Fys4150: Computational Physics

Project 1

Due date **19.th of September, 2016 - 23:59**

Øyvind B. Svendsen, Magnus Christopher Bareid
un: oyvinbsv, magnucb

September 18, 2016

Abstract

The aim of this project is for the students to get familiar with various vector and matrix operations, from dynamic memory allocation to the usage of programs in the library package of the course.

The students were invited to use either brute force-algorithms to calculate linear algebra, or to use a set of recommended linear algebra packages, i.e. Armadillo, that simplify the syntax of linear algebra. Additionally, dynamic memory handling is expected.

The students will showcase necessary algebra to perform the tasks given to them, and explain the way said algebra is implemented into algorithms. In essence, we're asked to simplify a linear second-order differential equation from the form of the Poisson equation, seen as

$$\nabla^2\Phi = -4\pi\rho(\mathbf{r})$$

into a one-dimensional form bounded by Dirichlet boundary conditions.

$$-u''(x) = f(x)$$

so that discretized linear algebra may be committed unto the equation, yielding a number of numerical methods for aquiring the underivated function $u(x)$.

Contents

1 Computational Physics, first project

1.1 The fundamental math

1.1.1 Introduction

The production of this document will inevitably familiarize its authors with the programming language `C++`, and to this end mathematical groundwork must first be elaborated to translate a Poisson equation from continuous calculus form, into a discretized numerical form.

The Poisson equation is rewritten to a simplified form, for which a real solution is given, with which we will compare our numerical approximation to the real solution.

The real motivation for this project, though, is to find a viable numerical method for double integration and the implementation of such.

1.1.2 Problem

1.1.3 Method

Reviewing the Poisson equation:

$$\begin{aligned}
&\nabla^2\Phi = -4\pi\rho(\mathbf{r}), \text{ which is simplified one-dimensionally by } \Phi(r) = \phi(r)/r \\
\Rightarrow &\frac{d^2\phi}{dr^2} = -4\pi r\rho(r), \text{ which is further simplified by these substitutions:} \\
&r \to x, \\
&\phi \to u, \\
&4\pi r\rho(r) \to f, \qquad \text{which produces the simplified form}
\end{aligned}$$

$$\begin{aligned}
&-u''(x) = f(x), \qquad \text{for which we assume that} \qquad f(x) = 100e^{-10x}, \\
\Rightarrow &u(x) = 1 - (1 - e^{-10})x - e^{-10x}, \text{ with bounds: } x \in [0,1],\ u(0) = u(1) = 0
\end{aligned} \tag{1}$$

From here on and out, the methods for finding the doubly integrated function $u(x)$ numerically will be deduced.

To more easily comprehend the syntax from a programming viewpoint, one may refer to the each discretized representation of x and u; we know the span of x, and therefore we may divide it up into appropriate chunks. Each of these x_i will yield a corresponding u_i.

We may calculate each discrete x_i by the form $x_i = ih$ in the interval from $x_0 = 0$ to $x_{n+1} = 1$ as it is linearly increasing, meaning we use $n+1$ points in our approximation, yielding the step length $h = 1/(n+1)$. Of course, this also yields the discretized representation of $u(x_i) = u_i$.

Through Euler's teachings on discretized numerical derivation methods, a second derivative may be constructed through the form of

$$\begin{aligned}
&\left(\frac{\partial}{\partial x}\right)_{fw} u(x) = \frac{u_{i+1} - u_i}{h}\ , \qquad \left(\frac{\partial}{\partial x}\right)_{bw} u(x) = \frac{u_i - u_{i-1}}{h}\ , \\
&\left(\frac{\partial}{\partial x}\right)^2 u_i = \left(\frac{\partial}{\partial x}\right)_{bw}\left(\frac{\partial}{\partial x}\right)_{fw} u_i = \left(\frac{\partial}{\partial x}\right)_{bw}\left(\frac{u_{i+1} - u_i}{h}\right) = \frac{\left(\frac{\partial}{\partial x}\right)_{bw} u_{i+1} - \left(\frac{\partial}{\partial x}\right)_{bw} u_i}{h} \\
&\left(\frac{\partial}{\partial x}\right)^2 u_i = \frac{u_{+1} - 2u_i + u_{i-1}}{h^2}\ , \qquad \text{which we then use for the problem in question, (1).} \\
\Rightarrow &-\left(\frac{\partial}{\partial x}\right)^2 u(x) = -\frac{u_{+1} - 2u_i + u_{i-1}}{h^2} = \frac{2u_i - u_{i+1} - u_{i-1}}{h^2} = f_i, \qquad \text{for } i = 1, ..., n
\end{aligned} \tag{2}$$

The discretized prolem can now be solved as a linear algebra problem. Looking closer at the discretized problem:

$$
\begin{aligned}
-u''(x_i) = \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} &= f_i \ , \qquad && \text{for } i = 1, \ldots, n. \\
\Rightarrow \qquad -u_{i+1} + 2u_i - u_{i-1} &= h^2 f_i \ , && \text{substitute } h^2 f_i = y_i, \text{ and test for some values:}
\end{aligned}
$$

$$
\begin{aligned}
i = 1: \qquad & -u_2 + 2u_1 - u_0 = y_1 \\
i = 2: \qquad & -u_3 + 2u_2 - u_1 = y_2 \\
i = 3: \qquad & -u_4 + 2u_3 - u_2 = y_3 \\
& \vdots \\
i = n: \qquad & -u_{n+1} + 2u_n - u_{n-1} = y_n
\end{aligned}
$$

By now it should be obvious to recognize that the coefficients corresponding to each of these terms and their corresponding values of $u(x)$ looks very similar to a tridiagonal matrix multiplication problem which could be represented such as this:

$$
-\left(\frac{\partial}{\partial x}\right)^2 u(x) = f(x) \qquad \Rightarrow \qquad \hat{\mathbf{A}}\hat{\mathbf{u}} = \hat{\mathbf{y}} \qquad \Rightarrow \qquad
\begin{pmatrix}
2 & -1 & 0 & \ldots & \ldots & 0 \\
-1 & 2 & -1 & 0 & & \vdots \\
0 & -1 & 2 & \ddots & \ddots & \vdots \\
\vdots & 0 & \ddots & \ddots & \ddots & 0 \\
\vdots & & \ddots & \ddots & \ddots & -1 \\
0 & \ldots & \ldots & 0 & -1 & 2
\end{pmatrix}
\begin{pmatrix} u_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ u_{n+1} \end{pmatrix}
=
\begin{pmatrix} y_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ y_{n+1} \end{pmatrix}
$$

This matrix equation will not be valid for the first, and last, values of $\hat{\mathbf{y}}$ because they would require elements of $\hat{\mathbf{u}}$ that are not defined; u_{-1} and u_{n+1}, respectively. Given this constraint we see that the matrix-equation gives the same set of equations that we require.

$$
\begin{aligned}
i = 1: \quad & -u_2 + 2u_1 - u_0 = y_1 \\
i = 2: \quad & -u_3 + 2u_2 - u_1 = y_2 \\
i = 3: \quad & -u_4 + 2u_3 - u_2 = y_3 \\
& \vdots \\
i = n: \quad & -u_{n+1} + 2u_n - u_{n-1} = y_n
\end{aligned}
$$

The original problem at hand (the simplified Poisson equation) has now been reduced to a numerical linear algebra problem. Solving a tridiagonal matrix-problem like this is done by Gaussian elimination of the tridiagonal matrix $\hat{\mathbf{A}}$, and thereby solving $\hat{\mathbf{u}}$ for the resulting diagonal-matrix, as presumably $\hat{\mathbf{A}}$ and $\hat{\mathbf{y}}$ are the knowns in this set.

Firstly the tridiagonal matrix $\hat{\mathbf{A}}$ is rewritten to a series of three vectors $\hat{\mathbf{a}}$, $\hat{\mathbf{b}}$, and $\hat{\mathbf{c}}$ that will represent a general tridiagonal matrix. This will make it easier to include other problems of a general form later.

The tridiagonal matrix $\hat{\mathbf{A}}$ with the vector $\hat{\mathbf{y}}$ included now looks like:

$$\begin{pmatrix} b_0 & c_0 & 0 & \dots & \dots & 0 & y_0 \\ a_1 & b_1 & c_1 & \ddots & & \vdots & \vdots \\ 0 & a_2 & b_2 & c_2 & \ddots & \vdots & \vdots \\ \vdots & \ddots & a_3 & b_3 & \ddots & 0 & \vdots \\ \vdots & & \ddots & \ddots & \ddots & c_n & \vdots \\ 0 & \dots & \dots & 0 & a_{n+1} & b_{n+1} & y_{n+1} \end{pmatrix}$$

, but we only work with rows from $i = 1$ to $i = n$ because of the Dirichlet conditions, as explained above. The matrix which we row-reduce thus looks like this

$$\begin{pmatrix} b_1 & c_1 & 0 & \dots & \dots & 0 & y_1 \\ a_2 & b_2 & c_2 & \ddots & & \vdots & \vdots \\ 0 & a_3 & b_3 & c_3 & \ddots & \vdots & \vdots \\ \vdots & \ddots & a_4 & b_4 & \ddots & 0 & \vdots \\ \vdots & & \ddots & \ddots & \ddots & c_n & \vdots \\ 0 & \dots & \dots & 0 & a_n & b_n & y_n \end{pmatrix}$$

The Gaussian elimination can be split into two parts; a forward substitution were the matrix-elements a_i are set to zero, and a backward substituion were the vector-elements u_i are calculated from known values.

Starting the Gaussian elimination with the second row, row II, a row operation is performed to maintain the validity of the system. The goal is to remove element a_2 from the row. This is done by subtracting row II, multiplied with some constant k from row I. For every next row operation, there will then be a new k_i calculated.

$$\begin{pmatrix} b_1 & c_1 & 0 & \dots & \dots & 0 & y_1 \\ \tilde{a}_2 & \tilde{b}_2 & \tilde{c}_2 & \ddots & & \vdots & \tilde{y}_2 \\ 0 & a_3 & b_3 & c_3 & \ddots & \vdots & \vdots \\ \vdots & \ddots & a_4 & b_4 & \ddots & 0 & \vdots \\ \vdots & & \ddots & \ddots & \ddots & c_n & \vdots \\ 0 & \dots & \dots & 0 & a_n & b_n & y_n \end{pmatrix}$$

$$\tilde{\text{II}} = \text{II} - k_{\text{I}} \times \text{I}$$

where k_{I} is determined by

$$\tilde{a}_2 = 0 = a_2 - k_{\text{I}} b_1 \quad \Rightarrow k_{\text{I}} = \frac{a_2}{b_1}$$

$$\tilde{b}_2 = b_2 - \frac{a_2}{b_1} c_1$$

$$\tilde{c}_2 = c_2 - \frac{a_2}{b_1} \times 0 = c_2$$

$$\tilde{y}_2 = y_2 - \frac{a_2}{b_1} y_1$$

Moving on to row 3, and performing a similar operation:

$$\begin{pmatrix} b_1 & c_1 & 0 & \dots & \dots & 0 & y_1 \\ 0 & \tilde{b}_2 & c_2 & \ddots & & \vdots & \tilde{y}_2 \\ 0 & \tilde{a}_3 & \tilde{b}_3 & \tilde{c}_3 & \ddots & \vdots & \tilde{y}_3 \\ \vdots & \ddots & a_4 & b_4 & \ddots & 0 & \vdots \\ \vdots & & \ddots & \ddots & \ddots & c_n & \vdots \\ 0 & \dots & \dots & 0 & a_n & b_n & y_n \end{pmatrix}$$

$$\tilde{\tilde{\text{II}}} = \text{II} - k_{\text{II}} \times \text{II}$$

where k_{II} is determined by

$$\tilde{a}_3 = 0 = a_3 - k_{\text{II}} \tilde{b}_2 \quad \Rightarrow k_{\text{II}} = \frac{a_3}{\tilde{b}_2}$$

$$\tilde{b}_3 = b_3 - \frac{a_3}{\tilde{b}_2} c_2$$

$$\tilde{c}_3 = c_3 - \frac{a_3}{\tilde{b}_2} \times 0 = c_3$$

$$\tilde{y}_3 = y_3 - \frac{a_3}{\tilde{b}_2} \tilde{y}_2$$

Having repeated this procedure, a pattern emerges and an algorithm can be formulated:

$$\tilde{b}_{i+1} = b_{i+1} - \frac{a_{i+1}}{\tilde{b}_i} c_i$$
$$\tilde{y}_{i+1} = y_{i+1} - \frac{a_{i+1}}{\tilde{b}_i} \tilde{y}_i$$
$$i = 1, 2, \ldots, n-1$$

After this procedure, the tridiagonal matrix $\hat{\mathbf{A}}$ is transformed into an uppertriangular matrix. This sort of set of equations can be solved iteratively for $\hat{\mathbf{u}}$, since the last equation has one unknown and the other equations has only two unknowns.

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2 Appendix - Program list

This is the code used in this assignment. Anything that was done by hand has been implemented into this pdf, above. `plot_stuff.py`

```
import pylab as pyl
import os
import sys

curdir = os.getcwd()
data_dict = {} #dictionary of files
n_range_LU = pyl.logspace(1,3,num=3)
n_range_tridiag = pyl.logspace(1, 4,num=7)

for n in n_range_tridiag:
    #loop through different n's
    with open(curdir+"/data/dderiv_u_c++_n%d_tridiag.dat"%(int(n)), 'r') as infile:
        full_file = infile.read() #read entire file into text
        lines = full_file.split('\n') #separate by EOL-characters
        lines = lines[:-1] #remove last line (empty line)
        keys = lines.pop(0).split(',  ') #use top line as keys for dictionary
        dict_of_content = {}
        for i,key in zip(range(len(keys)), keys): #loop over keys, create approp. arrays
            dict_of_content[key] = [] #empty list
            for j in range(len(lines)): #loop though the remaining lines of the data-set
                line = lines[j].split(',  ') #split the line into string-lists
                word = line[i] # append the correct value to the correct list with the correct key
                try:
                    word = float(word) #check if value can be float
                except ValueError: #word cannot be turned to number
                    print word
                    sys.exit("There is something wrong with your data-file \n'%s' cannot be turned to numbers"%word)
                dict_of_content[key].append(word)
        data_dict["n=%d"%n] = dict_of_content #add complete dictionary to dictionary of files

def u_exact(x):
    u = 1.0 - (1.0 - pyl.exp(-10.0))*x - pyl.exp(-10.0*x)
    return u

def compare_methods(n):
    """
    For a specific length 'n' compare both methods
    with the exact function.
    """
    x = pyl.array(data_dict["n=%d"%n]["x"])
    gen = pyl.array(data_dict["n=%d"%n]["u_gen"])
    spec = pyl.array(data_dict["n=%d"%n]["u_spec"])
    exact = u_exact(x)
    pyl.figure("compare methods")
    pyl.grid(True)
    pyl.hold(True)
    pyl.xlabel("x")
    pyl.ylabel("u(x)")
    pyl.title("function u for three different methods (n=%d)"%n)

    pyl.plot(x, exact, 'k-', label="exact")
    pyl.plot(x, gen, 'b--', label="general tridiagonal")
    pyl.plot(x, spec, 'g-', label="specific tridiagonal")
    pyl.legend(loc='best', prop={'size':9})
    pyl.savefig(curdir+"/img/compare_methods_n%d.png"%n)
```

```
56
57 def compare_approx_n(n_range=[10,100,1000], approx_string="general"):
58     """
59     For all n's available, plot the general approximation and
60     exact solution
61     """
62     if approx_string == "general":
63         approx_key = "u_gen"
64     elif approx_string == "specific":
65         approx_key = "u_spec"
66     else:
67         sys.exit("In function 'compare_approx_n', wrong argument 'approx_string'")
68     pyl.figure("compare %s"%approx_string)
69     pyl.grid(True)
70     pyl.hold(True)
71     pyl.xlabel("x")
72     pyl.ylabel("u(x)")
73     pyl.title("approximation by %s tridiagonal method"%approx_string)
74
75     for n in n_range:
76         n = int(n)
77         x = pyl.array(data_dict["n=%d"%n]["x"])
78         u_approx = pyl.array(data_dict["n=%d"%n][approx_key])
79         pyl.plot(x, u_approx, '--', label="n=%1.1e"%n)
80
81     x = pyl.linspace(0,1,1001)
82     exact = u_exact(x)
83     pyl.plot(x, exact, '-', label="exact")
84     pyl.legend(loc='best', prop={'size':9})
85     pyl.savefig(curdir+"/img/compare_%s_n_n%d.png"%(approx_string,n))
86
87 def epsilon_plots(n_range=[10,100,1000]):
88     eps_max = pyl.zeros(len(n_range))
89     h = pyl.zeros(len(n_range))
90     for i, n in enumerate(n_range):
91         x = pyl.array(data_dict["n=%d"%n]["x"])
92         u = u_exact(x)
93         v = pyl.array(data_dict["n=%d"%n]["u_gen"])
94         #calculate eps_max by finding max of |v_i - u_i|
95         max_diff_uv = 0; jmax = 0;
96         for j in range(n):
97             diff_uv = abs(v[j]-u[j])
98             if diff_uv > max_diff_uv:
99                 max_diff_uv = diff_uv
100                jmax = j
101        if jmax == 0 or jmax == n-1:
102            sys.exit("There is an error in calculating the max_epsilon")
103        eps_max[i] = pyl.log10(max_diff_uv/float(abs(u[jmax])))
104        h[i] = pyl.log10(1.0/(n+1))
105    pyl.figure("epsilon")
106    pyl.grid(True)
107    pyl.hold(True)
108    pyl.xlabel(r"\log_{10}(h)")
109    pyl.ylabel(r"$\epsilon = \log_{10}\left(\frac{u_{approx}-e_{exact}}{u_{exact}}\right)$")
110    pyl.title("log-plot of epsilon against step-length h")
111    pyl.plot(h, eps_max, 'ko')
112    pyl.legend(loc='best')
113    pyl.savefig(curdir+"/img/epsilon.png")
114
115 #make plots
```

```
compare_methods(n=10)
#compare_approx_n(approx_string="general")
#compare_approx_n(approx_string="specific")
#epsilon_plots()
pyl.show()
```