Lab Assignment 5
Solvers for Nonlinear Equations

ACS II

Spring 2020

Assigned: February 8

Due: February 20

Introduction

This lab will explore numerical methods for solving algebraic equations which are possibly nonlinear. This is a ubiquitous task in computational science, and it is important to be able to implement several numerical methods and understand what their properties are. Such problems are typically presented in the form

$$F(u) = 0$$

where F is nonlinear in u. Generally, the roots of such a function cannot be computed in closed-form, and numerical algorithms are required to obtain an approximation.

Bisection Method

The first and most simple method for obtaining the roots of a function is the bisection method. In this method, it is assumed that there exists an interval $[a, b]$ such that $F(a)$ and $F(b)$ have opposite signs. If the function is continuous, this indicates that at least one value u^* exists with $a \le u^* \le b$, that corresponds to the desired solution $F(u^*) = 0$. If such a sign change is present, the algorithm proceeds by creating two new intervals $[a, c]$ and $[c, b]$, where $c = \frac{1}{2}(a + b)$, and determing which now contains the root in the same fashion as before. This pattern repeats until the function $F(u)$ has been reduced below some tolerance.

Newton-Raphson Method

A much more powerful algorithm is the Newton-Raphson method, which uses information about the function's gradient to locate the root. The method is derived by simply setting a truncated Taylor series of $F(u)$ to zero, and solving for the root. For a scalar equation this produces a simple iterative formula

$$u^{k+1} = u^k - \frac{F(u^k)}{F'(u^k)},$$

given that the derivative is available.

Secant Method

The secant method provides an alternate way of incorporating gradient information. If an analytic derivative is unavailable, or expensive to compute, a numerical approximation may be made using finite differences. In the secant method, the derivative is approximated as

$$F'(u) \approx \frac{F(u^k) - F(u^{k-1})}{u^k - u^{k-1}},$$

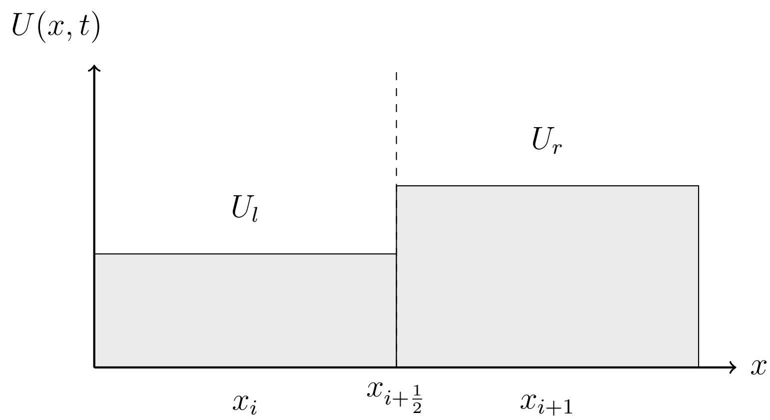
where values u^{k-1} and u^k are supplied. The iterates then proceed as

$$u^{k+1} = u^k - F(u^k)\frac{u^k - u^{k-1}}{F(u^k) - F(u^{k-1})}.$$

Methods that approximate the gradient in any way are known as quasi-Newton methods.

The Riemann Problem

An important application of solvers for nonlinear equations is the Riemann problem, which is encountered in the simulation of fluid dynamics. Within the context of the finite-volume method, the Riemann problem arises when computing the intermediate values between two constant states, as shown in the figure below.



The Riemann problem is to determine the evolution of the two constant states separated by the discontinuity. The states are given by (ρ, u, P), which are the density, velocity and pressure, respectively. There will be two characteristic waves traveling from the discontinuity: one to the left and the other to the right. The objective is to determine the pressure and velocity in the region between the two waves. For a gamma-law gas, the left-moving and right-moving waves yield

$$P^* - P_l + W_l(u^* - u_l) = 0$$
$$P^* - P_r + W_r(u^* - u_r) = 0,$$

where the wave speeds W_s are given by

$$W_s = C_s \left[1 + \frac{\gamma + 1}{2\gamma} \left(\frac{P^* - P_s}{P_s} \right) \right]^{\frac{1}{2}}.$$

Here γ is the ratio of specific heat and C_s is the sound speed,

$$C_s = (\gamma P_s \rho_s)^{\frac{1}{2}}.$$

Fortunately it is possible to decouple P^* and u^* in the previous equations, yielding a nonlinear equation for only pressure,

$$P^* = P_l + \frac{W_l}{W_l + W_r} \left[P_r - P_l - W_r(u_r - u_l) \right].$$

To solve this equation iteratively using Newton's method, the gradient with respect to P^*

must be supplied. The full Newton iteration is ultimately given by

$$P^{*(k+1)} = P^{*(k)} - \frac{Q_r Q_l}{Q_r + Q_l}\left(u_r^{*(k)} - u_l^{*(k)}\right),$$

where

$$Q_s = \left|\frac{dP^*}{du^*}\right|_s = \frac{2W_s^3}{W_s^2 + C_s^2},$$

and

$$u_l^{*(k)} = u_l - \frac{P^{*(k)} - P_l}{W_l},$$
$$u_r^{*(k)} = u_r + \frac{P^{*(k)} - P_r}{W_r},$$
$$W_s = C_s\left[1 + \frac{\gamma+1}{2\gamma}\frac{P^{*(k)} - P_s}{P_s}\right]^{\frac{1}{2}}.$$

Deliverable

Consider the following table of initial conditions for the left and right states.

Test	ρ_l	u_l	P_l	ρ_r	u_r	P_r
1	1.0	0.0	1.0	0.125	0.0	0.1
2	1.0	0.0	1000.0	1.0	0.0	0.01
3	1.0	0.0	0.01	1.0	0.0	100.0
4	5.99924	19.5975	460.894	5.99242	-6.19633	46.0950

These are the 4 seperate test setups that you will evaluate, and you will compute the pressure, P^*, for each. Take the ratio of specific heat to be $\gamma = 1.4$ in all cases. Perform the following tasks:

- Compute the solution P^* for each of the four cases using the bisection method and create a log-log plot of the residual $r^k = \frac{|u^k - u^{k-1}|}{|u^k|}$ versus the number of iterations. You must determine a suitable search bracket for each case in order to begin the algorithm. Specify the stopping criteria for your code to be $r^k < \epsilon$, where $\epsilon = 10^{-7}$. (25 points)

- Repeat the previous exercise but using Newton's method described above. Determine an appropriate initial guess to begin the algorithm. (25 points)

- Repeat the same exercise but now using the secant method. (25 points)

- Compute the rate of convergence of each of the methods, for each test case using the formula
$$\alpha \approx \frac{\log |(P^{*(k+1)} - P^{*(k)})/(P^{*(k)} - P^{*(k-1)})|}{\log |(P^{*(k)} - P^{*(k-1)})/(P^{*(k-1)} - P^{*(k-2)})|}$$
and make a table with your results. Comment on the rates of convergence. (25 points)

Remember that your solution should be physically relevant and obey positivity constraints (e.g. positive pressure).

Submission and Grading

To get credit for this assignment, you must submit the following information to the lab instructor by 11:59pm, February 20, 2020:

- Separate files for the implementation of the bisection method, Newton's method, and the secant method.
- A main file calling each of the methods, for each test case.
- A single `.pdf` file which includes the figures and results from your work, as well as relevant discussion of your observations, results, and conclusions.

This information must be received by 11:59pm, February 20 through Canvas. As stated in the course syllabus, late assignment submissions will be subject to a 10% point penalty per 24 hours past the due date at time of submission, to a maximum reduction of 50%, according to the formula:

*[final score] = [raw score] - min(0.5, 0.1 * [# of days past due]) * [maximum score]*