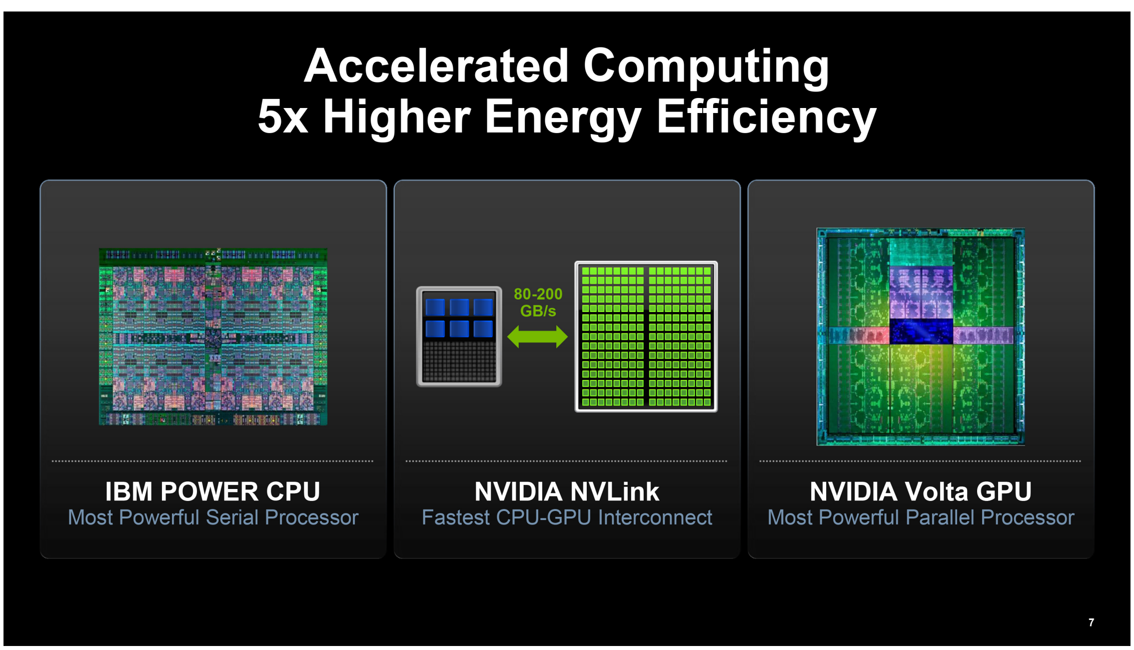
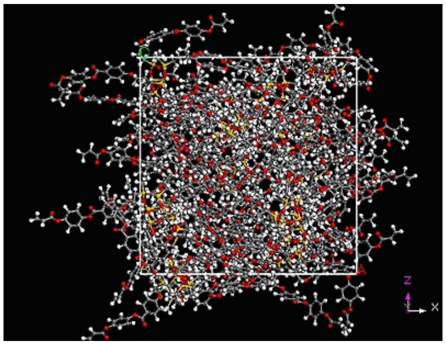
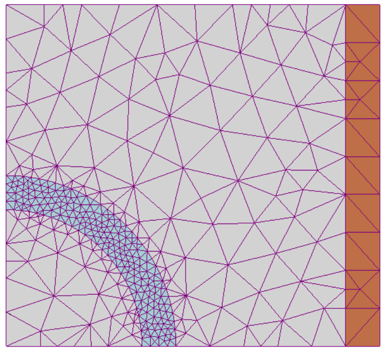
EC500 Paralllel Software for High Performance Computing

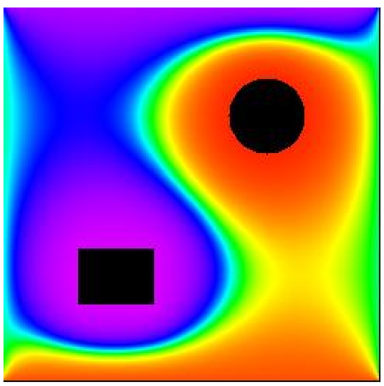
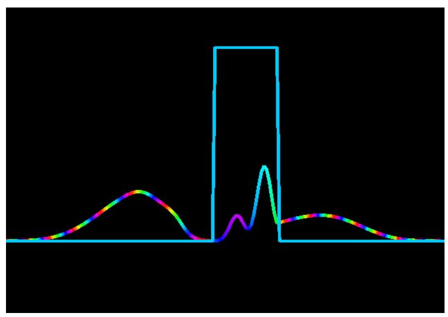
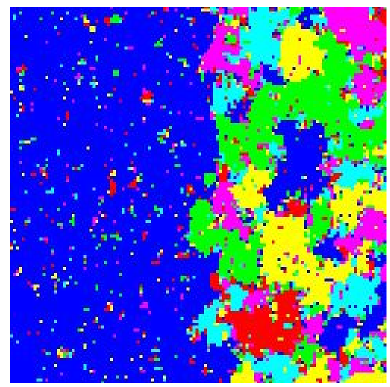
Rich Brower + Evan Weinberg

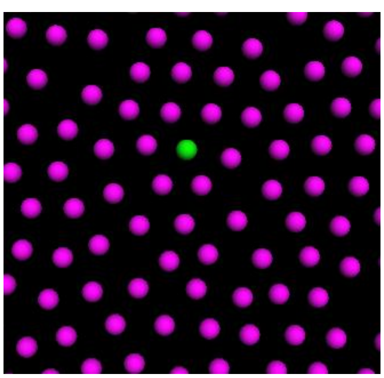
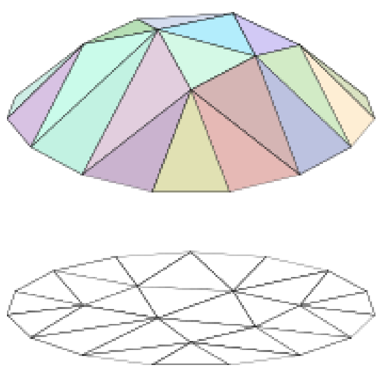
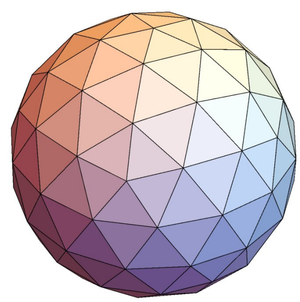
Course Description: The explosive advance in High Performance Computing (HPC) and advances in Big Data/Machine Learning and Cloud Computing now provides a fundamental tool in all scientific, engineering and industrial advances. Software is massively parallel so parallel algorithms and distributed data structures are required. Examples will be drawn from FFTs, Dense and Sparse Linear Algebra, Structured and unstructured grids. Techniques will be drawn from real applications to simple physical systems using Multigrid Solvers, Molecular Dynamics, Monte Carlo Sampling and Finite Elements with a final student project and team presentation to explore one example in more detail. Coding exercises will be in C++ in the UNIX environment with parallelization using MPI message passing, OpenMP threads and QUDA for GPUs. Rapid prototypes and graphics may use scripting in Python or Mathematica. (**Instructor: Prof. Richard Brower and Postdoctoral Fellow Evan Weinberg**)



Seven Dwarf: **Dense & Sparse linear algebra, Spectral methods, N-body methods, Structured & Unstructured grids and Monte Carlo methods**. These dwarfs have been identified as patterns, or motifs, which are the most important algorithm classes in numerical simulation

This is a "Hands on Course". Exercises will be started during class MW 12:20 - 2:05PM in the High Performance Computing Laboratory PHO 207. The "text" is on line lecture notes on Github and with access and documentation for advanced architecture: Programming guides for Intel Phi and Nvidia GPU. Prerequisite is programming experience in C at the level of EC327 or EC602 or consent of the instructor.

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1 Lecture Notes: Introduction

`These Lecture notes will be revised chapter by chapter to reflect the 2017 course and to respond to the interest and question of the students!`

REVISION For Spring 2017: Lecture 1 & 2 Sun Jan 22 11:54:35 EST 2017

Preliminary Course Outline

1. First Third Week 1-4 (4 weeks)
   - Intro to HPC and Engineering impact
   - Numerical algebra for calculus
   - Differentiation & Integration (Gauss and Monte Carlo)
   - Newtons method for root finding & Non-linear optimization
   - Curve fitting &Error analysis
   - FFT as recursion for divide and conquer
   - Simple ODEs (oscillation vs relaxation)
2. Second Third Weeks 5-9 (inclusive 5 weeks)
   - Projects & Parallelization Method
   - MPI
   - OpenMP
   - CUDA and Data Parallel
   - Submitting to HPC systems.
   - Use of Libraries. ETC
3. Second Third Week 10-14 (5 weeks): Class Projects
   - Image Processing and Smoothness
   - CG and iterative solvers
   - MG solvers
   - MD short range (neighborhood tables) vs long range Coulomb
   - MonteCarlo for Magenets: Cluster and Graphs
   - FEM in 2D

References

There is no Text – Amazingly it hash't been written! The course materials and exercies will be posted on github. There are useful pieces in some books that I will try provide as a library in the Lab in PHO 207.

Grading

The grade is based on HW exercies (2/3) , a final project and participation in the class (1/3). The project will include code, performance analysis and write up and a presentation in the last week. The HW must be done individually but the project can be in a small team of 2 to 3 individuals.

Assignment 1: Floating Point Numbers
due: Jan 30, 2017 – 11:59 PM

GOAL: The main purpose of this exercise is to make sure everyone has access to the necessary computation and software tools for this class: a C compiler, a Python interpreter, the graphing program gnuplot, and for future use the symbolic and numeric evaluator Mathematica (though we won't be using that in this exercise). In this class, there will be help to make sure everyone's system is functional.

1 Background

1.1 Numerical Calculations

LANGUAGES & BUILT IN DATA FORMATS: The primary language at present used for high performance numerical calculations is C or C++. The standard environment is the Unix or Linux operating system. For this reason, C and Unix tools will be emphasized. We will introduce some common tools such as Makefiles and gnuplot.

That said, modern software practices take advantage of a (vast) variety of high level languages as well. We will use a bit of two interpreted/symbolic languages, Mathematica and Python, because of the power they have to develop, test, and visualize simple algorithms. Little prior knowledge except familiarity with C will be assumed.

In large scale computing all data must be *represented* somehow—for numerical computing, this is often as a *floating point* number. Floats don't cover every possible real number (there are a lot of them between negative and positive infinity, after all). They can't even represent the fraction 1/3 exactly. Nonetheless, they can express a vast expanse of numbers both in terms of precision as well as the orders of magnitude they span.

As you'll learn in this exercise, round off error, stability, and accuracy will always be issues you should be aware of. As a starting point, you should be aware of how floating points are represented. Each language has some standard built in data formats. Two common ones are 32 bit `float`s and 64 bit `double`s, in C lingo. To get an idea of how these formats work on a bit-by-bit level, give a look at https://en.wikipedia.org/wiki/Single-precision_floating-point_format and https://en.wikipedia.org/wiki/Double-precision_floating-point_format.

You'll notice we're not shy about hopping off to the web to supplement the information we've put in this document and will discuss in class, and we expect you to do the same when you need to. **Searching the web is part of this course.**

As a last remark before we hop into some math, bear in mind that data types keep evolving. **Big Data** applications (deep learning!) are now using **smaller** 16 bit floats for a lot of applications. Why? Images often use 8 bit integer RGB formats. Some very demanding high precision science and engineering applications use 128 bit floats (quad precession). There are lots of tricks in code.

Symbolic codes represent some numbers like $\boldsymbol{\pi}$ and $\boldsymbol{e}$ as a special token since there are no finite bit representations! See for more about these issues: https://en.wikipedia.org/wiki/Floating_point.

1.2 Finite Differences

A common operation in calculus is the *derivative*: the local slope of a function. With pencil and paper, it's straightforward to evaluate derivative analytically for well known functions. For example:

$$\frac{d}{dx}\sin(x)\bigg|_{x=x_0} = \cos(x_0) \tag{1}$$

On a computer, however, it's a bit of a non-trivial exercise to perform the analytic derivative (you'd need a text parser, you'd need to encode implementations of many functions... there's a reason there are only a few very powerful analytic tools, such as Mathematica, that handle this). In numerical work the standard method is to approximate the limit,

$$\frac{df(x)}{dx} \equiv \lim_{h\to 0}\frac{f(x+h)-f(x)}{h} \tag{2}$$

with a finite but small enough difference h. The good news is this is completely general... the bad news is this is only an approximation and it is prone to errors. Due to round off, it's dangerous for h to get close to zero. $0/0$ is an ill-defined quantity!

One approximation of a derivative is the *forward finite difference*, which should look familiar:

$$D_h^+ f(x) = \frac{f(x+h)-f(x)}{h} \tag{3}$$

Two other methods are the backward difference and the central difference. The point of this exercise is to implement different types of differences, as well as test the effect of the step size h.

2 Programming Exercises

2.1 Part 1: Simple C++ Exercise

For this first exercise we've included the shell of a program below; it's your job to fill in the missing bits. The purpose of this program is to look at the forward, backward, and central difference of the function $\sin(x)$ at the point $x = 1$ as a function of the step size h. You should also print the exact dervative $\cos(x)$ at $x = 1$ in each column.

```
#include <iostream>
#include <iomanip>
#include <cmath>

using namespace std;
```

```
double function(double x) {
  return sin(x);
}

double derivative(double x) {
  return cos(x);
}

double forward_diff(double x, double h) {
  return (function(x+h)-function(x))/h;
}

double backward_diff(double x, double h) {
  // return the backward difference.
}

double central_diff(double x, double h) {
  // return the central difference.
}

int main(int argc, char** argv)
{
  double h;
  const double x = 1.0;

  // Set the output precision to 15 decimal places (the default is 6)!

  // Loop over 17 values of h: 1 to 10^(-16).
  for (h = /*...*/; h /*...*/; h *= /*...*/)
  {
    // Print h, the forward, backward, and central difference of sin(x) at 1,
    // as well as the exact derivative cos(x) at 1.
    // Should you use spaces or tabs as delimiters? Does it matter?
    cout << /*...*/ << cos(1.0) << "\n";
  }
  return 0;
}
```

Don't be afraid to search online for any information you don't know! I'm not good at programming, I'm good at Googling and I'm good at debugging. You should name your C++ program `asgn1_findiff.cpp`. You can compile it with:

```
g++ -O2 asgn1_findiff.cpp -o asgn1_findiff
```

2.2 Part 2: Finite Differences, Python

Once you've written this program in C++, your next task is to rewrite it in Python! You should name your Python program `asgn1_findiff.py`. You should verify that the outputs agree exactly. If you save the output of each program to file (this is done with the character `>` on the bash command line), you can quickly verify the outputs agree with the bash program `diff`.

I'm currently learning Python myself from Codecademy. I'm developing my own scripts through a simple text editor, but for a more integrated development environment, you can look at Spypder: https://pythonhosted.org/spyder/. If you want an even more complete IDE, give a look at Anaconda: https://www.continuum.io/anaconda-overview. Stick with Python 3.5.

2.3 Part 3: Plotting using gnuplot

You have all of this data, now what? To visualize how the finite differences for different h compares with the analytic derivative, we can plot the data using the program `gnuplot`. Using the output file you generated with C or with Python (which should be equivalent!), plot the relative error in the forward, backward, and central difference as a function of h. This is similar to what is being plotted on the right hand side of Fig. 3 in the Lecture notes. As a reminder, the relative error is defined as:

$$\frac{|\text{approximate} - \text{exact}|}{|\text{exact}|} \tag{4}$$

Don't forget to set x and y labels on your graph, and titles for each curve in the key.

By default `gnuplot` will output to the screen. You'll want to submit an image at the end of the day; the commands `set terminal` and `set output` will be helpful in this regard! As an FYI: while it's best to play with making plots in the `gnuplot` terminal, it can get annoying to do everything there! `gnuplot` can just run a script file:

```
gnuplot -e "load \"[scriptname].gp\""
```

Where you should replace `[scriptname]` with, well, the name of your plotting script!

Extra Credit& Extra Fun: Once you have a program, it is good to see what else you can do. If you want to see a function that is difficult to numerically approximate, try the derivative of $\sin(1/x)$, which is exactly $-\frac{\cos(1/x)}{x^2}$, at some point close to zero, say $x = 0.0001$. Don't pass this in, but you can brag about in class for virtual extra credit.

2.4 Submitting Your Assignment

This first assignment is due at 11:59 pm on Monday, January 30. Please e-mail a **tarball** containing the assignment to the class e-mail, bualghpc@gmail.com. Include your name in the tarball filename.

If you're not familiar with tar, here's a sample instruction that perhaps I would use:

```
tar -cvf evan_weinberg_asgn1.tar asgn1_findiff.cpp asgn1_findiff.py asgn1_findiff.pdf
```

You may want to include other files (such as your gnuplot plotting script, though it's not required). **Do NOT include a compiled executable!** That's a dangerous, unsafe practice to get into.

A Software Tools: Nothing to Pass in!

A.0.1 Part I: Accessing BU Computing

Make sure you can access BU's "Linux Virtual Lab" by following the instructions here:

http://www.bu.edu/tech/services/support/desktop/computer-labs/unix/

These Linux machines aren't for running long calculations, but they are useful for small, interactive jobs. (I think any job will get killed after 15 minutes—don't quote me on that.) These machines also allow access to Mathematica.

Access to BU Computing is not a substitute for installing Mathematica and standard Unix compilers on your own machine, as described below.

A.0.2 Part II: Making sure you have a C++ compiler

In this class, we'll be using the standard compiler "g++". If you have a Mac or a Linux install, g++ may exist already. Try running the command:

```
which g++
```

from the terminal. On my machine, it returns:

```
/usr/bin/g++
```

But your mileage may vary. If it returns nothing, it means you don't have g++ installed, which you should go do! I'd be surprised if it wasn't installed, though.

If you're on Windows, you'll need to install Cygwin, which even I struggled with—other options are dual-booting, or a much better idea is installing Linux in a virtual box! If you're interested in that but not brave, send me (Evan) an e-mail at `weinbe2@bu.edu` and I'll help you out!

To make sure you understand compiling without an IDE (Integrated Development Environment), follow the quick tutorial here: https://en.wikibooks.org/wiki/C%2B%2B_Programming/Examples/Hello_world

Amazing Interactive Tutorias: C++

http://www.tutorialspoint.com/cplusplus/index.htm

A.0.3 Part Iii: Installing gnuplot

You may have gnuplot already installed on your machine. You can test this the same way we tested for g++:

```
which gnuplot
```

If it returns a path, you have gnuplot installed! If not, use your favorite package manager to install it. I'm an Ubuntu user, so I had to run:

```
sudo apt-get install gnuplot
```

If you're on a different distribution, you'll probably need to use `yum`, or some GUI tool. On Mac OS X, an optional package manager is Brew: http://brew.sh/, which will help you out.

By looking around on stackoverflow, I found a sample brew install command:

```
brew install gnuplot --wx --cairo --pdf --with-x --tutorial
```

Which will let you output PDFs as well as to the screen (that's the whole `with-x` and `wx`), I imagine. If you get stuck, let us know!

To test out gnuplot in OS X or Linux, run:

```
gnuplot
```

from the terminal. This will put you in an interactive gnuplot terminal. A few useful commands:

```
# Hashes aren't for twitter, they're for comments in gnuplot!
plot sin(x) # plot the sine function
f(x) = cos(x) # assign a function
plot sin(x), f(x) # plot two functions at once.
set xrange [0:2] # change the x axis.
set yrange [-2:2] # change the y axis range.
replot # update the plot with your new axis.
set yrange [-5:-2] # change the y axis range again.
replot # you won't see anything! So do...
reset # ... because you've messed up!
set xrange [-1:1]
plot x*sin(1/x) # This will lootk really bad!
set samples 1000 # sample the function more frequently.
replot # it should look a lot better now
exit # and we're done!
```

Your will want to save a figure from time to time. In this case before you exit add in these instructions.

```
set term postscript color  #one option that gives a .ps figure.
set output "myfigure.ps"   #whatever you want to name it
```

```
replot                      #send it to the output
set term x11                #return to interactive view.
                            #On linux, you may need ``wxt'' instead of x11.
```

A.0.4 Part IV: Installing Mathematica

As students, you can luckily install Mathematica on your own computer without much pain. Follow this link and install Mathematica:

http://www.bu.edu/tech/support/desktop/distribution/mathsci/mathematica/student/step-1/

We've tested this on both Windows and Mac OS X. Mathematica will also work on standard Linux distros, we've just never tried installing it there ourselves—please try and let us know asap if you have issues.

After installing Mathematica, you should go through the following quick tutorials. They cover very simple topics, such as plotting, differentiation, and integration. The differentiation and integration articles go into much deeper mathematical detail than you'll need in this class! Just gleam out how to take a simple derivative and perform a simple integral. Don't let the word "Hessian" scare you.

- Plotting functions: https://reference.wolfram.com/language/tutorial/BasicPlotting.html
- Plotting data: https://reference.wolfram.com/language/howto/PlotData.html
- Differentiation: https://reference.wolfram.com/language/tutorial/Differentiation.html
- Integration: https://reference.wolfram.com/language/tutorial/Integration.html

We will suggest further reading as the need arises!

A.0.5 Part IV: Installing Anaconda for Python

You can get Anaconda distribution of python at

https://www.continuum.io/downloads

Get the one for Python 3.5 for your computer(s).

https://docs.python.org/2/tutorial/index.html

Amazing Interactive Tutorials:

https://docs.python.org/2/tutorial/index.html

http://www.tutorialspoint.com/python3/index.htm

http://docs.python-guide.org/en/latest/writing/style/#zen-of-python

2 Lecture Notes: Derivative to Finite Differences

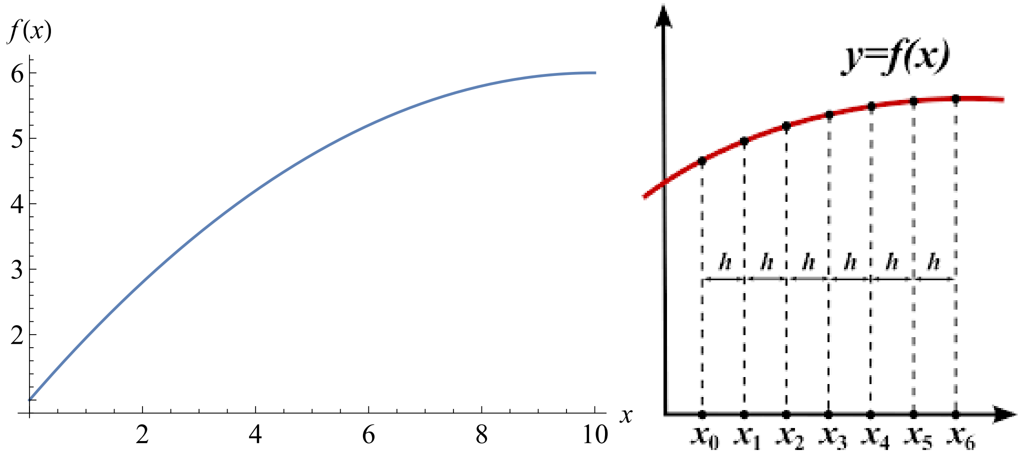


Figure 1: On left a function of x. On right the discrete points evalueted on a grid

We begin with the **1 D problems – The Derivative and the Anti-Derivative**: A smooth function $f(x)$ can be expanded in a power series around $x = 0$ expanded at x =0, (see Fig.1)

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots \ . \tag{1}$$

What is a_0? What is a_1? Hint:

$$\frac{dx^n}{dx} = n x^{n-1} \quad \text{or map} \quad Dx^n \to n x^{n-1} \tag{2}$$

So setting $x = 0$ we have $a_0 = f(0)$ taking the derivative and then setting $x = 0$ we get $df(0/dx = f'(0) = a_1$ and the next derivative $f''(0) = 2a_1$ etc. Ok now we have “derived” the Taylor series!

$$f(x) = f(0) + x f'(0) + \frac{1}{2!} x^2 f''(0) + \cdots + \frac{1}{n!} x^n f^{(n)}(0) + \cdots \ . \tag{3}$$

This is almost the only tool we will need from most of the course. In fact we will almost never use more than the first couple of terms.

Now we need to approximate a derivative on a computer. How? Define forward and backward difference approximation (see Fig.2)

$$\Delta_h f(x) = \frac{f(x+h) - f(x)}{h} \quad \text{and} \quad \widetilde{\Delta}_h f(x) = \frac{f(x) - f(x-h)}{h} \equiv \Delta_{-h} f(x) \tag{4}$$

NOTE: It is sometime convenient to take “units” where $h = 1$ (Much like just as in array notation in programming where x is a integer and the next element is $x + 1$). In this case I will woud write,

$$\Delta f(x) = f(x+1) - f(x) \quad \text{and} \quad \widetilde{\Delta} f(x) = f(x) - f(x-1) \tag{5}$$

If you are “smart” enough you can always figure out when and where to put back in the “lattice spacing” h.

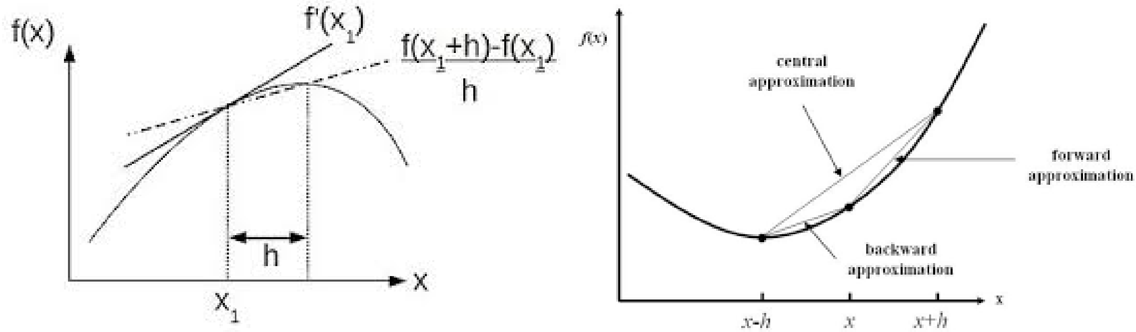


Figure 2: On left, finite difference. On right, central difference.

Note The second derivative is $\widetilde{\Delta}\Delta f(x) = \widetilde{\Delta}(f(x+1) - f(x)) = f(x+1) - 2f(x) + f(x-1) \simeq h^2 f''(x)$. Central difference is $\Delta + \widetilde{\Delta}$. As we will see later $\widetilde{\Delta} = -D^{\dagger}$.

2.1 Higher order and Undetermined Coefficients

Higher order approximations add $(\Delta_h + \Delta_h)/2h$ and $(\Delta_{2h} + \Delta_{2h})/4h$ to cancel $O(h^4)$ term.

2.2 Avoid Round off for $D_h f(x)$

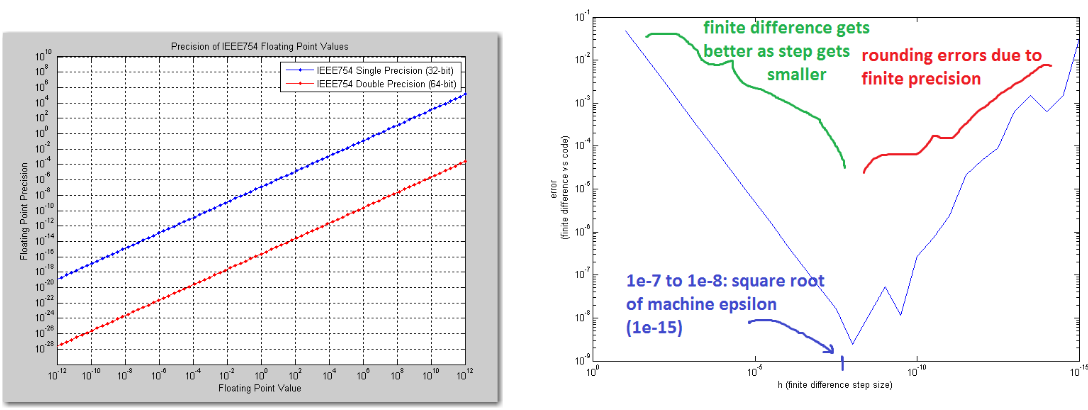


Figure 3: On the Right the error in the finite difference approximation to a deriative (y-axis) relative to size set size h (x-axis).

See IEEE floating point single (float) 32 bit is in this link:

https://en.wikipedia.org/wiki/Single-precision_floating-point_format

Consider the approximate derivative

$$df(x)/dx \simeq D_h f(x) = \frac{f(x+h) - f(x)}{h} \tag{6}$$

It is very vulnerable to round off error. Let do this with no round off for x^N. (See NR Page 186 Sec 5.7) So to avoid round cancel the factor of h in the numerator and denominator explicitly,

$$\begin{aligned} D_h x^N &= [x^N + Nhx^{N-1} + \cdots h^N - x^N]/h \\ &= Nx^{N-1} + \frac{N(N-1)}{2} hx^{N-1} + \cdots + h^{N-1} \,. \end{aligned} \tag{7}$$

The general expression for the coefficient in the expansion is the number of ways to put n things in i boxes: the coefficients in the expansion are

$$C[n][i] = \frac{n!}{(n-i)!i!} \quad \text{for} \quad i = 0, 1, \cdots, n \tag{8}$$

This is the way to get coefficients of: $(a+b)^0 = 1; (a+b)^1 = a+b; (a+b)^2 = a^2 + 2ab + b^2$, $(a+b)^3 = a^3 + 3a^2b + 3a^2b + b^3$ etc, which are just the values in the famous Pascal triangle:

$$C[n][i] = \begin{array}{c} n\backslash i= \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ \cdots \end{array} \begin{array}{c} \begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 & \cdots \end{array} \\ \left[\begin{array}{cccccc} 1 & 0 & 0 & 0 & 0 & \cdots \\ 1 & 1 & 0 & 0 & 0 & \cdots \\ 1 & 2 & 1 & 0 & 0 & \cdots \\ 1 & 3 & 3 & 1 & 0 & \cdots \\ 1 & 4 & 6 & 4 & 1 & \cdots \\ 1 & 5 & 10 & 10 & 5 & \cdots \\ \cdots & & & & & \end{array} \right] \end{array} \tag{9}$$

So we can avoid round off and compute (almost) exactly the finite difference form:

$$D_h x^N = \sum_{i=1}^{N} C[N][i] x^{N-1} h^{i-1} = Nx^{N-1} + \frac{N(N-1)}{2!} x^{N-2} h + \cdots + h^{N-1} \tag{10}$$

computing coef $C[n][i]$'s recursively:

```
C[n][i] = 0;
for(n = 0; n<N+1; n++) C[n][0] = 1;
C[n+1][i+1] = C[n][i] +C[n][i+1];
```

Knuth's Concrete Mathematics Text has the same Pascal triangle format in Table 155 page 155 and the "addition formula" above in Eq 5.8 see Concrete Math(There is also a totally over the top number of random identities in this text. Fun but not that useful.)

Similarly we can define $\widetilde{D}_h$ as an explicit expansion of $\widetilde{\Delta}_h$. What is? (Hint: Think what happen if $h \to -h$.) So the central difference cancels all term odd in h.

$$\frac{1}{2}(D_h + \widetilde{D}_h) x^N \tag{11}$$

This is good for any finite difference $\frac{1}{2}(D_h + \widetilde{D}_h) f(x)$ of course so the central difference has its first error in $O(h^2)$. See notes and code at https://github.com/BU-EC-HPC-S16/EC500-High-Performance-Computing

Assignment 2: Newton's Method and Root Finding
due: Feb 6, 2017 – 11:59 PM

GOAL: The purpose of Problem Set #2 is twofold: one purpose is to investigate searching and root-finding, but the other is to lay the groundwork for Problem Set #3: numerical integration, which has a lot to borrow from root finding, of all things!

The ultimate focus of this assignment looking for the zeroes of Legendre polynomials... this isn't made to scare you, but it's meant to emphasize how far you'll go in just a week. Finding the zeroes requires root finding, and if you're wondering what a Legendre polynomial is, well, it's a function we'll build recursively.

As a warm up to this impressive feat, we'll start of with simpler tasks: using *bisection* and *Newton's method* to find zeros of simple polynomials (which will apply to any continuous function, such as those pesky Legendre polynomials). And as a warm up to the warm up, we'll first point out that root finding is similar to searching in a sorted array!

Let's say you have a *sorted* array `c[0], c[1], ...`, and you want to find which index `i` satisfies `c[i] = b` for some `b`, that is, you want to find where `b` resides in the array. This is similar to finding the zero of a function—you're (discretely) solving:

```
c[i]-b = 0
```

With that in mind, let's get to it!

1 Warm Up Exercise : Searching an Array

To see the array version you should run the code `search.cpp` with the dependent `.h` files:

```
#include "search.h"
#include "sort.h"
```

that is on `github`. Read the code so you understand it. First set `Nsizse = 100` to see that it is all working. Then go back `= 10000000` to really see the differences between the different algorithms. This is a fun way to appreciate the advantages of better algorithms: LinearSearch, BinarySearch, and DictionarySearch are O(N), O(Log(N) and O(Log Log N) algorithms respectively. Or if you wish 3 algorithms: `Stupid, Smart, Brilliant!` Each has it corresponding version for root finding!

Modify the code `search.cpp` to run for a range of values of N (no larger than `10^8`) and output the results into a file `search_timing.dat`. The file should have four columns:

1. The value of N.
2. The number of iterations for linear search.
3. The number of iterations for binary search.
4. The number of iterations for dictionary search.

Using `gnuplot`, fit the curve to N, Log N and Log Log N to convince yourself that these estimates are right: See Problem Set #1 for how to fit with gnuplot. The deliverables for this exercise are:

- Your modified code, `search.cpp`.
- Your data file, `search_timing.dat`.
- Plots of your data with fit curves.

Do not stress too much about the plots of the data with fit curves. Don't worry about error bars and properly weighted fits, just do the simple fits we showed in Problem Set #1! Later we will discuss proper weighted fits.

(Also note that MergeSort is a smart fast $O(NLog(N))$ sort. Try using a stupid $O(N^2)$ Selection Sort. It is so terrible you will have to run it over spring break or longer!)

2 Coding Exercise #1: Taking a Square Root

Again, we have a prewritten program for simple root finding. The code in `bisection_vs_newton.cpp` explicitly solves $f(x) = x^2 - A$, giving the positive square root of A. Just compile `bisection_vs_newton.cpp` and run. This program is a contest between bisection search, a `Log(N)` method, and Newton's method (think Dictionary search!), a `LogLog(N)` method. Try it for various values of A.[1]

[1] There are some weird cases where bisection will beat Newton's method—for example, the way the code is currently written, bisection will win for $A = 1024$. This is a special case due to how we set our initial guess and because 1024 is an even power of 2, namely 2^{10}. These cases are special!

This exercise has two pieces.

First, modify the code `bisection_vs_newton.cpp` to find the n-th root of A, instead of just the square root. This requires modifying the functions `bisection` and `newton` appropriately to take and use an additional numerical argument, `int n`, which you should prompt the user for. Once you are done, the code will find the zero of $f(x) = x^n - A$. For Newton, this requires the iteration

$$x \leftarrow x \times (1.0 - 1.0/n) + A/(n \times \mathrm{pow}(x, n-1)). \tag{1}$$

Next, we'll focus specifically on square roots and third (cube) roots for $A = 2$. Instead of having the tolerance (`TOL`) fixed at the top of the code, make the tolerance a variable. Your goal is to study the iteration count as a function of the tolerance for `bisection` only. Sweep in N, where $N = 1/$`TOL`, for $N = 10, 100, \cdots 10^{15}$. Plot the iteration count as a function of N using gnuplot, and fit it to the form $c_0 + c_1 \log(N) + c_2 \log(\log(N))$, where c_0, c_1 and c_1 are free fit parameters.

The deliverables for this exercise are:

- Your modified code, `bisection_vs_newton.cpp`, which prompts the user for and computes arbitrary integer n-th roots using both `bisection` and `Newton's` method.
- Two plots showing the iteration count for computing the square root and cube root, respectively, of 2 using `bisection`. Your plots should include an overlaid fit curve.

For bit of extra credit and fun try to find the only zero of $f(x) = x^3(1 + \cos(10x)/2 - 1/4$ starting in the interval $[0, 3]$ starting with $x = 2$. Newton's method fails but bisection works. Why? (Are you having fun yet? https://www.englishforums.com/English/WhatMeantHaving/chll/post.htm)

3 Coding Exercise #2: Polynomials

3.1 Part #1: Generating Legendre Polynomials with Recursion

As a first step, we will generate the Legendre polynomials. Recall that an n-th ordefr polynomial is defined by a coefficients, $a_n[i0] \equiv a[n][i]$ for $i = 0, \cdots, n$. More specifically given these coefficients, a polynomial of degree n (such as $P_n(x)$!) can be evaluated as:

$$P_n(x) = a_n[0] + a_n[1]x + a_n[2]x^2 + \cdots + a_n[n]x^n \tag{2}$$

so all we need it to find the array $a[n][i]$. This is found by using the Legendre Polynomials which satisfy a recurrence relation:

$$nP_n(x) = (2n-1)xP_{n-1}(x) - (n-1)P_{n-2}(x)\ . \tag{3}$$

starting from

$$P_0(x) = 1 \qquad\qquad P_1(x) = x \tag{4}$$

As an example, let's review how to find the coefficients of $P_2(x)$. In general, we can write $P_2(x)$ as:

$$P_2(x) = a_2[0] + a_2[1]x + a_2[2]x^2, \tag{5}$$

where the subscript 2 implies that we're talking about $P_2(x)$. Similarly, we can write:

$$P_0(x) = a_0[0] = 1, \tag{6}$$
$$P_1(x) = a_1[0] + a_1[1]x = 0 + (1)x, \tag{7}$$

where $a_0[0] = 1$, $a_1[0] = 0$, $a_1[1] = 1$. Let us plug $n = 2$ into the recursion relation:

$$\begin{aligned}
nP_n(x) &= (2n-1)xP_{n-1}(x) - (n-1)P_{n-2}(x) \\
2P_2(x) &= 3xP_1(x) - 1P_0(x) \\
2\left(a_2[0] + a_2[1]x + a_2[2]x^2\right) &= 3x\left(a_1[0] + a_1[1]x\right) - 1\left(a_0[0]\right) \\
2\left(a_2[0] + a_2[1]x + a_2[2]x^2\right) &= 3x\left(x\right) - 1\left(1\right) \\
2\left(a_2[0] + a_2[1]x + a_2[2]x^2\right) &= 3x^2 - 1 \\
a_2[0] + a_2[1]x + a_2[2]x^2 &= \frac{3}{2}x^2 - \frac{1}{2}
\end{aligned}$$

We can now match powers of x on each side. This is known as *linear independence*: We thus get $a_2[0] = -\frac{1}{2}, a_2[1] = 0, a_2[2] = \frac{3}{2}$ and conclude:

$$P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$$

Comparing the coefficients for each power x^i in Eq. 3, we have a recursion relation

$$n\ a[n][i] = (2n-1)\ a[n-1][i-1] - (n-1)\ a[n-2][i] \tag{8}$$

Why? Your task in this programming exercise is to write a function in C that finds the coefficients $a_n[0], a_n[1], \cdots, a_n[n]$ for a general n. If you carefully follow the steps I've given for $n = 2$, you'll see I already wrote it for you! You just have to generalize the upper limits of your `for` loops. In reality, the values $a_n[i]$ satisfy a recursion relationship, similar to Pascal's triangle, except each $a_n[i]$ depends on $a_{n-1}[i-1]$ and $a_{n-2}[i]$, that is, it depends on values from two levels. Assume that $a_n[i] = 0$ if $i > n$. Note that we can really write this internally as a 2D array, `atemp[n][i]`$= a_n[i]$. All we care about is the array a for a fixed n, not all n, so this is only an internal structure.

The function should be declared as:

```
int getLegendreCoeff(double* a, int n);
```

where:

- `a` is an array of `double`s, already allocated, of length `n`+1.
- `n` indicates the order of Legendre polynomial.

- The return value is 1 if there are no errors, 0 if there are errors. Some errors include:
  - `n`< 0, since we have only defined the Legendre polynomials of integer order. (Yes, there are non-integer extensions. Check them out in Mathematica!)
  - `a` is a null pointer.

This function should be included in a file `legendre.c`, with a main function that prompts the user for a value n, allocates an array, finds the coefficients of $P_n(x)$, and prints the polynomial. As an example, here's how the code may run, where > indicates lines with user input. Assume we've started from a bash shell.

```
> ./legendre
What order Legendre polynomial?
> 5
7.875 x^5 + 0 x^4 + -8.75 x^3 + 0 x^2 + 1.875 x^1 + 0 x^0
```

We're not stressed about how many decimal points your output exhibits (as long as it's at least 6 if there are more than 6 non-zero digits).

The deliverables for this exercise are:

- Your own code file `legendre.c` as defined above with the function `getLegendreCoeff`.

3.2 Part #2: Finding Zeros of Legendre Polynomials

As a next step, we need to find the zeros of the Legendre polynomial. There are many different ways to do this, but for this assignment we will focus on the Newton-Rhapson's method. (Note IF you wish you can do this part first. Just using the values of the coefficients from Mathematica for $P_n(x)$. This is perfectly fine. Always smart to break up a problem first into simpler separate codes. In the future we will integrate the separate pieces into a single code.)

Unfortunately, the Newton-Rhapson method will not always converge to a zero of the function. We won't go very in depth on this; for more details, check out:

- https://en.wikipedia.org/wiki/Newton%27s_method, namely the section "Failure of the method to converge to the root".

Luckily, the roots of the Legendre polynomial are "well-behaved," in large fact because they are orthogonal polynomials. They are so well-behaved that there are high-quality approximate expressions for the roots of general Legendre polynomials. We will state without proof that the kth root of $P_n(x)$ is approximated by the expression:

$$\xi[n][k] \simeq \left(1 - \frac{1}{8n^2} + \frac{1}{8n^3}\right) \cos\left(\pi \frac{4k-1}{4n+2}\right). \tag{9}$$

Since the roots are almost equallly space in $[-1, 1]$ starting from this guess will quickly converge. Write a routine ,

```
int getLegendreZero(double* zero, double* a, int n);
```

that in the array of coefficient $a_n[i]$ for the Legendre Polynomial and uses this smart guess to report an array $zero[i]$ for the n zeros. Test for n =5, n = 6, n = 7.

```
> ./getZeros
What order Legendre polynomial?
> 5
-0.9061798459386640 -0.5384693101056831 0.0000000000000000
0.5384693101056831 0.9061798459386640
```

Of course you can verify the program to the known values. https://pomax.github.io/bezierinfo/legendre-gauss.html You can hard code the input arrays $a[n]$ for n = 5, 6, 7 to test it. If you are ambitious make it call `int getLegendreCoeff(double* a, int n);` as defined in the previous problem so it works for arbitrary n. In Problems set # 3, we will use the function to construct arbitrarily accurate Gaussian quadrature functions.

The deliverables for this exercise are:

- Your own code file `getZeros.c` as defined above with the function `getLegendreZero`.

3.3 Submitting Your Assignment

This assignment is due at 11:59 pm on Monday, February 6. Please e-mail a **tarball** containing the assignment to the class e-mail, bualghpc@gmail.com. Include your name in the tarball filename.

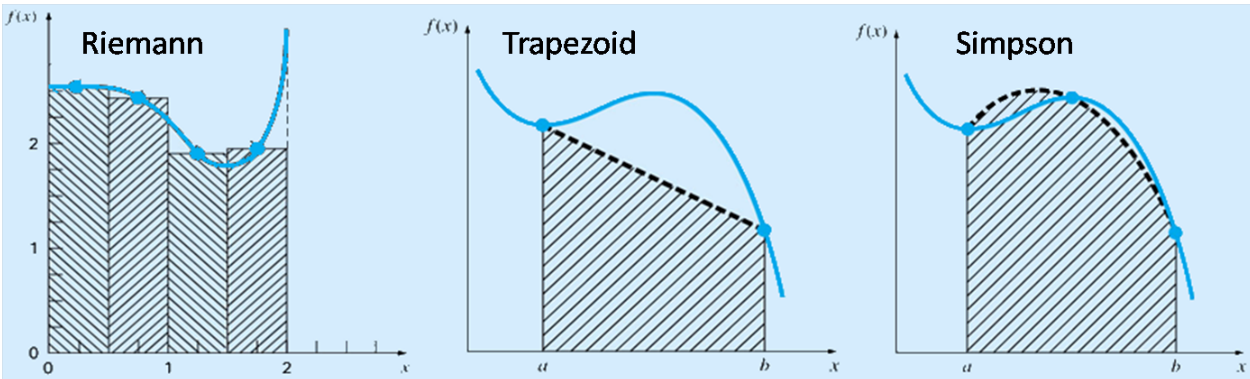
If you're not familiar with tar, here's a sample instruction that perhaps I would use:

```
tar -cvf evan_weinberg_asgn2.tar [directory with files]
```

You may want to include other files. **Do NOT include a compiled executable!** That's a dangerous, unsafe practice to get into.

3 Lecture Notes: Integrals to Sums

In **Numerical Recipes in C** at http://apps.nrbook.com/c/index.html there is a nice introduction to numerical integration: the trapazoidal rule, Simpson's rule and Gaussian Integration.See Ch 4 Sec 4.1 - 4.2 and theses lecture on Gaussian integration.



The solution(s) to the equation

$$Dy(x) = \frac{dy}{dx} = f(x) \quad \Longrightarrow \quad y(x) = \int_0^x f(x')dx' + c; \tag{12}$$

We define D^{-1} to be the integral up to an unknown constant. We can call this an "inverse Derivative"

$$D^{-1}f(x) = \int_0^x f(x')dx' + c \tag{13}$$

Check it (aka prove it!) : $D(D^{-1})f(x) = D\int_0^x f(x')dx' = f(x)$.

Now lets do this for finite steps. For sums we can solve the analagous expression:

$$\Delta_h y(x) = f(x) \quad \Longrightarrow \quad y(Nh) = \sum_{i=0}^{N-1} f(ih)h + c; \tag{14}$$

Why ? Ok how do we integrate in general? Setting $h = 1$ the expression our guess for Δ^{-1} is

$$\Delta^{-1}f(x) = f(x-1) + f(x-2) + \cdots + f(0) + c \tag{15}$$

Is this right? Let's check it.

$$\begin{aligned} D\Delta^{-1}f(x) &= D[f(x-1) + f(x-2) + \cdots + f(0) + c] \\ &= \quad (f(x) - f(x-1)) + (f(x-1) - f(x-2) + \cdots f(1) - f(0) + f(0) - f(-1) \\ &= f(x) \end{aligned} \tag{16}$$

All terms cancel except the first, if we take $f(-1) = 0$ as a convention. *After all it gives no contribution to the integral since is not in the interval. This is in fact what we assume below doing the trapezoidal rule.*

Now let's be more systematic about looking for a good approximation to the integral. To approximate the integral

$$I = \int_b^a f(x)dx \to I_N = \sum_{i=1}^{N} w_i f(x_i) \tag{17}$$

We can pick good points x_i in the interval $[a, b]$ and nice weights.

The first method is call the Trapezoidal rule. Let's try it for a regular spacing $\Delta x \equiv h = (b-a)/N$ or $x_i = a + i\Delta$ for $(x_0, x_1, ..., x_N)$

$$\begin{aligned} y &= \sum_{i=0}^{N-1} h[f(a+ih) + f(a+(i+1)h)]/2 \\ &= h[\frac{1}{2}f(x_0) + f(x_1) + f(x_2)\cdots f(a+x_{N-1}) + \frac{1}{2}f(x_N)] \end{aligned} \tag{18}$$

(see NR page 131, 4.1). Or in general Newton-Cotes for trapezoidal rule:

$$\int_{x_1}^{x_2} f(x) = h[f_1 + f_2]/2 + O(h^3 f'') \tag{19}$$

Exact for any $f(x) = c_0 + c_1 x$ of course. With two free "weights," we can make any two terms exact: $\int_{-h}^{h} f(x) = h[c_{-1}f(-h) + c_1 f(h)]$ so $f = 1$ implies $2h = 2h[c_{-1} + c_1]$, and $f = x$ implies $c_{-1} = c_1 = 1/2$. Note x^{odd} gives zero automatically. This implies

$$y_N = \sum_{i=0}^{N-1} (x_{i+1} - x_i)\frac{f(x_i) + f(x_{i+1})}{2} \tag{20}$$

This only exact for a straight line (linear) function ($f(x) = c_0 + c_1 x$) There are better "higher order" fits. A next example is"Simpson's rule," which is good up to $O(x^3)$ exactly:

$$\int_{-h}^{h} f(x)dx = h\left[\frac{1}{3}f(-h) + \frac{4}{3}f(0) + \frac{1}{3}f(h)\right] + O(h^5 f^{(4)}) \tag{21}$$

Proof. Odd powers are zero so try $f = 1, x^2$ (drop 2 h factor)

$$\begin{aligned} 2 &= c_{-1} + c_0 + c_1 \\ (2/3)h^3 &= h^3(c_{-1} + c_1) \end{aligned} \tag{22}$$

3.1 Gaussian Integration

Figure 4: On left Gauss of course. On right Galois – whom lost a dual at age 22!

We see that adding points lets us get exact results for higher order polynomials. To this point, though, we've only let the weights in our approximations change. What if we let both the weights and the positions to be tuned to get a better approximation?

$$I_N = \int_{-1}^{1} f(x)dx = \sum_{i=1}^{N} w_i f(x_i) \tag{23}$$

This is known, in general, as "Gaussian integration," or more appropriately "Gaussian quadrature" (see https://en.wikipedia.org/wiki/Gaussian_quadrature). We have $2N$ variables to play with: x_i, w_i. So we can get rid of $2N$ integrals over $1, x, x^2, \cdots, x^{2N-1}$ exactly!

As a quick aside: thus far, we've only been concerning ourselves with intervals $-h < x < h$, or $-1 < x < 1$. This is not an issue: we can transform any arbitrary interval $a < x < b$ into $-1 < x < 1$ by the rescaling:

$$\int_{-a}^{b} f(x')dx' = \frac{(b-a)}{2} \int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right) dx \tag{24}$$

Going forward, we'll only talk about integrating over the interval $-1 < x < 1$. Let's try our idea of Gaussian quadrature for $N = 1$ terms: (ie. 1 to x)

$$I_1 = w_0 f(0) \tag{25}$$

so

$$2 = w_0 \quad \text{for } 1 \tag{26}$$

This is also known as midpoint integration:

$$I_1 = 2f(0), \tag{27}$$

where we just approximate the integral as the value of the function at the center of the interval multiplied by the width of the integral.

Let's now try it for $N = 2$ terms, that is, two points and two weights (ie. 1 to x^3)

$$I_2 = w_1 f(-\delta) + w_1 f(\delta) \tag{28}$$

where I used symmetry to get rid of x, x^3 by fixing x_1, x_2 to be equal in magnitude but opposite in sign and w_1, w_2 to be equal. This gives us:

$$\begin{aligned} 2 &= w_1 + w_1 \quad \text{for } 1 \\ 2/3 &= w_1\delta^2 + w_1\delta^2 \quad \text{for } x^2 \end{aligned} \tag{29}$$

This gives us $w_1 = 1$ and $w_1\delta^2 = 1/3$, $\delta = 1/\sqrt{3} = 0.57735$, Let's try it for $N = 3$ terms (i.e. 1 to x^5)

$$I_3 = w_1 f(-\delta) + w_0 f(0) + w_1 f(\delta) \tag{30}$$

where I used symmetry to get rid of x, x^3, x^5 fixing x_1, x_2, x_3 to one constants and w_i to 2

$$\begin{aligned} 2 &= w_1 + w_0 + w_1 \quad \text{for } 1 \\ 2/3 &= w_1\delta^2 + w_1\delta^2 \quad \text{for } x^2 \\ 2/5 &= w_1\delta^4 + w_1\delta^4 \quad \text{for } x^4 \end{aligned} \tag{31}$$

so $w_1\delta^2 = 1/3$, $w_1\delta^4 = 1/5$ so $\delta^2 = 3/5$ and $w_1 = 5/9, w_0 = 8/9$ and therefore

$$\int_{-1}^{1} f(x)dx \simeq \frac{1}{9}[5f(-\sqrt{3/5}) + 8f(0) + 5f(\sqrt{3/5})] \tag{32}$$

or

$$\begin{aligned} \int_{-a}^{b} f(x')dx' &= \frac{(b-a)}{18}\left[5f\left(-\frac{(b-a)}{2}\sqrt{3/5} + \frac{(b+a)}{2}\right)\right. \\ &+ \left. 8f\left(\frac{(b+a)}{2}\right) + 5f\left(\frac{(b-a)}{2}\sqrt{3/5} + \frac{(b+a)}{2}\right)\right] \end{aligned} \tag{33}$$

Magic a la Gauss. Who else! General formulas can be found online easily, for example, at: https://pomax.github.io/bezierinfo/legendre-gauss.html.

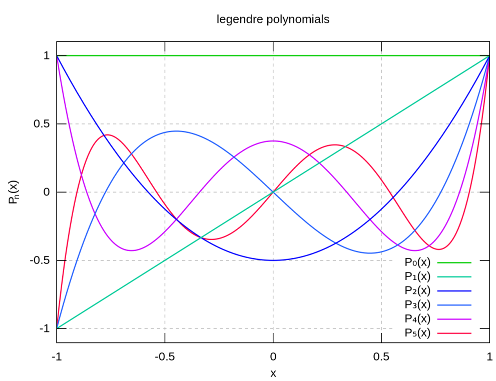
In class we discussed *Legendre* polynomials. The first few Legendre polynomials are:

$$P_1 = x$$
$$P_2 = \frac{1}{2}(3x^2 - 1)$$
$$P_3 = \frac{1}{2}(5x^3 - 3x)$$

As an interesting observation, the roots of these polynomials are exactly the positions where functions are sampled in I_1, I_2, and I_3 above. This generalizes for higher order Gauss-Legendre quadrature. The roots are always the position in the Gauss Lagrange methods, and the weights are given by:

$$w_i = \frac{2(1 - x_i^2)}{[(n+1)P_{n+1}(x_i)]^2} \tag{34}$$

See https://pomax.github.io/bezierinfo/legendre-gauss.html for roots and weights or just run the Mathematica program on the page.



n	$P_n(x)$
0	1
1	x
2	$\frac{1}{2}(3x^2 - 1)$
3	$\frac{1}{2}(5x^3 - 3x)$
4	$\frac{1}{8}(35x^4 - 30x^2 + 3)$
5	$\frac{1}{8}(63x^5 - 70x^3 + 15x)$
6	$\frac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5)$
7	$\frac{1}{16}(429x^7 - 693x^5 + 315x^3 - 35x)$
8	$\frac{1}{128}(6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35)$
9	$\frac{1}{128}(12155x^9 - 25740x^7 + 18018x^5 - 4620x^3 + 315x)$
10	$\frac{1}{256}(46189x^{10} - 109395x^8 + 90090x^6 - 30030x^4 + 3465x^2 - 63)$

Figure 5: On left, the plots of the Lengredre Polynomial listed on the right.

4 Lecture Notes: Root Finding

In **Numerical Analysis** by Burden & Fairs read Sec 2.1 for Bisection Method and Sec 2.3 for Newton's Method. for Trapezoidal and Simpson's rule of integration and Sec 4.7 to find zeros of Polynomial and Sec 3.1 for Lagrangian Interpolation.

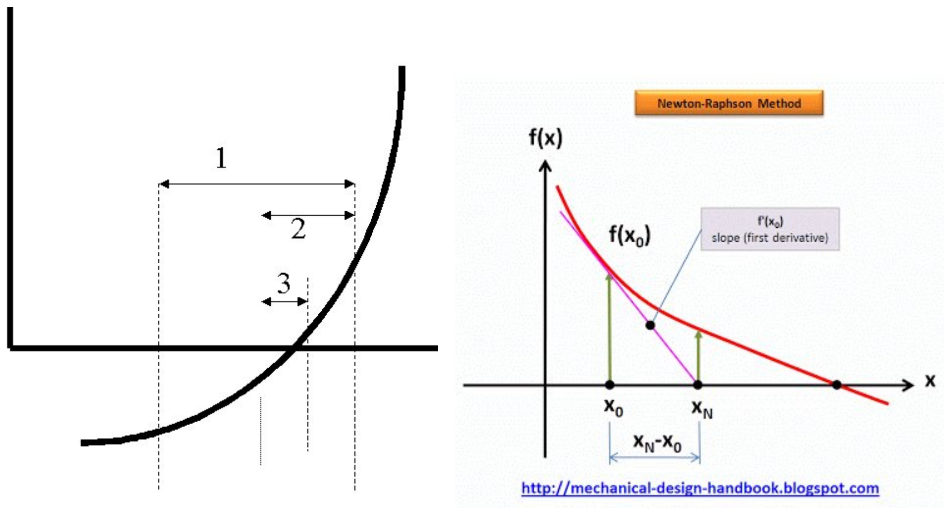


Figure 6: On left root finding by bisection. On the right root finding by Netwon-Raphson.

To find a root of a function you start with an interval $[x_{min}, x_{max}]$ where the function changes sign. For example, say $f(x_{min}) < 0$ and $f(x_{max}) > 0$, though we can switch this without too much effort. If the function is continuous (doesn't have any jumps in it, compare with the step function which does), there must be at least one zero between x_{min} and x_{max}: just one if the function monotonically increases/decreases, or more if the function oscillates

One way to find the zero is to bisect the interval repeatedly. To do this, look at $f\left(x_c \equiv \frac{x_{min}+x_{max}}{2}\right)$. If $f(x_c) < 0$, then a zero must be between $f(x_c)$ and $f(x_{max})$, so we replace our old x_{min} with x_c and repeat. If $f(x_c) > 0$, then a zero must be between $f(x_{min})$ and $f(x_c)$, so we replace our old x_{max} with x_c instead. By repeating this process, we can constrain a zero of the function $f(x)$ arbitrarily well.

Newton had a faster idea (smart computer scientist that Isaac). Start with a guess for the zero, x_0, approximate the function $f(x)$ as a straight line, and use the x intercept of that line, denoted x_1, as a new guess for the zero, then repeat.

More explicitly, we use a first order series for f(x),

$$f(x) \simeq f(x_0) + (x - x_0) f'(x_0), \tag{35}$$

and solve for the zero to get $x_1 = x_0 - f(x_0)/f'(x_0)$, or on the computer iterate

$$x \leftarrow x - f(x)/f'(x). \tag{36}$$

The classic example is to find the square root of a number A by finding the positive zero of $f(x) = x^2 - A$ using $f'(x) = 2x$. This gives us:

$$x - f(x)/f'(x) = x - \frac{x^2 - A}{2x} = \frac{x + x/A}{2} \to x$$

so the computer does the iteration,

$$x = (1/2) \times (x + x/A); \tag{37}$$

The problem set will show that this is fantastically fast relative to bisection... unless the method fails. That's life in the fastlane!