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AMATH 442 (Fall 2014 - 1149)

Numerical Solutions of Partial Differential Equations

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These notes are currently a work in progress, and as such may be incomplete or contain errors.

Fall 2014 ACKNOWLEDGMENTS

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Fall 2014 ABSTRACT

Abstract

The purpose of these notes is to provide the reader with a secondary reference to the material covered in AMATH 442. The formal prerequisite to this course is either AMATH 351 or AMATH 350.

Fall 2014 1 INTRODUCTION

Errata

6-7 Assignments Biweekly

25% Assignments, 25% Midterm, 50% Final Exam

Office hours: W, Th @ 2-3pm Midterm: Oct. 21st @ 4-5:30pm

1 Introduction

We begin with a quick review of the theoretical bases of **partial differential equations**.

1.1 Classification of 2nd Order Linear PDEs

There are 3 types of (linear) PDEs:

1. Parabolic PDEs (e.g. heat equation, diffusion equation)

(a) Has the form $u_t = \sigma u_{xx}$ or in the multivariate case, $u_t = \sigma (u_{xx} + u_{yy} + u_{zz})$

2. Elliptic PDEs (e.g. Laplace's equation, Poisson equation)

(a) Has the form $u_{xx} + u_{yy} = f(x, y)$ or $\Delta u = f(x, y)$

3. Hyperbolic PDEs (e.g. 1st, 2nd order wave equations)

(a) Has the form $u_{tt} - c^2 u_{xx} = 0$ or $u_t + a u_x = 0$

There are also non-linear PDEs:

• Burger's equation: $u_t + uu_x = 0$

• Non-linear heat equation: $u_t = (\sigma(u)u_x)_x$

• Higher-order PDEs: $u_t + uu_x = \sigma u_{xxx}$

Mixed types

1.2 Examples of Linear PDEs

(1) Let's begin by looking at the classic linear advection (a.k.a. wave) equation. The basic form is

$$u_t + au_x = 0, a \in \mathbb{R}, (x, t) \in \mathbb{R} \times \mathbb{R}$$

Claim 1.1. Any $\phi(x-at)$ is a solution.

Proof. Substitution and chain rule:

$$u = \phi(x - at) \implies u_t = \phi'(x - at)(-a), u_x = \phi'(x - at) \implies -a\phi' + a\phi' = 0$$

Therefore ϕ is a solution.

With the initial condition $u(x,0) = u_0(x)$, the solution is $u = u_0(x - at)$. The PDE with the aforementioned initial condition is called the **Cauchy problem**. We can interpret the parameter a as a speed parameter.

Now suppose that we introduce a finite domain $\Omega = [\alpha, \beta]$ and **boundary conditions**. Saying $u(\beta, t) = b_{right}(t)$ might lead to contradiction since $u_0(x-at) \neq b_{right}(\beta, t)$ or $u_0 = b_{right}$ (no new information is given). Instead, we provide $u(\alpha, t) = b_{left}(t)$ if a > 0 and we provide $u(\beta, t) = b_{right}(t)$ if a < 0.

Conclusion 1. Here are some conclusions regarding the above wave equation:

- [1] The solution of (1) does not grow or decay over time.
- [2] New extrema can be introduced only through boundary conditions.
- (2) Moving on, we have the diffusion (heat) equation. The basic form is

$$u_t = \sigma u_{xx}, \sigma \in \mathbb{R}$$

Assume that the initial conditions (I.C.) and boundary conditions (B.C.) are such that

$$u(x,t) = \hat{u}(k,t)\sin kx$$

is a solution, with k fixed. By substitution,

$$u_t = \hat{u}_t \sin kx$$

$$u_x = k\hat{u}\cos kx$$

$$u_{xx} = -k^2\hat{u}\sin kx$$

and so

$$\hat{u}_t \sin kx = -\sigma k^2 \hat{u} \sin kx \implies \hat{u}_t = -\sigma k^2 \hat{u} \implies \hat{u}(k,t) = ce^{-\sigma k^2 t} \implies u(x,t) = ce^{-\sigma k^2 t} \sin kx$$

If we set c = 1 then the I.C. should be

$$u(x,0) = e^{-\sigma k^2 \cdot 0} \sin kx = \sin kx$$

If the domain is $\Omega = [-1, 1]$ and $k = \pi$ then the B.C. is

$$\begin{cases} u(-1,t) &= 0\\ u(1,t) &= 0 \end{cases}$$

Remark 1.1. Here are some remarks about the solution:

- [1] If $\sigma > 0$ then u(x,t) decays with time (proper heat equation) and if $\sigma < 0$ then u(x,t) grows with time (inverse or backwards heat equation). For this course, we always assume that $\sigma > 0$.
- [2] The larger the σ , the faster the decay with respect to time. We call σ the **diffusion coefficient**.
- [3] The larger the k, the faster the decay \implies high frequencies decay faster.

2 Finite Difference Methods

Recall that

$$u_x := \lim_{\Delta x \to 0} \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x}$$

$$\Delta^+ u := \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x}$$

$$\Delta^- u := \frac{u(x, t) - u(x - \Delta x, t)}{\Delta x}$$

 $^{^{1}}x = \alpha$ is called inflow while $x = \beta$ is called outflow.

where we call the last two the **1st forward difference** and **1st backward difference** respectively. By convention, $\Delta x > 0$ and $\Delta t > 0$. Note that Δx is finite which is where the name "finite difference" comes from. u_x will be approximated by $\Delta^+ u$ or $\Delta^- u$. Similarly,

$$u_t \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t}$$

We then introduce a discretization of space where

$$\Delta x_j = x_{j+1} - x_j$$

$$\Delta t_n = t_{n+1} - t_n$$

For simplicity, assume uniform discretization. That is, $\Delta x_j = \Delta x, \Delta t_n = \Delta t$ for all j and t. In general $\Delta x \neq \Delta t$. We will use the notation

$$(x_j, t_n) \equiv (j, n)$$

 $u_j^n \equiv u(x_j, t_n)$

Finally, we denote the numerical solution as $U_i^n \approx u_i^n$. Now recall the Taylor series expansion of u about (x_j, t_n) in x:

$$u(x_{j} + \Delta x, t_{n}) = u(x_{j}, t_{n}) + \Delta x u_{x}(x_{j}, t_{n}) + \frac{\Delta x^{2}}{2} u_{xx}(x_{j}, t_{n}) + \dots$$
$$u(x_{j} - \Delta x, t_{n}) = u(x_{j}, t_{n}) - \Delta x u_{x}(x_{j}, t_{n}) + \frac{\Delta x^{2}}{2} u_{xx}(x_{j}, t_{n}) - \dots$$

or more compactly,

$$u_{j+1}^{n} = u_{j}^{n} + \Delta x (u_{x})_{j}^{n} + \frac{\Delta x^{2}}{2} (u_{xx})_{j}^{n} + \dots$$

$$u_{j-1}^{n} = u_{j}^{n} - \Delta x (u_{x})_{j}^{n} + \frac{\Delta x^{2}}{2} (u_{xx})_{j}^{n} - \dots$$

If we solve for $(u_x)_i^n$ in the first equation, then we get

$$(u_x)_j^n = \frac{u_{j+1}^n - u_j^n}{\Delta x} - \frac{\Delta x}{2} (u_{xx})_{j+\xi}^n, 0 < \xi < 1$$

by the mean value theorem. We call $\tau_j^n = -\frac{\Delta x}{2}(u_{xx})_{j+\xi}^n$ the **discretization (truncation) error**. Similarly from the second equation,

$$(u_x)_j^n = \frac{u_{j+1}^n - u_j^n}{\Delta x} + \frac{\Delta x}{2} (u_{xx})_{j-\xi}^n, 0 < \xi < 1$$

If we subtract the two equations together, then

$$(u_x)_j^n = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} \underbrace{-\frac{1}{6}(u_{xxx})_{j+\xi}^n \Delta x^2}_{\tau_i^n}, 0 < \xi < 1$$

We call the first term on the right side the **1st central difference**. Central difference is more accurate than forward and backward difference. More accuracy is achievable with more points x_{j+2}, x_{j+3} . Adding the two equations will give us

$$(u_{xx})_j^n = \frac{u_{j+1} - 2u_j^n + u_{j-1}^n}{\Delta x^2} - \frac{\Delta x^2}{12} (u_{xxxx})_{j+\eta}^n, 0 < \eta < 1$$

In general, higher derivatives and more accurate approximations require more points (i.e. larger stencil).

Using big-O notation, we can write:

$$(u_x)_j^n = \frac{u_{j+1}^n - u_j^n}{\Delta x} + O(\Delta x)$$

$$(u_t)_j^n = \frac{u_j^{n+1} - u_j^n}{\Delta t} + O(\Delta t)$$

$$(u_{xx})_j^n = \frac{u_{j+1} - 2u_j^n + u_{j-1}^n}{\Delta x^2} + O(\Delta x^2)$$

Example 2.1. Let's construct a finite difference (FD) scheme for the heat equation:

$$u_t = \sigma u_{xx}, -\infty < x < \infty$$

$$u(x,0) = \phi(x)$$

We have

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \sigma \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} \implies u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$

where $r = \sigma \Delta t/\Delta x^2$. If we know u_j^n for all j then we can compute u_j^{n+1} for all j. We need u_j^0 so we set $u_j^0 = u(x_j, 0) = \phi(x_j)$ for all j.

Let's plug in some values. Suppose that $\sigma=1$ and choose the I.C. such that $u_0^0=1, u_j^0=0, \forall j\neq 0$ and $\Delta x=1, \Delta t=1/4 \implies r=4$. This gives us

$$u_j^{n+1} = 4u_{j-1}^n - 7u_j^n + 4u_{j+1}^n$$

From stability analysis (CS 476), you will see that:

- 1. u_i^n grows
- 2. u_j^n oscillates (+ve, -ve, +ve, -ve, ...)

Instead, let's try: $\Delta x = 1/4$, $\Delta t = 1/64 \implies r = 1/4$ with:

$$u_j^{n+1} = \frac{1}{4}u_{j-1}^n + \frac{1}{2}u_j^n + \frac{1}{4}u_{j+1}^n$$

This will provide reasonable results. In general, we want u_0^n to be a good approximation of u_i^n .

Definition 2.1. A scheme is **convergent** on $0 < t \le T$ if

$$||u^n - U^n|| \to 0$$

as $\Delta x \to 0, \Delta t \to 0, n \to \infty, n\Delta t \le T$. Here, $\|\cdot\|$ is some norm with u^n as a vector of all the (u^n_j) 's. A scheme is **convergent** of order k if

$$||u^n - U^n|| = O(\Delta x^k)$$

Fact 2.1. Convergence is difficult to prove directly. Instead, we look at:

- Stability
- Convergence

Going back to our last example, consider $||u||_{\infty} = \max_{j} |u_{j}|$. From the general equation

$$|u_j^{n+1}| \le |r||u_{j-1}^n| + |1 - 2r||u_j^n| + |r||u_{j+1}^n|$$

 $\le (|r| + |1 - 2r| + |r|)||u^n||_{\infty}$

If $0 < r < \frac{1}{2}$ then $|u_j^{n+1}| \le \|u^n\|_{\infty}, \forall j \implies \|u^{n+1}\| \le \|u^n\|_{\infty}$. If $r > \frac{1}{2}$, then

$$|r| + |1 - 2r| + |r| = 2r - 1 + 2r = 4r - 1 \ge 1$$

and hence

$$|u_i^{n+1}| \le (4r-1)||u^n||_{\infty}$$

Definition 2.2. A scheme is **stable** if $\exists C > 0$ **independent** of $\Delta x, \Delta t, u^0$ such that

$$||u^n|| \le C||u^0||, \Delta x \to 0, \Delta t \to 0, n \to \infty, n\Delta t \le T$$

Note 1. (1) We allow some growth in the solution. Don't confuse this definition of stability with stability in ODE theory.

(2) Scheme is usually stable only for fixed values of some parameters. For example, Δt as a function of Δx or r.

In our example above, we showed that it was a stable scheme for the heat equation when $r < \frac{1}{2}$.

Definition 2.3. Alternatively, if u^n, v^n are solutions with $u^0 = \phi, v^0 = \psi$ (same problem, different I.C.), then a scheme is stable if $\exists C > 0$ independent of $\Delta x, \Delta t, u^0$ such that

$$||u^n - v^n|| \le C||u^0 - v^0||, \Delta x \to 0, \Delta t \to 0, n \to \infty, n\Delta t \le T$$

Example 2.2. Going back to heat equation, suppose we choose I.C.

$$u^0 = (..., -1, 1, -1, 1, ...) \implies u_i^0 = (-1)^{\gamma}$$

and hence

$$u_j^1 = 2r(-1)^{j+1} + (1-2r)(-1)^{\gamma}$$

$$= (-1)^{\gamma}(-2r+1-2r)$$

$$= -(4r-1)(-1)^{\gamma}$$

$$u_j^n = (-1)^{\gamma+1}(4r-1)^n$$

Taking norms, we have

$$||u^n||_{\infty} = (4r-1)^n ||u^0||_{\infty} = (4r-1)^n$$

We call this **exponential growth** in the case of $r > \frac{1}{2}$. As $\Delta x, \Delta t \to 0$ with fixed T and $n \to \infty$, we have

$$||u^n||_{\infty} \to \infty$$

So with $r > \frac{1}{2}$, the results are **unstable**.

Remark 2.1. Stability for numerical methods is equivalent to well-posedness for PDEs:

- Solution exists given suitable I.C. and B.C.
- Solution is unique
- Solution is continuously independent on initial data

2.1 Consistency

We now change our notation so that U^n is the finite difference estimate and u^n is the exact solution. We want to know how much u(x,t) satisfies the below equation

(2)
$$\frac{U_j^{n+1} - U_n^n}{\Delta t} = \sigma \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{\Delta x^2}$$

which is a discretization of the heat equation. Note that u(x,t) only exactly solves

(1)
$$u_t = \sigma u_{xx}$$

Define

$$P(v) = \frac{v_j^{n+1} - v_n^n}{\Delta t} - \sigma \frac{v_{j+1}^n - 2v_j^n + v_{j-1}^n}{\Delta x^2}$$

We have $P(U^n) = 0$. Define $\tau_j^n \equiv P(u)$ where u = u(x,t). We call τ_j^n the **truncation or discretization error**. Plug u(x,t) into (2) to get

$$\tau_{j}^{n} = \frac{u_{j}^{n} + \Delta t(u_{t})_{j}^{n} + \frac{\Delta t^{2}}{2}(u_{tt})_{j}^{n} + O(\Delta t^{3}) - u_{j}^{n}}{\Delta t} - \sigma \frac{u_{j}^{n} + \Delta x(u_{x})_{j} + \frac{\Delta x^{2}}{2}(u_{xx})_{j}^{n} + \frac{\Delta x^{3}}{6}(u_{xxx})_{j}^{n} + \frac{\Delta x^{4}}{24}(u_{xxxx})_{j}^{n} + O(\Delta x^{5})}{\Delta x^{2}} - \sigma \frac{-2u_{j}^{n} + \left(u_{j}^{n} - \Delta x(u_{x})_{j} + \frac{\Delta x^{2}}{2}(u_{xx})_{j}^{n} - \frac{\Delta x^{3}}{6}(u_{xxx})_{j}^{n} + \frac{\Delta x^{4}}{24}(u_{xxxx})_{j}^{n} + O(\Delta x^{5})\right)}{\Delta x^{2}}$$

This can be reduced to

$$\tau_{j}^{n} = \underbrace{(u_{t})_{j}^{n} - \sigma(u_{xx})_{j}^{n}}_{=0} + \frac{\Delta t}{2} (u_{tt})_{j}^{n} - \sigma \frac{\Delta x^{2}}{12} (u_{xxxx})_{j}^{n} + O(\Delta t^{2})$$

$$= \underbrace{\frac{\Delta t}{2} (u_{tt})_{j+\xi}^{n} - \sigma \frac{\Delta x^{2}}{12} (u_{xxxx})_{j+\eta}^{n}}_{=0}$$

Suppose that the function u(x,t) is smooth enough such that there exists M with the property $|u_{tt}|, |u_{xxxx}| \leq M$. We then get

$$|\tau_j^n| \le M\left(\frac{\Delta t}{2} + \frac{\Delta x^2}{12}\right)$$

and hence $(\tau_i^n) = O(\Delta t, \Delta x^2)$. Since we need $r < \frac{1}{2}$ for stability, we have

$$\sigma \frac{\Delta t}{\Delta x^2} < \frac{1}{2} \implies \Delta t < \frac{\Delta x^2}{2\sigma} \implies (\tau_j^n) = O(\Delta x^2) \text{ if } r < \frac{1}{2}$$

Definition 2.4. A scheme is called **consistent** if $\tau_j^n \to 0$ as $\Delta x \to 0, \Delta t \to 0$. A scheme is called **consistent of order** k in Δx and m in Δt if

$$\tau_j^n = O(\Delta x^k, \Delta t^m)$$

Remark 2.2. Regarding the truncation error:

- 1. τ_i^n measures how far (2) is from (1)
- 2. τ_j^n is a purely analytical tool. Don't try to find it in your code!
- 3. τ_j^n is easy to compute \implies the reason it is used
- 4. For many schemes (all ours) if $\tau_i^n = O(\Delta x^k, \Delta t^m)$ then

$$||e^n|| = ||u^n - U^n|| = O(\Delta x^k, \Delta t^m)$$

Note 2. We note that

$$\begin{cases} U_j^{n+1} &= rU_{j-1}^n + (1-2r)U_j^n + rU_{j+1}^n \\ u_i^{n+1} &= ru_{j-1}^n + (1-2r)u_j^n + ru_{j+1}^n + \Delta\tau_j^n \Delta t \end{cases}$$

and hence

$$\begin{array}{rcl} e_{j}^{n+1} & = & re_{j-1}^{n} + (1-2r)e_{j}^{n} + re_{j+1}^{n} + \tau_{j}^{n} \Delta t \\ |e_{j}^{n+1}| & \leq & (|r| + |1-2r| + |r|) \|e^{n}\| + \Delta t \|\tau^{n}\| \end{array}$$

and $r < \frac{1}{2}$ gives us

$$\begin{aligned} \|e^{n+1}\| & \leq & \|e^n\| + \Delta t \|\tau^n\| \\ & \leq & \|e^{n-1}\| + \Delta t (\|\tau^n\| + \|\tau^{n-1}\|) \\ & \leq & \|e^0\| + \Delta t \sum_{k=1}^n \|\tau^k\| \end{aligned}$$

Since $||e^0|| = 0$ because $U_j^0 = u_j^0$ if we let $\tau = \max ||\tau^k||$, then

$$||e^{n+1}|| \le \Delta t \sum_{k=1}^{n} \tau = \Delta t \cdot n \cdot \tau = t_n \cdot \tau$$

and hence

$$||e^{n+1}|| = ||u^n - U^n|| \le \underbrace{t_n}_{\text{finite}} \cdot C(\Delta x^2 + \Delta t) \le \bar{C}\Delta x^2$$

for some constants C, \bar{C} . We should expect quadratic convergence on smooth solutions of (1) using (2).

Remark 2.3. If $\tau_j^n = 0$ then $e_j^n = 0$ and hence if u(x,t) is linear in time and cubic in space, then (2) solves (1) exactly.

Recall

- 1. Stability doesn't grow with time uncontrollably
- 2. Consistency gives the convergence (and its rate)
- 3. Convergence is good

Theorem 2.1. (Lax Equivalence Theorem) We have

The forward direction is easy to prove, while the reverse direction is difficult to prove. This is true for most (and of all of our) methods.

2.2 Convergence in Practice and Error Estimation

From the previous section, we saw that

$$\|e_j^n\| \sim C \Delta x^2 \implies \|e_j^n\| = O(\Delta x^2)$$

Suppose we have two meshes with Δx and $\frac{\Delta x}{2}$ and we know that in general $e_i^n = O(\Delta x^k)$. We then have

$$\begin{cases} \|e_{\Delta x}^n\| & \sim C_1 \Delta x^k \\ \|e_{\Delta x}^n\| & \sim C_2 \left(\frac{\Delta x}{2}\right)^k \implies \frac{\|e_{\Delta x}^n\|}{\|e_{\Delta x}^n\|} \sim \frac{C_1 \Delta x^k}{C_2 \left(\frac{\Delta x}{2}\right)^k} \implies \log_2 \frac{\|e_{\Delta x}^n\|}{\|e_{\Delta x}^n\|} \sim k, \ (C_1 \approx C_2) \end{cases}$$

Convergence Tests when u(x,t) is not known

Suppose that we have three solutions $\{U_{\Delta x}, U_{\Delta x/2}, U_{\Delta x/4}\}$ which are methods of order k.

- 1. Pick a very fine mesh, say $\Delta x/64$ (arbitrary) and view if as an exact solution.
- 2. Consider

$$\log_2 \frac{\|U_{\Delta x} - U_{\Delta x/2}\|}{\|U_{\Delta x/2} - U_{\Delta x/4}\|} \le \log_2 \frac{\|U_{\Delta x} - u\| + \|u - U_{\Delta x/2}\|}{\|U_{\Delta x/2} - u\| + \|u - U_{\Delta x/4}\|} \sim \log_2 \frac{C_1 \Delta x^k + C_2 \left(\frac{\Delta x}{2}\right)^k}{C_2 \left(\frac{\Delta x}{2}\right)^k + C_3 \left(\frac{\Delta x}{4}\right)^k}$$

and simplifying with $C = C_1 \sim C_2 \sim C_3$, we we get

$$\log_2 \frac{C_1 \Delta x^k + C_2 \left(\frac{\Delta x}{2}\right)^k}{C_2 \left(\frac{\Delta x}{2}\right)^k + C_3 \left(\frac{\Delta x}{4}\right)^k} \sim \log_2 2^k = k$$

Richardson Extrapolation (Error Estimation)

Suppose we have two solutions $U_{\Delta x}^n, U_{\Delta x/2}^n$. Then,

$$U_{\Delta x}^n - U_{\Delta x/2}^n = \left(U_{\Delta x}^n - u^n\right) + \left(u_n - U_{\Delta x/2}^n\right) \approx c_1 \Delta x^k - c_2 \left(\frac{\Delta x}{2}\right)^k \approx C\left(1 - \frac{1}{2^k}\right) \Delta x^k$$

The error of the Δx grid is $e^n_{\Delta x} \approx C \Delta x^k$ and hence

$$e_{\Delta x}^n \sim C\Delta x^k \approx \frac{U_{\Delta x}^n - U_{\Delta x/2}^n}{1 - \frac{1}{2k}}$$

Similarly for the $\Delta x/2$ grid, we have $e^n_{\Delta x/2} \approx C \left(\frac{\Delta x}{2}\right)^k$ and hence

$$\frac{U_{\Delta x/2}^{n} - U_{\Delta x/4}^{n}}{2^{k} \left(1 - \frac{1}{2^{k}}\right)} = \frac{U_{\Delta x/2}^{n} - U_{\Delta x/4}^{n}}{2^{k} - 1} \sim e_{\Delta x/2}^{n}$$

So $e_{\Delta x}$ is more reliable than $e_{\Delta x/2}$ but $e_{\Delta x/2}$ is an estimate for a better solution.

3 Von-Neumann Stability Analysis

This is a general tool applicable to schemes other than finite difference methods.

Review. Recall Euler's formula

$$e^{\beta i} = \cos \beta + i \sin \beta \implies \cos \beta = \frac{1}{2} (e^{\beta i} - e^{-\beta i}), \sin \beta = \frac{i}{2} (e^{-\beta i} - e^{\beta i})$$

Given

$$g(t) = e^{(\alpha + i\beta)} = e^{\alpha t} (\cos \beta t + i \sin \beta t)$$

we have that α is responsible for the growth in g(t) w.r.t. (with respect to) time and β is the frequency.

Review. Suppose that f(x) is on $[-\pi, \pi]$. Then the **Fourier series** (F.S.) of f(x) is

$$f(x) \sim \frac{a_0}{2} + \sum_{k=1}^{\infty} (a_k \cos kx + b_k \sin kx)$$

Theorem 3.1. If f(x) is periodic and C^1 then the Fourier series of f(x) converges to f(x) in the infinity and L_2 norms.

Consider the exponential for the F.S. using Euler's formula as a substitution:

$$f(x) \sim \frac{a_0}{2} + \sum_{k=1}^{\infty} \frac{a_k}{2} (e^{kxi} + e^{-kxi}) + \sum_{k=1}^{\infty} \frac{ib_k}{2} (e^{-kxi} - e^{kxi})$$

$$= \frac{a_0}{2} + \sum_{k=1}^{\infty} \frac{1}{2} (a_k - ib_k) e^{kxi} + \sum_{k=1}^{\infty} \frac{1}{2} (a_k + ib_k) e^{-kxi}$$

$$= \sum_{k=-\infty}^{\infty} c_k e^{kxi}$$

It is easy to show that $c_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-kxi}$. In the discrete version, we first choose a function $[-\pi,\pi] \mapsto [0,J]$ using

$$x(\xi) = \frac{2\pi}{J}\xi - \pi$$

Then

$$e^{kxi} = e^{\frac{2\pi\xi k}{J}i}e^{-\pi ki} = (-1)^k e^{\frac{2\pi k}{J}\xi i}$$

If we substitute this into the exponential form, then we get the F.S. on [0, J]:

$$f(\xi) \sim \sum_{k=-\infty}^{\infty} c_k (-1)^k e^{\frac{2\pi k}{J}\xi i} = \sum_{k=-\infty}^{\infty} \hat{c}_k e^{\frac{2\pi k}{J}\xi i}, \hat{c}_k = c_k (-1)^k$$

Now U_i^n is a discrete function defined at $x = x_j, j \in [0, J], \xi = \delta$. We claim that

(*)
$$U_j = \sum_{k=0}^{J-1} A_k e^{\frac{2\pi k}{J} ji}$$

where we will call A_k the **discrete Fourier coefficients**. For the justification of (*), remark that:

1. The summation should be finite (stops at k = J - 1) because

$$e^{\frac{2\pi J}{J}ji} = e^{2\pi ji} = e^{0ji} = 1$$

Similar reasoning can be applied for any k = J + s, 0 < s < J.

2. If we rewrite (*) for U_j^n , then

$$(**) U_j^n = \sum_{k=0}^{J-1} A_k^n w_j^k, w_j^k = e^{\frac{2\pi j}{J}i}$$

where A_k^n is time-indexed with a superscript and w_j^k is of degree k (power k).

3. (Orthogonality relation) Note that

$$\sum_{j=0}^{J-1} w_j^k \bar{w}_j^m = \begin{cases} J & k \equiv m \mod J \\ 0 & \text{otherwise} \end{cases}$$

Multiply (**) by \bar{w}_j^m and sum over j (m is fixed) to get

$$\sum_{j=0}^{J-1} U_j^n \bar{w}_j^m = \sum_{j=0}^{J-1} \sum_{k=0}^{J-1} A_k^n w_j^k \bar{w}_j^m = \sum_{j=0}^{J-1} A_k^n \sum_{k=0}^{J-1} w_j^k \bar{w}_j^m = J A_m^n$$

and hence

$$A_m^n = \frac{1}{J} \sum_{i=0}^{J-1} U_j^n \bar{w}_j^m$$

4. (Discrete Parseval's Relation) It follows from above that

$$||U^n||_2^2 = J||A^n||_2^2$$

which follows from orthogonality. Compare this with the continuous case (very similar).

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Appendix

How to Check your Code

1. Manufacture a problem for which you know the exact solution and which you should be able to solve exactly.

(a) In the heat equation, we could try u(x,t) = 1 with I.C. u(x,0) = 1 and B.C. u(1,t) = 1, u(0,t) = 1.