Fall 2000: PHY 5157 Advanced Numerical Methods – Assignments

If not stated otherwise, each assignment counts ten points towards the homework score, which (see the outline) accounts for 50% of the final grade. An unexcused absence from class counts -10 points on the homework score.

1. Formulate your expectation for this course. Which numerical methods are you (most) interested in? Which do you expect to need most for your future work? Do you already have an idea in mind for your final project? (Approximately one handwritten page. Due date: Aug 31, 2000.)

2. Random Matrix Theory (RMT) plays a role in many branches of physics. In Quantum Chromodynamics (QCD) one used an RMT ansatz for the Dirac operators and the chiral condensate Σ becomes related to the expectation value of the smallest eigenvalue $\lambda_{\min}$ of the Dirac operator. In the sector of topological charge[1] ν one has

$$\Sigma = \Sigma^{\nu} = \frac{\langle z^{\nu} \rangle}{V \, \langle \lambda^{\nu}_{\min} \rangle} \tag{1}$$

where

$$\langle z^0 \rangle = \frac{1}{2} \int_0^{\infty} z^2 \, e^{-z^2/4} \,, \quad \langle z^1 \rangle = \frac{1}{2} \int_0^{\infty} z^2 \, e^{-z^2/4} \, I_2(z) \tag{2}$$

and

$$\langle z^2 \rangle = \frac{1}{2} \int_0^{\infty} z^2 \, e^{-z^2/4} \, \Big(I_2(z)^2 - I_1(z) \, I_3(z) \Big) \tag{3}$$

(I_1, I_2 and I_3 are modified Bessel functions). Use Maple to calculate the integrals (2) and (3) numerically. For (2) compare with the exact result. (Due date: Sep 5, 2000. The solution will be posted as rmt_int.mws.)

3. Read chapters 1 and 3 of **Numerical Recipes**. (Due date: Sep 5, 2000. **No points.**)

4. Use Fortran or C and determine the machine accuracy of your favorite computer for Real*4 and Real*8 floating point numbers.

   (a) Determine the smallest epsilon `eps` > 0 for which the IF statement does still distinguish between `1` and `1+eps`.

   (b) Find the smallest `eps` > 0 such that `abs(eps-dif)/eps` is smaller than 0.1, where `dif=(1+eps)-one`. Note: You will have to "outsmart" the compiler such that the `1+eps` sum is really done and stored by the program.

   (Due date: Sep 12, 2000. A Fortran solution will be posted as accuracy.f, a program which needs the files implicit.4 and implicit.8. The result obained by the program with the Linux g77 compiler will be posted as accuracy.txt.)

5. Read chapter 4 of **Numerical Recipes**. (Due date: Sep 12, 2000. **No points.**)

[1] A topological charge enters there through the Yang-Mills gluon fields. Reference: Edwards et al. Phys. Rev. Lett. 82 (1999) 4188 and citations therein.

6. Download the data set `dat_int.dat`. The x-values are given by the first column and three functions by columns two to four. Perform interpolations (extrapolations) for the range $0 \le x \le 1$ using the following *Numerical Recipes* routines: `POLINT`, `RATINT` and `SPLINE` with `SPLINT`. When applicable, make reasonable choices for the degrees. For each case use 101 values to plot the corresponding function for $x = 0, 0.01, 0.02, \ldots, 0.99, 1.0$ with **GNUPLOT** (install gnuplot if necessary). (Due date: Sep 19, 2000.)

7. Download the data set `Pqln3dl08.dj`, which actually belongs to a spin glass simulation (Berg, et al., PRB 61 (2000) 12143). The x-values are given by the first column and the function under investigation is given by the second column. Calculate the array `YA` of the *Numerical Recipes* routine `SPLINT` and plot the function

$$Y = \frac{y'(x)}{y''(x)}$$

with gnuplot. Limit the plot to the stable region $0.65 \le x \le 0.95$. (Due date: Sep 19, 2000.)

8. Caclculate the integral

$$\int_0^\pi dx\, x\, \sin(x)$$

(a) with Maple, (b) with Romberg integration and (c) with Gaussian integration. (Due date: Sep 26, 2000.)

9. (a) Assignment 2 of secion 1.2.1 of the script.

   (b) Translate the Fortran code of (a) into C.

   (Due date: Sep 26, 2000.)

10. Assignment 1 of secion 1.5.1 of the script. (Due date: Oct 3, 2000.)

11. Assignment 2 of section 1.7.5 of the script, **but** with `iseed2=1` (instead of `iseed2=0`) for the Marsaglia random number generator. (Due date: Oct 10, 2000.)

12. Assignment 2 of section 1.8.2 of the script. You find the Fortran program and gnuplot driver files in the `a0108_02` assignments subdirectory of picl-01. However, you have to complete the Fortran program file by include statements for the appropriate subroutines. (Due date: Oct 24, 2000.)

13. Read chapter 1 of the script (use the version posted on Oct 13). (Due date: Oct 24, 2000. **No points.**)

14. Assignment 1 of secion 2.1.4 of the script. (Due date: Oct 31, 2000.)

15. Assignment 8 of secion 2.1.4 of the script. (Due date: Oct 31, 2000.)

16. Assignment 2 of secion 2.9.3 of the script. (Due date: Nov 7, 2000.)

17. Read chapter 2 of the script. (Due date: Nov 7, 2000. **No points.**)

18. Write a Metropolis program to generate the normal distribution through the Markov process

$$x \to x' = x + 2\,a\,(x^r - 0.5)$$

where a is a real constant and x^r a uniformly distributed random number in the range $[0, 1)$. Use $a = 3.0$ and the initial value $x = 0.0$ to test your program. (1) Generate a chain of 2,000 events. Plot the empirical peaked distribution function for these event in comparison with the exact peaked normal distribution function. Monitor also the acceptance rate and give the result you find. (2) Repeat the above for a chain of 20,000 events.