Computational Applied Mathematics: Problems 1

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Instructions:	*Please explain your solutions carefully.*
Due Date:	*13 February 2008*

Consider the Sturm-Liouville problem given by

$$H\psi(x) = -\psi''(x) + |x|\psi(x) = E\psi(x), \tag{1}$$

where the eigenvalues $E_n > 0$ are to be determined so that $\psi \in L^2(\Re)$. You may assume if necessary that the bounded domain $\psi \in L^2[-L, L]$ with $L = 10$ is a good approximation: this squeeze constraint pushes the eigenvalues higher. One can show that the exact eigenfunctions have multiplicty one and are alternately even or odd functions of x. We have $E_0 < E_1 < E_2 \ldots$. The lowest eigenvalue E_0 is the bottom of the spectrum of the operator H, and the corresponding eigenfunction $\psi_0(x)$ is called the ground state. The spectrum of H can be characterized variationally. For the ground state, this means that for a suitable smooth 'trial function' $\phi(x)$, the ground-state energy is bounded above by the Rayleigh quotient, thus $E_0 \leq \mathcal{E} = (\phi, H\phi)/(\phi, \phi)$. If we assume that ϕ is symmetric, and we integrate by parts, we obtain

$$E_0 \leq \mathcal{E} = \frac{\int_0^\infty \left[(\phi'(x))^2 + x(\phi(x))^2)\right] dx}{\int_0^\infty \phi^2(x)dx}. \tag{2}$$

We can also express this by

$$E_0 \leq \mathcal{E} = (\phi, H\phi) = \int_{-\infty}^{\infty} \left[(\phi'(x))^2 + V(x)(\phi(x))^2)\right] dx \quad \text{with} \quad \int_{-\infty}^{\infty} \phi^2(x)dx = 1, \quad V(x) = |x|. \tag{3}$$

In this second form, a multiplicative constant is introduced into ϕ so that ϕ^2 becomes a probability density on $\Re$. Some optimization is possible if ϕ, and therefore $\mathcal{E}$, depend on parameters $\{a\}$.

(1.1) Suppose the trial function has the form $\phi(x; a) = \exp(-\frac{1}{2}ax^2)$, where a is a positive parameter. Find $\mathcal{E}(a)$ analytically and optimize this energy function with respect to a to find the best upper estimate $\mathcal{E}(\hat{a})$ obtainable with this 1-parameter family of Gaussian functions.

(1.2) Repeat the exercise (1.1) by doing the integrations and the optimization with respect to a numerically. It is very useful to explore the numerical approach by first looking at a problem whose solution is known.

(1.3) Now refine the upper estimate for E_0 by exploring the three-parameter trial function family given by

$$\phi(x; a, b, c) = e^{-\frac{1}{2}ax^2}(1 + bx^2 + cx^4), \quad a > 0.$$

Note that procedural simplifications can be obtained by first changing variables to $t = \sqrt{a}x$. Some careful thought is advised before a rush into computing. If the results are not eventually better (lower) than those of (1.1), then something is wrong, or incomplete. The integrations remove x, and we are left with dependences on the parameters; managing all this nicely is the point of the exercise. [After the integrations, the task could also be re-formulated as a matrix eigenvalue problem; in this alternative picture (based on (2))one speaks of 'looking at' H in a finite-dimensional Hilbert space; but this is not asked for here.]

(1.4) Now solve the eigenproblem by integrating the differential equation numerically (for example, buy using Runge-Kutta iterations). E is unknown initially, so we use a 'shooting method' to search. That is to say, convert to a finite boundary (say, $L = 10$), pick an E, and then start the integration from $x = 0$ and count the number ν of nodes as x increases to L (don't count a zero at 0). Suppose ν_g is the number of nodes sought (the node goal). If we reach L and $\nu < \nu_g$, then E is too small; if $\nu \geq \nu_g$, E is too large (or possibly exactly right if the last zero is at L). By repetition the eigenvalue can be found to high accuracy. For even states, start with $\{\psi(0) = 1,\ \psi'(0) = 0\}$ and set $n = 2\nu_g$, and for odd states use $\{\psi(0) = 0,\ \psi'(0) = 1\}$ and $n = 2\nu_g + 1$. Find in this way the first four eigenvalues and eigenfunctions. A very nice presentation of results is a single graph showing the potential $|x|$ on $[-L, L]$ and the four eigenfunctions $\{\psi_i\}$ placed on abscissae at heights $\{E_i\}$, $i = 0, 1, 2, 3$.

Notes:

(i) The convenient even-odd analysis is not valid if the original 'potential' $|x|$ is replaced by a function such as $V(x) = x^4 - x$ that is not even; in this more-general case, we should have to think again.

(ii) When we approach a problem numerically, we often end up solving an altogether new problem. With numerical integration, the results usually depend on the mesh or step size. For the present problem, if the Runge-Kutta iterations with step size h have global error of order $\sim h^4$, say, then it may be reasonable to presume a model for $E(h)$ of the form $E(h) \sim A + Bh^4$. By considering steps of sizes h and $h/2$, one can then extrapolate to find A, the best estimate for E from this data. What is the extrapolation formula in this case? I usually assume a more general model $E(h) = A + Bh^q$, and, by using three h values, I find the triple $\{A, B, q\}$; I need A and am always curious concerning q. I am not sure how best to do these extrapolations with Maple's `dsolve` since we don't seem to have access to h; it is not essential for the assignment to resolve these questions.