# PHYS 3142 Spring 2019
# Computational Methods in Physics
# Assignment 4
# Due: 1st April 2019

Before you submit your assignment, do remember:

1. the due day
2. submit a report which contains your figures and results
3. make sure your code can run
4. do not upload a compressed file(e.g. rar, zip, ...)

**(1) Relaxation** Consider the equation $x = 1 - e^{-cx}$, where c is a known parameter and x is unknown. This equation arises in a variety of situations, including the physics of contact processes, mathematical models of epidemics, and the theory of random graphs.

(1)Write a program to solve this equation for x using the relaxation method for the case $c = 3$. Calculate your solution to an accuracy of at least $10^{-6}$.

(2)Modify your program to calculate the solution for values of c from 0 to 4 in steps of 0.02 and make a plot of x as a function of c. You should see a clear transition from a regime in which $x = 0$ to a regime of nonzero x. This is another example of a phase transition. In physics this transition is known as the percolation transition; in epidemiology it is the $epidemicthreshold$.

**(2) Overrelaxation** You should do Q.1 before this one. The ordinary relaxation method involves iterating the equation $x' = f(x)$, starting from an initial guess, until it converges. As we have seen, this is often a fast and easy way to find solutions to nonlinear equations. However, it is possible in some cases to make the method work even faster using the technique of overrelaxation. Suppose our initial guess at the solution of a particular equation is, say, $x = 1$, and the final, true solution is $x = 5$. After the first step of the iterative process, we might then see a value of, say, $x = 3$. In the overrelaxation method, we observe this value and note that x is increasing, then we deliberately overshoot the calculated value, in the hope that this will get us closer to the final solution: in this case we might pass over $x = 3$ and go straight to a value of $x = 4$ perhaps, which is closer to the final solution of $x = 5$ and hence should get us to that solution quicker. The overrelaxation method provides a formula for performing this kind of overshooting in a controlled fashion and often, though not always, it does get us to our solution faster. In detail, it works as follows. We can rewrite the equation $x' = f(x)$ in the form $x' = x + \delta x$, where

$$\delta x = x' - x = f(x) - x \tag{1}$$

The overrelaxation method involves iteration of the modified equation

$$x' = x + (1 + w)\delta x \tag{2}$$

(keeping the definition of $\delta x$ the same). If the parameter w is zero, then this is the same as the ordinary relaxation method, but for $w > 0$ the method takes the amount $\delta$ x by which the value of x would have been changed and changes by a little more. Using $\delta x = f(x) - x$, we can also write $x'$ as

$$x' = x + (1 + w)[f(x) - x] = (1 + w)f(x) - wx \tag{3}$$

which is the form in which it is usually written. For the method to work the value of w must be chosen correctly, although there is some wiggle room: there is an optimal value, but other values close to it will typically also give good results. Unfortunately, there is no general theory that tells us what the optimal value is. Usually it is found by trial and error.

(a)For the ordinary relaxation method, the error on $x'$ is given by

$$\epsilon' \approx \frac{x - x'}{1 - \frac{1}{f'(x)}} \tag{4}$$

Derive an equivalent formula for the overrelaxation method and show that the error on $x'$ is given by

$$\epsilon' \approx \frac{x - x'}{1 - \frac{1}{(1+w)f'(x) - w}} \tag{5}$$

(b) Consider again the equation $x = 1 - e^{-cx}$ that we solved in Q.1. Take the program you wrote for part (a) of that exercise, which solved the equation for the case $c = 3$, and modify it to print out the number of iterations it takes to converge to a solution accurate to $10^{-6}$.

(c) Now write a new program (or modify the previous one) to solve the same equation $x = 1 - e^{-cx}$ for $c = 3$, again to an accuracy of $10^{-6}$, but this time using overrelaxation. Have your program print out the answers it finds along with the number of iterations it took to find them. Experiment with different values of w to see how fast you can get the method to converge. A value of $w = 0.5$ is a reasonable starting point. With some trial and error you should be able to get the calculation to converge about twice as fast as the simple relaxation method, i.e., in about half as many iterations.

(d)Are there any circumstances under which using a value $w < 0$ would help us find a solution faster than we can with the ordinary relaxation method? (Hint: The answer is yes, but why?)