

Examination, Computational Physics – FYTN03

October 29 2007

Allowed calculational aids: “TEFYMA” and pocket calculator. The examination consists of eight problems.

1. Assume you have a function, $f(x)$, which you know is everywhere well-behaved and smooth and behaves as

$$\lim_{|x| \rightarrow \infty} f(x) \propto e^{-x^2/2}.$$

Explain how to make a Monte Carlo estimate of the integral

$$\int_{-\infty}^{\infty} f(x) dx.$$

using importance sampling. Describe how to generate suitable random numbers according to the chosen weight function using the transformation method on uniformly distributed random numbers between 0 and 1.

2. For the same function and integral, devise a 2-point Gaussian quadrature formula using a suitable weight function.
3. Assuming you have generated 10 points in the Monte Carlo importance sampling in problem 1, and obtained the following weights

$$f(X)/\omega(X) = \{0.64, -0.44, 2.36, -1.63, 2.04, -0.21, -0.95, 0.45, 2.39, 1.98\}$$

give an estimate of the integral and an estimate of the error. Also estimate the number of points needed to obtain a relative error of 1%.

4. Calculate $\sum_{m=1}^n m^3$ using the Euler-Maclaurin formula

$$\frac{1}{2}f(a) + \sum_{m=1}^{n-1} f(a+hm) + \frac{1}{2}f(b) = \int_a^b f(x)dx + \sum_{k=1}^{\infty} c_k h^{2k}$$

where $h = (b-a)/n$ and

$$c_k = \frac{B_{2k}}{(2k)!} \left(f^{(2k-1)}(b) - f^{(2k-1)}(a) \right)$$

and where B_n are the Bernoulli numbers ($B_0 = 1, B_2 = 1/6, B_4 = -1/30, \dots$).

5. Consider a function $f(\mathbf{x}) = \frac{1}{2}\mathbf{x} \cdot \mathbf{A}\mathbf{x} - \mathbf{b} \cdot \mathbf{x}$, where $\mathbf{x}$ and $\mathbf{b}$ are n -component vectors and $\mathbf{A}$ is a symmetric, positive definite $n \times n$ -matrix. Suppose that $\mathbf{x}_0, \mathbf{x}_1, \dots$ and $\mathbf{h}_0, \mathbf{h}_1, \dots$ are two sequences of (n -component) vectors such that $\mathbf{x}_{i+1}$ is the minimum of the function f along the line $\lambda \rightarrow \mathbf{x}_i + \lambda \mathbf{h}_i$. Show that $\mathbf{h}_0 \cdot \nabla f(\mathbf{x}_2) = 0$ if $\mathbf{h}_0 \cdot \mathbf{A}\mathbf{h}_1 = 0$.

6. Consider a system of N Ising spins $\sigma_i \in \{\pm 1\}$ ($i = 1, \dots, N$) on a circle. Assign to each configuration $\sigma = (\sigma_1, \dots, \sigma_N)$ a probability

$$P(\sigma) \propto \exp \left(K \sum_{i=1}^N \delta(\sigma_i, \sigma_{i+1}) \right)$$

where $K > 0$ is a parameter, $\sigma_{N+1} = \sigma_1$ (cyclic boundary conditions), and $\delta(\sigma_i, \sigma_j) = 1$ if $\sigma_i = \sigma_j$ and $\delta(\sigma_i, \sigma_j) = 0$ if $\sigma_i \neq \sigma_j$. Suppose that this system is simulated by using an update where for a given configuration, σ , a random spin, i , is flipped ($\sigma_i \rightarrow -\sigma_i$), and the new configuration, σ' , is accepted with some probability $A(\sigma \rightarrow \sigma')$. Derive an A which will ensure that the update satisfies detailed balance. Also show that this means that $P(\sigma)$ is stationary.

7. Describe the Crank-Nicholson method for the system

$$i \frac{d\bar{\psi}}{dt} = \mathbf{H}\bar{\psi},$$

where $\bar{\psi}$ is a complex vector with components $\psi_i(t)$ ($i = 1, \dots, N$) and $\mathbf{H}$ is a constant Hermitian matrix (i.e., $H_{ij}^* = H_{ji}$, where $*$ means complex conjugation). Show that this method preserves the normalization

$$|\bar{\psi}|^2 = \sum_{i=1}^N |\psi_i|^2$$

8. The Levenberg-Marquardt method for minimizing $\chi^2(a_1, \dots, a_M)$ is based on the update

$$a_k \rightarrow a'_k = a_k + \delta a_k, \quad \text{with} \quad \sum_{l=1}^M \tilde{\alpha}_{kl} \delta a_l = \beta_k$$

$$\beta_k = -\frac{1}{2} \frac{\partial \chi^2}{\partial a_k} \quad \tilde{\alpha}_{kl} = \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_k \partial a_l} (1 + \lambda \delta_{kl})$$

where $\lambda > 0$ is a parameter ($\delta_{kl} = 1$ if $k = l$ and $\delta_{kl} = 0$ otherwise). Give a brief motivation for this update based on the behavior for small and large λ , respectively.