Homework 6.

Amath 301
Beginning Scientific Computing

Due: 5/9/23 at 11:59pm to Gradescope

Directions:

For the **written exercises** of the homework, please do the following:

- Write your name, student number, and section at the top of your written exercises. A half point will be deducted if these are not included.
- Complete all written exercises to the best of your ability and as neatly as possible.
- For those who are writing their answers by hand, please scan your work and save it as a pdf file.
- You are encouraged to type your written homework using LaTeX. Doing so will earn you a half bonus point. Check out my LaTeX beginner document and overleaf.com if you are new to LaTeX.

For the **coding exercises** of the homework, please do the following:

- Create a MATLAB script titled `hw6.m` and divide your script into sections according to the various coding exercises.
- Make sure your final answers in each coding exercise are assigned to the correct variable names.
- Publish your script as a pdf file. You can do this by typing `publish('hw6.m','pdf')` in the Command Window.
- Attach your published code to the end of your written exercises. Submit your entire homework assignment (written + coding exercises) to Gradescope.

Pro-Tips:

- You can check many of your answers to the written exercises of this homework by having MATLAB, Wolfram Alpha, or Chat GPT do the calculations for you.
- Teamwork makes the dream work, but please make sure you write up your solutions.
- Don't wait until the last minute. ☺

Written Exercises

(13 points total)

Exercise 1. (Component Skill 6.1)

A tornado passes over a weather station with a barometer that was recording atmospheric pressure as a function of time[1]. Several weeks after the storm passed and clean-up efforts concluded, meteorologists at the weather station fit the pressure data to a curve and found the following relationship:

$$p(t) = 1 - \frac{12t}{57 + 16(t-2)^2}.$$

Here, t is time in minutes after the tornado sirens first went off, and $p(t)$ is the atmospheric pressure (measured in standard atmospheres) at the weather station. The tornado destroyed the barometer after $t = 3$ minutes, so the relationship above is valid only for $0 \le t \le 3$.

a. Is $p(t)$ a unimodal function over $0 \le t \le 3$? Justify your answer by finding the critical point(s) of $p(t)$ over the interval $0 \le t \le 3$.

   Hint: Please use Wolfram Alpha to calculate $p'(t)$.

b. Show that your critical point from (b) is a local minimum using the second derivative test.

   Hint: Please use Wolfram Alpha to calculate $p''(t)$.

c. What is the minimum pressure recorded at the weather station over $0 \le t \le 3$? Don't forget to check the boundaries of the interval!

d. What is the maximum pressure recorded at the weather station over $0 \le t \le 3$? Don't forget to check the boundaries of the interval!

e. The tornado is right on top of the weather station when the pressure is minimized. At what time does the tornado arrive at the weather station?

Exercise 2. (Component Skills 6.2-6.3)

Consider the function

$$f(x) = |x - 1|$$

defined over the interval $-2 \le x \le 6$.

a. Perform three iterations of the three-point equal interval search by hand. What interval is guaranteed to contain the value of x that corresponds to the minimum of f after three iterations of the three-point equal interval search?

[1] Ironic, I know.

b. Perform one iteration of successive parabolic interpolation if f is sampled initially at $x_1 = 0$, $x_2 = 2$, and $x_3 = 4$. Based on this one iteration, at what value of x does f attain a minimum?

Exercise 3. (Component Skill 6.4)

Consider the quadratic polynomial

$$f(x) = ax^2,$$

with free parameter $a > 0$. Clearly, this quadratic has a global minimum at $x = 0$.

a. Set $a = 1$. Perform three iterations of gradient descent by hand with initial guess $x_0 = 1$ and learning rate $\gamma = 1/4$. Does gradient descent appear to be converging?

b. Set $a = 1$. Perform three iterations of gradient descent by hand with initial guess $x_0 = 1$ and learning rate $\gamma = 1$. Does gradient descent appear to be converging?

c. According to Theorem 6.4.1 in the weekly lecture notes, the learning rate γ must be strictly less than $1/L$ for gradient descent to converge, where L is the maximum of $|f''(x)|$. Use this theorem to explain why (a) converged and (b) did not.

d. According to Theorem 6.4.2 in the weekly lecture notes,

$$|f(x_k) - f(x_*)| \leq \frac{(x_0 - x_*)^2}{2\gamma k},$$

where x_* is the exact x-coordinate of the minimum, x_k is the kth iterate of gradient descent, x_0 is the initial guess, and γ is the learning rate. The expression on the LHS of this inequality can be thought of as the error between the exact minimum of f and what gradient descent predicts is the minimum of f after k iterations.

Given $f(x) = x^2$, $x_0 = 1$, $x_* = 0$, and $\gamma = 1/4$, how many iterations of gradient descent are necessary to guarantee that $|f(x_k) - f(x_*)| < 10^{-15}$?

Hint: Find the exact k such that the RHS of the inequality equals 10^{-15}.

Coding Exercises

(7 points total)

Exercise 1. (Component Skills 6.2-6.4)

A seminal breakthrough in HIV treatment was the use of multiple-drug combination therapy. The idea behind the therapy is that multiple drugs, when introduced to the body at specific times, fight the virus off better than one drug alone. A key step in the development of multiple-drug therapy was to determine the best time to take the next drug. One way this is done is to take the next drug when the previous drug is at its maximum concentration in the body.

Suppose the concentration of the first drug in the therapy is modeled by

$$x(t) = \frac{10}{3}\left(e^{-\frac{t}{24}} - e^{-\frac{t}{2}}\right).$$

Here, $x(t)$ represents the concentration of the first drug in the body (in mol/L) and t is time in hours since the initial injection of the first drug. Assume that we want to administer our second drug when $x(t)$ is at its maximum. Let's call this time $t_{\max}$.

a. In order to find $t_{\max}$, we need to convert this maximization problem into a minimization problem. This can be done by introducing

$$y(t) = -x(t).$$

Note that the minimum of $y(t)$ occurs at $t = t_{\max}$.

Copy my function file `threePtSearch` from the weekly lecture notes. Place this function file at the very bottom of your `hw6.m` script. Modify this function to return not only the variable `int`, but also the number of iterations `N` needed to achieve the desired error threshold. Use this function to compute a three-point equal interval search for the minimum of $y(t)$ over the interval $0 \leq t \leq 12$. Set the error threshold to $\varepsilon = 10^{-3}$.

Assign the variable `A1` to the interval returned by the `threePtSearch` function. Assign `A2` to the midpoint of `A1`. Assign the variable `A3` to the number of iterations of the three-point equal interval search.

Answers:

```
A1 =

   5.421386718750000   5.422119140625000


A2 =

   5.421752929687500


A3 =

    14
```

b. Copy my function file `succParInt` from the weekly lecture notes. Place this function file at the very bottom of your `hw6.m` script. Modify this function to return not only the variable `int`, but also the number of iterations `N` needed to achieve the desired error threshold. Use this function to compute find the minimum of $y(t)$ by successive parabolic interpolation. Set the initial sample points to be $t_1 = 3$, $t_2 = 6$, and $t_3 = 9$. Set the error threshold to $\varepsilon = 10^{-3}$.

Assign the variable `A4` to the interval returned by the `threePtSearch` function. Assign `A5` to the midpoint of `A4`. Assign the variable `A6` to the number of iterations of the successive parabolic interpolation.

Answers:

```
A4 =

   5.421500262090861   5.421629449508848


A5 =

   5.421564855799854


A6 =

     8
```

c. Copy my function file `gradDescent` from the weekly lecture notes. Place this function file at the very bottom of your `hw6.m` script. Calculate $y'(t)$ by hand. (You don't have to show your work for this.) Use $y'(t)$ to perform gradient descent on $y(t)$. Take the initial guess for the minimum to be $t_0 = 1$. Set the learning rate to be $\gamma = 20$ and the Cauchy error threshold to be $\varepsilon = 10^{-3}$.

Assign the variable `A7` to the value of the minimum of $y(t)$ according to gradient descent.

Answers:

```
A7 =

  5.421617885770670
```