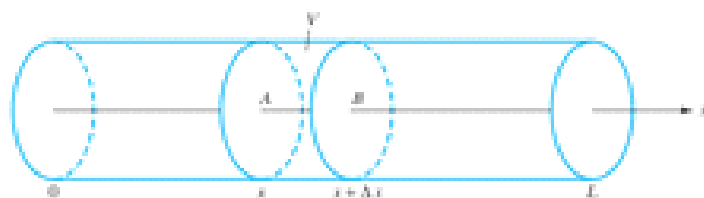


Nuevos métodos matemáticos y computacionales para las ciencias y la ingeniería

Oscar P. Bruno, Caltech

Warm-up and review. Separation of variables.

Simplest example: One-dimensional heat equation



$$\begin{cases} u_t(x,t) = \beta u_{xx}(x,t), & 0 < x < L, t > 0, \\ u(0,t) = u(L,t) = 0, & t > 0, \\ u(x,0) = f(x), & 0 < x < L. \end{cases}$$

Separation of variables

$$u(x,t) = X(x)T(t)$$

$$u_t = X(x)T'(t), \quad u_{xx} = X''(x)T(t)$$

$$\implies X(x)T'(t) = \beta X''(x)T(t), \text{ or}$$

$$\frac{T'(t)}{\beta T(t)} = \frac{X''(x)}{X(x)} = -\lambda$$

$$\rightarrow X'' = -\lambda X \quad \text{and} \quad T' = -\lambda \rho T$$

From the PDE boundary conditions we have

$$X(0) = X(L) = 0$$

Case $\lambda < 0$: General solution X is

$$X(x) = C_1 e^{\sqrt{-\lambda} \cdot x} + C_2 e^{-\sqrt{-\lambda} \cdot x}$$

Boundary conditions $\rightarrow C_1 = C_2 = 0 \rightarrow X = 0$

Case $\lambda = 0$: General solution X is

$$X(x) = C_1 + C_2 x$$

Boundary conditions $\rightarrow C_1 = C_2 = 0 \rightarrow X = 0$

Case $\lambda > 0$: General solution X is

$$X(x) = C_1 \cos(\sqrt{\lambda} x) + C_2 \sin(\sqrt{\lambda} x)$$

The boundary conditions now tell us that

$$C_1 = 0 \quad \text{and} \quad C_2 \sin(\sqrt{\lambda} L) = 0$$

$$\rightarrow \sqrt{\lambda} L = n\pi, \text{ or } \lambda = \left(\frac{n\pi}{L}\right)^2 \quad n \in \mathbb{N}$$

$$X = X_n(x) = a_n \sin\left(\frac{n\pi x}{L}\right)$$

and

$$T = T_n(t) = b_n e^{-\beta\left(\frac{n\pi}{L}\right)^2 t}$$

\rightarrow we have a PDE solution

$$u_n(x, t) = X_n(x) T_n(t) = c_n e^{-\beta\left(\frac{n\pi}{L}\right)^2 t} \sin\left(\frac{n\pi x}{L}\right)$$

This is a solution with initial condition function

$$f(x) = \sin\left(\frac{n\pi x}{L}\right) \quad (n=1, 2, \dots)$$

How about other functions f ?

We can easily obtain solutions for linear combinations

such as

$$f(x) = 3 \sin\left(\frac{\pi x}{L}\right) + 2 \sin\left(\frac{4\pi x}{L}\right)$$

→

$$u(x, t) = 3 e^{-\beta\left(\frac{\pi}{L}\right)^2 t} \sin\left(\frac{\pi x}{L}\right) + 2 e^{-\beta\left(\frac{4\pi}{L}\right)^2 t} \sin\left(\frac{4\pi x}{L}\right)$$

What is the most general function f we can

obtain in this manner?

ANS: "All" functions! (using, in general,

infinite sums):

$$f(x) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L}\right)$$

- Does this mean that, necessarily $f(0) = f(L) = 0$?
- How about cosines? How does the series converge?
- Can we differentiate the series termwise?
- How come we can do this for all f ?
- Can we do this for other equations? (Simplest example $\beta = \beta(x)$.) Higher dimensions?
- General domains?



Many important questions!

We will address these questions, and we will exploit the resulting answers to great effect — both theoretically and as a basis of powerful numerical methods.

Convergence of trigonometric Fourier Series

Guiding fact concerning the trigonometric functions in their periodicity interval: orthogonality

For example, assuming a periodicity interval of length 2π , the relevant trigonometric functions

are

$$1, \cos(x), \sin(x), \cos(2x), \sin(2x), \dots$$

They are pairwise orthogonal in any interval of

length 2π (we use $[-\pi, \pi]$); e.g.

$$\int_{-\pi}^{\pi} \cos(mx) \sin(nx) dx = 0,$$

$$\int_{-\pi}^{\pi} \cos(mx) \cos(nx) dx = 0 \quad (m \neq n)$$

etc.

Also

$$\int_{-\pi}^{\pi} 1^2 dx = 2\pi, \quad \int_{-\pi}^{\pi} \cos^2(nx) dx = \int_{-\pi}^{\pi} \sin^2(nx) dx = \pi$$

$n = 1, 2, \dots$

Orthogonality allows us to evaluate the necessary

coefficients easily (at least formally):

$$f(x) \sim \frac{1}{2} a_0 + a_1 \cos(x) + b_1 \sin(x) +$$

$$a_2 \cos(2x) + b_2 \sin(2x) + \dots =$$

$$= \frac{1}{2} a_0 + \sum_{n=1}^{\infty} (a_n \cos(nx) + b_n \sin(nx))$$

↪

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \cos(nt) dt, \quad b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \sin(nt) dt$$

$n = 0, 1, 2, \dots$

Convergence? To study this we proceed as follows.

The partial sum S_N is given by

$$\begin{aligned} S_N(x) &= \frac{1}{2}a_0 + \sum_{n=1}^N (a_n \cos(nx) + b_n \sin(nx)) = \\ &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \left\{ \frac{1}{2} + \sum_{n=1}^N (\cos(nx) \cos(nt) + \sin(nx) \sin(nt)) \right\} dt \\ &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \left\{ \frac{1}{2} + \sum_{n=1}^N \cos[n(x-t)] \right\} dt. \end{aligned}$$

The sum can be evaluated explicitly:

$$\begin{aligned}
 & \left\{ \frac{1}{2} + \sum_{n=1}^N \cos[n\gamma] \right\} \cdot \sin\left(\frac{1}{2}\gamma\right) = \\
 & = \frac{1}{2} \left\{ \sin\left(\frac{1}{2}\gamma\right) + \sum_{n=1}^N \left[\sin\left(\left(n + \frac{1}{2}\right)\gamma\right) - \sin\left(\left(n - \frac{1}{2}\right)\gamma\right) \right] \right\} \\
 & = \frac{1}{2} \sin\left(\left(N + \frac{1}{2}\right)\gamma\right) \rightarrow \\
 & \left\{ \frac{1}{2} + \sum_{n=1}^N \cos[n\gamma] \right\} = \frac{\sin\left(\left(N + \frac{1}{2}\right)\gamma\right)}{2 \cdot \sin\left(\frac{1}{2}\gamma\right)}
 \end{aligned}$$

$$\rightarrow S_N(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) \frac{\sin\left(N + \frac{1}{2}\right)(x-t)}{\sin\frac{1}{2}(x-t)} dt$$

$$\tau = t - x \rightarrow$$

$$S_N(x) = \frac{1}{2\pi} \int_{-\pi-x}^{\pi-x} f(x+\tau) \frac{\sin\left(N + \frac{1}{2}\right)\tau}{\sin\frac{1}{2}\tau} d\tau$$

The quotient of sin functions is 2π periodic.

Extending f by 2π -periodicity,

$$f(x + 2\pi n) = f(x)$$

the complete integrand becomes 2π -periodic

and we obtain

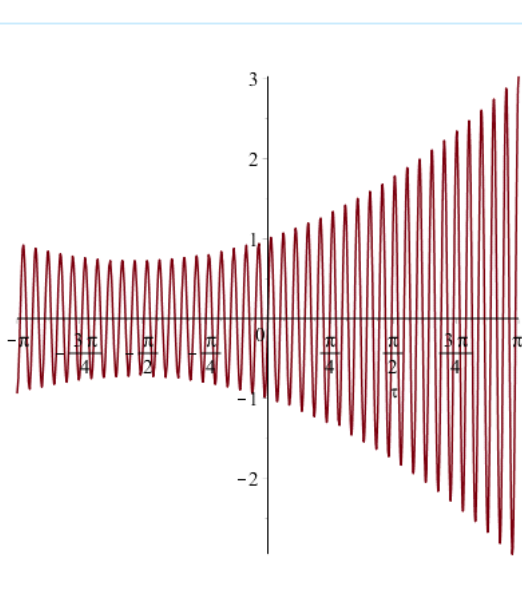
$$S_N(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x+z) \frac{\sin(N + \frac{1}{2})z}{\sin \frac{1}{2}z} dz. \quad (1)$$

Dirichlet kernel

We wish to obtain the limit of S_N as $N \rightarrow \infty$.

The integrand becomes more and more oscillatory as N grows.

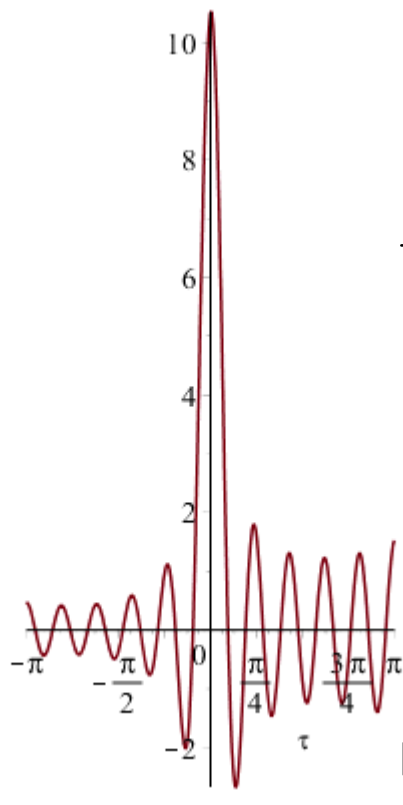
Let us look at a couple of related examples.



$$g(z) = \left(\frac{z^2}{10} + \frac{z}{3} + 1 \right) \cdot \sin\left(\left(N + \frac{1}{2}\right)z\right)$$

(No vanishing denominator.)

(N = 40)



$$\left(\frac{z^2}{10} + \frac{z}{3} + 1 \right) \cdot \frac{\sin\left(\left(N + \frac{1}{2}\right)z\right)}{2 \cdot \sin\left(\frac{1}{2}z\right)} =$$

$$= \frac{\frac{z^2}{10} + \frac{z}{3} + 1}{2 \cdot \sin\left(\frac{1}{2}z\right)} \sin\left(\left(N + \frac{1}{2}\right)z\right)$$

(Including a vanishing denominator.)

(N = 10)

In the first case the integral tends to zero, in view of cancellations. To see this we integrate

by parts:

$$\int_{-\pi}^{\pi} \overbrace{g(z) \cdot \sin\left(\left(N + \frac{1}{2}\right)z\right)}^{u'} dz = \left. \frac{\cos\left(\left(N + \frac{1}{2}\right)z\right)}{\left(N + \frac{1}{2}\right)} g(z) \right|_{z=-\pi}^{z=\pi} + \frac{1}{\left(N + \frac{1}{2}\right)} \int_{-\pi}^{\pi} \underbrace{g'(z)}_v \cdot \cos\left(\left(N + \frac{1}{2}\right)z\right) dz$$

$\xrightarrow{N \rightarrow \infty} 0$

(In fact, the Riemann Lebesgue's lemma, which we will establish later, tells us that the integral tends to zero for general functions g satisfying

$$\int_{-\pi}^{\pi} |g(z)| dz < \infty .)$$

We also see oscillations in the second function, but because of the vanishing denominator there is a peak at the origin. Note that the integrand is smooth! (The numerator vanishes too.)

But integration by parts as above \rightarrow infinite integrals.

While most oscillations may cancel each other out, the peak at the origin does not get cancelled! (Note: the width and height of the peak are $\sim \frac{1}{N}$ and N , respectively!)

We can slightly manipulate our integral (1) for $S_N(x)$ and reduce the problem to an integral determined by cancellations.

To do this we note that the representation (1) for the truncated sum

$$S_N(x) = \frac{1}{2}a_0 + \sum_{n=1}^N (a_n \cos(nx) + b_n \sin(nx))$$

is valid, in particular, for the function

$$f(x) = 1$$

(for which $S_N(x) = 1$ for all N). We thus have

$$1 = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\sin(N + \frac{1}{2})z}{\sin \frac{1}{2}z} dz, \quad (3)$$

and, therefore

$$f(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) \frac{\sin(N + \frac{1}{2})z}{\sin \frac{1}{2}z} dz \quad (2)$$

Subtracting (2) from (1) we obtain

$$S_N(x) - f(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\frac{f(x+z) - f(x)}{\sin \frac{1}{2}z} \right) \sin(N + \frac{1}{2})z dz$$

We now note that, provided f is smooth, the

factor $\frac{f(x+z) - f(x)}{\sin \frac{1}{2}z}$ is also smooth!

We can thus apply the integration by parts argument,

and we obtain $S_N(x) - f(x) \rightarrow 0$, or

$S_N(x) \rightarrow f(x)$ as desired!

We can also ensure convergence under milder assumptions.

Indeed, using the Riemann-Lebesgue lemma we see

that convergence is guaranteed **at the point x** provided

$$\int_{-\pi}^{\pi} \left| \frac{f(x+\tau) - f(x)}{\sin \frac{1}{2}\tau} \right| d\tau < \infty.$$

Since $\frac{\tau}{\sin(\frac{\tau}{2})}$ is bounded we may replace this

condition by

$$\int_{-\pi}^{\pi} \left| \frac{f(x+\tau) - f(x)}{\tau} \right| d\tau < \infty$$

This is Dini's test. If it holds for a point x

then the trigonometric expansion converges at x .

For example, if f is differentiable at x and

and

$$\int_{-\pi}^{\pi} |f(t)| dt < \infty$$

then we have convergence at the point x .

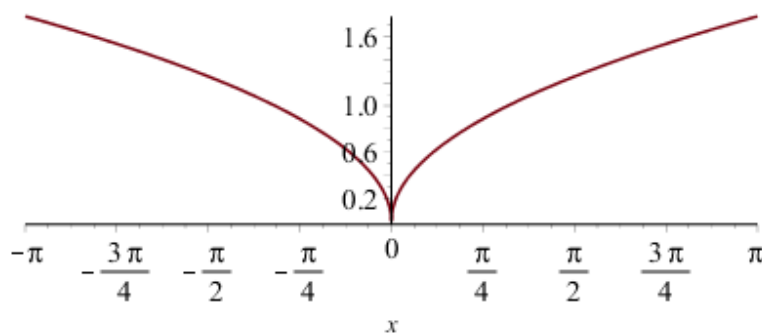
More generally, if f is Hölder α at x ,

$$|f(x) - f(y)| < M |x - y|^\alpha$$

for some α ($0 < \alpha \leq 1$) then there

is convergence at x . (Example:

$f(x) = \sqrt{|x|}$ even at $x = 0$!)



How about discontinuous f ? Say that the limits

$f(x+0)$ and $f(x-0)$ exist.

Instead of (3) (p. 14) we may also write

$$\frac{1}{2} = \frac{1}{2\pi} \int_0^{\pi} \frac{\sin(N + \frac{1}{2})z}{\sin \frac{1}{2}z} dz$$

and

$$\frac{1}{2} = \frac{1}{2\pi} \int_{-\pi}^0 \frac{\sin(N + \frac{1}{2})z}{\sin \frac{1}{2}z} dz.$$

Multiplying by $f(x+0)$ and $f(x-0)$ we

obtain

$$S_N(x) - \frac{1}{2} [f(x+0) + f(x-0)] =$$

$$= \frac{1}{2\pi} \int_{-\pi}^0 \frac{f(x+\sigma) - f(x-\sigma)}{\sin \frac{1}{2}\sigma} \sin(N + \frac{1}{2})\sigma \, d\sigma$$

$$+ \frac{1}{2\pi} \int_0^{\pi} \frac{f(x+\sigma) - f(x-\sigma)}{\sin \frac{1}{2}\sigma} \sin(N + \frac{1}{2})\sigma \, d\sigma =$$

$$= \frac{1}{2\pi} \int_0^{\pi} \frac{f(x+\sigma) - f(x-\sigma) + f(x-\sigma) - f(x+\sigma)}{\sin \frac{1}{2}\sigma} \sin(N + \frac{1}{2})\sigma \, d\sigma$$

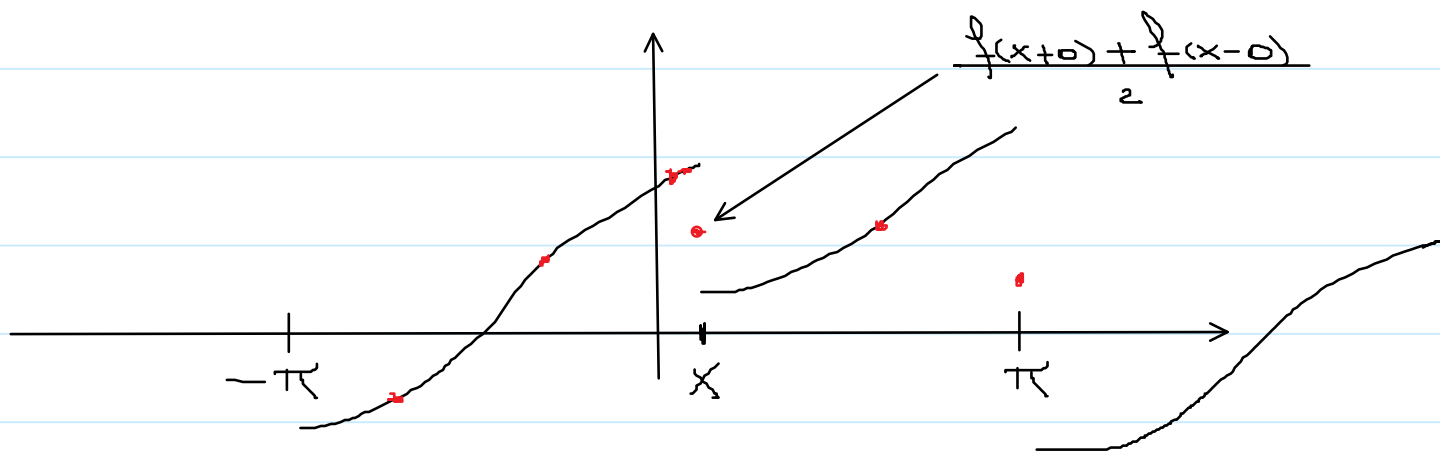
Improved version of Dini's test: if

$$\int_0^{\pi} \left| \frac{f(x+\sigma) - f(x-\sigma) + f(x-\sigma) - f(x+\sigma)}{\sigma} \right| d\sigma < \infty$$

$$\text{then } \lim_{N \rightarrow \infty} S_N(x) = \frac{f(x+0) + f(x-0)}{2}$$

The criterion is verified if

$$|f(x+\sigma) - f(x-\sigma)| < M \sigma^{\alpha} \quad \sigma \rightarrow 0_+^+ \\ (0 < \alpha \leq 1)$$



Convergence to the mid point of a discontinuity

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Gibbs Phenomenon

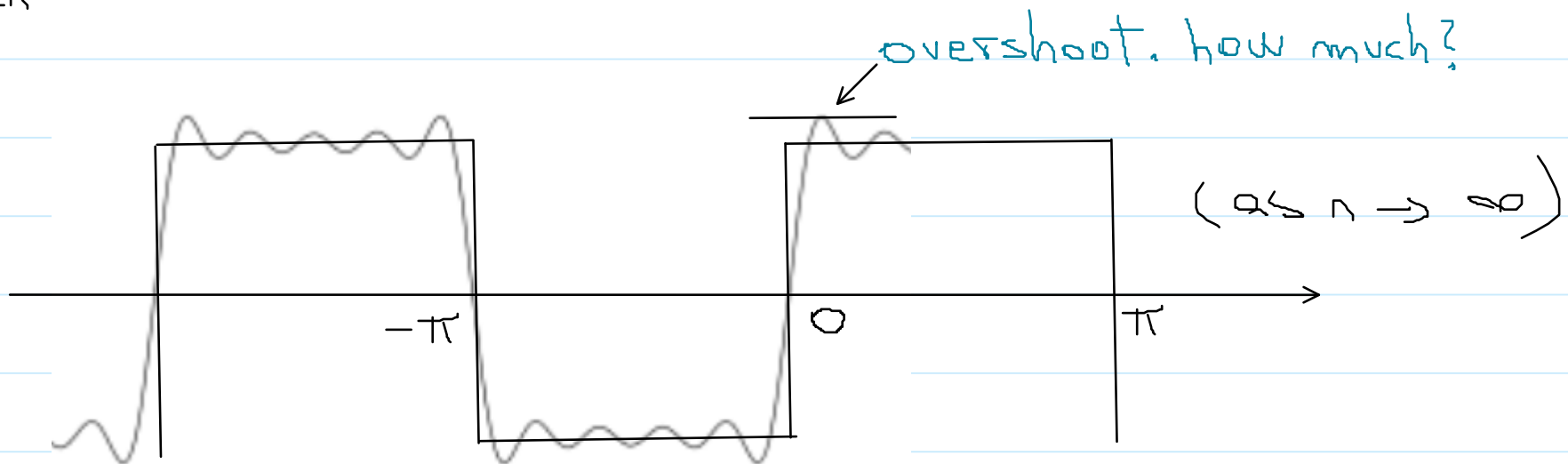
What sort of convergence results around a point of discontinuity?

To understand this we consider a particular case (from which the general case then follows, as shown in a homework problem).

$$\text{Let } f(x) = \begin{cases} -1 & -\pi \leq x < 0 \\ 1 & 0 \leq x \leq \pi \end{cases}$$

f is odd, the cosine is even \rightarrow only
sin coefficients arise (and, then, only
the odd ones):

$$S_{2n}(x) = \frac{4}{\pi} \left[\sin(x) + \frac{\sin(3x)}{3} + \dots + \frac{\sin((2n-1)x)}{2n-1} \right]$$



Let us compute the local maximum closest
to the origin:

$$0 = S'_{2n-1} =$$

$$= \frac{4}{\pi} [\cos(x) + \cos(3x) + \dots + \cos((2n-1)x)]$$

Mult. by $\sin(x)$ and using

$$\sin(x) \cos(kx) = \frac{1}{2} [\sin((k+1)x) - \sin((k-1)x)]$$

\implies

$$\pi \sin(x) S'_{2n-1}(x) = 2 \sin(2nx) = 0$$

$$\implies 2nx = \pm\pi, \pm 2\pi, \dots, \pm 2n\pi.$$

$$\implies x = \frac{\pi}{2n} \text{ is the } x\text{-coordinate of the}$$

maximum that is closest to the origin (for $x > 0$).

$$S_{2n-1} \left(\frac{\pi}{2n} \right) =$$

$$\frac{4}{\pi} \left[\sin \left(\frac{\pi}{2n} \right) + \frac{1}{3} \sin \left(\frac{3\pi}{2n} \right) + \dots + \frac{1}{2n-1} \sin \left(\frac{(2n-1)\pi}{2n} \right) \right]$$

$$\xrightarrow{n \rightarrow \infty} \frac{2}{\pi} \int_0^{\pi} \frac{\sin(x)}{x} dx \quad (b) \quad 1.18\dots$$

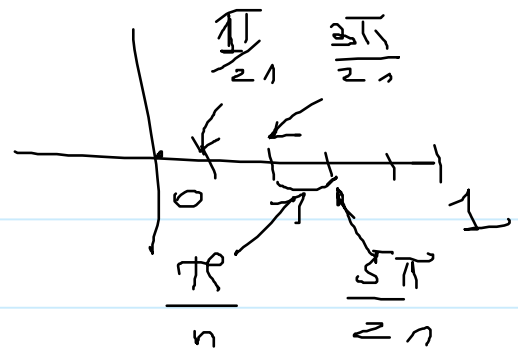
[(b) E.g., extending $\sin(x)$ in Taylor around

$x=0$ up to x^6 , the error in the integral is

★ smaller than 10^{-2} (first two digits right).]

This means that, as $n \rightarrow \infty$, the overshoot

approaches $0.18 = \underline{9\% \text{ of the jump}}$.



(a) Evaluation of sum

$$\frac{4}{\pi} \left[\sin\left(\frac{\pi}{2n}\right) + \frac{1}{3} \sin\left(\frac{3\pi}{2n}\right) + \dots + \frac{1}{2n-1} \sin\left(\frac{(2n-1)\pi}{2n}\right) \right]$$

$$= \frac{4}{\pi} \underbrace{\sum_{k=1}^n \sin\left(\frac{\pi(2k-1)}{2n}\right)}_S \cdot \frac{1}{2k-1}$$

But the sum S itself equals

$$S = \frac{1}{2} \sum_{k=1}^n \sin\left(\frac{\pi(2k-1)}{2n}\right) \cdot \frac{1}{\pi \frac{2k-1}{2n}} \cdot \frac{\pi}{n}$$

$\frac{\sin(x)}{x}$ at $x_k = \pi \frac{2k-1}{2n}$

$$\xrightarrow{n \rightarrow \infty} \frac{1}{2} \int_0^{\pi} \frac{\sin(x)}{x} dx.$$

PDE Discretization

Simplest approach to PDE discretization: finite differences

Example: let us consider the advection PDE

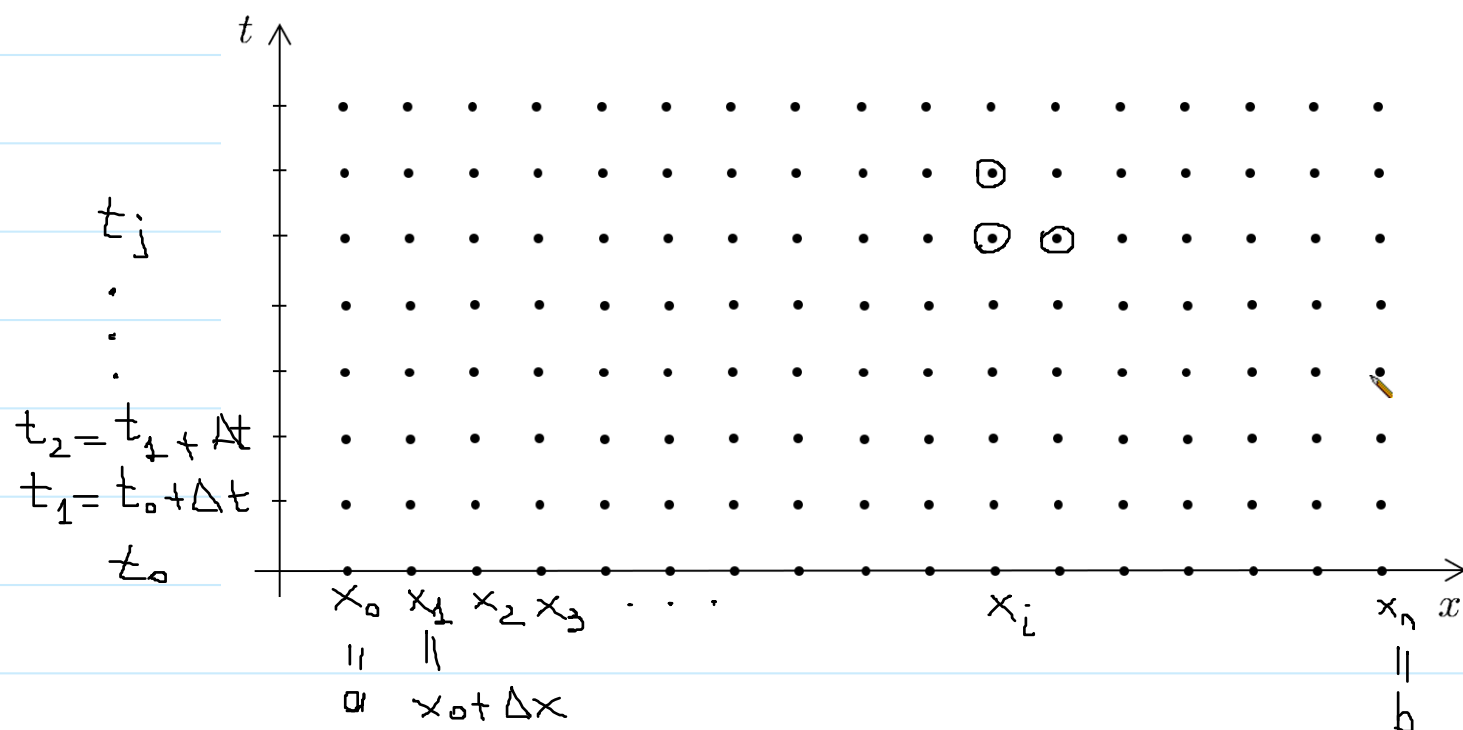
$$u_t(x,t) - u_x(x,t) = 0$$

for $a \leq x \leq b$; $t \geq t_0$

Finite difference paradigm: substitute

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

$$u_x(x,t) \sim \frac{u(x+\Delta x,t) - u(x,t)}{\Delta x}$$



Letting

$$u_{i,j} \approx u(x_i, t_j)$$

use of finite differences leads to the finite-difference

approximation

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x}$$

If we know

$$u_{i,0} = u(x_i, t_0) \quad (1 \leq i \leq n) \quad [\text{initial condition}]$$

and

$$u_{0,j} = u(x_0, t_j) \quad (j = 1, 2, \dots) \quad [\text{boundary cond.}]$$

we can obtain $u_{i,j}$ for all i, j :

$$u_{i,j+1} = u_{i,j} + \frac{\Delta t}{\Delta x} (u_{i+1,j} - u_{i,j})$$

Error? Convergence?

Let us now consider the somewhat more general

equation

$$\begin{cases} u_t + a u_x = 0 \\ u(x, 0) = f(x) \end{cases}$$

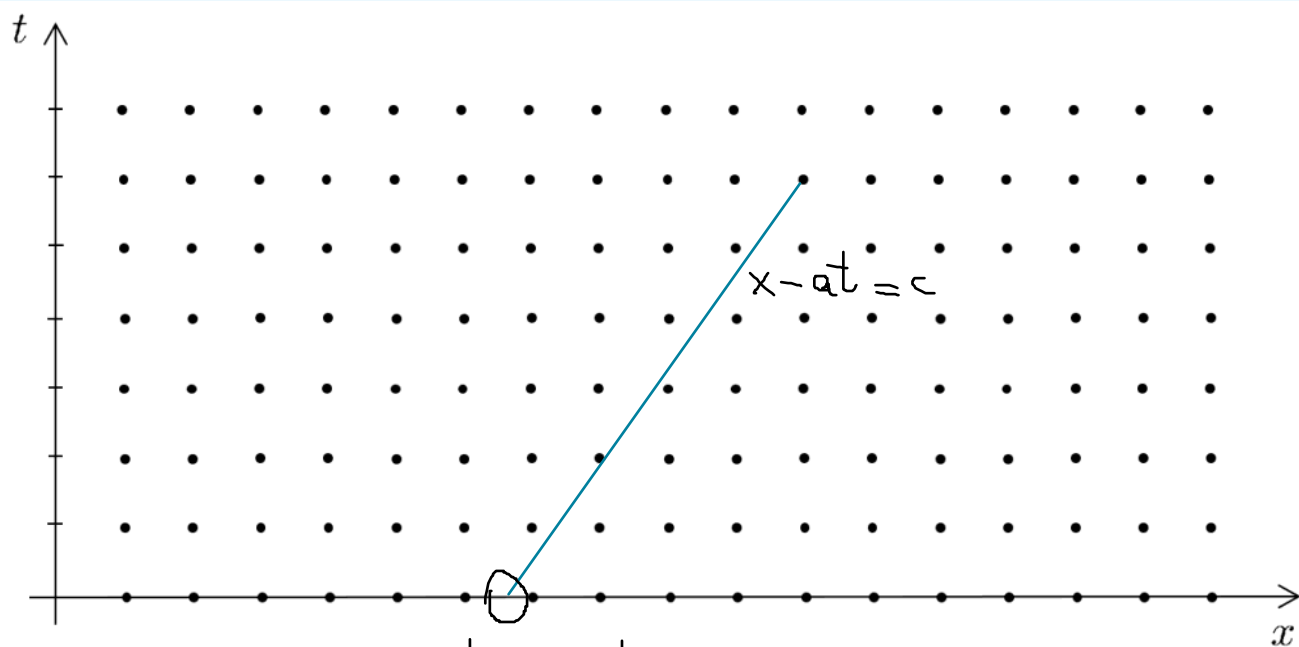
Exact solution

$$u(x,t) = f(x-at).$$

The solution is constant along the lines

$$x-at = c$$

for all c .

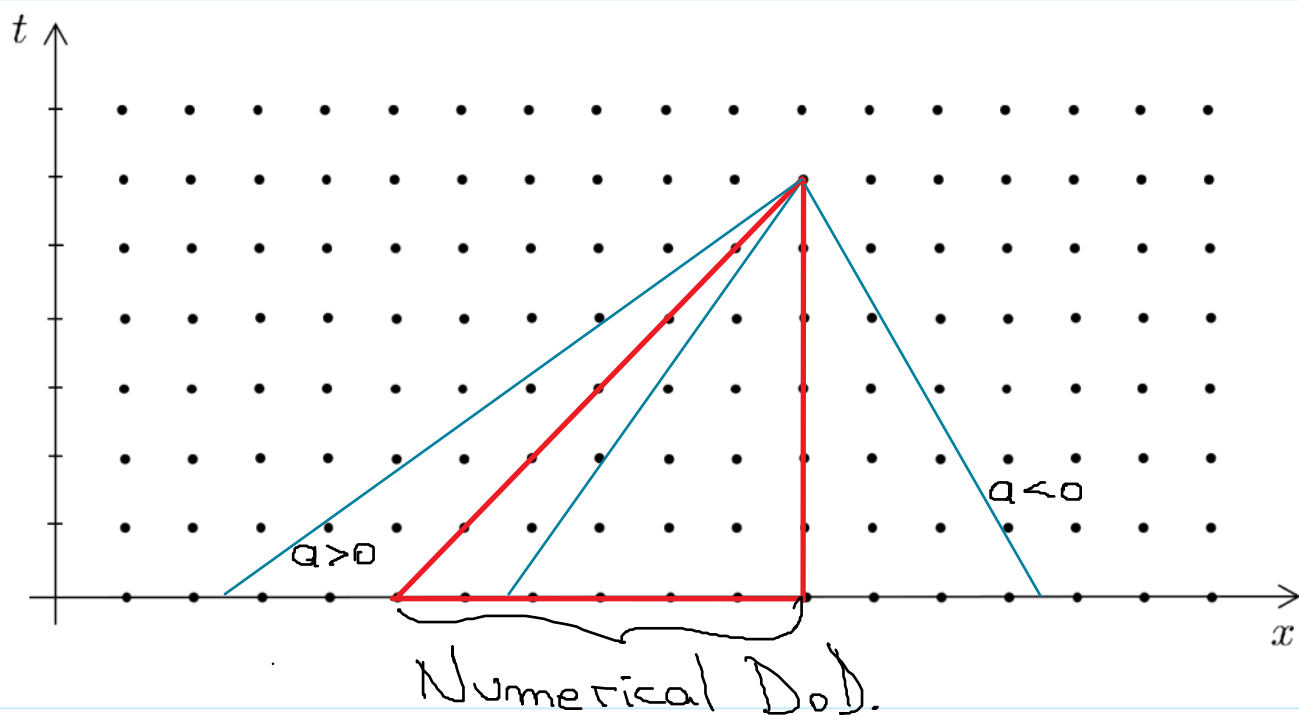


Domain of dependence

(one point, in this case, a region in the domain, for general time dependent PDE).

Numerical domain of dependence (in red).

and true PDE domain of dependence



$$\frac{u_{i,j,t+\Delta t} - u_{i,j}}{\Delta t} + a \frac{u_{i,j} - u_{i-1,j}}{\Delta x} = 0$$

(upwind, if $a > 0$)

For convergence to take place, the numerical DoD must contain the true PDE domain of dependence:

$$\text{upwind and } |a| \frac{\Delta t}{\Delta x} \leq 1.$$

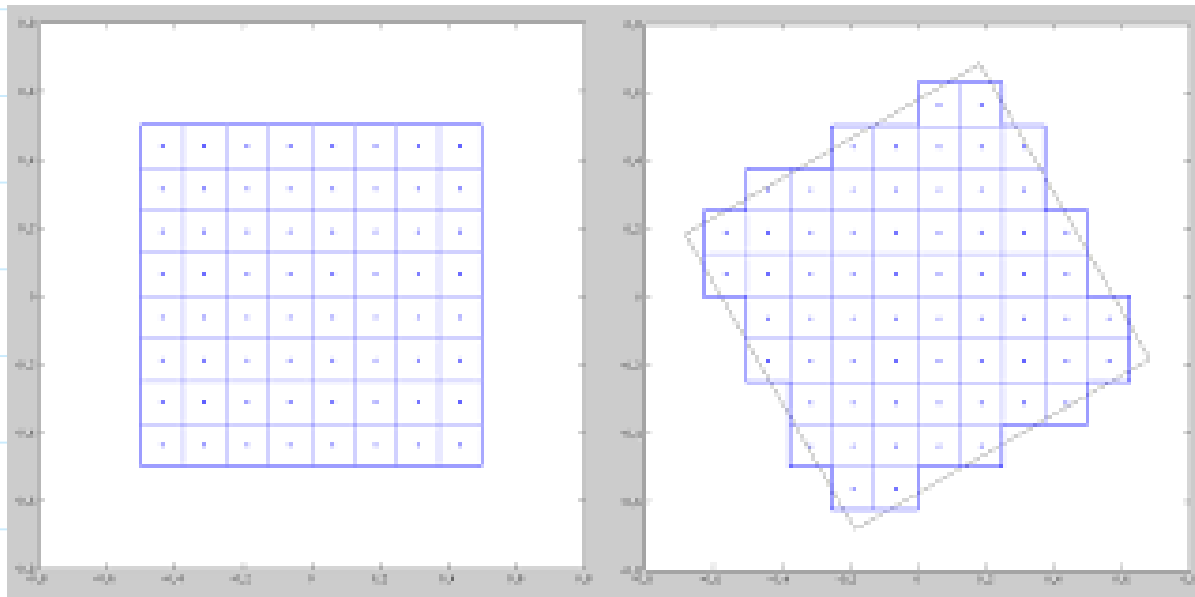
We cannot possibly expect convergence if this DoD condition is not satisfied: the numerical DoD must contain the exact DoD.

Yet, the error from one time-step to the next is (comparably) small, independently of whether the DoD condition is satisfied!

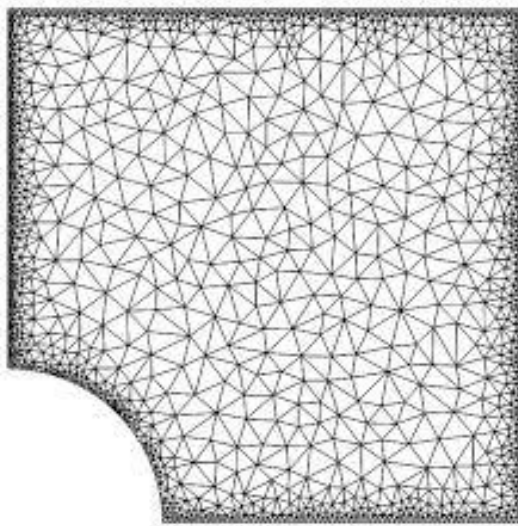
Rationale: the error factor grows without bound if the DoD condition is not satisfied.

How about higher spatial dimensions?

Eg. for a domain in two dimensions use
a two-dimensional grid



Note the "staircasing" that arises (except for a square domain). Alternative: finite element meshes



Error decay as the mesh-size tends to zero?

Issues: Accuracy, Stability and Speed.

1) Accuracy: Produce accurate derivatives from the available data.

2) Stability: how do errors accumulate?
Avoid catastrophic accumulation!

3) Speed/size: Fast numerical implementation.
Acceleration (e.g. FFT).

We will consider issues in all three categories.

We start by considering the accuracy of various finite difference differentiation strategies.

Differentiation I: finite differences
and differentiation of polynomial interpolants.

(See e.g. Leveque's text.)

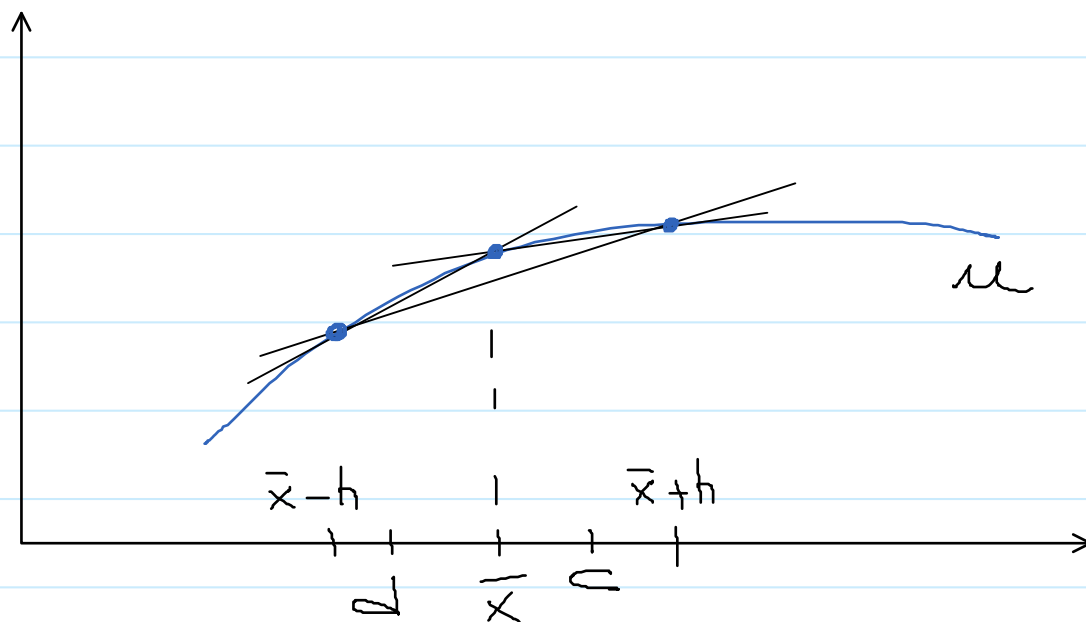
Define

$$D_+ u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x})}{h}$$

$$D_- u(\bar{x}) = \frac{u(\bar{x}) - u(\bar{x}-h)}{h}$$

$$D_0 u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h}$$

Are some of these alternatives more accurate
than the others?



How would we know?

Guiding principle:

"more accurate" \longleftrightarrow "converges faster to $u'(x)$ as $h \rightarrow 0$."

How fast do these approximations converge?

We can study this by considering Taylor expansions

around $x = \bar{x}$.

We have

$$u(\bar{x}+h) = u(\bar{x}) + u'(\bar{x})h + u''(c) \frac{h^2}{2}$$

$$u(\bar{x}-h) = u(\bar{x}) - u'(\bar{x})h + u''(d) \frac{h^2}{2}$$

\Rightarrow

$$\frac{u(\bar{x}+h) - u(\bar{x})}{h} = u'(\bar{x}) + \mathcal{O}(h)$$

$$\frac{u(\bar{x}) - u(\bar{x}-h)}{h} = u'(\bar{x}) + \mathcal{O}(h)$$

($\mathcal{O}(h)$ proportionality constant estimated by $\max\{u''\}$ in relevant regions.)

$$\frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h} = ?$$

Need to use one more term in the expansion.

$$u(\bar{x}+h) = u(\bar{x}) + u'(\bar{x})h + u''(\bar{x})\frac{h^2}{2} + u'''(\xi_1)\frac{h^3}{3!}$$

$$u(\bar{x}-h) = u(\bar{x}) - u'(\bar{x})h + u''(\bar{x})\frac{h^2}{2} - u'''(\xi_2)\frac{h^3}{3!}$$

⇒

$$\frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h} = u'(\bar{x}) + \mathcal{O}(h^2)$$

Better! (Although constant $\approx u'''$
could be worse)

Example: approximation of the derivatives of

$u(x) = \sin(x)$ at $\bar{x} = 1$. $u'(1) = \cos(1) = 0.5403023, \dots$

h	$D_+u(\bar{x})$	$D_-u(\bar{x})$	$D_0u(\bar{x})$	$D_3u(\bar{x})$
1.0e-01	-4.2939e-02	4.1138e-02	-9.0005e-04	6.8207e-05
5.0e-02	-2.1257e-02	2.0807e-02	-2.2510e-04	8.6491e-06
1.0e-02	-4.2163e-03	4.1983e-03	-9.0050e-06	6.9941e-08
5.0e-03	-2.1059e-03	2.1014e-03	-2.2513e-06	8.7540e-09
1.0e-03	-4.2083e-04	4.2065e-04	-9.0050e-08	6.9979e-11

$$D_3u(\bar{x}) = \frac{1}{6h} [2u(\bar{x}+h) + 3u(\bar{x}) - 6u(\bar{x}-h) + u(\bar{x}-2h)]$$

Easy to check

$$D_+u(\bar{x}) - u'(\bar{x}) \approx -0.42h,$$

$$D_0u(\bar{x}) - u'(\bar{x}) \approx -0.09h^2,$$

$$D_3u(\bar{x}) - u'(\bar{x}) \approx 0.007h^3,$$

Errors of order

1	D_+, D_-
2	D_0
3	D_3

In a log-log plot the errors are linear

functions of $\log(h)$, of slopes 1, 2 and 3, resp.:

If $E \approx Ch^p$, then

$$\log(E) \approx p \log h + \log(C)$$

