University of the Witwatersrand
Advanced Techniques in Physics : Part 2 - 2004
Tutorial 2 : 55 Marks
Numerical methods

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1. In the context of discretising partial differential equations :

   (a) Give the difference formula for the Laplacian. (5)

   (b) Using the Taylor Expansion, evaluate the error of the approximation explicitly to the next order. (5)

   (c) Suppose ϕ_1 and ϕ_2 are two solutions with the mesh size h and h/j respectively. Derive the Richardson extrapolation formula which shows that an improved solution is

   $$\phi_3 = (j^2\phi_2 - \phi_1)/(j^2 - 1)$$

   (Hint : $\phi_h = \phi + h^2 f + O(h^4)$.) (5)

[15]

2. In the context of investigating the stability of numerical solutions :

   (a) Write down the explicit discretised version of the Schrödinger equation directly from the differential equation. (3)

   (b) Use Von Neumann stability analysis (based on the local solution $\psi_j^n = \xi^n e^{-kj\Delta x}$) to show

   $$\xi = 1 - i\left[\frac{4\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right) + V_j\Delta t\right]$$

   (3)

(c) Show that $|\xi| > 1$ and that this approach is unstable. (3)

(d) Show that the the explicit discretised version of the Schrödinger equation corresponds to finite difference approximation to the formal solution which is first order in time,

$$\psi_j^{n+1} = (1 - iH\Delta t)\psi_j^n.$$

(3)

(e) Show that the operator is not unitary. (3)

(f) An implicit scheme resulting from the discretised version of the Schrödinger equation (after some re-arrangement) is by contrast

$$\psi_j^{n+1} = (1 + iH\Delta t)^{-1}\psi_j^n$$

which is also first order accurate in time and not unitary. Use Von Neumann stability analysis again to show that

$$\xi = \frac{1}{1 + i\left[\frac{4\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right) + V_j\Delta t\right]}$$

and that this is now unconditionally stable. (3)

(g) Cayley's approximation for the finite difference of e^{-iHt}

$$e^{-iHt} = \frac{(1 - \frac{1}{2}iH\Delta t)}{(1 + \frac{1}{2}iH\Delta t)}$$

leads to a finite difference scheme which is stable, unitary and second order accurate in both space and time. Suggest why it would become second order accurate. (2)

[20]

3. In the context of curve fitting :
Suppose both the dependent variables (x_i, y_i) in a two dimensional curve had errors (normally distributed) $\sigma^2_{x_i}$, $\sigma^2_{y_i}$. Derive a first order approximation to the variance σ^2_u of the function $u = f(x, y)$. [10]

4. In the context of Monte Carlo Methods :
A sequence of random events has a constant average rate μ, an exponential waiting time distribution for the time between each event and a Poisson frequency distribution for the number n of events in time T. The equation

$$\overline{n} = \mu\tau$$

links the two distributions, as $\overline{n}$ is the average of the Poisson frequency distribution for the number of events n in time T and τ characterises the mean life time of the exponential waiting time distribution. This can be exploited to derive a sampling method for Poisson Deviates n using

$$\Sigma_{i=1}^{k_{min}} t_i > T$$

and then setting $n = k_{min} - 1$ where the t_i are exponential deviates. Demonstrate this. [10]