

Homework Assignment: No tool is perfect.

The first objective of this assignment is to become aware that even well-written, commercial, tried-and-true software can produce wrong answers without any warning signs. The second objective is to learn how to recover once you understand what is going on. The moral of the homework is "Never use a numerical method until you understand how it works. No black boxes".

1 What to submit

Individual work: each student submits his or her own work. A single PDF file, 12 pt font. Each relevant part of the homework must be accompanied by graphics and plots. Descriptive figure captions are a must. At the graduate level you are expected to sort out all of those technicalities on your own.

2 Definitions

Let's call function $f(x)$ *nice* if it is defined everywhere on $[-1, 1]$, $-10 < f(x) < 10$, the function is infinitely differentiable on $[-1, 1]$, and has a single minimum on $(-1, 1)$ (trivial case of extrema at the ends are excluded). For example, $f(x) = x^2$ is a nice function, but $\sin(1/x^2)$ or x^3 are not. Suppose you use a numerical procedure to solve for the minimum, that is to find x^n for which $f(x^n) \rightarrow \min$. We call a numerical solution *right* if $|x^n - x^{exact}| < 10^{-3}$, x^{exact} being the exact answer. Otherwise, the solution is called *wrong*. Note that our definition is very generous: generically, one expects the correct solution to be within $\sqrt{\epsilon}$ of the exact, that is within $\sim 10^{-7}$.

2.1 Part I. Explore. 10 pts

Use Mathematica to explore the straightforward Newton's method for finding local minimum. First, read up and thoroughly understand the method. Wiki has a surprisingly good intro article on it. Follow up with any textbook. Nice functions have only one minimum by definition, so not to worry. Use `FindMinimum[]`; let Mathematica select all input parameters automatically, except the method "Newton", which you specify explicitly. You may use the template provided. Explore a nice function $f(x) = ax^2 + bx^4$, consider limiting cases such as $a = 0$, $b = 0$, and some intermediates. Present convergence graphs (use `FindMinimumPlot[]`). Make your conclusions.

2.2 Part II. Break. 20 pts

Now that you understand how Newton's method works, show it! **Come up with a nice function that breaks Newton's method** that is Mathematica, with default settings, gives a wrong solution (see above defs.) without so much as a peep - no warnings or errors. Present convergence graphs (use `FindMinimumPlot[]`). Explain the failure.

2.3 Part III. 10 pts

See if you can harness Mathematica's unique functionality and options to make it find the right solution, using the same Newton's. In fact, you may be able to get to it within $\sqrt{\epsilon}$ (Find what machine epsilon is for your machine. Use code on the class site). Explain why the solution, while useful in research, is not very useful in situations when you need to quickly find lots of minima as part of a larger code written in a standard language such as C.