18.303 Problem Set 5

Due Friday, 11 October 2013.

Problem 1: The min–max theorem and localization

Consider the operator $\hat{A} = -\frac{d^2}{dx^2} + c(x)$, for some real $c(x)$, acting on functions $u(x)$ on the whole real line with the inner product $\langle u, v\rangle = \int_{-\infty}^{\infty} \bar{u}v$.

The Hilbert space consists only of square-integrable functions ($\int |u|^2 < \infty$), but in such unbounded domains we typically look for "generalized" eigenfunctions that live in a "rigged" Hilbert space; very loosely speaking, these are functions that are *not exponentially growing* as $x \to \pm\infty$ (or rather, grow at *most* "polynomially" fast, i.e. no faster than some power of x). In case of $c(x) = 1$, the generalized eigenfunctions are $u_k(x) = e^{ikx}$ for any real k, with eigenvalues k^2. However, in this problem we will instead modify $c(x)$ and look for *localized* solutions: true square-integrable eigenfunctions that are decaying at infinity.

In particular, consider some $c(x)$ with $\int_{-\infty}^{\infty} c(x) < 0$ and $\int_{-\infty}^{\infty} |c(x)|dx < \infty$ (i.e. $|c|$ is integrable).

(a) Sketch two possible such $c(x)$: one that is nonzero everywhere and one that varies in sign.

(b) The Rayleigh quotient for this operator is

$$R\{u\} = \frac{\int_{-\infty}^{\infty} \left(|u'|^2 + c|u|^2\right) dx}{\int_{-\infty}^{\infty} |u|^2 dx}.$$

By a generalization of the min–max theorem from class to this operator for an unbounded domain (which you need not prove), it follows that $R\{u\}$ is $\geq$ the smallest eigenvalue (the "infimum of the spectrum of $\hat{A}$") for any square-integrable u (technically, for any u in the Sobolev space for $\hat{A}$). Consider $R\{e^{-|x|/L}\}$ for some $L > 0$ (i.e. plug in $u = e^{-|x|/L}$, which is *not* generally an eigenfunction). (This function is not differentiable at $x = 0$, but you can ignore that point when integrating $|u'|^2$: it is sufficient that the function is continuous and piecewise differentiable.) Focus on the numerator of R to show that $R\{e^{-|x|/L}\} < 0$ for some sufficiently large L:

(i) First, consider the specific case of $c(x) = -1$ for $x \in [-1, 1]$ and $c(x) = 0$ otherwise, and give a specific value of L_0 for which $R\{e^{-|x|/L}\} < 0$ for all $L > L_0$.

(ii) Now consider an arbitrary $c(x)$ satisfying $\int_{-\infty}^{\infty} c(x) < 0$ and $\int_{-\infty}^{\infty} |c(x)|dx < \infty$. Show that $\lim_{L\to\infty}$ of the numerator of $R\{e^{-|x|/L}\}$ is < 0. It follows that $R\{e^{-|x|/L}\} < 0$ for some sufficiently large but finite L.

You may quote the *Lebesgue dominated convergence theorem* in order to swap a limit with an integral: if you have some function $g_L(x)$, then $\lim_{L\to\infty} \left[\int g_L(x)dx\right] = \int \left[\lim_{L\to\infty} g_L(x)\right] dx$ if $|g_L(x)| \leq g(x)$ for some $g(x) \geq 0$ with $\int g < \infty$ (i.e. g is integrable). (Swapping limits and integrals doesn't work in general!)

(c) Since $R\{u\} < 0$ for some u, from above, it follows that the smallest eigenvalue λ_0 of $\hat{A}$ is < 0 as well. Suppose $c(x) = 0$ for $|x| > X$, for some X (i.e. c is "compactly supported"). Show that if $\hat{A}u_0 = \lambda_0 u_0$, then u_0 is exponentially decaying for $|x| > X$. (You can exclude solutions that are exponentially growing towards $\pm\infty$, which are not allowed by the "boundary conditions at ∞," and in any case aren't in the Hilbert space.)

Thus, for such a $c(x)$, the operator $\hat{A}$ has at least one exponentially localized eigenfunction. In quantum mechanics (where $\hat{A}$ is the Schrödinger operator), this is known as a "bound state."

Problem 2: Gridded cylinders

In this problem, we will solve the Laplacian eigenproblem $-\nabla^2 u = \lambda u$ in a 2d radius-1 cylinder $r \leq 1$ with Dirichlet boundary conditions $u|_{r=1\Omega} = 0$ by "brute force" in Julia with a 2d finite-difference discretization, and compare to the analytical Bessel solutions. You will find the IJulia notebooks posted on the 18.303 website for Lecture 9 and Lecture 11 extremely useful! (Note: when you open the notebook, you can choose "Run All" from the Cell menu to load all the commands in it.)

(a) Using the notebook for a 100×100 grid, compute the 6 smallest-magnitude eigenvalues and eigenfunctions of A with `λi, Ui=eigs(Ai,nev=6,which=’SM’)`. The eigenvalues are given by `λi`. The notebook also shows how to compute the exact eigenvalue from the square of the root of the Bessel function. Compared with the high-accuracy λ_1 value, compute the error $\Delta\lambda_1$ in the corresponding finite-difference eigenvalue from the previous part. Also compute $\Delta\lambda_1$ for $N_x = N_y = 200$ and 400. How fast is the convergence rate with Δx? Can you explain your results, in light of the fact that the center-difference approximation we are using has an error that is supposed to be $\sim \Delta x^2$? (Hint: think about how accurately the boundary condition on $\partial\Omega$ is described in this finite-difference approximation.)

(b) Modify the above code to instead discretize $\nabla \cdot c\nabla$, by writing A_0 as $-G^T C_g G$ for some G matrix that implements ∇ and for some C_g matrix that multiplies the gradient by $c(r) = r^2 + 1$. Draw a sketch of the grid points at which the components of ∇ are discretized—these will *not* be the same as the (n_x, n_y) where u is discretized, because of the centered differences. Be careful that you need to evaluate c at the ∇ grid points now! Hint: you can make the matrix $\begin{pmatrix} M_1 \\ M_2 \end{pmatrix}$ in Julia by the syntax `[M1;M2]`.

Hint: Notice in the IJulia notebook from Lecture 11 how a matrix `r` is created from a column-vector of `x` values and a row-vector of `y` values. You will need to modify these `x` and/or `y` values to evaluate r on a new grid(s). Given the r matrix `rc` on this new grid, you can evaluate $c(r)$ on the grid by `c = rc.^2 + 1`, and then make a diagonal sparse matrix of these values by `spdiagm(reshape(c, prod(size(c))))`.

(c) Using this $A \approx \nabla \cdot c\nabla$, compute the smallest-$|\lambda|$ eigensolution and plot it. Given the eigenfunction converted to a 2d $N_x \times N_y$ array `u`, as in the Lecture 11 notebook, plot $u(r)$ as a function of r, along with a plot of the exact Bessel eigenfunction $J_0(k_0 r)$ from the $c = 1$ case for comparison.

```
plot(r[Nx/2:end,Ny/2], u[Nx/2:end,Ny/2])
k0 = so.newton(x -> besselj(0,x), 2.0)
plot(0:0.01:1, besselj(0, k0 * (0:0.01:1))/50)
```

Here, I scaled $J_0(k_0 r)$ by 1/50, but you should change this scale factor as needed to make the plots of comparable magnitudes. Note also that the r array here is the radius evaluated on the original u grid, as in the Lecture 11 notebook.

Can you qualitatively explain the differences?