mathbf{A}_{n-1}(\mathbf{x}_n - \mathbf{x}_{n-1})](\mathbf{x}_n - \mathbf{x}_{n-1})^\top}{||\mathbf{x}_n - \mathbf{x}_{n-1}||^2} \\
&= \mathbf{A}_{n-1} + \frac{[\Delta\mathbf{f}_{n-1} - \mathbf{A}_{n-1}\Delta\mathbf{x}_{n-1}]}{||\Delta\mathbf{x}_{n-1}||^2}\Delta\mathbf{x}_{n-1}^\top
\end{aligned}$$

Using this formulation, we can write the inverse as:

$$\mathbf{A}_n^{-1} = \left(\mathbf{A}_{n-1} + \frac{[\Delta\mathbf{f}_{n-1} - \mathbf{A}_{n-1}\Delta\mathbf{x}_{n-1}]}{||\Delta\mathbf{x}_{n-1}||^2}\Delta\mathbf{x}_{n-1}^\top\right)^{-1}$$

Now, let us restate the Sherman Morris Theorem as:

$$\mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{x}\mathbf{y}^\top\mathbf{A}^{-1}}{1+\langle \mathbf{y}, \mathbf{A}^{-1}\mathbf{x}\rangle} = (\mathbf{A}+\mathbf{x}\mathbf{y}^\top)^{-1}$$

If we make substitutions into the Sherman Morris theorem, we can get the form of the inverse. Let $\mathbf{A} = \mathbf{A}_{n-1}$, $\mathbf{y} = \Delta\mathbf{x}_{n-1}$, $\mathbf{x} = \frac{\Delta\mathbf{f}_{n-1} - \mathbf{A}_{n-1}\Delta\mathbf{x}_{n-1}}{||\Delta\mathbf{x}_{n-1}||^2}$. We rewrite the theorem using these substitutions and make simplifications:

$$\begin{aligned}
&\left(\mathbf{A}_{n-1} + \frac{[\Delta\mathbf{f}_{n-1} - \mathbf{A}_{n-1}\Delta\mathbf{x}_{n-1}]}{||\Delta\mathbf{x}_{n-1}||^2}\Delta\mathbf{x}_{n-1}^\top\right)^{-1} \\
&= \mathbf{A}_{n-1}^{-1} - \frac{\mathbf{A}_{n-1}^{-1}(\frac{\Delta\mathbf{f}_{n-1} - \mathbf{A}_{n-1}\Delta\mathbf{x}_{n-1}}{||\Delta\mathbf{x}_{n-1}||^2})\Delta\mathbf{x}_{n-1}^\top\mathbf{A}_{n-1}^{-1}}{1 + \langle \Delta\mathbf{x}_{n-1}, \mathbf{A}_{n-1}^{-1}(\frac{\Delta\mathbf{f}_{n-1} - \mathbf{A}_{n-1}\Delta\mathbf{x}_{n-1}}{||\Delta\mathbf{x}_{n-1}||^2})\rangle} \\
&= \mathbf{A}_{n-1}^{-1} - \frac{(\mathbf{A}_{n-1}^{-1}\Delta\mathbf{f}_{n-1} - \Delta\mathbf{x}_{n-1})\Delta\mathbf{x}_{n-1}^\top\mathbf{A}_{n-1}^{-1}}{||\Delta\mathbf{x}_{n-1}||^2 + \langle \Delta\mathbf{x}_{n-1}, \mathbf{A}_{n-1}^{-1}(\Delta\mathbf{f}_{n-1} - \mathbf{A}_{n-1}\Delta\mathbf{x}_{n-1})\rangle} \\
&= \mathbf{A}_{n-1}^{-1} - \frac{(\Delta\mathbf{p}_{n-1} - \Delta\mathbf{x}_{n-1})\Delta\mathbf{x}_{n-1}^\top\mathbf{A}_{n-1}^{-1}}{||\Delta\mathbf{x}_{n-1}||^2 + \langle \Delta\mathbf{x}_{n-1}, \Delta\mathbf{p}_{n-1}\rangle - ||\Delta\mathbf{x}_{n-1}||^2} \\
&= \mathbf{A}_{n-1}^{-1} + \frac{(\Delta\mathbf{x}_{n-1} - \Delta\mathbf{p}_{n-1})\Delta\mathbf{x}_{n-1}^\top\mathbf{A}_{n-1}^{-1}}{\langle \Delta\mathbf{x}_{n-1}, \Delta\mathbf{p}_{n-1}\rangle}
\end{aligned}$$

Putting these two parts together, we get:

$$\mathbf{A}_n^{-1} = \mathbf{A}_{n-1}^{-1} + \frac{(\Delta\mathbf{x}_{n-1} - \Delta\mathbf{p}_{n-1})\,\Delta\mathbf{x}_{n-1}^{\top}\mathbf{A}_{n-1}^{-1}}{\langle \Delta\mathbf{x}_{n-1}, \Delta\mathbf{p}_{n-1}\rangle}$$

Problem 6. Use both Newton-Raphson and Broyden's methods for a starting vector $(x^{(0)}, y^{(0)}, z^{(0)}) = (-1, -1, 2)$ to approximate the solution of the following system of equations to tolerance $tol = 10^{-15}$:

$$\begin{cases} x + \cos(xyz) - 1 = 0 \\ (1-x)^{1/4} + y + \frac{1}{20}z^2 - \frac{3}{20}z - 1 = 0 \\ -x^2 - \frac{1}{10}y^2 + \frac{1}{100}y + z - 1 = 0 \end{cases}$$

Compare the number of iterations and also the wall clock time required for this accuracy with the two methods. In order to make a more accurate estimate of the relative clock time, repeat the root-finding a large number of times N_{repeat} for both methods (in the same loop) and average over the repeated trials.

Solution: Both method yield the same approximation: $x_* = [0, 0.1, 1]$. The Newton Raphson method takes 7 iterations to converge while Broyden's method takes 16. I ran both methods 100 times together in a loop. The average run times were as follows: Newton Raphson Average Time = 0.000642, Broyden Average Time = 0.000627. We can see that even through the Newton Raphson method converges in fewer iterations because of its higher order convergence, Broyden's method is generally faster because the inverse matrix is easier to calculate.