CS4414. Homework Assignment 4 - 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 her own work. A single PDF file, 12 pt font. Extra points for typesetting it in LaTex, see below. Each relevant part of the homework must be accompanies by graphics, plots must contain the key elements discussed in "Scientific visualization" lecture. Descriptive figure captions are a must. I highly recommend that you install GSL (below) on your own computer, but you can use "kuprin" as a last resort. Create a sub-directory (your last name) in your group's directory, and do your work there. Just be aware that it may be difficult or even impossible to make Mathematica send graphics over the X-connection. You can, of course, just save the plots on kuprin and then sftp them to your machine. At the 4000 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 $f(x^n) \to min$. 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. Fix. 20 pts

Reason which GSL or Numerical Recipes code may mitigates the problem, and test your solution. The algorithm should find a right solution by the definition above. Use `xmgrace` to make convergence plots. Give an intuitive explanation for why the alternative to Newton's works: simply testing a bunch of code won't bring you the points. In a few sentences, give at least one pro and one con for your alternative.

2.4 Part IV. Fix again. 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.

2.5 Part V. Make it pretty and earn 10 extra credit points

Use LaTex, which is a document preparation system designed for math, CS, and other "hard" sciences. Submit your PDF into the regular slot, and separately, using the "extra credit" slot, submit a single zip file the .tex, and all the figures in .eps format, as fig1.eps, etc. So that we can compile the document and get the same PDF. Use the template for the final report.