2.1 $u'' = f(x)$: the First Differential Equation

Differential equations are the fundamental equations governing numerous physical, chemical, and biological processes. In this section, we focus on the following differential equations

$$\begin{cases} -u'' & = f(x), x \in (0,1) \\ au + b\frac{du}{dx} & = g(x), x \in \{0,1\} \end{cases} \tag{2.1}$$

If $a \neq 0$ and $b = 0$, the boundary condition is called the Dirichlet boundary condition.

If $a = 0$ and $b \neq 0$, the boundary condition is called the Neumann boundary condition.

If both a and b are nonzero, then it is called Robin boundary condition.

We would like to explore the numerical solution to these problems.

2.1.1   Finite Difference

The key to solving differential equations is approximating derivatives-a process of infinitesimal division-with something finite, something that a computer can handle. To do that, we recall the definition of derivatives. For a function $f : \mathbb{R} \to \mathbb{R}$, the derivative of $f(x)$, denoted as $f'(x)$, is defined as

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \tag{2.2}$$

Hence, the first attempt to approximating $f'(x)$ would be

$$\frac{f(x+h) - f(x)}{h} \tag{2.3}$$

This is known as the forward difference approximation. However, there are equivalent definitions of derivatives, such as

$$f'(x) = \lim_{h \to 0} \frac{f(x) - f(x-h)}{h} \tag{2.4}$$

$$= \lim_{h \to 0} \frac{f(x+h) - f(x-h)}{2h} \tag{2.5}$$

Hence, we can also approximate $f'(x)$ as

$$\frac{f(x) - f(x - h)}{h} \tag{2.6}$$

$$\frac{f(x + h) - f(x - h)}{2h} \tag{2.7}$$

These are called, respectively, the backward difference approximation and centered difference approximation. The question is: how do they differ as valid approximations to derivatives? Is one more accurate than the other? To explore that question, let's take the function $f(x) = x^3$. We know that $f'(x) = 3x^2$. We compute

$$\frac{f(x + h) - f(x)}{h} = \frac{(x + h)^3 - x^3}{h} = 3x^2 + 3xh + h^2 \tag{2.8}$$

$$\frac{f(x) - f(x - h)}{h} = \frac{x^3 - (x - h)^3}{h} = 3x^2 + 3xh - h^2 \tag{2.9}$$

$$\frac{f(x + h) - f(x - h)}{2h} = \frac{(x + h)^3 - (x - h)^3}{h} = 3x^2 + h^2 \tag{2.10}$$

$$\tag{2.11}$$

Notice that in each case, the first term is $3x^2$, and the subsequent terms depend on h. This means that as h gets small, the approximation becomes more accurate. Secondly, for h small, $3xh$ is going to be a lot larger than h^2 as h gets smaller and smaller. Hence, the term with the lowest order of h determines the accuracy of each method. This term is also called the leading order. We can then conclude that, at least for the function $f(x) = x^3$,

- The forward difference is first-order, denoted as $O(h)$;

- The backward difference is first-order, denoted as $O(h)$;

- The center difference is second-order, denoted as $O(h^2)$

It is actually true that the forward difference and backward difference are first-order for any function $f(x)$. The key to proving this fact is Taylor expansion (https://en.wikipedia.org/wiki/Taylor_series). For a function $f(x)$, we can write

$$f(x + h) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x)h^n}{n!} \tag{2.12}$$

$$= f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \frac{1}{6}h^3 f'''(x) + \dots \tag{2.13}$$

$$f(x - h) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x)(-h)^n}{n!} \tag{2.14}$$

$$= f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) - \frac{1}{6}h^3 f'''(x) + \dots \tag{2.15}$$

Then we observe the following algebraic manipulations

$$\frac{f(x + h) - f(x)}{h} = f'(x) + \frac{1}{2}hf''(x) + \frac{1}{6}h^2 f'''(x) + \dots \tag{2.16}$$

Since the smallest/leading order of h is 1, this method is first-order. A similar calculation can be done for backward and centered difference approximations. This will be left as a homework exercise.

In fact, (2.14) and (2.15) provide us a powerful tool to find the suitable finite difference approximations for any orders of derivatives. To find the second order finite difference approximation, we notice that $(2.14) + (2.15) - 2f(x)$ gives us

$$f(x+h) + f(x-h) - 2f(x) = h^2 f''(x) + \frac{1}{12} h^4 f''''(x) + \dots \tag{2.17}$$

If we divide everything by h^2, we have

$$\frac{f(x+h) + f(x-h) - 2f(x)}{h^2} = f''(x) + \frac{1}{12} h^2 f''''(x) + \dots \tag{2.18}$$

This gives us an second-order approximation to the second derivative of a function $f(x)$. This is known as the second difference approximation.

2.1.2 Finite Difference Equation

Now that we know how to approximate $u''(x)$, let us solve (2.1), with the following boundary condition

$$u(0) = a \tag{2.19}$$
$$u(1) = b \tag{2.20}$$

First, let's do some preparation

- Divide the interval $(0, 1)$ into $N + 1$ pieces, so that each piece is of size $h = 1/(N + 1)$.

- Then at the ith grid point, we have $x_i = ih$, for $i = 0, \dots, N+1$.

- It is our goal to evaluate $u(x_i)$ for all $i = 1, \dots, N$ (note that $u(x = x_0 = 0)$ and $u(x = x_{N+1} = 1)$ are located at the boundary whose conditions have been specified as part of the problem setup)

Then we write the second difference to $u''(x)$ at each $x_1, \dots, x_N$

$$f(x_i) = \frac{-u(x_{i+1}) + 2u(x_i) - u(x_{i-1})}{h^2} \tag{2.21}$$

If we abbreviate $u(x_i)$ as u_i and $f(x_i)$ as f_i, we can rewrite the second difference equation as

$$f_i = \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} \tag{2.22}$$

Then if we write N of the equations above, we can recast all of them into a matrix equation

$$K\vec{u} = \vec{f} \tag{2.23}$$

where

$$\frac{1}{h^2} \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0\dots & & 0 \\ \vdots & \vdots & \vdots & \ddots & & & \\ \vdots & \vdots & \vdots & & \ddots & & \\ \vdots & \vdots & \vdots & & & \ddots & \\ 0\dots & \dots & \dots & \dots & \dots & \dots -1 & 2 \end{bmatrix} \tag{2.24}$$

$$\vec{u} = (u_1, ..., u_N)^T \tag{2.25}$$

$$\vec{f} = (f_1, ..., f_N)^T \tag{2.26}$$

$$\tag{2.27}$$

Now notice that the first and last row of the matrix equation read

$$\frac{2u_1 - u_2}{h^2} = f_1 \tag{2.28}$$

$$\frac{-u_{N-1} + 2u_N}{h^2} = f_N \tag{2.29}$$

which is not the same as the second order approximation. The correct one should be

$$\frac{-u_0 + 2u_1 - u_2}{h^2} = f_1 \tag{2.30}$$

$$\frac{-u_{N-1} + 2u_N - u_{N+1}}{h^2} = f_N \tag{2.31}$$

But since $u_0 = u(x = 0) = u(x_0) = a$ and $u_{N+1} = u(x = 1) = u(x_{N+1}) = b$, our equations become

$$\frac{-a + 2u_1 - u_2}{h^2} = f_1 \tag{2.32}$$

$$\frac{-u_{N-1} + 2u_N + -b}{h^2} = f_N \tag{2.33}$$

Hence, we need to correct the matrix equation (2.35) as follows

$$K\vec{u} - \vec{a} = \vec{f} \tag{2.34}$$

$$K\vec{u} = \vec{f} + \vec{a} \tag{2.35}$$

where $\vec{a} = (a, 0, ..., 0, b)/h^2$. The MATLAB command $K \backslash (\vec{f} + \vec{a})$ would give us $\vec{u}$ immediately.

2.1.3   Convergence Analysis

How do we know that our numerical method is accurate/converging? We benchmark it against cases where we already know the analytical solutions (ie. solutions that we can directly compute). As an example, suppose we want to solve

$$\begin{cases} -u''(x) & = \sin(x\pi), \text{ on } (0,1) \\ u(0) & = 0 \\ u(1) & = 0 \end{cases} \tag{2.36}$$

Then we know the solution to the differential equation would be $u(x) = \sin(x\pi)/\pi^2$ via direct integration. Then we apply the numerical method as described above to discretize the space, set up the matrix, and solve for the discrete values at the interior nodes, resulting in $\vec{u} = (u_1, u_2, ..., u_N)^T$ as approximations to the value of u at $\vec{x} = (x_1, x_2, ..., x_N)$. On the other hand, we can compute the analytical solution $\vec{v} = \frac{1}{\pi^2}(\sin(x_1\pi), \sin(x_2\pi), ..., \sin(x_N\pi))^T$, which are exact at $\vec{x}$. Now we just have to compute how much $\vec{u_a}$ and $\vec{u}$ differ. Out of many ways to compare vectors, we choose the L^2 distance measurement. The erros is henceforth called the L^2 error, defined as

$$error_2 = ||\vec{v} - \vec{u}||_{L_2} \tag{2.37}$$

$$= \sqrt{\frac{1}{N} \sum_{k=1}^{n} |u_n - v_n|^2} \tag{2.38}$$

Notice the scaling by N under the square root. The fact that the second derivative finite difference approximation is second-order implies that the error should be quadratic in h, the grid size, ie.

$$error_2 \propto h^2 \tag{2.39}$$

Taking the log on both sides, we have

$$\ln(error_2) \propto 2\ln(h) \tag{2.40}$$

This means that if we plot the natural log of the error with the natural log of the grid size, we should get a line, whose slope is the order-in this case equal to 2-of the numerical method. And they are indeed! See figures below
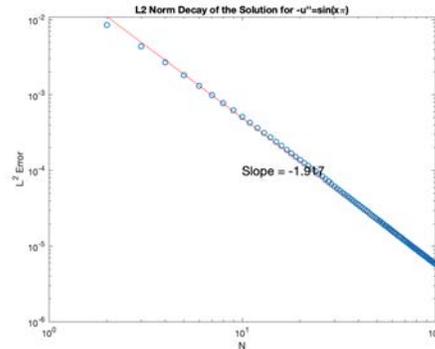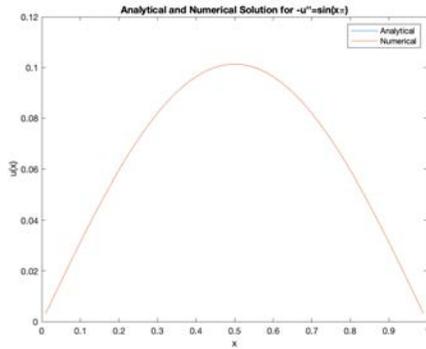
(a) Analytic and numerical solutions are almost identical for $N = 100$ (b) Log-Log Plot of Error vs. Number of Grids. The slope is about -2, since $h \propto \frac{1}{N}$

2.2 Inverses and Delta Functions

Often time the source of disturbance $f(x)$ is not smooth, but can be very abrupt. Sometimes it is as abrupt as a delta function

2.2.1 Delta Function

Here is how we define the delta function

Definition 2.1 *Delta function, denoted as $\delta_a(x) = \delta(x - a)$, is defined as*

$$\delta(x - a) = \begin{cases} 0, & if \ x \neq a \\ \infty, & if \ x = a \end{cases} \tag{2.41}$$

The motivation for the definition of the delta is the follows. Imagine taking the "derivative" of the heaviside function, defined as follows

$$H(x - a) = \begin{cases} 1, & \text{if } x < a \\ 0, & \text{if } x \geq a \end{cases} \tag{2.42}$$

The function does not change away from a, but at a, the function suddenly changes. This change is an finite change within zero time, henceforth producing an "infinite derivative". Here is an important fact about the delta function

Theorem 2.2 *Let $f(x)$ be a function and let $a \in \mathbb{R}$. Then for any finite interval I_a that contains the a,*

$$\int_{I_a} f(x)\delta(x-a) = f(a) \tag{2.43}$$

Here is how you "prove" it (note: it is not mathematically rigorous at all):

Proof: For any number ϵ, We define the function $h_\epsilon(x)$

$$h_\epsilon(x) = \begin{cases} \frac{1}{2\epsilon}, & \text{if } x \in [a-\epsilon, a+\epsilon] \\ 0, & \text{otherwise} \end{cases} \tag{2.44}$$

Then $h_\epsilon(x) \to \delta_a(x)$. But also note that

$$\int_{I_a} f(x)h_\epsilon(x) \approx f(a) \int_{I_a} h_\epsilon(x) \tag{2.45}$$

$$= f(a) \tag{2.46}$$

As $\epsilon \to 0$, the "$\approx$" will become "$=$". Henceforth,

$$f(a) = \lim_{\epsilon \to 0} \int_{I_a} f(x)h_\epsilon(x) \tag{2.47}$$

$$= \int_{I_a} f(x) \lim_{\epsilon \to 0} h_\epsilon(x) \tag{2.48}$$

$$= \int_{I_a} f(x)\delta(x-a) \tag{2.49}$$

$\blacksquare$

2.2.2   The Delta Function Source

We are interested in solving the following differential equation

$$\begin{cases} -u''(x) = \delta(x - 1/2) \\ u(0) = 0 \\ u(1) = 0 \end{cases} \tag{2.50}$$

The key to solving the problem is dividing up the region into separate parts. Obviously, something interesting happens at $1/2$, which then seems to be a natural point of division. Hence we solve

$$\begin{cases} -u_L''(x) = 0 \\ -u_R''(x) = 0 \end{cases} \tag{2.51}$$

Then we can write

$$\begin{cases} u_L(x) = Ax + B \\ u_R(x) = Cx + D \end{cases} \tag{2.52}$$

2.2.2.1 Step 1: Natural boundary conditions

We note that

$$u(x = 0) = u_L(x = 0) \tag{2.53}$$
$$= B \tag{2.54}$$
$$= 0 \tag{2.55}$$
$$u(x = 1) = u_R(x = 1) \tag{2.56}$$
$$= C + D \tag{2.57}$$
$$= 0 \tag{2.58}$$

Hence we know that $B = 0$ and $C = -D$

$$\begin{cases} u_L(x) = Ax \\ u_R(x) = -Dx + D \end{cases} \tag{2.59}$$

2.2.2.2 Step 2: Matching @ $x = 1/2$

Now let's focus on what's happening at $x = 1/2$. Whatever happens there, we assume that the solution is continuous there, ie. $u_L(1/2) = u_R(1/2)$. Hence

$$u_L(x = 1/2) = u_R(x = 1/2) \tag{2.60}$$
$$A/2 = -D/2 + D \tag{2.61}$$
$$A = D \tag{2.62}$$

Then we have

$$\begin{cases} u_L(x) = Ax \\ u_R(x) = -Ax + A \end{cases} \tag{2.63}$$

2.2.2.3 Step 3: Flux Conversation

So far, we have not used the information about the delta function. To take that into account, we perform an integration on both sides of the equation. Let $I_{1/2} = (1/2 - \epsilon, 1/2 + \epsilon)$, where $\epsilon > 0$ is a very small number. Then we can write

$$\int_{I_a} -u''(x) = \int_{I_a} \delta(x - 1/2) \tag{2.64}$$
$$-u'(x)|_{a+\epsilon} + u'(x)|_{a-\epsilon} = 1 \tag{2.65}$$
$$A + A = 1 \tag{2.66}$$
$$A = 1/2 \tag{2.67}$$

2.2.2.4 Write down the solution

We can now write

$$u(x) = \begin{cases} \frac{x}{2}, x \in (0, 1/2] \\ -\frac{1}{2}x + \frac{1}{2}, (1/2, 1) \end{cases} \tag{2.68}$$

2.2.2.5   A Numerical Note

When numerically implementing the solution for the equation with a delta source ($\delta(x-a)$), the discretized vector is such that it is all zeros except for at the node where $x = a$, when the vector should be 1.

2.2.3   Green's Function

Let's explore the solution to the following differential equations

$$\begin{cases} -u''(x) = \delta(x-a) \\ u(0) = 0 \\ u(1) = 0 \end{cases} \tag{2.69}$$

Repeating the process described below (by replacing $1/2$ with a), one can get

$$u(x) = \begin{cases} (1-a)x, x \in (0, a] \\ a(1-x), x \in (1/2, 1) \end{cases} \tag{2.70}$$

Since the solution depends on both x and a (which is a fixed number), we shall re-denote it as

$$u_G(x, a) = \begin{cases} (1-a)x, x \in (0, a] \\ a(1-x), x \in (1/2, 1) \end{cases} \tag{2.71}$$

$u_G(x, a)$ is known as the Green's function of 1-D Laplace's equation with Dirichlet boundary. Here is a nice property of Green's function

Theorem 2.3 $u(x)$, *defined as,*

$$u(x) = \int_0^1 u_G(x, a) f(a) da \tag{2.72}$$

solves the following differential equation

$$\begin{cases} -u''(x) = f(x) \\ u(0) = 0 \\ u(1) = 0 \end{cases} \tag{2.73}$$

where u_G is the Green's function

Proof: We plug in $u(x)$ into the differential equation

$$-u''(x) = -\frac{d^2u}{dx^2} \tag{2.74}$$

$$= -\frac{d^2u}{dx^2} \left(\int_0^1 u_G(x, a) f(a) da \right) \tag{2.75}$$

$$= \int_0^1 -\frac{d^2u}{dx^2} (u_G(x, a)) f(a) da \tag{2.76}$$

$$= \int_0^1 \delta(x-a) f(a) da \tag{2.77}$$

$$= f(x) \tag{2.78}$$

Lastly we observe that since $u_G(x,a)$ satisfies the problem with 0 Dirichlet boundary, $u_G(0,a) = u_G(1,a) = 0$, whence, $u(0) = u(1) = 0$ ∎

Here is an example with $f(x) = 1$

$$\begin{cases} -u''(x) = 1 \\ u(0) = 0 \\ u(1) = 0 \end{cases} \tag{2.79}$$

We know the solution is $u(x) = -x^2/2 + 1/2x$. Now let's compute

$$u(x) = \int_0^1 u_G(x,a)f(a)da \tag{2.80}$$

$$= \int_0^1 u_G(x,a)(1)da \tag{2.81}$$

$$= \int_0^x u_G(x,a)da + \int_x^1 u_G(x,a)da \tag{2.82}$$

$$= \int_0^x (1-x)ada + \int_x^1 (1-a)xda \tag{2.83}$$

$$= -x^2/2 + 1/2x \tag{2.84}$$

Note that this is kind of a silly example, but Green's function turns out to be extremely useful for general linear differential operators. We will not discuss this in more details here.

2.3 Application of Eigenvalues to First Order Differential Equations

We are switching gears a little and shall examine the relation between eigenvalues and differential equations. A quick review on solving the following linear differential equation:

$$\frac{du}{dt} = 3u \tag{2.85}$$

$$u(0) = 1 \tag{2.86}$$

We can solve it by separation of variable, ie.

$$du/(3u) = dt \tag{2.87}$$

$$1/3ln(u) = t + C \tag{2.88}$$

$$ln(u) = 3t + C \tag{2.89}$$

$$u(t) = C\exp(3t) \tag{2.90}$$

where C is the arbitrary constant. To solve for the constant, we use the initial condition $u(t = 0) = 1$ and get that $C = 1$, whence

$$u(t) = \exp(3t) \tag{2.91}$$

Now let's imagine the following systems of 2 differential equations

$$\begin{cases} \frac{du}{dt} = 2u - v \\ \frac{dv}{dt} = -u + 2v \end{cases} \tag{2.92}$$

subject to $u(0) = 7$ and $v(0) = 3$

These systems of linear differential equations often appear in chemical reaction and ecological modeling. Observe that we can re-cast the equation above into the following matrix form

$$\frac{dU}{dt} = AU(t) \tag{2.93}$$

where

$$U = (u(t), v(t))^T \tag{2.94}$$

$$A = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \tag{2.95}$$

Now let's formulate the general recipe for solving the system of n differential equations in the matrix form $\frac{dU}{dt} = AU(t)$, where $U = (u_1(t), u_2(t), ..., u_n(t))^T$, subject to initial conditions $U(0) = (u_0, ..., u_n)^T$.

2.3.1   Recipe for Solving Coupled System of Differential Equations

2.3.1.1   Step 1: Diagonalize the Matrix

Let diagonalize the matrix into the following form

$$A = V \Lambda V^{-1} \tag{2.96}$$

where V has n eigenvectors populate its columns and Λ has n eigenvalues populate its diagonal.

2.3.1.2   Step 2: Transform the system of differential equations

We plug the diagonalizing form of A into the system of differential equations and find

$$\frac{dU}{dt} = V \Lambda V^{-1} U(t) \tag{2.97}$$

$$V^{-1} \frac{dU}{dt} = \Lambda V^{-1} U(t) \tag{2.98}$$

$$\frac{d(V^{-1}U)}{dt} = \Lambda(V^{-1}U(t)) \tag{2.99}$$

$$\tag{2.100}$$

Let $W(t) = (w_1(t), ..., w_n(t))^T = V^{-1}U(t)$. Then we have

$$\frac{dW}{dt} = \Lambda W(t) \tag{2.101}$$

$$\tag{2.102}$$

The great thing about this is that because Lambda is diagonal, we have completely decoupled the system of equations. Hence we can write down immediately

$$w_i(t) = C_i exp(\lambda_i t) \tag{2.103}$$

where C_i is an arbitrary constant, for each $i = 1, ..., n$.

2.3.1.3   Step 3: Transform back to the original system of differential equations

Since $W(t) = V^{-1}U(t)$, $U(t) = VW(t)$

2.3.1.4   Step 4: Solve for the arbitrary constants using the initial condition

Solve for the C_i using the known value of $U(0)$.

Now let's solve for the specific case of A

2.3.1.5   Step 1

We can diagonalize matrix A as $A = V\Lambda V^{-1}$, where

$$V = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{2.104}$$

$$\Lambda = \begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix} \tag{2.105}$$

2.3.1.6   Step 2

We formulate $W = (w_1(t), w_2(t))^T = VU(t)$ and solve that $w_1(t) = C_1 \exp(t)$ and $w_2(t) = C_2 \exp(3t)$.

2.3.1.7   Step 3

We compute $U(t) = VW(t)$ and conclude that $U(t) = (C_1 \exp(t) + C_2 \exp(3t), C_1 \exp(t) - C_2 \exp(3t))^T$

2.3.1.8   Step 4

Using $U(0) = (7, 3)$, we get that $C_1 = 5$ and $C_2 = 2$. We are done.

2.3.2   An Expanded Notion of Eigenvalue and Eigenvector

We recall the definition of eigenvalues and eigenvectors. For a matrix A, eigenvalues λ and eigenvector v satisfy

$$Av = \lambda v \tag{2.106}$$

As we discussed, we can think of a matrix A as a mapping between two geometric spaces. But then if we expand the definition of mapping beyond matrices, we can also expand our notion of eigenvalues and eigenvectors. For example, consider the second derivative $-\frac{d^2}{dx^2}$. It is a mapping between a function and another function, eg. it takes x^2 and spits out $2x$. We can talk about the eigenvalue, η, and eigenvector of $-\frac{d^2}{dx^2} f(x)$ (which is a function) as

$$-\frac{d^2 u(x)}{dx^2} u = \eta u(x) \tag{2.107}$$

Hence a better term for $u(x)$ would be eigenfunctions. For the zero Dirichlet boundary conditions, $u(0) = u(1) = 0$, we know that $u(x) = \sin(k\pi x)$ and $\eta = k^2\pi^2$, for all $k = 1, 2, 3...$ Hence the second derivative

operator with zero Dirichlet boundary condition has an infinite number of eigenfunctions and eigenvalues.

Keep this concept in mind as it will become extremely useful later on in higher dimensional Laplace's equation and Fourier analysis.

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