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Relaxation: from Laplace's equation to the heat equation and discretely back again

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Abstract

We see how the relaxation method for Laplace's equation is related to a numerical solution of the heat equation, which is in turn motivated by thinking of the Hamiltonian as the the time evolution operator in quantum mechanics. This gives some physical insight into what the relaxation method is doing. We also use this to suggest investigative work for a student learning about computational methods in physics.

1 Introduction

An undergraduate course in quantum mechanics [1, 2] generally introduces to the student the notion that solutions to Schrödinger's equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle \tag{1}$$

can be expressed as

$$\exp(-iHt/\hbar)|\psi(0)\rangle \tag{2}$$

where $\exp(-iHt/\hbar)$ is defined as

$$1 + i\frac{t}{\hbar}H - \frac{t^2}{2\hbar^2}H^2 + \ldots \tag{3}$$

Because H is self-adjoint, this is a unitary operator and so has some highly desirable properties, which are subsequently explored and used to good effect throughout quantum mechanics: see, for example, Chapter 7 of Isham [2] for an overview of this.

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The same student is almost certain to meet at some point in his or her studies the heat equation

$$\frac{\partial u}{\partial t} = \Delta u \tag{4}$$

and Laplace's equation

$$\Delta u = 0 \tag{5}$$

and to learn some standard methods for solving them, often centred round separation of variables and Fourier or Laplace transform methods [3].

It is rather less likely that the student will meet numerical methods for solving these equations. One particularly simple approach to solving Laplace's equation is called the relaxation method [4], and in two dimensions it is this. First, we note that we can approximate $\Delta u(x, y)$ by

$$\begin{aligned}\tilde{\Delta} u(x,y) &= \frac{1}{h^2}(u(x+h,y) - 2u(x,y) + u(x-h,y) \\ &\quad + u(x,y+h) - 2u(x,y) + u(x,y-h)) \\ &= \frac{1}{h^2}(u(x+h,y) + u(x-h,y) + u(x,y+h) + u(x,y-h)) \\ &\quad - 4u(x,y)\end{aligned} \tag{6}$$

Rewriting this slightly by discretizing the x and y values to a grid given by $x_i = x_0 + hi$ and $y_j = y_0 + hj$ we have

$$\tilde{\Delta} u(i,j) = \frac{1}{h^2}\left(u(i+1,j) + u(i-1,j) + u(i,j+1) + u(i,j-1) - 4u(i,j)\right). \tag{7}$$

for interior grid points.

Then if u satisfies this discretized Poisson's equation, we have $\Delta u = 0$ and so

$$u(i,j) = \frac{1}{4}\left(u(i+1,j) + u(i-1,j) + u(i,j+1) + u(i,j-1)\right). \tag{8}$$

This, together with boundary values at the edge of the domain of the differential equation, gives a set of simultaneous equations to be solved for $u(i, j)$.

The only remaining question is, how to solve these equations? And one answer is, start off by setting all $u(i, j)$ (except the boundary values) to some arbitrary value (say 0), and then successively apply the iteration

$$u_{n+1}(i,j) = \frac{1}{4}\left(u_n(i+1,j) + u_n(i-1,j) + u_n(i,j+1) + u_n(i,j-1)\right).$$

This works remarkably well, and investigating it numerically is an excellent exercise to accompany the extraction of a Fourier series solution to a given problem.

The purpose of the following section is to give a more physical insight into why the relaxation method works.

2 Relaxing in the heat

Let's now recall the heat equation:

$$\frac{\partial u}{\partial t} = \Delta u.$$

We know on physical grounds that as $t \to \infty$, for any initial conditions and fixed boundary conditions, this approaches a steady state solution, and so in this limit we have

$$\Delta u = 0.$$

In other words, the long-time limit of the solution of the heat equation is the solution of Laplace's equation, for a given set of boundary conditions, and independent of the initial conditions.

Now, by analogy with the Schrödinger equation, we write

$$u(t+k,x,y) = \exp(k\Delta)u(t,x,y) \tag{9}$$

which, to first order in k, says

$$u(t+k,x,y) = u(t,x,y) + k\Delta u(t,x,y). \tag{10}$$

But now also making our discrete approximation to Δ this gives

$$\begin{aligned} u(t+k,i,j) = u(t,i,j) + \frac{k}{4}((u(t,i+1,j) + u(t,i-1,j) \\ + u(t,i,j+1) + u(t,i,j-1) - 4u(t,u,j)), \end{aligned} \tag{11}$$

or, more evocatively,

$$\begin{aligned} u_{n+1}(i,j) = (1-k)u_n(i,j) + \frac{k}{4}(u_n(i+1,j) \\ + u_n(i-1,j) + u_n(i,j+1) + u_n(i,j-1)) \end{aligned} \tag{12}$$

where $u_n(i,j) = u(nk,i,j)$. Therefore the relaxation method amounts to solving a discretized version of the heat equation with $k = 1$, and finding the steady state solution of this.

So, this gives us an alternative reason to believe that if the relaxation method converges, it does so to a solution of the discretized Laplace's equation. But why should we believe that it converges at all?

The argument in the preceding section can be split into several steps. First, we went from

$$\frac{\partial u}{\partial t} = \Delta u$$

to

$$\frac{\partial u(i,j)}{\partial t} = \tilde{\Delta} u(i,j) \tag{13}$$

where $\tilde{\Delta}$ represents the discretized Laplace operator (7) and finally to

$$u_{n+1}(i,j) = u_n(i,j) + \tilde{\Delta}u_n(i,j).$$

If the actual solution we are seeking is U, then we hope that $U = \tilde{U} + v$, where v is small and $\tilde{\Delta}\tilde{U} = 0$, so $\tilde{U}$ is the solution to the discretized Laplace's equation.

So, we now write the process (12) as

$$u_{n+1} = (I + \tilde{\Delta})u_n$$

where u_n is a vector composed of the values at each grid point at the nth time step, I is the identity matrix, and u_0 is arbitrary except at the boundary points, where it contains the boundary values. With this in mind, we see that the matrix $I + \tilde{\Delta}$ is composed of rows of one of the two types:

1. In rows corresponding to points on the boundary, there is a 1 on the main diagonal, and all other entries are 0, so that the boundary values are fixed.

2. In all other rows, $I + \tilde{\Delta}$ is 0 on the main diagonal, with four entries of $1/4$ and all the rest 0, so that values at interior points are replaced by the average of the four neighbouring values.

From the Gershgorin circle theorem [5], we see first that all eigenvalues are inside a disc centred on the origin and of radius 1, or are in a disc centred on 1 of radius 0, and so all eigenvalues are of modulus less than or equal to 1. Furthermore, any eigenvalue of modulus 1 must lie on the boundary of both discs, and so must in fact be 1. Thus, all eigenvalues are either exactly 1, or are less than 1 in modulus, and the solutions to $\tilde{\Delta}\tilde{U} = 0$ are the eigenvectors of $(I + \tilde{\Delta})$ of eigenvalue 1.

We have then used the difference equation

$$u_{n+1} = (I + \tilde{\Delta})u_n \tag{14}$$

from which we see that

$$\begin{aligned} u_n &= (I + \tilde{\Delta})^n u_0 \\ &= (I + \tilde{\Delta})^n (\tilde{U} + u_0 - \tilde{U}) \\ &= (I + \tilde{\Delta})^n \tilde{U} + (I + \tilde{\Delta})(u_0 - \tilde{U}) \\ &= \tilde{U} + (I + \tilde{\Delta})^n (u_0 - \tilde{U}) \end{aligned} \tag{15}$$

since $(I + \tilde{\Delta})\tilde{U} = \tilde{U}$.

Now, consider the second term. The vector $u_0 - \tilde{U}$ has zeros at all boundary components, and the only solution to $\tilde{\Delta}V = 0$ with zeros on all boundary components is $V = 0$. So, considered as a linear operator on the space of vectors vanishing at all boundary components, all eigenvalues of $I + \tilde{\Delta}$ must be less than 1 in magnitude. Therefore we must have $\|(I + \tilde{\Delta})(u_0 - \tilde{U})\| \leq k\|u_0 - \tilde{U}\|$, where k is the magnitude of the largest eigenvalue other than 1, so that $(I + \tilde{\Delta})^n(u_0 - \tilde{U}) \to 0$.

We therefore expect that for any boundary values, and any initial vector u_0 containing those boundary values, (12) will converge to $\tilde{U}$, the solution of $\tilde{\Delta}U = 0$ with those boundary values.

3 Comments

This has given us a way of understanding where the relaxation method comes from, together with an argument for the convergence of the method.

It also suggests various worthwhile investigations that might be undertaking by a student learning computational methods:

1. Check over a variety of boundary conditions that the system (12) does indeed converge when $k = 1$. Investigate the consequences of changing k. For which values is the procedure convergent? Does any other choice significantly improve the rate of convergence?

2. Investigate the effect of different choices of initial values u_0 for the iteration.

3. Pick some exact solution and investigate how the size of h affects the quality of the discrete solution obtained.

4. Investigate the power method for finding eigenvectors [4] and its relationship with the relaxation method.

Finally, we should note that use has made use of the discrete heat equation, and in particular its long time behaviour, to motivate the relaxation method for solving Laplace's equation, but we have not addressed the extent to which the iterative procedure gives an approximate solution to the actual heat equation. There is, of course, an extensive literature on this topic, and the reader interested in development along these lines can find a useful starting point in the Chapter 13 of the textbook of Iserles [6].

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References

[1] S Gasiorowicz (2003) *Quantum Physics, 3rd Ed*, John Wiley & Sons

[2] C Isham (1995) *Lectures on Quantum Theory*, Imperial College Press

[3] W Strauss (2008) *Partial Differential Equations*, John Wiley & Sons

[4] R Burden, J Faires (2011) *Numerical Analysis, 9th Ed*, Brooks/Cole

[5] A Quarteroni, R Sacco, F Saleri (1991) *Numerical Mathematics*, Springer

[6] A Iserles (1996) *A First Course in the Numerical Analysis of Differential Equations*, Cambridge University Press