18.336 Problem Set 4

Due Thursday, 20 April 2006.

Problem 1: Galerkin warmup

Consider a Galerkin method for a linear PDE $Pu = f$. We showed in class that this leads to a linear equation $A\mathbf{c} = \mathbf{f}$. Show that if P is positive-definite (i.e. if $(u, Pu) > 0$ for any function $u \neq 0$), then A is (i.e. $\mathbf{c} \cdot A\mathbf{c} > 0$ for any $\mathbf{c} \neq 0$).[1]

Problem 2: Galerkin FEM

You will implement a Galerkin finite-element method, with piecewise linear elements, for the Schrodinger eigen-equation in 1d:

$$[-\frac{d^2}{dx^2} + V(x)]\psi(x) = E\psi(x)$$

with a given potential $V(x)$ and for an unknown eigenvalue E and eigenfunction $\psi(x)$. As usual, we'll use periodic boundary conditions $\psi(x+2) = \psi(x)$ and only solve for $\psi(x)$ in $x \in [-1, 1]$.

As in class, we will approximate $\psi(x)$ by its value c_n at N points x_n $(n = 1, 2, \ldots, N)$ and linearly interpolate in between.

(a) A Galerkin method leads to a generalized Hermitian eigenproblem $A\mathbf{c} = E_N B\mathbf{c}$ with matrices A and B. Derive expressions for the matrix elements of A and B in terms of the x_n and $V(x)$.

(b) Implement a Matlab function that assembles the matrices A and B given an array `x` of the x_n and an arbitrary function `V` for $V(x)$. i.e. write a function of the form:
```
function [A,B] = schrodinger_galerkin(x, V)
```
Note that you can pass a function as an argument in Matlab by using the `@` command, for example `schrodinger_galerkin([-1:0.1:0.9], @(x) exp(-x))`. You can evaluate the Galerkin integrals numerically using Matlab's `quadl` function (adaptive Gaussian quadrature).

(c) Solve for the four smallest eigenvalues E_N and plot the corresponding eigenstates $\psi(x)$ by using `eig(A,B)` with $V(x) = 50 \cdot \sin(\pi x + \cos(3\pi x))$ and $N = 100$ points distributed as:

  (i) equally spaced points $x_n - x_{n-1} =$ constant.

  (ii) points spaced proportional to some function $\rho(x)$ that you think will be better: $x_n - x_{n-1} = \text{constant} \cdot \rho(x_{n-1})$, where the constant is chosen to give N points with $x_1 = -1$ and $x_{N+1} = 1$ (of course, x_{N+1} is not stored because of the periodic boundaries).

(d) Given your function $\rho(x)$ from above, compute the error $\Delta E_N = |E_N - E_{2N}|$ in the smallest eigenvalue as a function of N for $N = 32, 64, 128, 256, 512$. Plot your data and (using the last two points) fit to a power law $\Delta E_N = \alpha N^{-\gamma}$. Also give a table of your ΔE_N data. **A small prize and eternal glory will be awarded for the error/convergence that is judged the best.**

Problem 3: Orthogonal polynomials

In class we proved that all of the roots of the orthogonal polynomial $p_N(x)$ over $[a, b]$ lie strictly inside (a, b). Prove that there are no repeated roots. Hint: the proof is very similar...assume there are repeated roots and construct a lower-degree polynomial $s(x)$that would have non-zero inner product (s, p_N).

[1] I sort of proved this in class, but I think I went a little too quickly.