

Chapter 8 8 Linear Operators and Computing Spectra

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SUMMARY

The discussion focuses on the significance of linear operators and their spectra in mathematical physics and engineering, particularly in solving differential equations. It emphasizes the importance of eigenvalue problems, stability analysis, and computational methods for deriving spectra, which are crucial for understanding the behavior of complex systems.

- Linear operators, often involving derivatives, are central to solving differential equations in physics and engineering.*
- The eigenvalue problem helps determine the stability of solutions; positive eigenvalues indicate instability, while negative ones suggest stability.*
- The Sturm-Liouville problem is a key example of an eigenvalue problem with widespread applications in various fields.*
- Derivatives can be computed using finite difference methods, which can be represented as matrix operations for efficiency.*
- Different boundary conditions (zero, periodic) affect the formulation of derivative matrices used in spectral computations.*
- The process involves discretizing the operator and constructing matrices that represent the differential equations under specified boundary conditions.*
- Computational tools can be used to derive eigenvalues and eigenfunctions, enabling the analysis of complex systems.*
- The discussion concludes with an invitation to experiment with code for spectral computations, highlighting the practical applications of the concepts discussed.*

The last topic on really computing some of these values is going to come down to thinking about what are called linear operators and computing the spectra of linear operators. This actually turns out to be a really important thing we do in practice and a lot of engineering and mathematical physics which is to look at spectral content and EN values because they tell us quite a bit about often the underlying problem we're trying to solve. So this is the typical form of things we're going to look at for linear operators. The linear operator itself is L . It's typically made up of differential components. will show that that is in other words derivatives of things that often is some function of a function of x and so we're looking at this operator acting on v and essentially producing a constant λ and v . So this is a very interesting operator. This is an eigen value problem, right? That we would have a differential operator that when you hit something just basically takes V and makes it bigger or smaller according to λ .

That's it. So these are our eigen functions λ and our eigen values λ that we want to compute because they often dominate the solution structure of a problem. So the spectrum of an operator has been classically a really important thing to consider because it shows up everywhere across mathematical physics and engineering. So let's talk about where it actually shows up. So a lot of physics problems like very complex physics problems can be you know maybe comes from dynamics that comes from some partial differential equation that's nonlinear.

So like this is just a generic representation of a partial differential equation and often if it's a nonlinear differential equation we have recourse simply to do simulations on this. However there are cases where even with n being nonlinear we actually might find a solution to this system. So for instance we might find some u that satisfies the steady state problem. The steady state problem is just or it's not changing in time. So u of t is not changing in time, puts the duct is zero and if we can solve this problem that is a solution to this problem. So often times we've had luck traditionally especially in the 20th century when we were doing quite a bit of mathematical physics of finding some very complex equations that under certain conditions we could find exact solutions even for these nonlinear problems. But then we were asking questions like well does this problem actually show up in reality and a lot of times that comes down to understanding the stability of that problem by taking that solution u perturbing it slightly and asking what happens to that problem or what happens to that solution and this is where the eigen value problem comes in why spectrum of the eigen value is very important because what we really do is when we do that expansion it leads to this eigen value problem for the perturbation And what we really want to know is the eigen values if they are in fact if I right is if the values are real and have a real part that's positive then the solution is going to grow to infinity.

In other words when we perturb it the solution just grows and that solution is called unstable. If the λ s are negative that means the perturbations decay. We bump it it settles back to the solution. If they're complex things oscillate around there. So we would like to understand the qualitative behavior around these solutions. It's often called perturbation theory, weakly nonlinear theory. and the key to it is always understanding this eigen value problem. the most famous of the eigen value problems when it comes to differential equations is the Sturm-Liouville problem. Sturm-Liouville theory shows up everywhere. It shows especially electronics, quantum mechanics. This is like we got so much progress in the 20th century by understanding this problem here because many problems in physics and engineering come down to a Sturm-Liouville type problem here. So here's what the operator looks like. It's a derivative with p of x $\frac{d}{dx}$ so you have both here a first derivative and a second derivative non-constant coefficients p of x and q of x and on the right hand side λ with a w .

That's a generic representation of the Sturm-Liouville problem. And here's the left boundary condition, the right boundary condition. So this is a generic formulation. This problem's famous because what we know about this problem is that it's what's called self adjoint. And so that or Hermitian depending upon where you come from. So it means all the values for here are real and they're they're distinct. And so there's some really beautiful properties come out for this. We have special functions that often represent some of these solutions.

But generically, if I give you a p of x and q of x , that's not one of the special functions. You may not have an analytic solution form. And so you want to solve this thing computationally. So we can easily do that with the

methods we're going to talk about here. Okay. So let's talk about how we're going to do something like this. If you notice, go back. We have derivatives we have to compute. Well, what we're going to do is we're going to figure out how do we compute derivatives? Well, we know how to compute derivatives. They're rise over run formulas. We know how to compute a first derivative, second derivative through finite differences. And so, we're going to use that here. And in fact, I'm going to show you that essentially when we discretize, we can just think of differentiation as a matrix multiply. So, the derivative operator ddx is essentially a matrix multiply that looks like this. How do we get this? Well, this is this rise over run formula which is you use a point in front that's the one minus a point behind that's the minus one over the run which is $2 \Delta x$. So when you hit this essentially when you hit a vector with this you're going to take one derivative of it and here what we're assuming is the boundary conditions are zero at both edges because you see this run of negative one. What happens to negative 1's when you get up here? There's nothing here but if the derivative if the boundary condition is zero doesn't matter. Okay, so this matrix here is a representation of taking a vector and if I multiply it by this matrix A , I get out the derivative with the assumption that the boundary conditions are zero.

So it's very nice. Now we're starting to think about differentiation as not just doing finite differences across a vector, but doing it across the whole thing all at once by just a matrix multiplying. What if I had more complicated boundary conditions? So now we start thinking about well what if the boundaries are zero well we can handle that just as easily but now we have to take care of the boundaries itself. So let's first of all talk about what the boundary conditions are. When I when I do rise or run formulas I use my two neighbors all the way across. But if I am on the left side on one side of the boundaries and I need to use a forward difference formula to take derivatives here. So I don't just use this point. I use two neighbors internally and when I'm on on the other side you have to use the internal point.

So we can use forward and difference backwards formulas and we covered those in the differentiation section. So here is for instance if I'm at the first point V_{KN} v_{KN} is the end point. To take the derivative at V_{KN} I use a forward difference formula. So I not only use V , I use V_1 and V_2 . And here's the formula for it. So what if I wanted to set the derivative to zero? Well, here is this formula that has to hold.

But notice once I have this formula, I can easily solve for V_{KN} . V_{KN} is $\frac{4}{3} V_1$ minus $\frac{1}{3} V_2$. So in other words, if I know what V_1 and V_2 are, it determines V_{KN} for that zero boundary condition. So I don't have to actually solve for V_{KN} . I just solve for the internal points V_1 , V_2 , and so forth. And at the last boundary point, let's call it V_{N+1} . If I use the same idea, now I use a backward difference formula. So it relies on V_N and V_{N-1} .

Here's this formula that has to hold. Which means I can solve for the last point in terms of the interior points. V_N of N of $N-1$. So the first and the last point I don't have to solve for them. They are determined by the interior points. And so this gives me an architecture in which to determine the other formulas. So here's the interesting thing of how it's going to change my matrix operation. So dv/dx .

So v_1 relies on v_0 and v_2 . Well v_0 is given by here. So v when I do the rise over run formula. So it depends on v_2 minus v_0 . But v_0 now I just solve for it from right there and I plug it into here. And then I have this here in

my matrix in that first row of my matrix. So let me show you what this looks like. So this modifies. So this is now the derivative matrix dx with no flux boundary condition. In other words, zero boundary conditions at both the left and right. And it looks like this.

So you have on the diagonals your normal diagonal terms ex which are zeros because it's the first derivative. So you if you look from row two onwards point in front minus point behind by two Δx . the first row and the last row get modified by that zero boundary condition on both sides. So here I get $-4/3$ $4/3$ $-4/3$ $4/3$ and that all comes from using this formula right there and there it is right there. Okay. So now when I take a derivative of a vector multiply by this function here it gives me the derivative of a function with zero boundary conditions imposed.

Okay, that's the second one that's interesting. Third one is periodic boundary conditions, which is again same thing as before, but now the periodic boundary conditions. The ones that run along here, there should be a one over here, but it's periodic boundary condition. It then shows up over here. Same thing with the negative ones. The negative 1's come across here. There should be a negative to run out here. Periodic boundary conditions puts it over here. So now I've got these three derivative matrices. Here they are. This one here which has zero boundary conditions and no you know right this one here has no flux so derivative is zero at the boundary. This here is periodic boundary conditions. So this is how you would build up a suite of derivative operators and we're going to use these matrices to solve for the spectra of an operator. So now when I go back to that spectrum of an operator, that operator L , which is a bunch of differentials, all I got to do is replace those differentials by a matrix.

So a first derivative, there's a first derivative matrix. A second derivative have a has a second derivative matrix. And depending upon the boundary conditions, you would modify that matrix. But once you have that, you just say I and that gives you your spectrum. So it's how you would compute the spectrum. So let's go do an example here of how we would discretize this and make these matrices. So I pick the number of points. Let's say 200 points in my domain. dx is 0.1. Here's my matrix A that I'm building. And for instance here, all I'm going to do for this matrix is put one and minus one on the upper diagonal and the lower diagonal. That's it. And then take that matrix divide by $2 \Delta x$. So this is just rise over run formula. And this is gives me a derivative matrix with zero boundary conditions.

That's how easy it is to make that matrix. Okay. And so now when we go to something like this, here's a differential operator. So an operator L that I want to find its eigen values and functions. Notice what I've done here. I put X^2 here. This is a second derivative and it has zero boundary conditions. So this here again I can make this matrix which is a second derivative matrix, right? Okay. And we know how to do finite second derivatives and finite differences. It's -2 . So it's point in front, point behind, minus two for the diagonal. So all I have to do is make a matrix representing this. This is on the diagonals. Yikes. So let's go ahead and do this. Here's how we do it. So I'm going to pick a domain size of four. I'm chop it up to 200 points. And I'm So here's the domain L to L . And remember I do N plus two, which means I have n points in the interior. The first and last point are going to just be determined by the various boundary conditions.

Here's your dx. Here's the here's what the operator looks like. So I'm putting on the diagonal I'm putting down x^2 . Okay. And then once I have that I can take here this matrix B1 is basically the second derivative matrix. So it's second derivative matrix plus this extra diagonal term. I exit and that's that's it. So there it is. There's the command I for that linear operator and then I sort through the igen values. If you don't sort it, it won't usually come out maybe in the way you want it. So you I'm going to resort it into the biggest to largest. And here's my values. And these are the igen values what are called the harmonic oscillator in quantum mechanics. Okay. So I had a parabolic potential that was at x^2 . If you want to know what the igen values and functions look like here they are. We got these now computationally and we did it just through the ig command. So that's how you would do something like this. And of course if we do more complicated I value problems like for this one here the harmonic oscillator we actually know what the solutions look like. But now I can just put any function in that I want instead of x^2 I can make some complex function just iikes and I would get here's what the igen values and functions look like. So again you can compute this spectra which is the I values and I vectors very simply just using the IG command with appropriate discorization of the operator in the space and the derivatives themselves and the derivatives again are set up to satisfy the boundary conditions. So that's how you would do spectral computations really important in mathematical physics and engineering. always are solving value problems and here's a generic method for doing this very efficiently for boundary value problems computationally.

So play around with it. You have the code there. You can make some really interesting plots and and computations of spectra available for you and just all under discretization.