The Heat Equation

The Heat Equation

We study the heat equation:

$$u_t = u_{xx} \quad \text{for } x \in (0,1), t > 0,$$
 (1)

$$u(0,t) = u(1,t) = 0 \text{ for } t > 0,$$
 (2)

$$u(x,0) = f(x)$$
 for $x \in (0,1)$, (3)

where f is a given initial condition defined on the unit interval (0,1). We shall in the following study

- physical properties of heat conduction versus the mathematical model (1)-(3)
- "separation of variables" a technique, for computing the analytical solution of the heat equation
- analyze the stability properties of the explicit numerical method

We define the "energy" of the solution u at a time t by

$$E_1(t) = \int_0^1 u^2(x,t) dx$$
 for $t \ge 0$. (4)

- Note that this is not the physical energy
- This "energy" is a mathematical tool, used to study the behavior of the solution
- We shall see that $E_1(t)$ is a non-increasing function of time

 If we multiply the left and right hand sides of the heat equation (1) by u it follows that

$$u_t u = u_{xx} u$$
 for $x \in (0,1), t > 0$

By the chain rule for differentiation we observe that

$$\frac{\partial}{\partial t}u^2 = 2uu_t$$

Hence

$$\frac{1}{2}\frac{\partial}{\partial t}u^2 = u_{xx}u \quad \text{for } x \in (0,1), t > 0$$

• By integrating both sides with respect to x, and applying the rule of integration by parts, we get

$$\frac{1}{2} \int_{0}^{1} \frac{\partial}{\partial t} u^{2}(x,t) dx = \int_{0}^{1} u_{xx}(x,t) u(x,t) dx \qquad (5)$$

$$= u_{x}(1,t) u(1,t) - u_{x}(0,t) u(0,t)$$

$$- \int_{0}^{1} u_{x}(x,t) u_{x}(x,t) dx$$

$$= - \int_{0}^{1} u_{x}^{2}(x,t) dx \quad \text{for } t > 0,$$

where the last equality is a consequence of the boundary condition (2)

• We assume that u is a smooth solution of the heat equation, which implies that we can interchange the order of integration and derivation in (5), that is

$$\frac{\partial}{\partial t} \int_0^1 u^2(x,t) \, dx = -2 \int_0^1 u_x^2(x,t) \, dx \quad \text{for } t > 0$$
 (6)

Therefore

$$E'_1(t) = -2 \int_0^1 u_x^2(x,t) dx$$
 for $t > 0$

This implies that

$$E_1'(t) \leq 0$$

• Thus E_1 is a non-increasing function of time t, i.e.,

$$E_1(t_2) \le E_1(t_1)$$
 for all $t_2 \ge t_1 \ge 0$

In particular

$$\int_0^1 u^2(x,t) \, dx \le \int_0^1 u^2(x,0) \, dx = \int_0^1 f^2(x) \, dx$$
for $t > 0$ (7)

- This means that the energy, in the sense of $E_1(t)$, is a non-increasing function of time
- The integral of u_x^2 with respect to x, tells us how fast the energy decreases
- From a physical point of view it seems reasonable that a the energy will decrease in a system without any heat source
- In the following we study another energy function which can be analyzed in a similar manner

Define the new "energy" function

$$E_2(t) = \int_0^1 u_x^2(x, t) \, dx$$

• Similar to above, we can multiply by u_t and integrate with respect to x and get

$$\int_0^1 u_t^2(x,t) \, dx = \int_0^1 u_{xx}(x,t) u_t(x,t) \, dx$$

Integration by parts leads to

$$\int_0^1 u_t^2(x,t) dx = [u_x(x,t)u_t(x,t)]_0^1 - \int_0^1 u_x(x,t)u_{tx}(x,t) dx$$

$$= u_x(0,t)u_t(0,t) - u_x(1,t)u_t(1,t)$$

$$- \int_0^1 u_x(x,t)u_{xt}(x,t) dx$$

By the chain rule we get

$$\frac{\partial}{\partial t}u_x^2 = 2u_x u_{xt}$$

Hence

$$\int_{0}^{1} u_{t}^{2}(x,t) dx = u_{x}(0,t)u_{t}(0,t) - u_{x}(1,t)u_{t}(1,t)$$

$$- \int_{0}^{1} u_{x}(x,t)u_{xt}(x,t) dx$$

$$= u_{x}(0,t)u_{t}(0,t) - u_{x}(1,t)u_{t}(1,t)$$

$$- \frac{1}{2} \int_{0}^{1} \frac{\partial}{\partial t} u_{x}^{2}(x,t) dx$$

 We can interchange the order of integration and differentiation and thereby conclude that

$$\frac{1}{2} \frac{\partial}{\partial t} \int_0^1 u_x^2(x,t) \, dx = -\int_0^1 u_t^2(x,t) \, dx - u_x(0,t) u_t(0,t) + u_x(1,t) u_t(1,t)$$

- According to the boundary condition (2), u(0,t) = u(1,t) = 0 for all t > 0
- Since u(0,t) and u(1,t) are constant with respect to time, we can conclude that

$$u_t(0,t) = u_t(1,t) = 0 \quad \text{for } t > 0$$
 (8)

Thus, we get that

$$E_2'(t) = \frac{\partial}{\partial t} \int_0^1 u_x^2(x,t) \, dx = -2 \int_0^1 u_t^2(x,t) \, dx \le 0,$$

• This means that E_2 is a non-increasing function of time, i.e.

$$E_2(t_2) \le E_2(t_1)$$
 for all $t_2 \ge t_1 \ge 0$ (9)

$$\int_0^1 u_x^2(x,t) \, dx \le \int_0^1 u_x^2(x,0) \, dx = \int_0^1 f_x^2(x) \, dx, \quad t > 0$$

- We will now study how modifications of the initial condition (3) influence on the solution
- Consider the problem with a modified initial condition

$$v_t = v_{xx} \quad \text{for } x \in (0,1), t > 0$$
 (10)

$$v(0,t) = v(1,t) = 0 \quad \text{for } t > 0$$
 (11)

$$v(x,0) = g(x) \quad \text{for } x \in (0,1)$$
 (12)

If g is close to f, will v be approximately equal to u?

• Let *e* denote the difference between *u* and *v*, i.e.

$$e(x,t) = u(x,t) - v(x,t)$$
 for $x \in [0,1], t \ge 0$

From equations (1) and (10) we find that

$$e_t = (u - v)_t = u_t - v_t = u_{xx} - v_{xx} = (u - v)_{xx} = e_{xx}$$

• Furthermore from (2)-(3) and (11)-(12) we get

$$e(0,t) = u(0,t) - v(0,t) = 0 - 0 = 0$$
 for $t > 0$
 $e(1,t) = u(1,t) - v(1,t) = 0 - 0 = 0$ for $t > 0$
 $e(x,0) = u(x,0) - v(x,0) = f(x) - g(x)$ for $x \in (0,1)$

- Thus, e solves the heat equation with homogeneous Dirichlet boundary conditions at x=0,1 and with initial condition h=f-g
- From the above discussion, we therefore get that

$$\int_0^1 e^2(x,t) \, dx \le \int_0^1 h^2(x) \, dx, \quad t > 0,$$

$$\int_{0}^{1} (u(x,t) - v(x,t))^{2} dx \le \int_{0}^{1} (f(x) - g(x))^{2} dx, \quad t > 0$$
(13)

- Thus, if g is close to f then the integral of $(u-v)^2$, at any time t>0, must be small
- Hence, we conclude that minor changes in the initial condition of (1)-(3) will not alter its solution significantly
- The problem is stable with respect to changes in the initial condition

Uniqueness

- We will now prove that (1)-(3) can have at most one smooth solution
- Assume that both u and v are smooth solutions of this problem
- Using the above notation, this means that g(x) = f(x), $x \in (0,1)$
- (13) implies that

$$\int_0^1 (u(x,t) - v(x,t))^2 dx = 0, \quad t > 0$$

Uniqueness

• Note that the function $(u-v)^2$ is continuous, and furthermore

$$(u(x,t) - v(x,t))^2 \ge 0$$
 for all $x \in [0,1]$ and $t \ge 0$

We can therefore conclude that

$$u(x,t) = v(x,t)$$
 for all $x \in [0,1]$ and $t \ge 0$

- We know that the solution of (1)-(3), will be more and more smooth, and that it will approach zero, as time increases
- Physically it is reasonable that the maximum temperature must appear either initially or at the boundary
- We now study the initial-boundary value problem

$$u_t = u_{xx} \quad \text{for } x \in (0,1), t > 0$$
 (14)

$$u(0,t) = g_1(t)$$
 and $u(1,t) = g_2(t)$ for $t > 0$ (15)

$$u(x,0) = f(x)$$
 for $x \in (0,1)$ (16)

• We shall see that the maximum value of the solution u(x,t) will occur initially or on the boundary

- First, we recall an important theorem from calculus
- Let q(x), $x \in [0,1]$ be a smooth function of one variable, which attains its maximum value at an interior point x^* , i.e.

$$x^* \in (0,1)$$
 and $q(x) \le q(x^*)$ for all $x \in [0,1]$

- Then q must satisfy
 - $q'(x^*) = 0$
 - $q''(x^*) \le 0$

• Consequently, if a smooth function h(x), defined on [0,1], is such that

$$h'(x) \neq 0$$
 for all $x \in (0,1)$

or

$$h''(x) > 0$$
 for all $x \in (0,1)$,

then h must attain its maximum value at one of the endpoints

Hence, we conclude that

$$h(0) \ge h(x)$$
 for all $x \in [0, 1]$ (17)

or

$$h(1) \ge h(x)$$
 for all $x \in [0, 1]$ (18)

• Furthermore, if (17) hold, then h must satisfy

$$h'(0) \le 0, \tag{19}$$

and if (18) is the case, then it follows that

$$h'(1) \ge 0 \tag{20}$$

- Let v = v(x,t) be a smooth function of space $x \in [0,1]$ and time $t \in [0,T]$
- That is, we assume that the partial derivatives of all orders of v with respect x and t are continuous, and that

$$\nu:\overline{\Omega}_{T}
ightarrow \mathrm{I\!R},$$

where

$$\Omega_{T} = \{(x,t) | 0 < x < 1 \text{ and } 0 < t < T\},$$

$$\partial \Omega_{T} = \{(x,0) | 0 \le x \le 1\} \cup \{(1,t) | 0 \le t \le T\}$$

$$\cup \{(x,T) | 0 \le x \le 1\} \cup \{(0,t) | 0 \le t \le T\}$$
(21)

and

$$\overline{\Omega}_T = \Omega_T \cup \partial \Omega_T \tag{23}$$

• Assume that $(x^*,t^*) \in \Omega_T$, an interior point, is a maximum point for v in $\overline{\Omega}_T$, i.e.,

$$v(x,t) \leq v(x^*,t^*)$$
 for all $(x,t) \in \overline{\Omega}_T$

• Then, as in the single variable case, v must satisfy

$$v_x(x^*, t^*) = 0, \quad v_t(x^*, t^*) = 0,$$
 (24)

$$v_{xx}(x^*, t^*) \le 0$$
 and $v_{tt}(x^*, t^*) \le 0$ (25)

• Thus, a smooth function $w=w(x,t), \ (x,t)\in \overline{\Omega}_T$ such that either

$$w_x(x,t) \neq 0, \quad w_t(x,t) \neq 0,$$
 $w_{xx}(x,t) > 0 \quad \text{or} \quad w_{tt}(x,t) > 0, \quad \text{for all } (x,t) \in \Omega_T, \quad (26)$

must attain its maximum value at the boundary $\partial\Omega_T$ of Ω_T

• We also have that if the maximum is achieved for t = T, say at (x^*, T) , then w must satisfy the inequality

$$w_t(x^*, T) \ge 0 \tag{27}$$

- Assume that u is a smooth solution of (14)-(16), and that u achieves its maximum value at an interior point $(x^*, t^*) \in \Omega_T$
- From (14) it follows that

$$u_t(x^*,t^*) = u_{xx}(x^*,t^*)$$

By (24) we conclude that

$$u_{xx}(x^*,t^*)=0$$

• If there were strict inequalities in (25), we would have had a contradiction, and we could have concluded that u must achieve its maximum at $\partial\Omega_T$

• Define a family of auxiliary functions $\{v_{\varepsilon}\}_{{\varepsilon}>0}$ by

$$v^{\varepsilon}(x,t) = u(x,t) + \varepsilon x^2 \quad \text{for } \varepsilon > 0,$$
 (28)

where u solves (14)-(16)

Note that

$$v_t^{\varepsilon}(x,t) = u_t(x,t),$$

$$v_{xx}^{\varepsilon}(x,t) = u_{xx}(x,t) + 2\varepsilon > u_{xx}(x,t)$$
(29)

• Now, if v^{ε} achieves its maximum at an interior point, say $(x^*, t^*) \in \Omega_T$, then the property (24) implies that

$$v_t^{\varepsilon}(x^*, t^*) = 0 \quad \Rightarrow \quad u_t(x^*, t^*) = 0$$

We can apply the heat equation (14) to conclude that

$$u_{xx}(x^*,t^*) = u_t(x^*,t^*) = 0$$

Therefore

$$v_{xx}^{\varepsilon}(x^*,t^*) = u_{xx}(x^*,t^*) + 2\varepsilon = 2\varepsilon > 0$$

- This violates the property (25), which must hold at a maximum point of v^{ε}
- Hence, we conclude that v^{ε} must attain its maximum value at the boundary $\partial \Omega_T$ of Ω_T , i.e.,

$$v^{\varepsilon}(x,t) \leq \max_{(y,s)\in\partial\Omega_T} v^{\varepsilon}(y,s)$$
 for all $(x,t)\in\overline{\Omega}_T$

- Can v^{ε} reach its maximum value at time t = T and for $x^* \in (0,1)$?
- Assume that (x^*, T) , with $0 < x^* < 1$, is such that

$$v^{\varepsilon}(x,t) \leq v^{\varepsilon}(x^*,T)$$
 for all $(x,t) \in \overline{\Omega}_T$

• Then, according to property (27), $v_t^{\varepsilon}(x^*, T) \ge 0$, which implies that

$$u_t(x^*,T) \geq 0$$

see (29)

Consequently, since u satisfies the heat equation

$$u_{xx}(x^*,T) = u_t(x^*,T) \ge 0$$

It follows that

$$v_{xx}^{\varepsilon}(x^*,T) = u_{xx}(x^*,T) + 2\varepsilon \ge 0 + 2\varepsilon > 0$$

- This contradicts the property (25) that must be fulfilled at such a maximum point
- This means that

$$v^{\varepsilon}(x,t) \le \max_{(y,s)\in\Gamma_T} v^{\varepsilon}(y,s) \quad \text{for all } (x,t)\in\overline{\Omega}_T,$$
 (30)

where

$$\Gamma_T = \{(0,t) \mid 0 \le t \le T\} \cup \{(x,0) \mid 0 \le x \le 1\} \cup \{(1,t) \mid 0 \le t \le T\}$$

Let

$$M = \max\left(\max_{t\geq 0} g_1(t), \max_{t\geq 0} g_2(t), \max_{x\in(0,1)} f(x)\right)$$

And let

$$\Gamma = \{(0,t) \mid t \ge 0\} \cup \{(x,0) \mid 0 \le x \le 1\} \cup \{(1,t) \mid t \ge 0\}$$

• Since $\Gamma_T \subset \Gamma$, (30) and the definition (28) of v^{ϵ} , we have that

$$v^{\varepsilon}(x,t) \leq \max_{(y,s)\in\Gamma} v^{\varepsilon}(y,s) \leq M + \varepsilon \quad \text{for all } (x,t) \in \overline{\Omega}_T$$

• By (28), it follows that

$$u(x,t) \leq v^{\varepsilon}$$
 for all $(x,t) \in \overline{\Omega}_T$

Therefore

$$u(x,t) \leq M + \varepsilon$$
 for all $(x,t) \in \overline{\Omega}_T$ and all $\varepsilon > 0$

• This inequality is valid for all $\epsilon > 0$, hence it must follow that

$$u(x,t) \le M \quad \text{for all } (x,t) \in \overline{\Omega}_T$$
 (31)

• Since T > 0 was arbitrary chosen, this inequality must hold for any t > 0, i.e.,

$$u(x,t) \le M$$
 for all $x \in [0,1], t > 0$ (32)

Minimum principle

- The maximum principle above can be used to prove a similar minimum principle
- Let u(x,t) be a solution of the (14)-(16), and define w(x,t) = -u(x,t) for all $x \in [0,1], t > 0$
- Note that w satisfies the heat equation, since

$$w_t = (-u)_t = -u_t = -u_{xx} = (-u)_{xx} = w_{xx}$$

Moreover

$$w(0,t) = -g_1(t)$$
 and $w(1,t) = -g_2(t)$ for $t > 0$, $w(x,0) = -f(x)$ for $x \in (0,1)$

Minimum principle

Thus, from the analysis presented above we find that

$$\begin{split} w(x,t) & \leq & \max\left(\max_{t\geq 0}(-g_1(t)), \max_{t\geq 0}(-g_2(t)), \max_{x\in (0,1)}(-f(x))\right) \\ & = & -\min\left(\min_{t\geq 0}g_1(t), \min_{t\geq 0}g_2(t), \min_{x\in (0,1)}f(x)\right), \\ & \text{for all } x\in [0,1], t>0 \end{split}$$

We can write this

$$u(x,t) \geq \min\left(\min_{t\geq 0} g_1(t), \min_{t\geq 0} g_2(t), \min_{x\in(0,1)} f(x)\right),$$
 for all $x\in[0,1], t>0$

A smooth solution of the problem (14)-(16) must satisfy the bound

$$m \le u(x,t) \le M$$
 for all $x \in [0,1], t > 0,$ (33)

where

$$m = \min\left(\min_{t \ge 0} g_1(t), \min_{t \ge 0} g_2(t), \min_{x \in (0,1)} f(x)\right), \quad (34)$$

$$M = \max\left(\max_{t\geq 0} g_1(t), \max_{t\geq 0} g_2(t), \max_{x\in(0,1)} f(x)\right).$$
(35)

- Separation of variables is a technique for computing the analytical solution of the heat equation
- First, we study functions satisfying

$$u_t = u_{xx} \quad \text{for } x \in (0,1), t > 0,$$
 (36)

$$u(0,t) = u(1,t) = 0 \quad \text{for } t > 0$$
 (37)

We guess that we have solutions on the form

$$u(x,t) = X(x)T(t), \tag{38}$$

where X(x) and T(t) only depend on x and t

The boundary conditions imply that

$$u(0,t) = 0 = X(0)T(t)$$
 and $u(1,t) = 0 = X(1)T(t)$

• Consequently, X(x) must satisfy

$$X(0) = 0$$
 and $X(1) = 0$, (39)

provided that $T(t) \neq 0$ for t > 0

• By using (38) for u(x,t) in the heat equation (36) we find that X and T must satisfy the relation

$$X(x)T'(t) = X''(x)T(t)$$
 for all $x \in (0,1), t > 0$

• Thus, if $X(x) \neq 0$ for $x \in (0,1)$ and $T(t) \neq 0$ for t > 0, we get

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} \quad \text{for all } x \in (0,1), t > 0$$
 (40)

 Since the left hand side of (40) only depends on t and the right hand side only depends on x, we conclude that there must exist a constant λ such that

$$\frac{T'(t)}{T(t)} = \lambda \tag{41}$$

$$\frac{X''(x)}{X(x)} = \lambda \tag{42}$$

 We have studied problems on the form (41) earlier and have seen that a solution is given by

$$T(t) = ce^{\lambda t}, \tag{43}$$

where c is an arbitrary constant

• We write (42) on the form

$$X''(x) = \lambda X(x), \tag{44}$$

with the boundary conditions

$$X(0) = 0 \text{ and } X(1) = 0$$
 (45)

- We have that: $\sin''(k\pi x) = -k^2\pi^2\sin(k\pi x)$
- Therefore

$$X(x) = X_k(x) = \sin(k\pi x), \tag{46}$$

$$\lambda = \lambda_k = -k^2 \pi^2 \tag{47}$$

satisfy (44) and (45), for k = ..., -2, -1, 0, 1, 2, ...

We can now summarize that

$$u_k(x,t) = c_k e^{-k^2 \pi^2 t} \sin(k\pi x)$$
 for $k = \dots, -2, -1, 0, 1, 2, \dots$ (48)

satisfy both the heat equation (36) and the boundary condition (37)

• Note that, $\{c_k\}$ are arbitrary constants

Consider the problem

$$u_t = u_{xx} \quad \text{for } x \in (0,1), t > 0,$$
 (49)

$$u(0,t) = u(1,t) = 0 \quad \text{for } t > 0,$$
 (50)

$$u(x,0) = \sin(\pi x)$$
 for $x \in (0,1)$. (51)

We have that

$$u(x,t) = e^{-\pi^2 t} \sin(\pi x)$$

satisfies (49) and (50). Furthermore,

$$u(x,0) = e^{-\pi^2 0} \sin(\pi x) = \sin(\pi x)$$

and thus this is the unique smooth solution of this problem.

Our second example is

$$u_t = u_{xx}$$
 for $x \in (0,1), t > 0,$
 $u(0,t) = u(1,t) = 0$ for $t > 0,$
 $u(x,0) = 7\sin(5\pi x)$ for $x \in (0,1).$

Putting k = 5 and $c_5 = 7$ in equation (48) we find that

$$u(x,t) = 7e^{-25\pi^2 t}\sin(5\pi x)$$

satisfies the heat equation and the boundary condition of this problem. Furthermore,

$$u(x,0) = 7e^{-25\pi^2 0}\sin(5\pi x) = 7\sin(5\pi x)$$

and hence the initial condition is also satisfied.

Super-positioning

• Assume that both v_1 and v_2 satisfy equations (36) and (37), and let

$$w = v_1 + v_2$$

Observe that

$$w_t = (v_1 + v_2)_t = (v_1)_t + (v_2)_t = (v_1)_{xx} + (v_2)_{xx} = (v_1 + v_2)_{xx} = w_{xx}$$

Furthermore

$$w(0,t) = v_1(0,t) + v_2(0,t) = 0 + 0 = 0$$
 for $t > 0$,

and

$$w(1,t) = v_1(1,t) + v_2(1,t) = 0 + 0 = 0$$
 for $t > 0$,

hence w also satisfies (36) and (37)

Super-positioning

• For an arbitrary constant a_1 consider the function

$$p(x,t) = a_1 v_1(x,t)$$

• Since a_1 is a constant and v_1 satisfy the heat equation it follows that

$$p_t = (a_1v_1)_t = a_1(v_1)_t = a_1(v_1)_{xx} = (a_1v_1)_{xx} = p_{xx}$$

Furthermore

$$p(0,t) = a_1 v_1(0,t) = 0$$
 for $t > 0$,
 $p(1,t) = a_1 v_1(1,t) = 0$ for $t > 0$.

Thus we conclude that p satisfy both (36) and (37)

Super-positioning

• We can now conclude that, if v_1 and v_2 satisfy (36)-(37) then any function on the form

$$a_1v_1 + a_2v_2$$
,

also solves this problem for all constants a_1 and a_2

More generally, for any sequence of numbers

$$c_0, c_1, c_2, \ldots$$

such that the series of functions

$$\sum_{k=1}^{\infty} c_k e^{-k^2 \pi^2 t} \sin(k\pi x)$$

converges, this sum forms a solution of (36)-(37)

This is called super-positioning

Fourier series and the initial condition

We now have that, for any sequence of numbers

$$c_1, c_2, \ldots$$

the function

$$u(x,t) = \sum_{k=1}^{\infty} c_k e^{-k^2 \pi^2 t} \sin(k\pi x)$$
 (52)

defines a formal solution of (36)-(37), provided that the series in (52) converges

- Therefore, if we drop the initial condition, we can find infinitely many functions satisfying the heat equation
- We shall now see how our model problem (1)-(3) (including the initial condition) can be solved

Consider the problem

$$u_t = u_{xx} \quad \text{for } x \in (0,1), t > 0,$$
 (53)

$$u(0,t) = u(1,t) = 0 \quad \text{for } t > 0,$$
 (54)

$$u(x,0) = 2.3\sin(3\pi x) + 10\sin(6\pi x) \quad \text{for } x \in (0,1). \tag{55}$$

This fit into (52) with

$$c_k = 0$$
 for $k \neq 3$ and $k \neq 6$, $c_3 = 2.3$ and $c_6 = 10$.

Thus, the unique smooth solution is given by

$$u(x,t) = 2.3e^{-9\pi^2t}\sin(3\pi x) + 10e^{-36\pi^2t}\sin(6\pi x).$$

Let us determine a formula for the solution of the problem

$$u_t = u_{xx}$$
 for $x \in (0,1), t > 0$,
 $u(0,t) = u(1,t) = 0$ for $t > 0$,
 $u(x,0) = 20\sin(\pi x) + 8\sin(3\pi x) + \sin(67\pi x) + 1002\sin(10^4\pi x)$.

By putting

$$c_k = 0$$
 for $k \neq 1, 3, 67, 10^4$,
 $c_1 = 20, c_3 = 8, c_{67} = 1, c_{10^4} = 1002$,

in formula (52), we get the solution

$$u(x,t) = 20e^{-\pi^2 t} \sin(\pi x) + 8e^{-9\pi^2 t} \sin(3\pi x) + e^{-(67\pi)^2 t} \sin(67\pi x) + 1002e^{-(10^4\pi)^2 t} \sin(10^4\pi x).$$

Sums of sine functions

We can generalize as follows:

- Let S be any finite set of positive integers and let $\{c_k\}_{k\in S}$ be arbitrary given constants
- Consider an initial condition on the form

$$f(x) = \sum_{k \in S} c_k \sin(k\pi x)$$

• Then the solution of (1)-(3) is given by

$$u(x,t) = \sum_{k \in S} c_k e^{-k^2 \pi^2 t} \sin(k\pi x)$$

Sums of sine functions

This is valid because

$$u_{t}(x,t) = \sum_{k \in S} -k^{2}\pi^{2}c_{k}e^{-k^{2}\pi^{2}t}\sin(k\pi x)$$

$$u_{xx}(x,t) = \sum_{k \in S} -k^{2}\pi^{2}c_{k}e^{-k^{2}\pi^{2}t}\sin(k\pi x)$$

$$u(0,t) = \sum_{k \in S} c_{k}e^{-k^{2}\pi^{2}t}\sin(0) = 0$$

$$u(1,t) = \sum_{k \in S} c_{k}e^{-k^{2}\pi^{2}t}\sin(k\pi) = 0$$

$$u(x,0) = \sum_{k \in S} c_{k}e^{0}\sin(k\pi x) = \sum_{k \in S} c_{k}\sin(k\pi x) = f(x)$$

Sums of sine functions

What about infinite series?
For any initial condition on the form

$$f(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x) \quad \text{for } x \in (0,1),$$

where the sum on the right hand side is an convergent infinite series. The solution of (1)-(1) is given by

$$u(x,t) = \sum_{k=1}^{\infty} c_k e^{-k^2 \pi^2 t} \sin(k\pi x).$$
 (56)

• For a given function f(x), does there exist constants c_1, c_2, c_3, \ldots such that

$$f(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x) \quad \text{for } x \in (0,1)?$$
 (57)

- If so, how can the constants $c_1, c_2, c_3,...$ be determined?
- Let us first assume that the answer to the first question is yes

 Recall the trigonometric identity that, for any real numbers a and b

$$\sin(a)\sin(b) = \frac{1}{2}(\cos(a-b) - \cos(a+b))$$
 (58)

Therefore it follows that

$$\int_0^1 \sin(k\pi x) \sin(l\pi x) \, dx = \begin{cases} 0 & k \neq l, \\ 1/2 & k = l \end{cases}$$
 (59)

Now

$$\int_0^1 f(x) \sin(l\pi x) dx = \int_0^1 \left(\sum_{k=1}^\infty c_k \sin(k\pi x)\right) \sin(l\pi x) dx$$
$$= \sum_{k=1}^\infty c_k \int_0^1 \sin(k\pi x) \sin(l\pi x) dx$$
$$= \frac{1}{2} c_l$$

Therefore

$$c_k = 2 \int_0^1 f(x) \sin(k\pi x) dx$$
 for $k = 1, 2, ...$ (60)

• We conclude that, if the function f can be written on the form (57), then the coefficients must satisfy (60)

Usually, a function can be written on the form (57), and we refer to such functions as "well-behaved".

We can now summarize

The Fourier coefficients for a "well-behaved" function f(x), $x \in (0,1)$, is defined by

$$c_k = 2 \int_0^1 f(x) \sin(k\pi x) dx$$
 for $k = 1, 2, ..., (61)$

and the associated Fourier sine series by

$$f(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x)$$
 for $x \in (0,1)$. (62)

Furthermore, if f satisfies (62) then

$$u(x,t) = \sum_{k=1}^{\infty} c_k e^{-k^2 \pi^2 t} \sin(k\pi x)$$
 (63)

defines a formal solution of the problem

$$u_t = u_{xx} \quad \text{for } x \in (0,1), t > 0,$$
 (64)

$$u(0,t) = u(1,t) = 0$$
 for $t > 0$, (65)

$$u(x,0) = f(x)$$
 for $x \in (0,1)$. (66)

• For a given integer N, we can approximate u by the Nth partial sum u_N of the Fourier series, i.e.,

$$u(x,t) \approx u_N(x,t) = \sum_{k=1}^{N} c_k e^{-k^2 \pi^2 t} \sin(k\pi x)$$
 (67)

Determine the Fourier sine series of the constant function

$$f(x) = 10$$
 for $x \in (0,1)$.

From formula (61) we find that

$$c_k = 2\int_0^1 f(x)\sin(k\pi x) \, dx = 2\int_0^1 10\sin(k\pi x) \, dx$$

$$= 20\left[-\frac{1}{k\pi}\cos(k\pi x)\right]_0^1 = -\frac{20}{k\pi}(\cos(k\pi) - 1) = \begin{cases} 0 & \text{if k is even} \\ \frac{40}{k\pi} & \text{if k is odd} \end{cases}$$

Thus we find that the Fourier sine series of this function is

$$f(x) = 10 = \sum_{k=1}^{\infty} \frac{40}{(2k-1)\pi} \sin((2k-1)\pi x) \quad \text{for } x \in (0,1) \quad (68)$$

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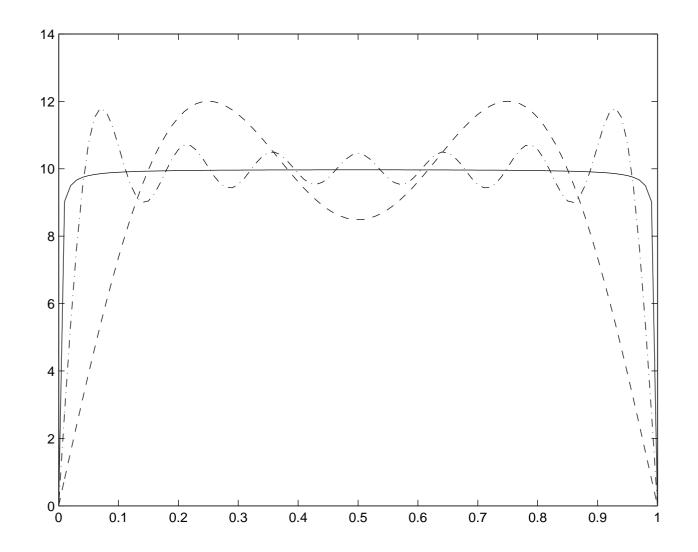


Figure 1: The first 2 (dashed line), 7 (dashed-dotted line) and 100 (solid line) terms of the Fourier sine series of the function f(x) = 10.

Solve

$$u_t = u_{xx}$$
 for $x \in (0,1), t > 0$,
 $u(0,t) = u(1,t) = 0$ for $t > 0$,
 $u(x,0) = 10$ for $x \in (0,1)$.

The formal solution is given by

$$u(x,t) = \sum_{k=1}^{\infty} \frac{40}{(2k-1)\pi} e^{-(2k-1)^2 \pi^2 t} \sin((2k-1)\pi x)$$
 (69)

In figures 2 and 3 we have graphed the function given by the 100th partial sum of the series (69) at time t = 0.5 and t = 1, respectively.

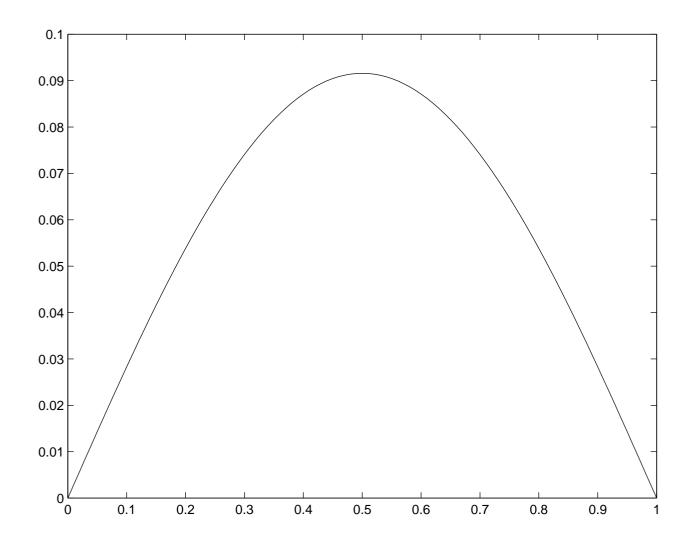


Figure 2: A plot of the function given by the sum of the 100 first terms of the series defining the formal solution of the problem studied in Example 26. The figure shows a "snapshot" of this function at time t = 0.5.

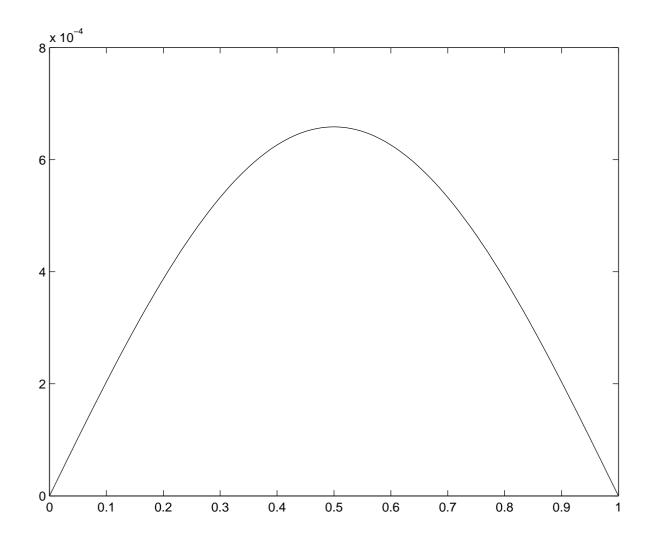


Figure 3: A plot of the function given by the sum of the 100 first terms of the series defining the formal solution of the problem studied in Example 26. The figure shows a "snapshot" of this function at time t = 1.

Note that

A Fourier sine series, finite or infinite,

$$g(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x),$$

will have the property that

$$g(0) = g(1) = 0$$

- So, if a function f(x) is not zero at the endpoints, it can not be written as a sum of sine series on the closed interval [0,1]
- But the Fourier sine series of f, will in most cases still converge to f(x) in the open interval (0,1)

Compute the Fourier coefficients $\{c_k\}$ of the function

$$f(x) = x(1-x) = x - x^2$$
.

According to formula (61)

$$c_k = 2\int_0^1 (x - x^2) \sin(k\pi x) \, dx = 2\int_0^1 x \sin(k\pi x) \, dx - 2\int_0^1 x^2 \sin(k\pi x) \, dx.$$

We have

$$\int_{0}^{1} x \sin(k\pi x) dx = \left[-x \frac{1}{k\pi} \cos(k\pi x) \right]_{0}^{1} - \int_{0}^{1} -\frac{1}{k\pi} \cos(k\pi x) dx$$
$$= -\frac{1}{k\pi} \cos(k\pi) + \frac{1}{k\pi} \left[\frac{1}{k\pi} \sin(k\pi x) \right]_{0}^{1}$$
$$= -\frac{1}{k\pi} \cos(k\pi) = \frac{(-1)^{k+1}}{k\pi}.$$

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$$\int_{0}^{1} x^{2} \sin(k\pi x) dx = \left[-x^{2} \frac{1}{k\pi} \cos(k\pi x) \right]_{0}^{1} - \int_{0}^{1} -2x \frac{1}{k\pi} \cos(k\pi x) dx$$

$$= -\frac{1}{k\pi} \cos(k\pi) + \frac{2}{k\pi} \left[x \frac{1}{k\pi} \sin(k\pi x) \right]_{0}^{1}$$

$$-\frac{2}{k\pi} \int_{0}^{1} \frac{1}{k\pi} \sin(k\pi x) dx$$

$$= -\frac{1}{k\pi} \cos(k\pi) + \frac{2}{(k\pi)^{2}} \left[\frac{1}{k\pi} \cos(k\pi x) \right]_{0}^{1}$$

$$= -\frac{1}{k\pi} \cos(k\pi) + \frac{2}{(k\pi)^{3}} \cos(k\pi) - \frac{2}{(k\pi)^{3}}$$

$$= \frac{(-1)^{k+1}}{k\pi} + \frac{2(-1)^{k}}{(k\pi)^{3}} - \frac{2}{(k\pi)^{3}}.$$

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Thus

$$c_k = 2\left(\frac{2}{(k\pi)^3} - \frac{2(-1)^k}{(k\pi)^3}\right) = \begin{cases} 0 & \text{if } k \text{ is even,} \\ \frac{8}{(k\pi)^3} & \text{if } k \text{ is odd,} \end{cases}$$

and we find that

$$f(x) = x - x^2 = \sum_{k=1}^{\infty} \left(\frac{8}{((2k-1)\pi)^3} \right) \sin((2k-1)\pi x).$$

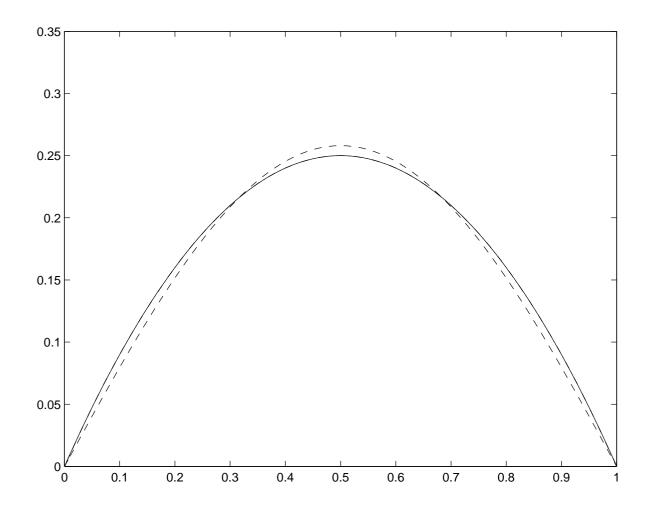


Figure 4: The first (dashed line), 7 first (dashed-dotted line) and 100 first (solid line) terms of the Fourier sine series of the function $f(x) = x - x^2$. It is impossible to distinguish between the figures representing the 7 first and 100 first terms. They are both accurate approximations of $x - x^2$.

Solve the problem

$$u_t = u_{xx}$$
 for $x \in (0,1), t > 0,$
 $u(0,t) = u(1,t) = 0$ for $t > 0,$
 $u(x,0) = x(1-x) = x - x^2$ for $x \in (0,1).$

According to (63) the function

$$u(x,t) = \sum_{k=1}^{\infty} \left(\frac{8}{((2k-1)\pi)^3} \right) e^{-(2k-1)^2\pi^2 t} \sin((2k-1)\pi x)$$
 (70)

defines a formal solution of this problem.

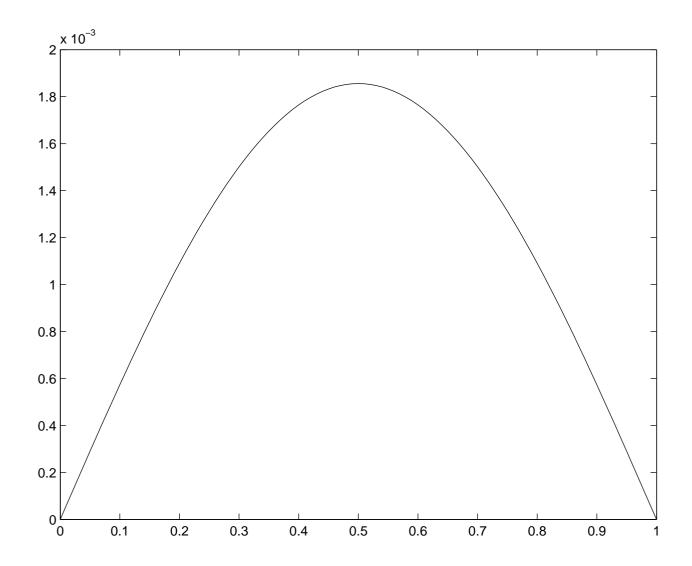


Figure 5: A "snapshot", at time t = 0.5, of the function given by the sum of the 100 first terms of the series defining the formal solution of the problem studied in Example 28.

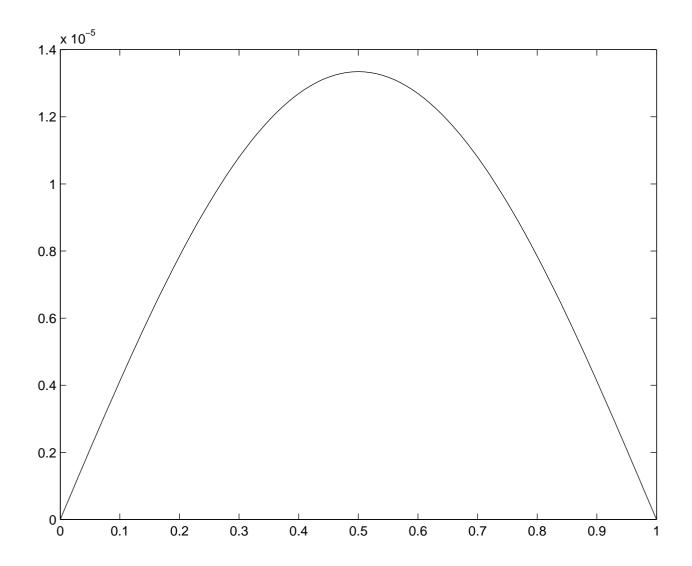


Figure 6: A "snapshot", at time t = 1, of the function given by the sum of the 100 first terms of the series defining the formal solution of the problem studied in Example 28.

Stability analysis of the num. sol.

- We shall now study the stability properties of the explicit finite difference scheme for heat equation presented earlier
- As above, the discretization parameters are defined by

$$\Delta t = \frac{T}{m}$$
 and $\Delta x = \frac{1}{n-1}$,

and functions are only defined in the gridpoints

$$u_i^{\ell} = u(x_i, t_{\ell}) = u((i-1)\Delta x, \ell \Delta t)$$

for $i = 1, ..., n$ and $\ell = 0, ..., m$

Stability analysis of the num. sol.

The numerical scheme is written

$$u_{i}^{\ell+1} = u_{i}^{\ell} + \frac{\Delta t}{\Delta x^{2}} (u_{i-1}^{\ell} - 2u_{i}^{\ell} + u_{i+1}^{\ell})$$

$$= \alpha u_{i-1}^{\ell} + (1 - 2\alpha)u_{i}^{\ell} + \alpha u_{i+1}^{\ell}$$
(71)

for $i=2,\ldots,n-1$ and $\ell=0,\ldots,m-1$, where

$$\alpha = \frac{\Delta t}{\Delta x^2} \tag{72}$$

- Boundary conditions are $u_0^\ell = u_1^\ell = 0$ for $\ell = 1, \dots, m$
- We shall see that this numerical scheme is only conditionable stable, and the stability depends on the parameter α

Example 29

Consider the following problem

$$u_t = u_{xx}$$
 for $x \in (0,1), t > 0,$
 $u(0,t) = u(1,t) = 0$ for $t > 0,$
 $u(x,0) = \sin(3\pi x)$ for $x \in (0,1),$

with the analytical solution

$$u(x,t) = e^{-\pi^2 t} \sin(3\pi x).$$

In Figures 7-9 we have graphed this function and the numerical results generated by the scheme (71) for various values of the discretization parameters in space and time. Notice how the solution depends on α .

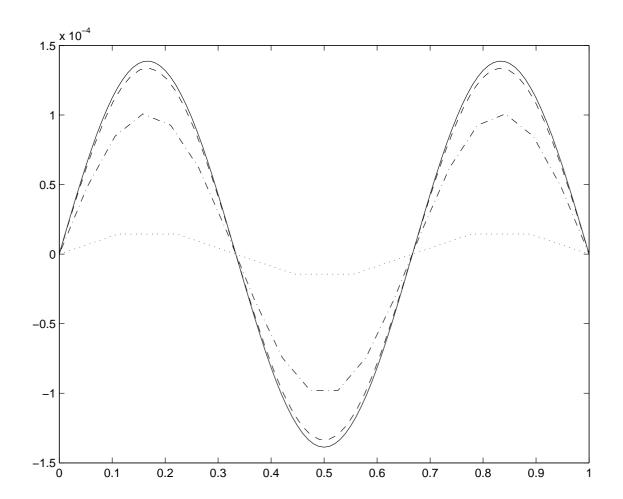


Figure 7: The solid line represents the solution of the problem studied in Example 29. The dotted, dash-dotted and dashed lines are the numerical results generated in the cases of n = 10 and m = 17 ($\alpha = 0.4765$), n = 20 and m = 82 ($\alpha = 0.4402$), n = 60 and m = 706 ($\alpha = 0.4931$), respectively.

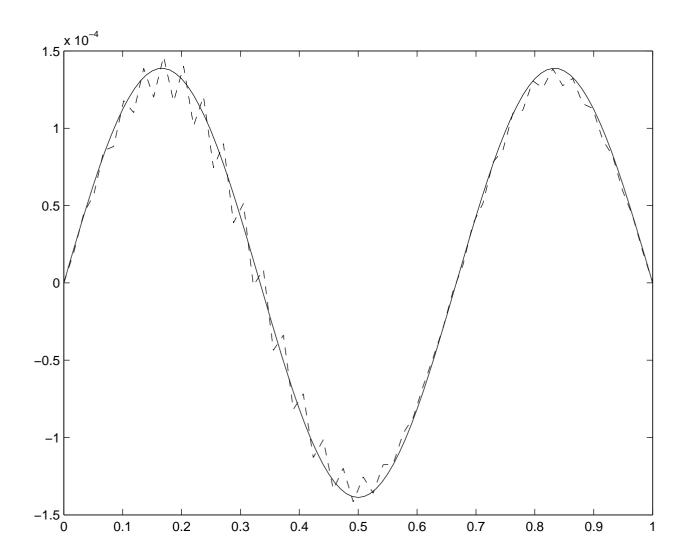


Figure 8: The dashed line represents the results generated by the explicit scheme (71) in the case of n = 60 and m = 681, corresponding to $\alpha = 0.5112$, in Example 29. The solid line is the graph of the exact solution of the problem studied in this example.

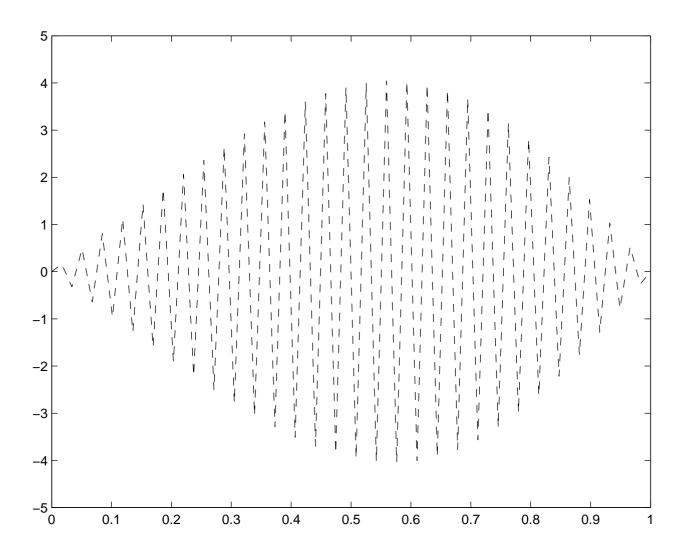


Figure 9: A plot of the numbers generated by the explicit scheme (71), with n=60 and m=675, in Example 29. Observe that $\alpha=0.5157>0.5$ and that, for these discretization parameters, the method fails to solve the problem under consideration!

Example 30

We reconsider the problem analyzed Example 28, and study the performance of the explicit scheme (71) applied to

$$u_t = u_{xx}$$
 for $x \in (0,1), t > 0,$
 $u(0,t) = u(1,t) = 0$ for $t > 0,$
 $u(x,0) = x(1-x) = x - x^2$ for $x \in (0,1).$

We compare the numerical approximations generated by (71) with the formal solution (70) for various discretization parameters Δt and Δx

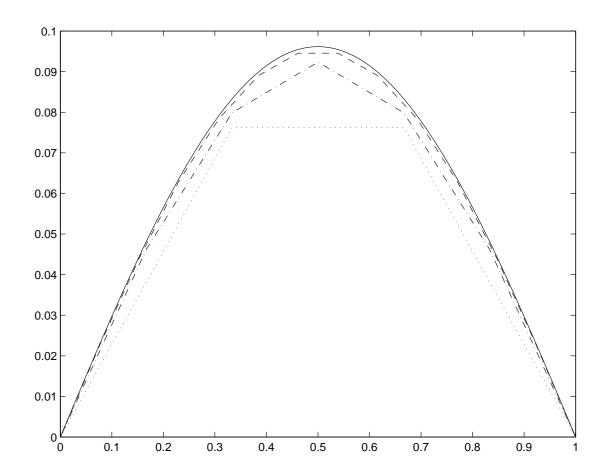


Figure 10: Numerical results from Example 30. The solid line represents the sum of the 100 first terms of the sine series of the formal solution of the problem studied in this example. The dotted, dash-dotted and dashed curves are the numerical results generated in the cases of n = 4 and m = 3 ($\alpha = 0.3$), n = 7 and m = 8 ($\alpha = 0.45$), n = 14 and m = 34 ($\alpha = 0.4971$), respectively.

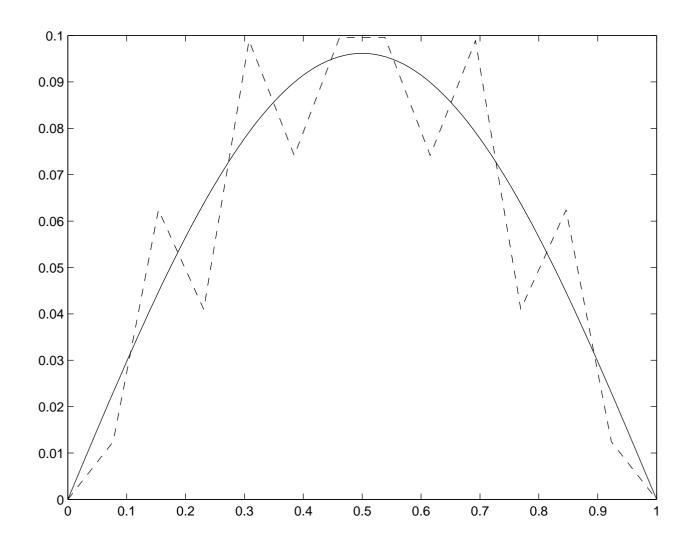


Figure 11: The dashed line represents the results generated by the explicit scheme (71) in the case of n = 14 and m = 29, corresponding to $\alpha = 0.5828$, in Example 30. The solid line is the graph of the Fourier based approximation of the solution.

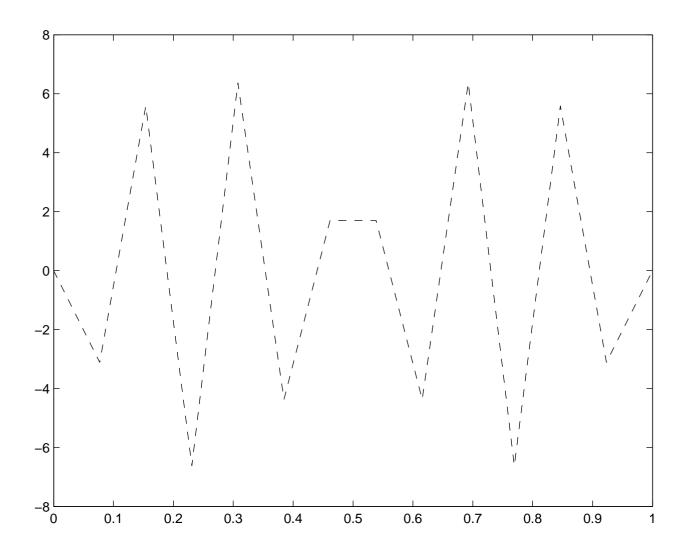


Figure 12: A plot of the numerical results produced by the explicit scheme (71), using n=25 grid points in the spatial dimension and m=25 time steps, in Example 30. In this case $\alpha=0.6760>0.5$ and the method fails to solve the problem.

- We have observed that the explicit scheme (71) works fine, provided that $\alpha \leq 1/2$
- For small discretization parameters Δt and Δx , it seems to produce accurate approximations of the solution of the heat equation
- However, for $\alpha>1/2$ the scheme tends to "break down", i.e., the numbers produced are not useful. Our goal now is to investigate this property from a theoretical point of view
- We will derive, provided that $\alpha \le 1/2$, a discrete analogue to the maximum principle
- Note that, for (1)-(3), the maximums principle implies $|u(x,t)| \le \max_{x} |f(x)|$ for all $x \in (0,1)$ and $t \ge 0$

• Assume that Δt and Δx satisfy

$$\alpha = \frac{\Delta t}{\Delta x^2} \le \frac{1}{2}$$

Then

$$1 - 2\alpha \ge 0 \tag{73}$$

We introduce

$$\bar{u}^{\ell} = \max_{i} |u_{i}^{\ell}| \quad \text{for } \ell = 0, \dots, m$$

Note that

$$\bar{u}^0 = \max_i |f(x_i)|$$

- Recall that $u_i^{\ell+1} = \alpha u_{i-1}^{\ell} + (1-2\alpha)u_i^{\ell} + \alpha u_{i+1}^{\ell}$
- It now follows from the triangle inequality that

$$|u_{i}^{\ell+1}| = |\alpha u_{i-1}^{\ell} + (1 - 2\alpha)u_{i}^{\ell} + \alpha u_{i+1}^{\ell}|$$

$$\leq |\alpha u_{i-1}^{\ell}| + |(1 - 2\alpha)u_{i}^{\ell}| + |\alpha u_{i+1}^{\ell}|$$

$$= \alpha |u_{i-1}^{\ell}| + (1 - 2\alpha)|u_{i}^{\ell}| + \alpha |u_{i+1}^{\ell}|$$

$$\leq \alpha \bar{u}^{\ell} + (1 - 2\alpha)\bar{u}^{\ell} + \alpha \bar{u}^{\ell}$$

$$= \bar{u}^{\ell}$$
(74)

for i = 2, ..., n - 1

Note that

$$u_1^{\ell+1} = u_n^{\ell+1} = 0$$

• Since (74) is valid for i = 2, ..., n-1, we get

$$\max_{i} |u_i^{\ell+1}| \le \bar{u}^{\ell}$$

or

$$\bar{u}^{\ell+1} \leq \bar{u}^{\ell}$$

Finally, by a straightforward induction argument we conclude that

$$\bar{u}^{\ell+1} \le \bar{u}^0 = \max_i |f(x_i)|$$

Assume that the discretization parameters Δt and Δx satisfy

$$\alpha = \frac{\Delta t}{\Delta x^2} \le \frac{1}{2}.\tag{75}$$

Then the approximations generated by the explicit scheme (71) satisfy the bound

$$\max_{i} |u_i^{\ell}| \le \max_{i} |f(x_i)| \quad \text{for } \ell = 0, \dots, m,$$
 (76)

where f is the initial condition in the model problem (1)-(3).

Consequences

For a given n, m must satisfy

$$m \ge 2T(n-1)^2$$

- Hence, the number of time steps, m, needed increases rapidly with the number of grid points, n, used in the space dimension
- If T = 1 and n = 101, then m must satisfy $m \ge 20000$, and in the case of n = 1001 at least $2 \cdot 10^6$ time steps must be taken!
- This is no big problem in 1D, but in 2D and 3D this problem may become dramatic