Homework 3 - Methods in Theoretical Physics (Physics 5350)

I. **DUE DATE**: February 28, 09:00 AM (PLEASE SHOW YOUR WORK)

Problem 1) Linear Interpolation

a) State the error term for 1st order linear interpolation.

b) A 2nd order polynomium is used to estimate $e^{0.2}$ by interpolation among the values of $e^0 = 1$, $e^{0.1} = 1.1052$, and $e^{0.3} = 1.3499$. Find the estimate for $e^{0.2}$ and use the error formula to find an estimate of the **maximum and minimum error.** Is the actual error within these bounds?

Problem 2) Program for Neville's Algorithm

2a) ***Write a function (or subroutine)*** that performs ***Neville's algorithm*** for polynominal interpolation. Assume that the values of $n+1$ support points (x and y vectors) are passed to the function (subroutine). Furthermore, the location x_{inter} (the location where you want to interpolate to) should be passed to the function (subroutine) and the interpolated value at this location should be returned.

Choose your path through the interpolation tree so as to stay close to a "straight line" as discussed in class.

Keep track of the corrections $C_{m,,i}$ and/or $D_{m,\,i}$ and return their last value, $C_{n,0}$, and/or $D_{n,0}$, as an estimate for the error of the interpolation.

2b) Write a program that uses (calls) your Neville interpolation algorithm (2a).
Generate support points using the following do loop:

```
n=11
do i = 0, 10
  x(i) = 2.*3.1415*i/(n-1.)
  y(i) = cos(x(i))
end do
```

Using your interpolation evaluate the function at x = π/4 and x = 5π/4 and compare to the actual results.

Using the error formula for interpolation, evaluate if the error is consistent with your expectations?

3) Program for Kaczmarz Algorithm

Consider you have a square of 3x3 boxes as shown below containing 9 numbers x_1 to x_9.

Let's say that the only thing we know about these numbers are the sums along each row, each column, and along the two diagonals.

X_1	X_2	X_3
X_4	X_5	X_6
X_7	X_8	X_9

$$X_1 + X_2 + X_3 = 6$$
$$X_4 + X_5 + X_6 = 15$$
$$X_7 + X_8 + X_9 = 24$$
$$X_1 + X_4 + X_7 = 12$$
$$X_2 + X_5 + X_8 = 15$$
$$X_3 + X_6 + X_9 = 18$$
$$X_1 + X_5 + X_9 = 15$$
$$X_3 + X_5 + X_7 = 15$$

The first thing you notice is that we have 8 equations and 9 unknowns. So the problem is underdetermined and we will have not just one solution that solves the above equations. Such problems, for example, occur often in tomographic inversions.

But let's organize the above equations in a matrix form: Ax = b, where A is a matrix, x is our solution vector, and b is the right-hand side vector.

Underdetermined inversion problems like the one above are often solved using correction algorithms. These are iterative techniques in which an assumed solution is gradually improved upon through successive iterations which approach some approximate solution to a linear system. Most modern correction algorithms and a significant number of imaging technologies rely on this process. The mathematical foundation of these algorithms is derived from the work of Polish mathematician Stefan Kaczmarz and was developed in 1937 for solving large systems of equations.

The method states that given a real or complex mxn matrix A and a real or complex vector b, an approximate solution to the system Ax = b can be found using the expression

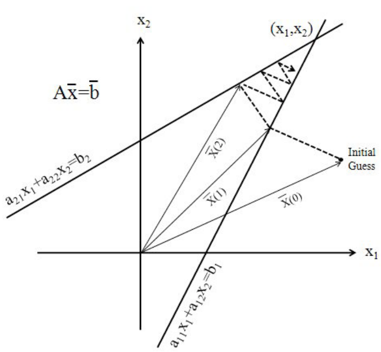
$$x^{k+1} = x^k + \frac{b_i - \langle a_i, x^k \rangle}{\|a_i\|^2} a_i$$

The iteration value is represented by k and i = modulo(k, m)+1. The ith row of matrix A is given by a_i and the ith component of vector b by b_i. In this notation <-,-> refers to the inner product of two vectors and $\|\cdot\|$ to the euclidian norm of a vector.

The Kaczmarz method is an alternating projection algorithm in which a given point is alternately projected onto the hyperplanes defined by the system of equations

This process is illustrated in the figure below for a 2x2 system and demonstrates the concept of an iterative solution. Suppose that a set of two equations in two variables contains a single unique solution. This system can be represented by two lines intersecting at one point in two dimensional space as seen in the figure. A point is selected as the initial guess for the solution. The inner product $\langle a_i, x^k \rangle = b_i^k$ serves as a projection operator. The computed value of the vector b_i^k obtained from the initial guess differs from the known value b_i. As a result, the point is projected onto the line (hyperplane) defined by a_i. The process is repeated as the point is successively projected onto the hyperplanes defined by each row of the matrix A. In the example seen in the figure, the repeated projection of the initial point results in its convergence to an approximate solution, which is equivalent to the exact solution in the limit that the number of projections becomes infinite. The process is less intuitive for large matrices although it utilizes the same principles. When the system is underdetermined a unique solution does not exist and, as a result, the Kazcmarz method cannot converge to a single point. The question naturally arises as to how the algorithm behaves when presented with an infinite number of solutions. If an infinite set of solutions exists, the algorithm will converge to the smoothest solution.

Write a program (Hint: This is a rather short program) to use the algorithm to solve the set of 8 equations given above. Start from an initial guess that the entire x vector is zero. Test your program first on a simple 2x2 system as indicated in the figure below. I recommend to first try out the algorithm for a simple 2x2 example on a piece of paper to see how it works before programming it.



Hand in your programs, and functions, from problems 1, 2 and 3.
(Email to Ludger.Scherliess@usu.edu)