Math 126 – Supplemental Lecture Notes

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These lecture notes are meant to supplement the course textbook

Partial Differential Equations: An Introduction. Walter A. Strauss.

1 Where do PDE come from?

Multi-variable calculus review

- Subscript notation for partial derivatives: $u_x = \frac{\partial u}{\partial x}$.
- Divergence div $\mathbf{v} = v_x^1 + v_y^2 + v_z^3$, where $\mathbf{v}(x, y, z) = (v^1(x, y, z), v^2(x, y, z), v^3(x, y, z))$.
- Divergence of gradient is the Laplace operator

$$\operatorname{div} \nabla u = u_{xx} + u_{yy} + u_{zz} = \Delta u.$$

• Divergence theorem in 2D:

$$\iint_D \operatorname{div} \mathbf{v} \, dx \, dy = \int_{\partial D} \mathbf{v} \cdot \mathbf{n} \, dS,$$

where **n** is the unit outward normal vector field to ∂D .

• Divergence theorem in 3D:

$$\iiint_D \operatorname{div} \mathbf{v} \, dx \, dy \, dz = \iint_{\partial D} \mathbf{v} \cdot \mathbf{n} \, dS,$$

where **n** is the unit outward normal vector field to ∂D .

• Normal derivative

$$\frac{\partial u}{\partial \mathbf{n}} := \nabla u \cdot \mathbf{n}$$

Let us now give some motivating examples of applications of PDE.

Example 1 (Traffic Flow). Let u(x,t) be the density of cars (in, say, cars per mile) on a street at position x and time t. Let f(x,t) denote the traffic flow (or flux) at position x and

time t in, say, cars per hour. Let us suppose that the velocity v of the traffic depends on the density u. The fundamental equation of traffic flow is then

$$\underbrace{f(x,t)}_{\text{Flow (cars/hr)}} = \underbrace{u(x,t)}_{\text{Density (cars/mile)}} \times \underbrace{v(u(x,t))}_{\text{Velocity (miles/hr)}}.$$

We also note that

Cars between
$$x = a$$
 and $x = b$ is $\int_a^b u(x,t) dx$

Supposing there are no on-ramps or off-ramps on our ideal highway, we have

$$\frac{d}{dt} \int_a^b u(x,t) \, dx = \underbrace{u(a,t)v(u(a,t)) - u(b,t)v(u(b,t))}_{\text{Flow in - Flow out}} = -\int_a^b [u(x,t)v(u(x,t))]_x \, dx.$$

Dividing by b - a and sending $b \rightarrow a$ yields

$$u_t + [u \cdot v(u)]_x = 0.$$
(1)

This is an example of a scalar conservation law. If the cars are moving at a constant speed v (miles/hr) independent of u (which is unrealistic), then v(u) = v is constant and we obtain

$$u_t + vu_x = 0.$$

This is called a *transport* equation.

The velocity function v(u) can actually be (and is) determined experimentally by measuring flow and density of cars on highways. As you might expect, v(u) is a decreasing function of u, which leads to traffic jams when u is large. We used v(u) = 1 - u in the simulations shown in class.

Evidently, the conservation law (1) holds for any conserved quantity (not just traffic), provided we have an expression for the flux (or flow).

Example 2 (Diffusion). Consider the diffusion of heat along a thin insulated rod. Let u(x,t) be the temperature at position x along the rod at time t. Fourier's law of heat conduction states that the heat flow (or flux) is proportional to the negative gradient, so $f(x,t) = -k(x)u_x(x,t)$. The constant of proportionality k(x) is called the *thermal conductivity*, and it may vary along the rod if it were composed of different materials. Proceeding as in the traffic jam example

$$\int_{a}^{b} u_t \, dx = \frac{d}{dt} \int_{a}^{b} u \, dx = \underbrace{-k(a,t)u_x(a,t) - (-k(b,t)u_x(b,t))}_{\text{Flow in - Flow out}} = \int_{a}^{b} [k(x)u_x(x,t)]_x \, dx.$$

Since a and b are arbitrary, we arrive that the heat diffusion equation

$$u_t - [ku_x]_x = 0. (2)$$

When k is constant along the rod, we get the usual diffusion equation

$$u_t - ku_{xx} = 0.$$

The diffusion equation applies in other settings as well. Consider a motionless liquid in a thin tube containing a substance (e.g., a dye). The dye moves by diffusing from high concentrations to low concentrations. Let u(x,t) be the concentration of the dye at position xof the tube at time t. Fick's law of diffusion states that the rate of motion (or flux) of the dye is proportional to the negative of the concentration gradient, i.e., $f = -ku_x$ for some k > 0. Proceeding as above yields the same diffusion equation (2).

Example 3 (Vibrating String). Consider a flexible elastic string of length l and let u(x, t) be the displacement from equilibrium at (x, t). Assume there is a tension force of T in the tangential direction of the string, independent of x and t. This assumption is valid for small displacements u. Let ρ be the (constant) density of the string. Then Newton's law F = ma applied to the vertical forces over an interval $[x, x + \Delta x]$ says that

$$\rho\Delta x u_{tt}(x,t) \approx \frac{T u_x(x+\Delta x,t)}{\sqrt{1+u_x^2}} - \frac{T u_x(x,t)}{\sqrt{1+u_x^2}} \approx T(u_x(x+\Delta x,t) - u_x(x,t)),$$

when the displacement and its gradient u_x are small. Dividing by Δx and sending $\Delta x \to 0$ yields

$$u_{tt}(x,t) - c^2 u_{xx}(x,t) = 0,$$

where $c = \sqrt{T/\rho}$. This is the one dimensional wave equation.

Example 4 (Schrödinger's equation). Consider a Hydrogen atom, which is a single electron orbiting a proton. Let m be the mass of the electron, e its charge, and h Planck's constant divided by 2π . Let $r = \sqrt{x^2 + y^2 + z^2}$ and suppose the proton is at the origin. The motion of the electron is governed by a *wave function* u(x, y, z, t) which satisfies Schrödinger's equation

$$-ihu_t = \frac{h^2}{2m}\Delta u + \frac{e^2}{r}u.$$

This is usually taken as an axiom and is generally not derived from any other physical principles. Note u is complex valued. The probability of finding the electron in a region D at time t is

$$\iiint_D |u|^2 \, dx \, dy \, dz.$$

Example 5 (Diffusion in higher dimensions). We consider heat flow in higher dimensions. Diffusion of a substance gives the same equation. Let u(x, y, z, t) be the temperature and let H(t) be the amount of heat contained in a region D. Then

$$H(t) = \iiint_D k u \, dx \, dy \, dz,$$

where k is the thermal conductivity of the material. The rate of change of the total heat in D is

$$\frac{dH}{dt} = \iiint_D ku_t \, dx \, dy \, dz$$

By Fourier's law of heat conduction, the heat flux through ∂U is proportional to the negative gradient of the temperature. Since heat is conserved, the total heat in D can only change by flowing through the boundary. Therefore

$$\frac{dH}{dt} = \iint_{\partial D} k(\nabla u \cdot \mathbf{n}) \, ds = \iiint_{D} \operatorname{div} \left(k \nabla u \right) \, dx \, dy \, dz.$$

Since D is arbitrary

$$u_t - \operatorname{div}\left(k\nabla u\right) = 0.$$

This is the heat, or diffusion equation in higher dimensions. When k is constant, we get the heat equation

$$u_t - k\Delta u = 0.$$

Example 6 (Wave equation in higher dimensions). Consider in 2 dimensions a vibrating drumhead with density ρ . Let D be a small set, say a circle or square, and let |D| be the area of D. Newton's law applied to D states that

$$ma = \rho |D| u_{tt} \approx \int_D T \frac{\partial u}{\partial \mathbf{n}} \, dS = F.$$

Using the divergence theorem we have

$$u_{tt} \approx \frac{1}{\rho |D|} \iint_D T(u_{xx} + u_{yy}) \, dx dy.$$

Making D arbitrarily small yields the 2-dimensional wave equation

$$u_{tt} - c^2 \Delta u.$$

The wave equation above describes waves in higher dimensions (i.e., $n \ge 3$), such as sound or electromagnetic waves.

The examples we have seen so far are all linear PDE. Let us see one nonlinear example.

Example 7 (Distance function). Let Γ be a subset of the (x, y) plane, and let

u(x, y) =Minimal distance to Γ .

For any r > 0 and $x \notin \Gamma$, u satisfies

$$u(x,y) = r + \min_{(x',y') \in \partial B_r(x,y)} u(x',y').$$

Using a Taylor series

$$u(x',y') \approx u(x,y) + u_x(x,y)(x'-x) + u_y(x,y)(y'-y).$$

Substituting this above gives

$$0 = r + \min_{(x',y') \in \partial B_r(x,y)} (u_x(x,y)(x'-x) + u_y(x,y)(y'-y)).$$

Set $v_1 = (x' - x)/r$, $v_2 = (y' - y)/r$, and $v = (v_1, v_2)$ we have

$$0 = 1 + \min_{\|v\|=1} \nabla u(x, y) \cdot v.$$

The minimum is attained when $v = -\nabla u(x, y) / \|\nabla u(x, y)\|$, and we have

$$u_x(x,y)^2 + u_y(x,y)^2 = \|\nabla u(x,y)\|^2 = 1.$$

This should be satisfied when $(x, y) \notin \Gamma$, and u(x, y) = 0 for $(x, y) \in \Gamma$. This PDE is referred to as *Eikonal's equation*.

2 Initial/boundary conditions and well-posedness

As we have seen, a partial differential equation is an equation involving the partial derivatives of an unknown function. The most general first order PDE in dimension n = 2 is

$$F(x, y, u(x, y), u_x(x, y), u_y(x, y)) = F(x, y, u, u_x, u_y) = 0,$$

for a given function F. A second order PDE is of the form

$$F(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}) = 0.$$

We can of course pose PDE in dimensions $n \ge 3$, and with higher derivatives. We can write an arbitrary PDE in the form

$$\mathcal{L}(u) = 0,$$

where

$$\mathcal{L}(u) = F(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}).$$

For example, the heat equation corresponds to $\mathcal{L}(u) = u_t - \Delta u$.

Definition 1. A PDE is *linear* if

$$\mathcal{L}(u+v) = \mathcal{L}(u) + \mathcal{L}(v) \text{ and } \mathcal{L}(cu) = c\mathcal{L}(u),$$

for all function u, v and $c \in \mathbb{R}$.

Example 8. Which of the following equations are linear?

(i)
$$\mathcal{L}(u) = u_x + 2u_y + u_{xy}$$

(ii)
$$\mathcal{L}(u) = u_{xx} + u_{yy}$$

(iii) $\mathcal{L}(u) = u_t + 3u^2 - u_x.$

Remark 1. If \mathcal{L} is linear, and u_1, \ldots, u_n are solutions of $\mathcal{L}(u) = 0$, then the linear combination

 $u = c_1 u_1 + \dots + c_n u_n$

is a solution of $\mathcal{L}(u) = 0$, for any real numbers c_1, \ldots, c_n .

Definition 2. If \mathcal{L} is linear, then an equation of the form $\mathcal{L}(u) = 0$ is called a *homogeneous* linear equation, while $\mathcal{L}(u) = g$ is called *inhomogeneous* linear.

ODE vs PDE

Recall that the general solutions of ODE involve a number of arbitrary constants.

Example 9. Consider the simple ODE u'(x) + 2xu(x) = 0. The general solution is

$$u(x) = Ce^{-x^2},$$

for an arbitrary constant C.

In contrast, the general solutions of PDE involve one or more arbitrary functions.

Example 10. Consider the PDE

$$u_{xy} + 2xu_y = 0$$

The general solution of this PDE is

$$u(x,y) = e^{-x^2}(F(x) + G(y)),$$

for arbitrary functions F and G.

Initial/Boundary conditions

To single out one solution, we need to impose boundary or initial conditions. The conditions are usually motivated by physics, and depend on the particular PDE.

• Initial conditions: When the PDE involves time, one often specifies and initial condition of the form

$$u(x,t_0) = \varphi(x),$$

where $\varphi(x)$ is a given function. For diffusion equations, φ represents the concentration or heat profile at time t_0 . For the wave equation, there is a pair of initial conditions

$$u(x,t_0) = \varphi(x)$$
 and $\frac{\partial u}{\partial t}(x,t_0) = \psi(x),$

where φ is the initial position and ψ is the initial velocity.

- Boundary conditions: Physical problems usually have a domain $D \subseteq \mathbb{R}^n$ in which the PDE is valid. It is physically obvious that we need to specify some type of boundary condition. Three common boundary conditions are
 - 1. Dirichlet condition: The value of u is specified on the boundary ∂u . For the heat equation, this is equivalent to fixing the temperature at the boundary of the object. For the wave equation, it amounts to holding the string or membrane and moving it in some specified way.
 - 2. Neumann condition: The normal derivative is specified on the boundary, i.e. $\frac{\partial u}{\partial n} = g(x,t)$ for $x \in \partial U$ and $t > t_0$. For the heat equation, g = 0 corresponds to insulating the object on the boundary so that heat is not allowed to flow through the boundary, and $g \neq 0$ corresponds to adding or removing heat at the boundary. For the wave equation, g = 0 corresponds to allowing the string or membrane to move freely at the boundary (say on a track).
 - 3. Robin condition: The robin condition is a combination of Dirichlet and Neumann conditions, where

$$\frac{\partial u}{\partial n} + au$$

is specified on the boundary. For the wave equation, imagine the end of the string is free to move along a track, but is attached to a coiled spring that tends to pull it back to equilibrium. For the heat equation, this amounts to submersing the boundary of the object into a reservoir of temperature g(t). Then by Newton's law of cooling

$$\frac{\partial u}{\partial x}(x,t) = -a(u(x,t) - g(t)),$$

for all $x \in \partial U$.

Well-posed problems

We expect that the physically correct boundary/initial conditions should determine exactly one unique solution of the PDE. Whether or not this is true can be determined mathematically, and this is one question we shall address in this course. WE say a PDE in a domain with boundary/initial conditions is *well-posed* if it enjoys the properties

- (i) **Existence:** There exists at least one solution of the PDE satisfying all conditions.
- (ii) Uniqueness: There is at most one solution.
- (iii) **Stability:** The unique solution u(x,t) depends in a stable manner on the boundary conditions, initial conditions, and any other data in the problem. This means that if the data are changed by a small amount, the solution u changes by a correspondingly small amount.

Example 11. Consider the diffusion equation

$$u_{t}(x,t) - k\Delta u(x,t) = f(x,t) \quad \text{for } (x,t) \in U \times (0,T)$$

$$u(x,0) = \varphi(x) \quad \text{for } x \in U$$

$$\frac{\partial u}{\partial n}(x,t) = \psi(x,t) \quad \text{for } (x,t) \in \partial U \times (0,T).$$

$$(3)$$

The data for this problem are the functions f, φ and ψ , and the positive constant c > 0. Existence and uniqueness mean that for any choice of data, there exists exactly one solution u(x,t) of (3). Stability means that if any of these data change slightly, the solution u also changes slightly. Mathematically, this requires defining a notion of distance between functions, which we will discuss later.

3 Differentiating under an integral

We have seen many examples in the course so far where a function u(x) is expressed in the form

$$u(x) = \int_{a}^{b} f(x, y) \, dy, \tag{4}$$

where f is an arbitrary given function, a < b (we allow $a = -\infty$ and/or $b = +\infty$), and $x, y \in \mathbb{R}$. For example, the solution of the heat equation on the entire real line is of the form

$$u(x,t) = \int_{-\infty}^{\infty} S(x-y,t)\varphi(y) \, dy,$$

where S is the fundamental solution of the heat equation.

The question addressed in these notes is the following: Under what circumstances is it valid to differentiate under the integral sign in (4)? Namely, we are asking when the following formula is valid:

$$u'(x) = \int_{a}^{b} f_{x}(x, y) \, dy.$$
(5)

Let us proceed by first principles and write

$$\frac{u(x+h) - u(x)}{h} = \int_{a}^{b} \frac{f(x+h,y) - f(x,y)}{h} \, dy,$$

which holds by linearity of the integral. Evidently, u'(x) exists if and only if the limit

$$\lim_{h \to 0} \int_a^b \frac{f(x+h,y) - f(x,y)}{h} \, dy$$

exists and is finite. Suppose that f is continuously differentiable in x so that

$$\lim_{h \to 0} \frac{f(x+h,y) - f(x,y)}{h} = f_x(x,y).$$

The question of the validity of (5) then boils down to whether we exchange limits with integrals. In particular, is it true that

$$\lim_{h \to 0} \int_{a}^{b} \frac{f(x+h,y) - f(x,y)}{h} \, dy = \int_{a}^{b} \lim_{h \to 0} \frac{f(x+h,y) - f(x,y)}{h} \, dy?$$

The following theorem is particularly useful in this context.

Theorem 1 (Dominated Convergence Theorem). Let a < b, allowing $a = -\infty$ and/or $b = +\infty$. Let f and f_n for n = 1, 2, 3, ... be functions on the interval (a, b) such that

$$f(x) = \lim_{n \to \infty} f_n(x) \quad \text{for all } x \in (a, b).$$
(6)

Suppose there exists a function g on (a, b) such that

$$|f_n(x)| \le g(x) \quad \text{for all } n \ge 1 \quad and \ x \in (a, b)$$
 (7)

and

$$\int_{a}^{b} g(x) \, dx < \infty. \tag{8}$$

Then

$$\lim_{n \to \infty} \int_a^b f_n(x) \, dx = \int_a^b f(x) \, dx. \tag{9}$$

We are omitting some details in the theorem statement related to measurability, but these are purely technical. The essence of the result is contained in the statement above. We will not prove the Dominated Convergence theorem here; this would normally be covered in a second undergraduate course on real analysis or in graduate real analysis.

We first note that the integrability condition (8) is in general necessary.

Example 12. Recall the fundamental solution of the heat equation is

$$S(x,t) = \frac{1}{\sqrt{4\pi kt}} e^{-x^2/4kt}$$

Notice that $\lim_{t\to\infty} S(x,t) = 0$ for all x. However

$$\lim_{t \to \infty} \int_{-\infty}^{\infty} S(x,t) \, dx = 1,$$

since $\int_{-\infty}^{\infty} S(x,t) dx = 1$ for all t > 0. The Dominated Convergence theorem does not hold in this case because a dominating function g does not exist.

Remark 2. When (a, b) is a bounded interval (so $a \neq -\infty$ and $b \neq +\infty$), we usually choose g(x) to be a constant function $g(x) \equiv M$. Then $\int_a^b g(x) dx = (a - b)M$ and the integrability condition (8) is clearly satisfied. In this case the Dominated Convergence Theorem holds whenever there exists M > 0 such that

$$|f_n(x)| \le M \quad \text{for all } n \ge 1 \quad \text{and } x \in (a, b).$$
(10)

Theorem 2 (Differentiating under an integral). Let a < b, allowing $a = -\infty$ and/or $b = +\infty$. Let f(x, y) be continuously differentiable in x and suppose there exists a function g(y) such that

$$|f_x(x,y)| \le g(y) \quad for \ all \ x \in \mathbb{R} \quad and \quad y \in (a,b),$$
(11)

and

$$\int_{a}^{b} g(y) \, dy < \infty. \tag{12}$$

Then u'(x) exists for each $x \in \mathbb{R}$ and

$$u'(x) = \int_{a}^{b} f_{x}(x, y) \, dy.$$
(13)

Proof. Fix $x \in \mathbb{R}$. Let h_n be a sequence of nonzero real numbers converging to 0 and write

$$\frac{u(x+h_n) - u(x)}{h_n} = \int_a^b \frac{f(x+h_n, y) - f(x, y)}{h_n} \, dy.$$

Define

$$f_n(y) := \frac{f(x+h_n, y) - f(x, y)}{h_n} \quad \text{for } y \in (a, b).$$

Then we have

$$\lim_{n \to \infty} f_n(y) = f_x(x, y).$$

Fix $n \ge 1$ and suppose that $h_n > 0$. By the fundamental theorem of calculus we have

$$|f_n(y)| = \frac{1}{h_n} \left| \int_x^{x+h_n} f_x(t,y) \, dt \right| \le \frac{1}{h_n} \int_x^{x+h_n} |f_x(t,y)| \, dt \stackrel{(11)}{\le} \frac{1}{h_n} \int_x^{x+h_n} g(y) \, dt = g(y),$$

for all $y \in (a, b)$. If $h_n < 0$, the same estimate $|f_n(y)| \le g(y)$ can be obtained by a similar argument. Therefore, we can apply the Dominated Convergence Theorem to obtain

$$\lim_{n \to \infty} \frac{u(x+h_n) - u(x)}{h_n} = \lim_{n \to \infty} \int_a^b f_n(y) \, dy = \int_a^b f_x(x,y) \, dy$$

Since $h_n \to 0$ was an arbitrary sequence, we have

$$\lim_{h \to 0} \frac{u(x+h) - u(x)}{h} = \int_{a}^{b} f_{x}(x,y)$$

Therefore u'(x) exists and (13) holds.

Remark 3. It is sometimes useful to note that the dominating condition (11) need not hold for all $x \in \mathbb{R}$. Indeed, inspecting the proof, we see that for computing $u'(x_0)$, we need only require that (11) hold for $x \in (x_0 - \delta, x_0 + \delta)$ for some fixed small number $\delta > 0$.

Example 13. Let us consider the solution of the heat equation

$$u(x,t) = \int_{-\infty}^{\infty} S(x-y,t)\varphi(y) \, dy,$$

where φ is assumed to be bounded, that is there exists M > 0 such that $|\varphi(y)| \leq M$ for all $y \in \mathbb{R}$. We will show how to use Theorem 2 to compute u_x .

Fix $x_0 \in \mathbb{R}$. Then we have

$$S_x(x-y,t) = \frac{-2(x-y)}{(4kt)^{3/2}\sqrt{\pi}} \exp\left(\frac{-(x-y)^2}{4kt}\right).$$

Therefore

$$|S_x(x-y,t)\varphi(y)| \le \frac{2M|x-y|}{(4kt)^{3/2}\sqrt{\pi}} \exp\left(\frac{-(x-y)^2}{4kt}\right).$$
 (14)

Suppose that $x \in (x_0 - 1, x_0 + 1)$ so that $|x - x_0| < 1$. Then by the triangle inequality

$$|x - y| = |x - x_0 + x_0 - y| \le |x - x_0| + |x_0 - y| < 1 + |x_0 - y|,$$
(15)

and $|x_0 - y| \le |x_0 - x| + |x - y| < 1 + |x - y|$, which is equivalently

$$|x - y| > |x_0 - y| - 1.$$
(16)

Inserting (15) and (16) into (14) we have

$$|S_x(x-y,t)\varphi(y)| \le \frac{2M(1+|x_0-y|)}{(4kt)^{3/2}\sqrt{\pi}} \exp\left(\frac{-(|x_0-y|-1)^2}{4kt}\right) =: g(y),$$

whenever $x \in (x_0 - 1, x_0 + 1)$. As an exercise, check that g is integrable, i.e., $\int_{-\infty}^{\infty} g(y) dy < \infty$. By Theorem 2 we have

$$u_x(x,t) = \int_{-\infty}^{\infty} S_x(x-y,t)\varphi(y) \, dy.$$

All other derivatives of u can be shown to exist with similar arguments.

4 Gibb's Phenomenon

The Fourier series for the function

$$f(x) = \begin{cases} \frac{1}{2}, & \text{if } 0 < x < \pi \\ -\frac{1}{2}, & \text{if } -\pi < x < 0, \end{cases}$$

is

$$f(x) = \sum_{\substack{n=1\\n \text{ odd}}}^{\infty} \frac{2}{\pi n} \sin(nx).$$

The Fourier series partial sums

$$S_N(x) = \sum_{\substack{n=1\\n \text{ odd}}}^N \frac{2}{\pi n} \sin(nx), \qquad (17)$$

converge pointwise to f provided we set f(0) = 0. We will show that the convergence here is *not* uniform, and furthermore, the partial sums S_N consistently overshoot the unit 1 jump by about 9% in the limit as $N \to \infty$. See Figure 1 for an illustration of the overshoot, which is called *Gibb's Phenomenon*.

We will argue that

$$\lim_{N \to \infty} \max S_N = \frac{1}{\pi} \int_0^\pi \frac{\sin(\theta)}{\theta} \, d\theta \approx 0.59.$$
(18)

by viewing the sum in (17) as a Riemann sum for an integral similar to the one above. For a completely different proof, refer to Strauss 5.5.

To establish (18), we first consider the question of where the maximum of S_N is attained. If N is even, then $S_{N-1} = S_N$, and we can replace N by the odd number N-1. Therefore we may assume N is odd. We note that the highest frequency sine wave in the partial sum S_N is $\sin(Nx)$, and this function has a maximum at $Nx = \pi/2$. Thus, it is reasonable to suspect that the maximum of S_N is attained at some point x_N^* of the form $x_N^* = x/N$. Let's plug this into S_N and see what we get:

$$S_N\left(\frac{x}{N}\right) = \sum_{\substack{n=1\\n \text{ odd}}}^N \frac{2}{\pi n} \sin\left(\frac{n}{N}x\right).$$

Let us rewrite this in a slightly different form:

$$S_N\left(\frac{x}{N}\right) = \frac{1}{\pi} \sum_{\substack{n=1\\n \text{ odd}}}^N \left(\frac{n}{N}\right)^{-1} \sin\left(\frac{n}{N}x\right) \frac{2}{N}.$$

Let us set $\Delta \theta = 2/N$ and $\theta_n = n/N$. Then we have

$$S_N\left(\frac{x}{N}\right) = \frac{1}{\pi} \sum_{\substack{n=1\\n \text{ odd}}}^N \frac{\sin(\theta_n x)}{\theta_n} \Delta \theta.$$



Figure 1: Depiction of Gibb's Phenomenon for a unit step function.

Since the sum is over all *odd* n, we have that $\Delta \theta = 2/N = \theta_{n+2} - \theta_n$ is the difference of two subsequent values of θ_n . Furthermore, $\theta_1 = 1/N$ and $\theta_N = 1$. Therefore, this is exactly a Riemann sum for the integral

$$\frac{1}{\pi} \int_0^\pi \frac{\sin(\theta x)}{\theta} \, d\theta.$$

Therefore

$$\lim_{N \to \infty} S_N\left(\frac{x}{N}\right) = \frac{1}{\pi} \int_0^\pi \frac{\sin(\theta x)}{\theta} \, d\theta = \frac{1}{\pi} \int_0^x \frac{\sin\theta}{\theta} \, d\theta =: \operatorname{Si}(x)$$

The function Si(x) is called the *Sine Integral*. Like the error function, there is no closed form expression for Si(x). The integrand of the Sine Integral is often called the *cardinal sine function* or the *sinc* function and denoted

$$\operatorname{sinc} \theta := \frac{\sin \theta}{\theta}.$$

See Figure 2 for a plot of the sinc function.

We claim the maximum value of $\operatorname{Si}(x)$ occurs at $x = \pi$. To see this, we first note that $\operatorname{sinc} \theta$ has the same sign as $\sin \theta$ for $\theta > 0$. So for $n\pi < \theta < (n+1)\pi$, $\operatorname{sinc} \theta > 0$ for n even, and $\operatorname{sinc} \theta < 0$ for n odd. This tells us that $\operatorname{Si}(x)$ has local maximums at $x = n\pi$ for odd n. Since $\theta \mapsto 1/\theta$ is decreasing, and $|\sin \theta|$ is π -periodic, we have

$$\int_{n\pi}^{(n+1)\pi} |\operatorname{sinc} \theta| \, d\theta \ge \int_{(n+1)\pi}^{(n+2)\pi} |\operatorname{sinc} \theta| \, d\theta$$

Therefore, for odd $n \in \mathbb{N}$ we have

$$\operatorname{Si}((n+2)\pi) = \int_{0}^{(n+2)n\pi} \operatorname{sinc} \theta \, d\theta$$
$$= \operatorname{Si}(n\pi) + \int_{n\pi}^{(n+1)\pi} \operatorname{sinc} \theta \, d\theta + \int_{(n+1)\pi}^{(n+2)\pi} \operatorname{sinc} \theta \, d\theta$$
$$= \operatorname{Si}(n\pi) - \int_{n\pi}^{(n+1)\pi} |\operatorname{sinc} \theta| \, d\theta + \int_{(n+1)\pi}^{(n+2)\pi} |\operatorname{sinc} \theta| \, d\theta$$
$$\leq \operatorname{Si}(n\pi).$$



Figure 2: Plot of the function sinc $\theta = \frac{\sin \theta}{\theta}$.

By induction, $\operatorname{Si}(n\pi) \leq \operatorname{Si}(\pi)$ for all odd $n \in \mathbb{N}$. This establishes the claim that the maximum of Si occurs at $x = \pi$. As an exercise, you may also wish to verify that $x = n\pi$ with n odd is a local maximum of Si by computing $\operatorname{Si}'(x) = 0$ and checking the sign of $\operatorname{Si}''(x)$.

Therefore, we have established that

$$\lim_{N \to \infty} S_N\left(\frac{\pi}{N}\right) = \frac{1}{\pi} \operatorname{Si}(\pi) = \frac{1}{\pi} \int_0^{\pi} \frac{\sin\theta}{\theta} \, d\theta \approx 0.58949,$$

where the value ≈ 0.58949 can be obtained by numerical integration. Since $f(0^+) = 0.5$, the overshoot is approximately 9% of the entire unit jump from $f(0^-) = -0.5$ to $f(0^+) = 0.5$.

To be entirely rigorous, we have actually only shown that

$$\liminf_{N \to \infty} \max S_N \ge \frac{1}{\pi} \operatorname{Si}(\pi) \approx 0.58949,$$

which shows that the overshoot is at least 9% in the limit as $N \to \infty$. To show that the limit exists, so that

$$\lim_{N \to \infty} \max S_N = \frac{1}{\pi} \operatorname{Si}(\pi),$$

takes a bit more work (but not too much). We can differentiate S_N to find that

$$S'_N(x) = \sum_{\substack{n=1\\n \text{ odd}}}^N \frac{2}{\pi} \cos(nx) = \frac{2}{\pi} \sum_{n=0}^{(N-1)/2} \cos((2n+1)x),$$

assuming N is odd. Using Euler's formula $e^{i\theta} = \cos \theta + i \sin \theta$ we can derive a simpler expression for this sum in a similar way to our derivation of Dirichlet's kernel K_N in class. We have

$$S'_N(x) = \frac{\sin(x(N+1))}{\pi \sin x}.$$

As an exercise, you should fill in the details above. From this we can show that S_N attains its maximum at $x = \pi/(N+1)$, and using the argument above yields

$$\lim_{N \to \infty} S_N\left(\frac{\pi}{N+1}\right) = \frac{1}{\pi} \operatorname{Si}(\pi).$$

5 Regularity and decay of Fourier Series coefficients

We define

$$L^{2}\left(\left(-\pi,\pi\right)\right) := \left\{ \text{functions } f \text{ on } \left(-\pi,\pi\right) \text{ such that } \|f\| < \infty \right\}$$

where $||f||^2 = \int_{-\pi}^{\pi} f(x)^2 dx$, and

 $C_{per}^{k} := \Big\{ 2\pi \text{-periodic functions } f \text{ that are } k \text{-times continuously differentiable} \Big\}.$

We recall that f is k-times continuously differentiable if the derivatives $f', f'', \ldots, f^{(k)}$ all exist and are continuous.

In this lecture, we examine the relationship between the rate of decay of the Fourier coefficients and the regularity of f. We consider the full Fourier series on $(-\pi, \pi)$

$$\frac{1}{2}A_0 + \sum_{n=1}^{\infty} A_n \cos(nx) + B_n \sin(nx)$$

with coefficients

$$A_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(nx) \, dx$$
 and $B_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(nx) \, dx.$

Lemma 1 (Riemann-Lebesgue). If $f \in L^2((-\pi, \pi))$ then

$$\lim_{n \to \infty} A_n = 0 \quad and \quad \lim_{n \to \infty} B_n = 0.$$
⁽¹⁹⁾

Proof. By Bessel's inequality we have

$$\frac{\pi}{2}A_0^2 + \sum_{n=1}^{\infty} \pi (A_n^2 + B_n^2) \le \|f\|^2 < \infty.$$

Therefore $\sum A_n^2 < \infty$ and $\sum B_n^2 < \infty$, from which (19) immediately follows.

The Riemann-Lebesgue Lemma tells us that the Fourier coefficients decay to zero as $n \to \infty$, but it gives us no information about the rate of convergence. If we have more information about the regularity of f, then we can get information on the rate.

Theorem 3. If $f \in C_{per}^k$, then there exists a constant C > 0 such that

$$|A_n| \le \frac{C}{n^k} \quad and \quad |B_n| \le \frac{C}{n^k}.$$
(20)

Proof. The case of k = 0 is trivial, so we assume $k \ge 1$. We will prove the theorem for A_n ; the case of B_n is strictly similar. Integrating by parts we have

$$A_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(nx) \, dx = \frac{-1}{\pi} \int_{-\pi}^{\pi} f'(x) \frac{\sin(nx)}{n} \, dx + \frac{1}{\pi} f(x) \frac{\sin(nx)}{n} \Big|_{-\pi}^{\pi}.$$

The boundary term on the right vanishes due to the periodicity of f and sin. Therefore

$$A_n = \frac{-1}{\pi n} \int_{-\pi}^{\pi} f'(x) \sin(nx) \, dx.$$

We can continue (if $k \ge 2$) and integrate by parts again to find that

$$A_n = \frac{-1}{\pi n} \int_{-\pi}^{\pi} f''(x) \frac{\cos(nx)}{n} \, dx + \frac{1}{\pi n} f'(x) \frac{\cos(nx)}{n} \Big|_{-\pi}^{\pi}$$

The boundary terms again vanish due to periodicity and we have

$$A_n = \frac{-1}{\pi n^2} \int_{-\pi}^{\pi} f''(x) \cos(nx) \, dx.$$

If we continue k times, it is clear that

$$|A_n| = \frac{1}{\pi n^k} \left| \int_{-\pi}^{\pi} f^{(k)}(x) g(nx) \, dx \right|,$$

where $g(x) = \cos(x)$ when k is even, and $g(x) = \sin(x)$ when k is odd. Either way, $|g(x)| \le 1$. Therefore

$$|A_n| \le \frac{1}{\pi n^k} \int_{-\pi}^{\pi} |f^{(k)}(x)g(nx)| \, dx \le \frac{1}{n^k} \left(\frac{1}{\pi} \int_{-\pi}^{\pi} |f^{(k)}(x)| \, dx\right).$$

Setting

$$C = \frac{1}{\pi} \int_{-\pi}^{\pi} |f^{(k)}(x)| \, dx$$

completes the proof.

Remark 4. The direct converse of Theorem 3 is not true. For example, recall that for the step function

$$f(x) = \begin{cases} \frac{1}{2}, & \text{if } 0 < x < \pi \\ -\frac{1}{2}, & \text{if } -\pi < x < 0, \end{cases}$$

the Fourier series is

$$f(x) = \sum_{\substack{n=1\\n \text{ odd}}}^{\infty} \frac{2}{\pi n} \sin(nx).$$

In this case $A_n = 0$ for all n and

$$|B_n| \le \frac{2}{\pi n} = \frac{C}{n}$$

However, f is discontinuous at x = 0, so $f \notin C_{per}^0$, much less C_{per}^1 .

We can prove a converse to Theorem 3 if we assume slightly stronger decay of the Fourier coefficients. Before presenting this result, we present a version of the Dominated Convergence Theorem for series.

Theorem 4 (Dominated Convergence Theorem for Series). Let $\{a_{n,k}\}_{n,j=1}^{\infty}$ and $\{b_n\}_{n=1}^{\infty}$ such that

$$\lim_{j \to \infty} a_{n,j} = b_n \quad \text{for all } n.$$

Suppose there exists $\{c_n\}_{n=1}^{\infty}$ such that

$$|a_{n,j}| \le c_n \quad \text{for all } n, j \ge 1, \quad and \quad \sum_{n=1}^{\infty} c_n < \infty.$$
 (21)

Then

$$\lim_{j \to \infty} \sum_{n=1}^{\infty} a_{n,j} = \sum_{n=1}^{\infty} \lim_{j \to \infty} a_{n,j} = \sum_{n=1}^{\infty} b_n.$$
 (22)

We can now prove a converse to Theorem 3.

Theorem 5. Let $\{A_n\}_{n=0}^{\infty}$ and $\{B_n\}_{n=1}^{\infty}$ be sequences of real numbers satisfying

$$|A_n|, |B_n| \le \frac{C}{n^{k+1+\varepsilon}} \qquad (k \ge 0, \, C > 0, \, \varepsilon > 0), \tag{23}$$

and define the partial sums

$$S_N(x) = \frac{1}{2}A_0 + \sum_{n=1}^N A_n \cos(nx) + B_n \sin(nx).$$
(24)

Then S_N converges uniformly to a function $f \in C_{per}^k$ as $N \to \infty$ and

$$f^{(k)}(x) = \sum_{n=1}^{\infty} \frac{d^k}{dx^k} \left(A_n \cos(nx) + B_n \sin(nx) \right).$$
(25)

Proof. We will sketch the proof, as it relies on some results from real analysis (besides the dominated convergence theorem). We note that for N > M we have

$$|S_N(x) - S_M(x)| = \left| \sum_{n=M+1}^N A_n \cos(nx) + B_n \sin(nx) \right|$$
$$\leq \sum_{n=M+1}^N |A_n| + |B_n|$$
$$\leq 2C \sum_{n=M+1}^\infty \frac{1}{n^{k+1+\varepsilon}}.$$

Since $\sum_{n=1}^{\infty} \frac{1}{n^{k+1+\varepsilon}} < \infty$, we have

$$\lim_{M \to \infty} \sum_{n=M+1}^{\infty} \frac{1}{n^{k+1+\varepsilon}} = 0.$$

Therefore the sequence $\{S_N\}_{N=1}^{\infty}$ is uniformly Cauchy. Since each S_N is a continuous function, it follows from standard results in real analysis that S_N converges uniformly to a continuous function $f \in C_{per}^0$. Therefore we have

$$f(x) = \frac{1}{2}A_0 + \sum_{n=1}^{\infty} A_n \cos(nx) + B_n \sin(nx).$$
 (26)

We will prove the rest of the theorem by induction. Let h_j be sequence of nonzero real numbers converging to zero. Then

$$\frac{f(x+h_j) - f(x)}{h_j} = \sum_{n=1}^{\infty} A_n \frac{\cos(n(x+h_j)) - \cos(nx)}{h_j} + B_n \frac{\sin(n(x+h_j)) - \sin(nx)}{h_j}.$$
 (27)

Define

$$a_{n,j} := A_n \frac{\cos(n(x+h_j)) - \cos(nx)}{h_j} + B_n \frac{\sin(n(x+h_j)) - \sin(nx)}{h_j}.$$

As an exercise, show using the fundamental theorem of calculus that

 $|\cos(x) - \cos(y)| \le |x - y|$ and $|\sin(x) - \sin(y)| \le |x - y|$.

Therefore

$$|a_{n,j}| \le |A_n| \frac{n|h_j|}{|h_j|} + |B_n| \frac{n|h_j|}{|h_j|} = n|A_n| + n|B_n|.$$

Using the decay estimates (23) for k = 1 we have

$$|a_{n,j}| \le \frac{2C}{n^{1+\varepsilon}} =: c_n.$$

Since $\sum c_n < \infty$, we may use the Dominated Convergence Theorem and (27) to find that

$$\lim_{j \to \infty} \frac{f(x+h_j) - f(x)}{h_j} = \sum_{n=1}^{\infty} \lim_{j \to \infty} a_{n,j} = \sum_{n=1}^{\infty} -nA_n \sin(nx) + nB_n \cos(nx).$$

Therefore f' exists and

$$f'(x) = \sum_{n=1}^{\infty} -nA_n \sin(nx) + nB_n \cos(nx).$$

This establishes the base case. Since $n|A_n|, n|B_n| \leq 1/n^{1+\varepsilon}$, the argument at the start of the proof shows that f' is a continuous function. Hence $f \in C_{per}^1$.

The inductive hypothesis is as follows: Let $k \ge 2$, and suppose that if $|A_n|, |B_n| \le C/n^{k+\varepsilon}$ then $f \in C_{per}^{k-1}$ and

$$f^{(k-1)}(x) = \sum_{n=1}^{\infty} \frac{d^{k-1}}{dx^{k-1}} \left(A_n \cos(nx) + B_n \sin(nx) \right).$$

We need to show that if (23) holds, then $f \in C_{per}^k$ and (25) holds.

For simplicity, let us assume that k is odd; the case where k is even is strictly similar. Since k - 1 is even, we have

$$f^{(k-1)}(x) = \sum_{n=1}^{\infty} (-1)^{\frac{k-1}{2}} n^{k-1} \left(A_n \cos(nx) + B_n \sin(nx) \right).$$

Let h_j be sequence of nonzero real numbers converging to zero and consider the difference quotient

$$\frac{f^{(k-1)}(x+h_j) - f^{(k-1)}(x)}{h_j} = \sum_{n=1}^{\infty} a_{n,j},$$
(28)

where

$$a_{n,j} := (-1)^{\frac{k-1}{2}} n^{k-1} \left(A_n \frac{\cos(n(x+h_j)) - \cos(nx)}{h_j} + B_n \frac{\sin(n(x+h_j)) - \sin(nx)}{h_j} \right)$$

As before, we have the estimate

$$|a_{n,j}| \le n^{k-1} \left(\frac{n|A_n||h_j|}{|h_j|} + \frac{n|B_n||h_j|}{|h_j|} \right) \le \frac{2Cn^k}{n^{k+1+\varepsilon}} = \frac{2C}{n^{1+\varepsilon}} = c_n,$$

where we used the decay estimates (23) in the middle step. Since $\sum c_n < \infty$, the Dominated Convergence Theorem yields

$$\lim_{j \to \infty} \frac{f^{(k-1)}(x+h_j) - f^{(k-1)}(x)}{h_j} = \sum_{n=1}^{\infty} \lim_{j \to \infty} a_{n,j}$$
$$= \sum_{n=1}^{\infty} (-1)^{\frac{k-1}{2}} n^{k-1} \left(-nA_n \sin(nx) + nB_n \cos(nx) \right).$$

Therefore, $f^{(k)}(x)$ exists and

$$f^{(k)}(x) = \sum_{n=1}^{\infty} (-1)^{\frac{k+1}{2}} n^k \left(A_n \sin(nx) - B_n \cos(nx) \right).$$

By (23), the coefficients $\overline{A}_n := (-1)^{\frac{k+1}{2}} n^k A_n$ and $\overline{B}_n := -(-1)^{\frac{k+1}{2}} n^k A_n$ of the series for $f^{(k)}$ satisfy

$$|\overline{A}_n|, |\overline{B}_n| \le \frac{Cn^k}{n^{k+1+\varepsilon}} \le \frac{C}{n^{1+\varepsilon}}.$$

By the first part of the proof, $f^{(k)}$ is continuous, hence $f \in C_{per}^k$. This completes the proof. \Box

5.1 An application to the heat equation

Let us give an application of these results to the heat equation with Dirichlet boundary conditions

(H)
$$\begin{cases} u_t(x,t) - u_{xx}(x,t) = 0 & 0 < x < \pi, t > 0 \\ u(0,t) = u(\pi,t) = 0 & t > 0 \\ u(x,0) = \varphi(x) & 0 < x < \pi. \end{cases}$$

Recall we had previously used separation of variables to find the Fourier series solution

$$u(x,t) = \sum_{n=1}^{\infty} B_n e^{-n^2 t} \sin(nx), \quad (0 \le x \le \pi, t \ge 0)$$
(29)

where

$$B_n = \frac{2}{\pi} \int_0^\pi \varphi(y) \sin(ny) \, dx. \tag{30}$$

Theorem 6. Assume $\varphi \in L^2((0,\pi))$. Then u defined by (29) is infinitely differentiable in the rectangle $0 < x < \pi$ and t > 0, and solves the heat equation (H).

Remark 5. Since $\varphi \in L^2((0,\pi))$, the Fourier sine series for φ converges in L^2 , but may not converge pointwise. Hence, the initial condition $u(x,0) = \varphi(x)$ is interpreted in the sense that

$$\lim_{N \to \infty} \|S_N - \varphi\| = 0,$$

where

$$S_N(x) = \sum_{n=1}^N B_n \sin(nx).$$

If φ is Lipschitz continuous, then the Fourier sine series converges pointwise in $0 < x < \pi$, and the initial condition is satisfied in the usual sense

$$u(x,0) = \sum_{n=1}^{\infty} B_n \sin(nx) = \varphi(x) \qquad (0 < x < \pi).$$

Notice we have

$$u(0,0) = u(\pi,0) = 0.$$

Hence, $u(x,0) = \varphi(x)$ for all $0 \le x \le \pi$ if and only if φ satisfies the Dirichlet boundary conditions $\varphi(0) = \varphi(\pi) = 0$.

Proof of Theorem 6. The series representation of u(x,t) is of the form

$$u(x,t) = \sum_{n=1}^{\infty} A_n \sin(nx),$$

where

$$A_n = B_n e^{-n^2 t}$$

Since $\lim_{n\to\infty} n^{k+2}e^{-n^2t} = 0$ for any k and all t > 0, there exists a constant C > 0 depending on k and t such that $e^{-n^2t} \leq C/n^{k+2}$. By Theorem 5, the function $x \mapsto u(x,t)$ belongs to C_{per}^k for all k. Therefore u is infinitely differentiable in x and

$$u_{xx}(x,t) = \sum_{n=1}^{\infty} \frac{\partial^2}{\partial x^2} B_n e^{-n^2 t} \sin(nx) = -\sum_{n=1}^{\infty} n^2 e^{-n^2 t} \sin(nx).$$

We claim that u is infinitely differentiable in x and t and all partial derivative are continuous. We'll just sketch the proof here. Let h_j be a sequence of real numbers converging to zero and consider

$$\frac{u(x,t+h_j) - u(x,t)}{h_j} = \sum_{n=1}^{\infty} B_n \sin(nx) \left(\frac{e^{-n^2(t+h_j)} - e^{-n^2t}}{h_j}\right).$$

Define

$$a_{n,j} = B_n \sin(nx) \left(\frac{e^{-n^2(t+h_j)} - e^{-n^2t}}{h_j} \right) = B_n \sin(nx) e^{-n^2t} \left(\frac{e^{-n^2h_j} - 1}{h_j} \right).$$

As an exercise, show that

$$|e^x - 1| \le |x|e^{|x|}$$
 for all $x \in \mathbb{R}$.

Hence

$$|a_{n,j}| \le Ce^{-n^2t}e^{n^2|h_j|} = Ce^{-n^2(t-|h_j|)}$$

Since $h_j \to 0$, we may assume that $|h_j| \le t/2$. Then

$$|a_{n,j}| \le Ce^{-n^2t/2}$$
, and $\sum_{n=1}^{\infty} e^{-n^2t/2} < \infty$.

By the Dominated Convergence Theorem

$$\lim_{j \to \infty} \frac{u(x, t+h_j) - u(x, t)}{h_j} = \sum_{j=1}^{\infty} \lim_{j \to \infty} B_n \sin(nx) \left(\frac{e^{-n^2(t+h_j)} - e^{-n^2t}}{h_j} \right).$$

It follows that u_t exists and

$$u_t(x,t) = -\sum_{n=1}^{\infty} n^2 e^{-n^2 t} \sin(nx).$$

Recalling the expression for u_{xx} above, we see that u solves the heat equation (H).

We finally note that the same argument shows that all derivatives in t of all orders exist (including the mixed partials in t and x) and the formula

$$\frac{\partial^{k+j}}{\partial x^k \partial t^j} u(x,t) = \sum_{n=1}^{\infty} \frac{\partial^{k+j}}{\partial x^k \partial t^j} B_n e^{-n^2 t} \sin(nx)$$

holds for all k and j. As we did in the proof of Theorem 5, we can show that for fixed $\sigma > 0$, the series on the right hand side is uniformly Cauchy on the rectangle $0 \le x \le \pi$ and $t \ge \sigma$. Therefore it converges uniformly to the mixed partial on the left hand side (which is therefore continuous). Since $\sigma > 0$ is arbitrary, this shows that all partial derivatives are continuous on the rectangle $0 \le x \le \pi$ and t > 0. Regularity cannot be extended to t = 0, as φ may not even be continuous.

6 Convergence rates for numerically solving the heat equation

Consider the Dirichlet problem for the heat equation

(P)
$$\begin{cases} u_t = u_{xx} & \text{if } 0 < x < 1, t > 0\\ u(0,t) = u(1,t) = 0 & \text{if } t > 0\\ u(x,0) = \varphi(x) & \text{if } 0 < x < 1, \end{cases}$$

and the finite difference approximation

$$\begin{cases} u_j^{n+1} = s \left(u_{j-1}^n + u_{j+1}^n \right) + (1-2s) u_j^n & \text{if } n \ge 1 \text{ and } 1 \le j \le J-1 \\ u_0^n = u_J^n = 0 & \text{for } n \ge 1 \\ u_j^0 = \varphi(j\Delta x) & \text{for } 1 \le j \le J-1, \end{cases}$$

where $\Delta x > 0$ is a positive number for which $J = 1/\Delta x$ is a positive integer, and $s = \Delta t/\Delta x^2$. If we set $\mathbf{u}^n = [u_1^n, \dots, u_{J-1}^n]^T$, then we can rewrite the finite difference scheme as

(S)
$$\begin{cases} \mathbf{u}^{n+1} = A_s \mathbf{u}^n & \text{for } n \ge 1\\ \mathbf{u}^0 = \boldsymbol{\varphi}, \end{cases}$$

where $\boldsymbol{\varphi} = [\varphi(\Delta x), \dots, \varphi((J-1)\Delta x)]^T$ and A_s is the $(J-1) \times (J-1)$ matrix

$$A_{s} = \begin{bmatrix} 1-2s & s & 0 & 0 & \dots & 0 \\ s & 1-2s & s & 0 & \dots & 0 \\ 0 & s & 1-2s & s & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & s & 1-2s & s \\ 0 & 0 & \dots & 0 & s & 1-2s \end{bmatrix}$$
(31)

For two vectors \mathbf{u} and \mathbf{v} in \mathbb{R}^{J-1} we write $\mathbf{u} \leq \mathbf{v}$ whenever $u_i \leq v_i$ for all *i*. When $s \leq \frac{1}{2}$, all the entries of A_s are positive and we have

$$\mathbf{u} \ge \mathbf{0} \implies A_s \mathbf{u} \ge \mathbf{0}$$

Therefore, whenever $\mathbf{u} \leq \mathbf{v}$ we have $\mathbf{v} - \mathbf{u} \geq 0$ and hence

$$A_s \mathbf{v} - A_s \mathbf{u} = A_s (\mathbf{v} - \mathbf{u}) \ge 0.$$

Therefore, we have the useful monotonicity condition

$$\mathbf{u} \le \mathbf{v} \implies A_s \mathbf{u} \le A_s \mathbf{v},\tag{32}$$

which holds whenever $s \leq \frac{1}{2}$. As an aside, a general, possibly nonlinear scheme $\mathbf{u}^{n+1} = F(\mathbf{u}^n)$ is said to be monotone if $F(\mathbf{u}) \leq F(\mathbf{v})$ whenever $\mathbf{u} \leq \mathbf{v}$. There is a very general theory establishing convergence of monotone finite difference schemes. Here we will illustrate the classical theory for the heat equation (P).

The monotonicity property (32) allows us to prove the following lemma.

Lemma 2. Let $s \leq \frac{1}{2}$ and let K > 0. Suppose that $\mathbf{v}^0 = \mathbf{0}$ and $\mathbf{v}^n = (v_i^n)_j$ satisfies

$$|v_j^{n+1} - [A_s \mathbf{v}^n]_j| \le K \tag{33}$$

for all $n \ge 0$ and all $1 \le j \le J - 1$. Then

$$|v_j^n| \le Kn \tag{34}$$

for all $n \ge 0$ and $1 \le j \le J - 1$.

If K = 0, then \mathbf{v}^n solves the scheme (S) with $\varphi = \mathbf{0}$. Therefore $\mathbf{v}^n = A_s^n \mathbf{0} = \mathbf{0}$. The lemma is a perturbation result, which says that if \mathbf{v}^n has zero initial condition $\varphi = \mathbf{0}$ and \mathbf{v}^n is close to solving the scheme (S) (i.e., within K) then \mathbf{v}^n is close to zero (i.e., within Kn of zero).

Proof. The proof is by induction. For n = 0 the result is true due to the fact that $\mathbf{v}^0 = \mathbf{0}$. Suppose the result (34) holds for $n \ge 0$. Then $-Kn \le v_j^n \le Kn$ for all j, which in vector form is

$$-Kn\mathbf{1} \le \mathbf{v}^n \le Kn\mathbf{1},$$

where $\mathbf{1} = [1, \ldots, 1]^T$. Using the monotonicity of A_s (32) we have

$$-KnA_s\mathbf{1} \le A_s\mathbf{v}^n \le KnA_s\mathbf{1}.$$

Furthermore, we can compute that $A_s \mathbf{1} \leq \mathbf{1}$. Therefore

$$-Kn\mathbf{1} \leq A_s \mathbf{v}^n \leq Kn\mathbf{1}.$$

This is equivalent to $|[A_s \mathbf{v}^n]_j| \leq Kn$ for all $1 \leq j \leq J - 1$. Using (33) we have

$$\begin{aligned} |v_j^{n+1}| &= |v_j^{n+1} - [A_s \mathbf{v}^n]_j + [A_s \mathbf{v}^n]_j| \\ &\leq |v_j^{n+1} - [A_s \mathbf{v}^n]_j| + |[A_s \mathbf{v}^n]_j| \\ &\leq K + Kn = K(n+1), \end{aligned}$$

for all j. The proof is completed by induction.

We now prove that solutions \mathbf{u}^n of the scheme (S) converge to the solution u(x,t) of (P) as $\Delta t \to 0$, when the ratio $\Delta t/\Delta x^2 = s$ is fixed. We assume that φ is a smooth 1-periodic function satisfying $\varphi(0) = \varphi(1) = 0$.

Theorem 7. Fix $s \leq \frac{1}{2}$ and set $\Delta t = s\Delta x^2$. Let $\mathbf{u}^n = (u_j^n)_j$ be the solution of (S) and let u(x,t) be the solution of (P). Then there exists a constant C > 0, depending only on φ , such that

$$|u(x,t) - u_i^n| \le Ct\Delta x^2$$

for all $n \ge 0$ and $1 \le j \le J - 1$, where $x = j\Delta x$ and $t = n\Delta t$.

Proof. Set $w_j^n = u(j\Delta x, n\Delta t)$. By our assumptions on φ and our previous study of Fourier series and the Dirichlet problem for the heat equation (P), we know that u is infinitely differentiable, and each derivative of u is uniformly bounded. Expanding u via a Taylor series, as we did in class, there exists a constant C > 0 such that

$$\left|\frac{w_{j+1}^n - 2w_j^n + w_{j-1}^n}{\Delta x^2} - u_{xx}(x,t)\right| \le C\Delta x^2,\tag{35}$$

and

$$\left|\frac{w_j^{n+1} - w_j^n}{\Delta t} - u_t(x, t)\right| \le C\Delta t \tag{36}$$

for all $n \ge 0$ and $1 \le j \le J-1$, where $x = j\Delta x$ and $t = n\Delta t$. Since u solves the heat equation (P) we can write

$$\begin{split} |w_{j}^{n+1} - [A_{s}\mathbf{w}^{n}]_{j}| &= \left| w_{j}^{n+1} - w_{j}^{n} - s(w_{j+1}^{n} - 2w_{j}^{n} + w_{j-1}^{n}) \right| \\ &= \Delta t \left| \frac{w_{j}^{n+1} - w_{j}^{n}}{\Delta t} - \frac{w_{j+1}^{n} - 2w_{j}^{n} + w_{j-1}^{n}}{\Delta x^{2}} \right| \\ &= \Delta t \left| \frac{w_{j}^{n+1} - w_{j}^{n}}{\Delta t} - u_{t}(x, t) + u_{xx}(x, t) - \frac{w_{j+1}^{n} - 2w_{j}^{n} + w_{j-1}^{n}}{\Delta x^{2}} \right| \\ &\leq \Delta t \left| \frac{w_{j}^{n+1} - w_{j}^{n}}{\Delta t} - u_{t}(x, t) \right| + \Delta t \left| u_{xx}(x, t) - \frac{w_{j+1}^{n} - 2w_{j}^{n} + w_{j-1}^{n}}{\Delta x^{2}} \right| \\ &\leq C\Delta t^{2} + C\Delta t\Delta x^{2}, \end{split}$$

where the last line follows from (35) and (36). Since $\Delta t = s \Delta x^2$ we have

$$|w_j^{n+1} - [A_s \mathbf{w}^n]_j| \le C(1+s)\Delta t \Delta x^2, \tag{37}$$

for all $n \ge 0$ and $1 \le j \le J - 1$. Now set $\mathbf{v}^n = \mathbf{w}^n - \mathbf{u}^n$. Since \mathbf{u}^n solves the scheme (S), so $\mathbf{u}^{n+1} = A_s \mathbf{u}^n$, we have that

$$\mathbf{v}^{n+1} - A_s \mathbf{v}^n = \mathbf{w}^{n+1} - A_s \mathbf{w}^n - (\mathbf{u}^{n+1} - A_s \mathbf{u}^n) = \mathbf{w}^{n+1} - A_s \mathbf{w}^n.$$

Therefore

$$|v_j^{n+1} - [A_s \mathbf{v}^n]_j| = |w_j^{n+1} - [A_s \mathbf{w}^n]_j| \le C(1+s)\Delta t \Delta x^2.$$

Since $\mathbf{v}^0 = \mathbf{w}^0 - \mathbf{u}^0 = 0$, we can invoke Lemma 2 to find that

$$|w_j^n - u_j^n| = |v_j^n| \le C(1+s)n\Delta t\Delta x^2.$$

Since $t = n\Delta t$ and $w_j^n = u(x, t)$

$$|u(x,t) - u_j^n| \le C(1+s)t\Delta x^2 \le \frac{3C}{2}t\Delta x^2.$$