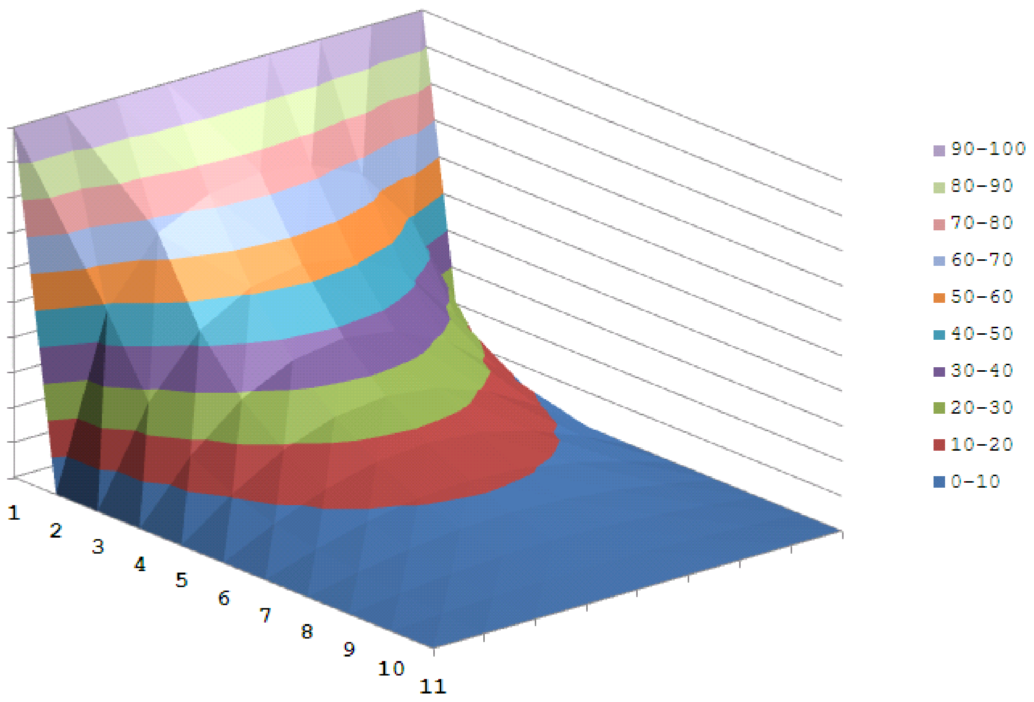


EP 208

Computational Methods in Physics
Lab Sheets

Feb 2014

SOURCES OF ERRORS

Task 1 - Truncation Errors

The first derivative (gradient) of a function can be approximated by the Forward Difference Approximation:

```
FDA = (f(x+h)-f(x))/h + O(h)
```

where h is small but not zero. Write a program that computes, using the FDA, at x = 4.0, for h = 0.01, the first derivative of the function:

$$f(x) = 3.4 + 18.7x - 1.6x^2$$

Hint: use double precision to avoid significant round-off errors confusing the results.

Task 2 - Round-off Errors

1. What is the result of your FDA program with all the variables in single-precision (float) for $h = 10^k$ where $k = 1,2,\ldots,9$

2. What is the result of your FDA program with all the variables in double-precision for $h = 10^k$ where $k = 1,2,\ldots,9$

3. What do you expect to be the output of the following programs?

```
#include <iostream>
#include <iomanip>
#include <cmath>
using namespace std;

int main()
{
  float x = 45 * M_PI/180.0;
  float a = cos(x);
  float b = sin(x);
  float c = sqrt(a*a + b*b);

  cout << setprecision(10)
       << fixed << c << endl;
}
```

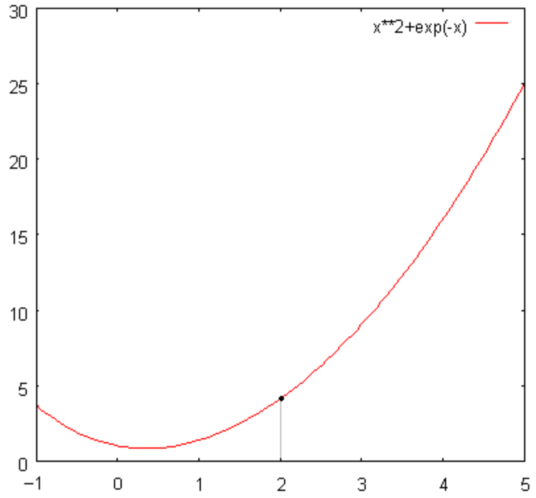
```
#include <iostream>
#include <iomanip>
#include <cmath>
using namespace std;

int main()
{
  double a=0.0;

  while(true) {
     a = a + 0.1;
     cout << setprecision(20)
          << fixed << a << endl;
     if ( a == 1.0 ) break;
     getchar();
  }
}
```

NUMERICAL DIFFERENTIATION

Consider the function $f(x) = x^2 + e^{-x}$.



Task 1
Evaluate F'(2) and F''(2) analytically.

Task 2
Write a computer program to evaluate first derivative and compare the accuracy of FDA, CDA and REA.For this use h = 0.01, and double precision data.

Task 4
Write a computer program to evaluate second derivative and compare the accuracy of FDA, CDA and REA.For this use h = 0.01, and double precision data.

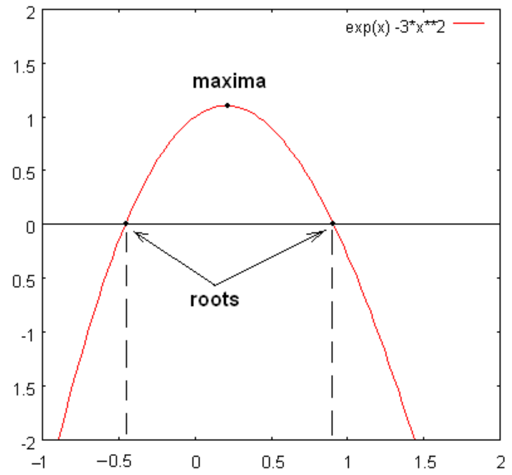
Task 5
The file **`rockect.txt`** contains two columns of data for a rocket.
First column is time in seconds and second is upward velocity in m/s.
By using CDA, compute the acceleration of the rocket as a function of time.
Also plot acceleration vs time graph of the rocket.

Download: http://www1.gantep.edu.tr/~bingul/ep208/data/rocket.txt

ROOT FINDING

For the function $f(x) = \exp(x) - 3x^2$

Task 1
Roughly, determine the roots of F(x) graphically.



Task 2
Using the bisection method, write a program evaluate to at least 6 decimal place accuracy the root of f(x). Let the initial bracket be [0.5, 1.5].

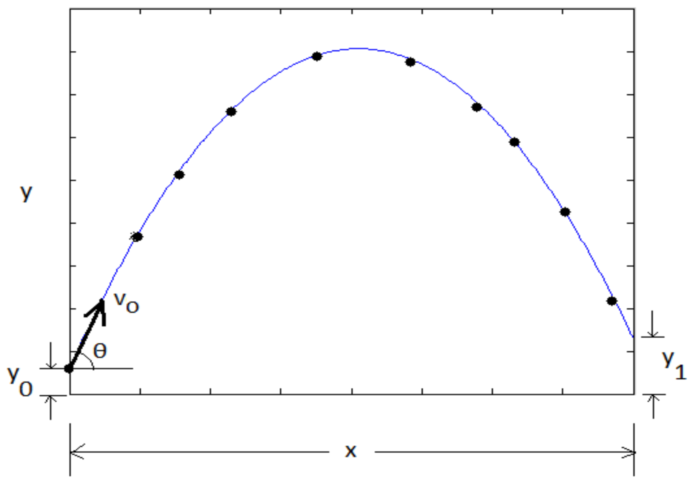
Question: *For the bisection method, theoretically, how many iterations is expected for the required accuracy of 6 dp? (Answer: 19 iterations).*

Task 3
Implement the *Newton-Raphson* root-finding algorithm given in the lecture into computer program. Using the program, evaluate to at least 6 decimal place accuracy the root of the function F(x) starting from $x_1 = 1.5$.

Task 4
Aerospace engineers sometimes compute the trajectories (path) of projectiles like rockets. A trajectory of a rocket is defined by a (x, y) coordinates and is modeled by

$$y = y_0 + (\tan\theta)x - \frac{g}{2v_0^2\cos^2\theta}x^2$$

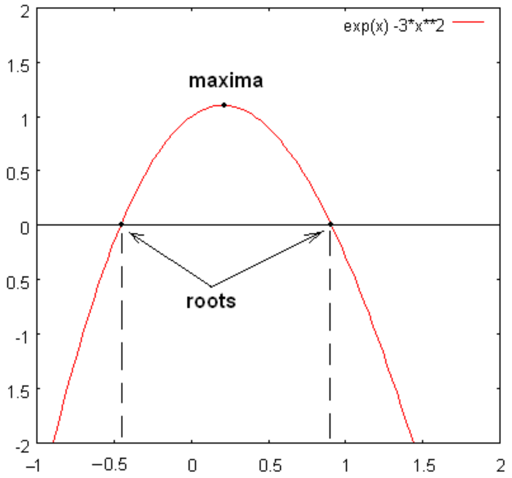
Write a program to find the appropriate initial angle θ for v_0 = 200 m/s , x = 1950 m , y_0 = 28 m and y_1 = 123 m.



Taks 5
Implement the *Newton's Square-Root* algorithm given in the lecture into a program. Use your program to evaluate, to at least 9 decimal place accuracy, the square root of 133.
Check the results against your pocket calculator or sqrt(x) intrinsic function.

OPTIMIZATION

Given the function f(x) = exp(x) – 3x^2.



Task 1

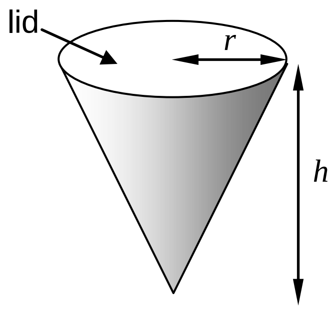
Roughly, determine the extremum point of f(x) graphically. Is is maxima or minima?

Task 2

Implement *Newton's method* and *Modified Newton's method* for finding extrema of a function f(x) given in the lecture into computer programs. Using your computer programs, find extremum of the function f(x) (for –0.5 < *x* < 1.5) to 6 decimal place accuracy.

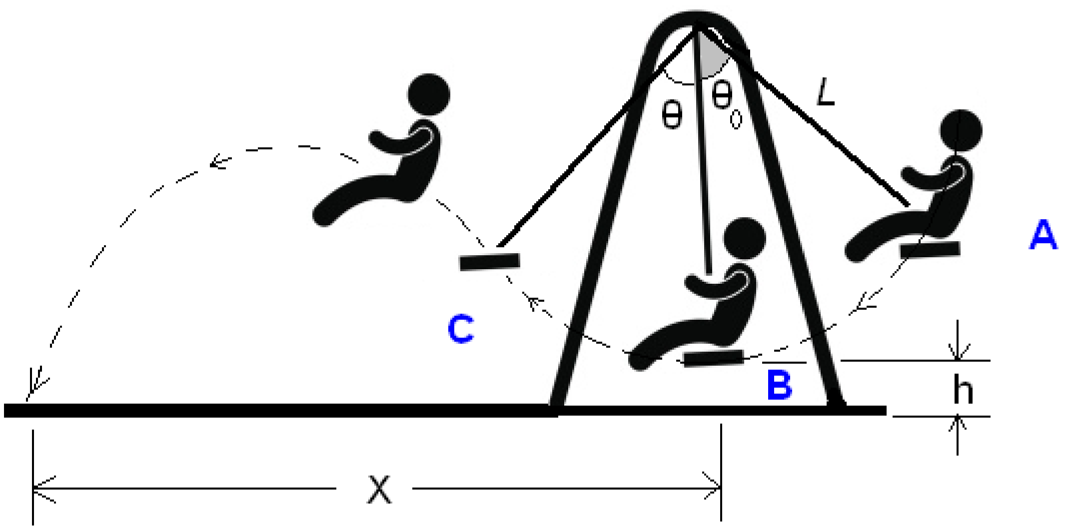
Task 3

Design an optimum conical container that has a cover and walls of negligible thickness. The container is to hold 0.2 m^3 waste water. Write a program that minimizes the area of its top and sides.



Task 4

As shown in figure, a child starts to swing at an initial angle $\theta_0 = 60^o$ from point A. Then, he passes though the minimum point B. At point C where the angular position is $\theta < \theta_0$ he jumps from swing and falls down at a distance x from point B. Write a program to find the optimal value of θ such that he can reach the maximum distance from the minimum point of the swing. Assume that the height and length of the swing are *h* = 0.5 m and *L* = 2.5 m respectively.



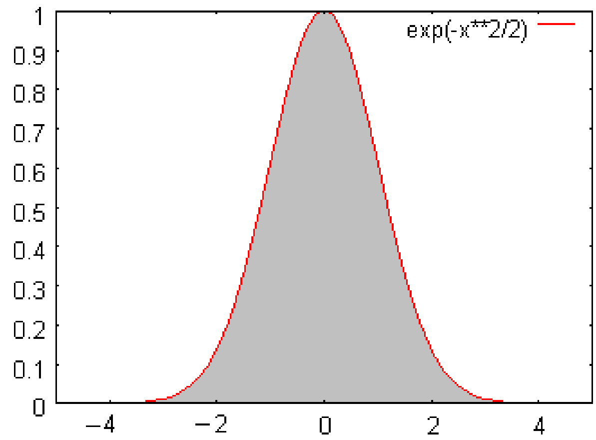
NUMERICAL INTEGRATION

Task 1

Write a computer program to integrate the following functions for n = 100 equally spaced segments using the Trapezoidal Formula and the Simpson's Formula.

(a) $\int_{-4}^{+4} \sqrt{4 - x^2}\, dx$

(b) $\int_{-3}^{+3} \exp(-x^2/2)\, dx$



Task 2

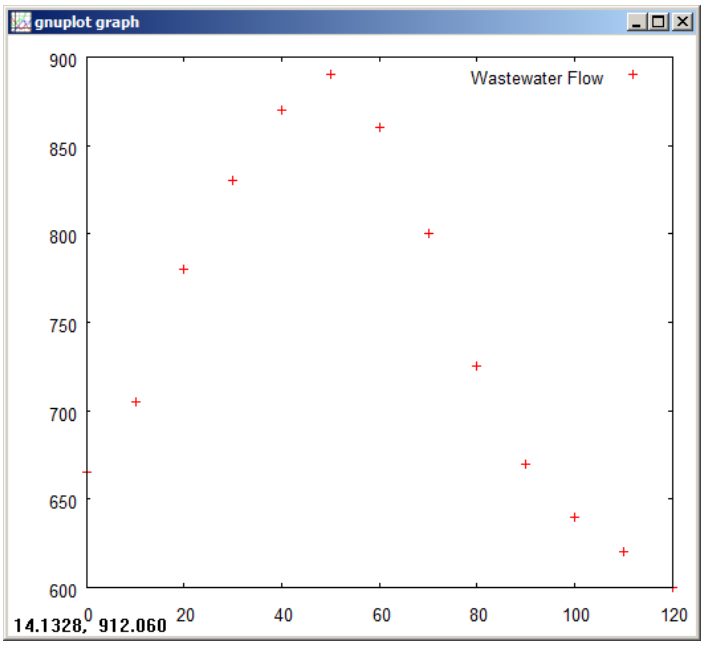
The rate of flow of wastewater in an open channel has been measured and the data given right obtained.

Determine the total flow in m^3 for 120 min using
(a) Trapezoidal method
(b) Simpson's method

Time (min)	Flow (m^3/min)
0	665
10	705
20	780
30	830
40	870
50	890
60	860
70	800
80	725
90	670
100	640
110	620
120	600

You can plot the data using gnuplot program:

```
gnuplot> plot "data.txt" title "Wastewater Flow"
```



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SOLUTIONS OF DIFFERENTIAL EQUATIONS (INITIAL VALUE PROBLEMS)

Task 1

Solve the initial value problem via the simple-Euler method for the range: $1 \le x \le 5$ with $h = 0.4$.

$$\frac{dy}{dx} = \frac{y}{x} + x \;;\; y(1) = 0$$

Compare the results with the analytical solution: $y(x) = x^2 - x$.

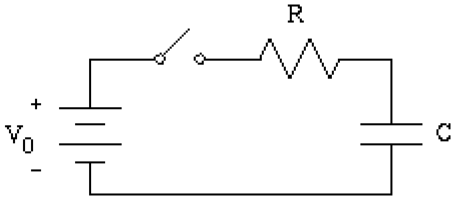
Task 2

Solve the same initial value problem in Task 1 by using second and forth order Runge-Kutta methods.

Task 3

A charging R-C circuit is governed by the 1st order D.E.

$$\frac{dq}{dt} = \frac{V_0 C - q}{RC} \quad ; \quad q\ \ 0\ \ = 0$$



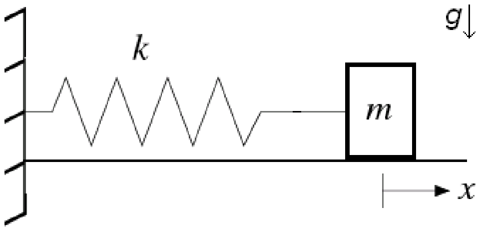
where R = 100 kΩ, C = 1 μF, charging voltage V_o = 12 V. Using the time step of $h = dt$ = 0.01 seconds and evolve the system for 1 seconds. Save your data (t and q) into file (say capacitor.txt). Use gnuplot to construct a graph of *t* vs *q*. Type:

```
gnuplot > plot "capacitor.txt" with lines
```

Task 4

A spring-mass system is governed by the 2nd order D.E.

$$m\frac{d^2x}{dt^2} + kx = 0 \quad ; \quad v\ \ 0\ \ = 0, x\ \ 0\ \ =\ 0.2\,m$$



where the mass is m = 1.01 kg, the spring constant is k = 10 N/m, $v = dx/dt$ is the velocity in m/s and x is the displacement in m. Using a time step of $h = dt$ = 0.05 s, evolve the system for 10 seconds.

Save your data (t, x, v) into file (say spring.txt). Using gnuplot, construct a graphs of t-x and t-v and t-x-v. Type

```
gnuplot > plot "datafile.txt" using 1:2
gnuplot > plot "datafile.txt" using 2:3
gnuplot > splot "datafile.txt" using 1:2:3
```

(*) More information about "*using gnuplot plotting numerical data in a data file*" can be found at:
http://t16web.lanl.gov/Kawano/gnuplot/datafile-e.html

LEAST SQUARE FITTING

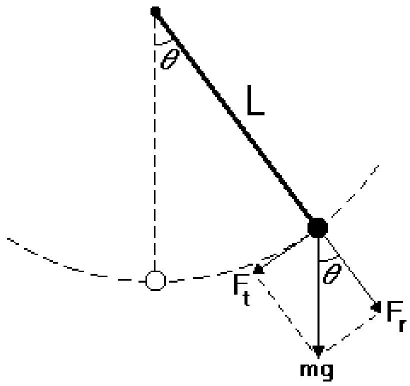
Task 1
Write a computer program
a) to fit the data given right into function f(x) = ax + b
b) to calculate the regression coefficient

x	y
1	12
2	9
3	8
4	5
5	3

Task 2
Write a computer program
a) to fit the data given right into function f(x) = ax + b
b) to calculate the regression coefficient

x	y
1	12 +- 3
2	9 +- 2
3	8 +- 2
4	5 +- 1
5	3 +- 1

Task 3
Table given below shows an experimental result of measured length (L) and corresponding measured period (T) of a simple pendulum.



Using least square fitting method, write a computer program
a) to determine the gravitational acceleration g in meter/s^2.
b) to calculate the regression coefficient.
Note that the period of a pendulum is given by $T = 2*\mathrm{pi}*(L/g)^{1/2}$

L (m)	0.150	0.160	0.170	0.180	0.190	0.200	0.210	0.220	0.230	0.240
T (s)	0.777	0.802	0.830	0.849	0.897	0.918	0.941	0.963	0.985	0.985

PROBABILITY AND FREQUENCY EXPERIMENTS

Task 1
Write a computer program to simulate tossing a coin and output probability of getting head.

Task 2
Write a computer program to simulate tossing four coins at a time and output probability of getting at least two heads.

Task 3
Write a computer program to simulate tossing a dice and output probability of getting six.

Task 4
Write a computer program to simulate tossing five dice at a time and output probability of getting at least two six.

Task 5
Suppose 1% of items made by a factory are defective. Write a program to find the probability that 6 defective items in a sample of 300 items.

MONTE CARLO METHODS

Task 1
The following C++ program can be used to estimate the area of a circle of unit radius.

```
#include <iostream>
using namespace std;

int main()
{
  int i, m=0, n=1000;
  double  x, y;
  for (i = 1; i<=n; i++){
    x = rand()/(RAND_MAX+1.0);
    y = rand()/(RAND_MAX+1.0);
    if ( x*x+y*y < 1.0 ) m++;
  }
  cout << 4.0*m/n << endl;
}
```

a) Copy the program, run and check it.
   How many random trials (n) does it take to achieve an accuracy of three decimal places?
b) See also:
   http://www1.gantep.edu.tr/~bingul/seminar/monte-carlo/src/pi.html
   http://www1.gantep.edu.tr/~bingul/seminar/monte-carlo/src/pi.exe
c) Modify it to estimate the volume of a sphere of unit radius.

Task 2
MC integration of a function f(x) = 10 sin(x) over the range x = 0 to x = π.

a) Write a Monte Carlo integration program to integrate the function f(x).
b) Compare your computed result with the analytical result: *20*.
c) How many trials (n) are required to achieve an accuracy of three decimal places?
d) See also:
   http://www1.gantep.edu.tr/~bingul/seminar/monte-carlo/src/mc-int.exe

Task 3
Write a program to evaluate the following integral:

$$\int_0^1 \int_{-3}^{+2} (x+y)\,dx\,dy$$