10.001 Introduction to Computer Methods
Final Examination
December 17, 2001

Open Book, Notes and Calculator

There is a total of 6 problems on this exam. Be sure to write your answer to each problem in a separate blue book, and to write both your name and your username on each blue book. Please take a moment to review the problems before you start answering. Try not to spend too much time on any single problem. You have 3 hours to finish the exam. Total number of points: 100.

Problem 1 (10 points)

Write down your answer to each part of this problem in your blue book.

(a) What would you type at the command prompt in unix to find out how to use the `undelete` command?

(b) What is the maximum value that can be assigned to a variable of type `unsigned int`, if the datum is stored in 2 bytes?

(c) What is meant by the statement "an algorithm using Simpson's Rule converges quartically"?

(d) If Santa's elves are attempting to fabricate toys while a howling North Pole gale shakes their workshop, are the resulting errors likely to be systematic or random?

(e) Write a single line in C that creates storage space for M float values when the value of M is not known to the person writing the code, and initializes them all to zero.

(f) How many roots will the Newton-Raphson algorithm find, each time it is invoked?

(g) If the boolean expression which controls a `do-while` statement evaluates to zero when first met, do the statements within the `do-while` nevertheless get evaluated at least once?

(h) Is the following equation linear or nonlinear?

$$f(x_1, x_2, x_3) = y_1 x_1 + \sin(y_2) x_2 - y_3^2 x_3$$

(i) Assuming that the function f(x) is continuous and has at least one root, what condition has to be true in order for the bisection algorithm converge towards a root?

(j) Name a numerical <u>algorithm</u> you could use to solve the following problem:
  "given values for the annual the production rate of floppy disks in the US, how many floppy disks were produced between 1990 and 2000?"

Problem 2 (20 points).

The moment of inertia for an object is defined as

$$I_z = \sum_{i=1}^{N} m_i \left[\left(x_i - \langle x \rangle \right)^2 + \left(y_i - \langle y \rangle \right)^2 \right]$$

where x_i and y_i are the coordinate in the xy-plane for the N point masses m_i which make up the object, <x> and <y> are the mean (i.e. average) values of x_i and y_i, and I_z is the moment of inertia about an axis perpendicular to the xy-plane and passing through the point [<x>,<y>].

Write the prototype, definition and sample invocation for a C function which computes the moment of inertia for an object consisting of N point masses, where N is specified by the user in the calling routine. The coordinates used in the calling routine are stored in two 1-dimensinal arrays, as are the masses.

Your function should adhere strictly to the following guidelines:
(a) the name of the function is *moment_of_inertia*
(b) the function receives information only through its argument list
(c) all the data in the calling routine have been declared to be of type *double*
(d) your code should be formatted and documents to be user-friendly

Indicate each part of your answer in the blue book:

Part (a): prototype

Part (b) definition

Part (c) invocation

Problem 3. (15 points)

Answer the following questions in your blue book.

(a) Write a piece of Matlab code to multiply matrix **A,** having dimensions **m** and **n** (ie. an **m** x **n** matrix), with matrix **B** (a **p** x **q** matrix). Your code should take advantage of Matlab syntax which operates with rows and columns of **A** and **B**, not with matrices as a whole or with single elements. The code should check for the matrix dimensions to agree. (10 points)

Given the column vector **A** = $(1\ \ 2\ \ 4)^T$ and the row vector **B** = (3 0 2), compute the result of the following three Matlab operations (5 points):

(b) A*B

(c) B*A

(d) A.*B

Problem 4. (15 points)

Answer the following questions on the statistical analysis of experimental errors:

(a) What are the main parameters that characterize the Gaussian distribution, and how are they calculated for a set of data, $\{x_i, i=1 \text{ to } N\}$? (6 points)

(b) Suppose that you are collecting experimental data for a particular measurement, and you know that the data is Gaussian-distributed. What must you do if you wish to decrease the *absolute* error of the measurement? How quickly does the error decrease if you do this? (3 points)

(c) Suppose that you measure g, the acceleration due to gravity, using a simple pendulum with period known to be $T = 2\pi\sqrt{l/g}$, where l is pendulum length. Thus $g = \dfrac{4\pi^2 l}{T^2}$.

The measured values of T and l are:

$$l = 46.48 \pm 0.1\,\text{cm}$$
$$T = 1.37 \pm 0.004\,\text{s}$$

Estimate the absolute and relative experimental errors of g, and give the final result in the two different forms using these estimates. (6 points)

Problem 5. (20 points)

In order to monitor the diffusion of pollutants from a smoke stack, an inert tracer gas (SF_6) is released continuously with the smoke from the stack, and you measure the concentration of the tracer gas (at a fixed height above ground level) as a function of distance (y) downwind of the smoke stack. Using a GPS (global positioning satellite) dish and an SF_6 detector, you can measure concentration (C) and distance (y) once a second for 2 hours, for a total of 7200 data points (time, Y-coordinate, and SF_6 concentration). Therefore the data is a matrix (called "Data") with 7200 rows and 3 columns. The data has been saved in your Athena locker as a Matlab file called tracer.dat

Pollutant dispersion from a continuous point source can be accurately modeled using the *Gaussian Plume Equation:*

$$C = \frac{kq}{2\pi u \sigma_y} \exp\left\{ \frac{-y^2}{2\sigma_y^2} \right\}$$

where:

- k = numerical constant = 3.712 [m^{-1}];
- C is the concentration of SF_6 [$\mu g/m^3$];
- q = SF_6 source strength = 10 μg/s;
- u = average wind speed = 6.2 m/s;
- y is the Y-coordinate [m];
- σ_y is the standard deviation of the concentration in the y direction [m]. (The standard deviation can be related to the diffusivity of the gas.)

It is believed that reasonable guess for σ_y is 150 m. Your job is to perform a regression of the data to obtain a more accurate estimate of this parameter. Answer the following two questions in your blue book:

(a) Write a Matlab function that calculates the sum of the square of the residuals. Your function should have two arguments: a vector containing your initial guess for σ_y and and the matrix of data. (10 points)

(b) Write a Matlab script file that loads the data and minimizes the square of the residuals. (10points)

Problem 6. (20 points)

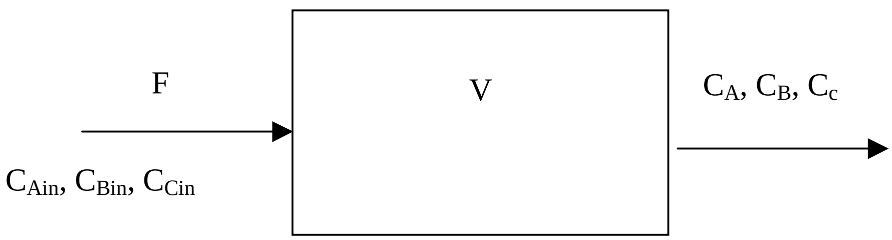
A chemical reaction is performed in a continuous stirring tank reactors (CSTR) to produce compound C from compounds A and B, according to the following reaction:

$$A + B \rightarrow C$$

The rate at which A and B are converted to C may be written as follows:

$$-\frac{dC_A}{dt} = -\frac{dC_B}{dt} = \frac{dC_C}{dt} = kC_A C_B$$

k is a reaction rate constant, C_A, C_B and C_C are the concentrations of A, B and C, respectively, in the reactor. One of the features of a CSTR is that the concentrations of compounds leaving the reactor are the same as those inside the reactor. Inlet pipes deliver a mixture of A, B & C into the reactors at concentrations C_{Ain}, C_{Bin}, C_{Cin} and flow rate F. Outlet pipes bring out the mixture of the same compounds with concentrations C_A, C_B, C_C.



A mass balance on compound A requires that the amount of A which flows into the reactor, minus the amount of A consumed by the reaction, equals the amount of A which leaves the reactor:

$$FC_{Ain} - V k\, C_A C_B = FC_A$$

Similar equations can be written for the mass balances on B and C.

You are given the following information:

Input concentrations:	$C_{Ain} = 0.5$, $C_{Bin} = 0.4$, $C_{Cin} = 0.2$,
output concentration for A:	$C_A = 0.1$,
reaction rate constant k:	$k = 1.0\ \text{min}^{-1}$

and wish to solve for the output concentrations C_B and C_C, and the ratio $\theta = F/V$, where F is the flow rate (liters/min) and V is the reactor volume (liters). Answer the following questions:

a) What classification of numerical problems that we covered in 10.001 does this problem belong to? (1 point)

b) Write the mass balance equations for A, B, and C in the form $\mathbf{f}(\mathbf{x})=0$, where $\mathbf{f}(\mathbf{x})$ is a 3-component vector and $\mathbf{x} = (C_B \;\; C_C \;\; \theta)^T$. (5 points):

c) Calculate the Jacobian matrix J for the system of equations created in part (b) (5 points):

d) Write the linearized equations required to solve this probem by Newton's method, in matrix form with the unknown vector $\mathbf{x} = (C_B \;\; C_C \;\; \theta)^T$ and the initial guess $\mathbf{x}_0=(C_{B0} \;\; C_{C0} \;\; \theta_0)^T$ (4 points):

e) Using $\mathbf{x}_0=(0.4 \;\; 0.1 \;\; 0.1)^T$ as an initial estimate of $\mathbf{x}$, calculate the correction to this estimate obtained in one iteration by solving the linearized system of equations. Hint: Swapping some rows and/or columns in the matrix makes this problem easier to solve. (5 points)