PHYS 325 Scientific Computing — Fall 2018

Solutions Exam 1

Problem 1: Short questions

a) 10^{-6} =`1e-6` [1 point]
   0.0022 =`2.2e-3` [1 point]
b) `1.25e2`= 125 [1 point]
   `1e-1`= 0.1 [1 point]
c) `n` is a string in `n='5'` because of the quotes. [1 point]
d) The output of `print(3 >= 3)` is `True`. [1 point]
e) The output of the program is 12, because we add $0 + 2 + 4 + 6$ via the loop. [2 points]

Problem 2: Python

```
import numpy as np              # alternatively, use numpy.sign(...) later

def f(x):
    return 2 - np.exp(-x) - x   # wrong indentation; either np.exp or import math

a = -2
b = 0
counter = 0

accuracy = float( input("Please enter the desired accuracy, for example 1e-10") )

# Check that the root is indeed bracketed
if( np.sign(f(a)) != np.sign(f(b)) ):
    while( abs(a-b) > accuracy ):
        counter += 1
        midpoint = (a+b)/2
        if( np.sign(f(midpoint)) == np.sign(f(a)) ):
            a = midpoint
        else:
            b = midpoint

print("Bisection converged to ", (a+b)/2, " after ", counter, " iterations")
```

The errors were corrected in the code in red:

- referred to numpy module incorrectly
- used function from the math module which was not imported
- wrong indentation
- forgot to initialize counter
- confused integer and float
- forgot quotes around input promt text

- forgot `#` before comment
- forgot `:` in two places
- comparison needs to be done with the `==` operator
- missing bracket
- misspelled a variable name

Problem 3: Numerical Stability

a) For small values of x the value of y approaches $1-1=0$. Subtraction of two similar numbers suffers from large roundoff errors.

b) Rewrite

$$y = \frac{1}{1-3x} - \frac{1+2x}{1-x} = \frac{1-x-(1-3x)(1+2x)}{(1-3x)(1-x)} = \frac{1-x-1-2x+3x+6x^2}{(1-3x)(1-x)} = \frac{6x^2}{(1-3x)(1-x)}$$

This expression is numerically stable.

c) The exact value of the sum is 0.110002

d) The numerical value is 0.01. Step by step:

```
1e20 + 1e-1 = 1e20      # insufficient machine precision
1e20 - 1e20 = 0.0
0.0 + 1e12  = 1e12
1e12 + 1e-6 = 1e12      # insufficient machine precision
1e12 + 1e-6 = 1e12      # insufficient machine precision
1e12 - 1e12 = 0.0
0.0 + 1e-2  = 1e-2 = 0.01
```

e) For example:

```
1e20 - 1e20 + 1e12 - 1e12 + 1e-1 + 1e-2 + 1e-6 + 1e-6
```

Problem 4: LU decomposition

$$A = \begin{pmatrix} 2 & 2 & 3 \\ 2 & 8 & 9 \\ 8 & 0 & 10 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 4 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 2 & 3 \\ 0 & 6 & 6 \\ 0 & -8 & -2 \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 4 & -4/3 & 1 \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} 2 & 2 & 3 \\ 0 & 6 & 6 \\ 0 & 0 & 6 \end{pmatrix}}_{U}$$

The determinant of A is the same as the determinant of U, namely the product of the diagonal elements of U: $\det A = 2 \cdot 6 \cdot 6 = 72$.
The matrix is invertible: for example, its determinant is not zero.

Problem 5: Nonlinear equations
See lecture notes.