MATHEMATICAL TRIPOS, PART II COMPUTATIONAL PROJECT

Parabolic Partial Differential Equations



University of Cambridge

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Contents

1	Analytic Solution	2
2	Numerical Methods	4
\mathbf{A}	Codes	8
	A.1 P1	8
	A 2 P2	10

1 Analytic Solution

Question 1

(i) Write $\theta = f(t)(1-x) + \phi(x,t)$, and substitute into the diffusion equation, we have the following governing equation:

$$2(3t-1)(1-x) + \phi_t = \phi_{xx}$$

on the interval $0 \le x \le 1$, with boundary conditions:

$$\phi(0,t) = \phi(1,t) = 0$$

for $0 \le t \le \infty$, and initial condition:

$$\phi(x,t) = -(3t-2)t(1-x)$$

for $t \leq 0$, $0 \leq x \leq 1$.

Write ϕ in a Fourier Sine Series in x: $\phi(x,t) = \sum_{n=1}^{\infty} g_n(t) \sin(n\pi x)$, and $1-x = \sum_{n=1}^{\infty} \frac{2}{n\pi} \sin(n\pi x)$ Then we have:

$$\frac{4}{n\pi}(3t-1) + g_n' = -n^2\pi^2 g_n$$

for $n=1,2,3\cdots$ with initial condition: $\phi(x,0)=0$ for $0\leqslant x\leqslant 1$. and the solution is

$$g_n(t) = \frac{4}{n^3 \pi^3} (1 - 3t) + \frac{12}{n^5 \pi^5} - \frac{4}{n^3 \pi^3} (1 + \frac{3}{n^2 \pi^2}) e^{-n^2 \pi^2 t}$$

for $t \ge 0$, $n = 1, 2, 3 \cdots$.

(ii) Known that

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

$$2\int_{0}^{1} x^{2} \sin(n\pi x) dx = \frac{4((-1)^{n} - 1)}{n^{3}\pi^{3}} + 2\frac{(-1)^{n+1}}{n\pi}$$

$$2\int_{0}^{1} x^{3} \sin(n\pi x) dx = \frac{12(-1)^{n}}{n^{3}\pi^{3}} + 2\frac{(-1)^{n+1}}{n\pi}$$

$$2\int_{0}^{1} x^{4} \sin(n\pi x) dx = \frac{48(1 - (-1)^{n})}{n^{5}\pi^{5}} + \frac{24(-1)^{n}}{n^{3}\pi^{3}} + 2\frac{(-1)^{n+1}}{n\pi}$$

$$2\int_{0}^{1} x^{5} \sin(n\pi x) dx = (-\frac{240}{n^{5}\pi^{5}} + \frac{40}{n^{3}\pi^{3}} - \frac{2}{n\pi})(-1)^{n}$$

From the Fourier Series Solution, as $t \to \infty$,

$$g_n(t) \to -\frac{12}{n^3 \pi^3} t + \frac{4}{n^3 \pi^3} (1 + \frac{3}{n^2 \pi^2})$$

and the functions are:

$$\alpha(x) = -\sum_{n=1}^{\infty} \frac{12}{n^3 \pi^3} \sin(n\pi x) = -(x^3 - 3x^2 + 2x)$$

$$= -x(x-2)(x-1)$$

$$\beta(x) = \sum_{n=1}^{\infty} \frac{4}{n^3 \pi^3} (1 + \frac{3}{n^2 \pi^2}) \sin(n\pi x) = -\frac{x^5}{20} + \frac{x^4}{4} - x^2 + \frac{4}{5}x$$

$$= -\frac{1}{20} x(x-1)(x-2)(x+2)(x-4)$$

- (iii) The programme is in A.1.
- (iv) Plot at times t = 0.1, 2/3 and 1 ,according to the initial condition (3t-2)t.

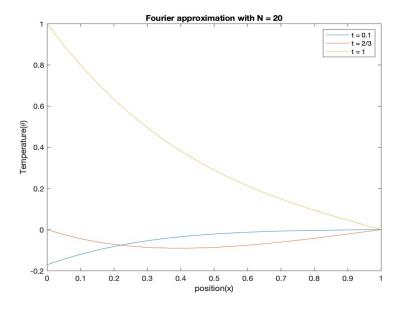


Figure 1.1: Fourier series solution at given times

(v) The convergence is sufficiently accurate as we used a truncated sum of the first 6 terms. By using a Fourier Sine Series we actually extended ϕ to $-1 \leqslant x \leqslant 1$, with ϕ odd, and computed its Fourier series. Since we have periodic boundary condition for ϕ , and by knowledge from Numerical Analysis II the N point Fourier approximation of an analytic periodic function converges at spectral speed. i.e. the error is $O(N^{-p})$, for any $p=1,2,3\cdots$.

(vi) The evolution of temperature in space consists with the second law of Thermodynamics. The heat flows from the hot spot to the cold spot. By the Fourier law of heat conduction, the heat flux is proportional to the temperature difference when the length of material is fixed, i.e. we have

$$q = -D\nabla\theta$$

, where D is the diffusivity, which is a positive constant. The rate of change of the internal energy is proportional to that of the temperature by

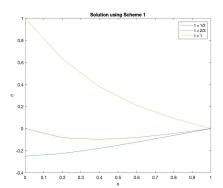
$$\frac{\partial E}{\partial t} = \rho c \frac{\partial \theta}{\partial t}$$

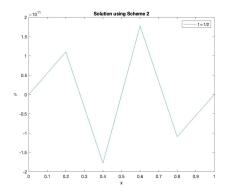
where ρ is the density and c is the specific heat capacitance. Both are positive constants. Then from conservation of energy and divergence theorem, after rescaling, we reach the diffusion equation as given. The time evolution is due to the initial condition at x=0. When $t\leqslant \frac{2}{3}$, the hot spot is x=1. Otherwise it is x=0. So the direction of heat flow is right to left before $t=\frac{2}{3}$ and is left to right after that. As time goes by, the left end is heated up and the temperature rises quadratically with time. But the temperature still drops fast close to the right end.

2 Numerical Methods

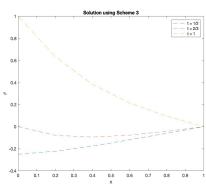
Question 2

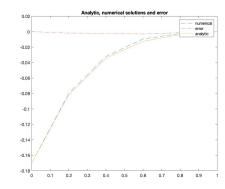
(i) On next page. v = 1/2 in each case.



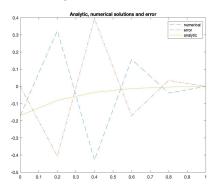


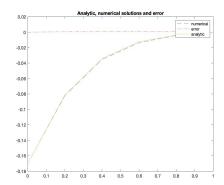
(a) Figure 2.1: numerical solutions with (b) Figure 2.2: numerical solutions with scheme 1 at given times $\begin{array}{c} \text{scheme 2 at given times} \\ \end{array}$





(c) Figure 2.3: numerical solutions with (d) Figure 2.4: Analytic, numerical soluscheme 3 at given times tion and error of scheme 1 at t=0.1





(e) Figure 2.5: Analytic, numerical solution and error of scheme 2 at t=0.1 tion and error of scheme 3 at t=0.1

•	u1	e1	u2	e2	u3	e3	analytic
x = 0	-0.1700	0.0000	-0.1700	0.0000	-0.1700	0.0000	-0.1700
x = h	-0.0798	-0.0018	0.3248	-0.4064	-0.0821	0.0005	-0.0816
x = 2h	-0.0322	-0.0022	-0.4292	0.3949	-0.0353	0.0010	-0.0343
x = 3h	-0.0094	-0.0031	0.1576	-0.1701	-0.0135	0.0010	-0.0125
x = 4h	-0.0024	-0.0013	-0.0388	0.0351	-0.0043	0.0006	-0.0037
x = 1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 1: analytic, numerical solutions and errors

- (ii) A few more plots were made by considering different values of ν and ρ .
- (iii) Firstly, we analyze the stability of each scheme. A more precise definition of stability is that the norm of \underline{u}^m is uniformly bounded for all m. We define the Fourier Transform(FT) of a series: $\hat{u}^m = \sum_{n \in \mathbb{Z}} e^{-in\theta} u_n^m$. Then by Parseval's theorem, Fourier Transform preserves the norm. In scheme 1 and 3, after taking FT of the whole equation, we obtain equations of the form: $u^{m+1} = H(\theta)u^m$. And clearly we need $\|H(\theta)\|\leqslant 1, \forall \ |\theta|\leqslant \pi.$

Specifically, in scheme 1 we have $H(\theta) = 1 - 4\nu \sin^2(\frac{\theta}{2})$ and in scheme 3 we have

$$H(\theta) = 1 - \frac{4\nu \sin^2 \frac{\theta}{2}}{1 + 4\nu\rho \sin^2 \frac{\theta}{2}}$$

Therefore, For scheme 1 to be stable, we need $\nu \leqslant \frac{1}{2}$. For scheme 3 to be stable, we need $\nu \leqslant \frac{1}{2(1-2\rho)}$.

Scheme 2 is different as we need to solve a difference equation of second order and make sure both of its roots have absolute value ≤ 1 . The two roots are

$$-4\nu\sin^2(\frac{\theta}{2}) \pm \sqrt{16\nu^2\sin^4(\frac{\theta}{2}) + 1}$$

And the minus root has an absolute value greater than 1 when $\sin(\frac{\theta}{2}) = 1$ for all positive ν . Consequently, the scheme is not stable for all positive ν , as we can see from 2b

The order of each scheme is calculated by Taylor expansion about about u(nh, mk). The we consider the coefficient of leading order term.

Scheme 2 has order 4 for any values of ν . Since the coefficient of h^4 is $\frac{\nu(6\nu-1)}{12}$, scheme 1 has order 4 unless $\nu=\frac{1}{6}$, at which value the order is 6. Similarly, since the coefficient is $\frac{\nu((6(1-2\rho))\nu-1)}{12}$, scheme 3 has order 4 unless $\nu=\frac{1}{6(1-2\rho)}$, at which the

order is 6 again.

Particularly, in scheme 3 we have the additional parameter ρ . From the previous stability analysis, if $\rho=1/2$, this scheme is stable for all positive ν . However, the order of accuracy cannot be higher than h^4 as ν is supposed to be a bounded positive constant. With $\rho=1/2$, if we fix $k=\mu$ instead, then the stability is preserved for all positive μ as $\mu=h\nu$. We cannot gain the same accuracy as the order is dropped to 3, unless when

$$\frac{\mu(\mu^2 - \frac{1}{4})}{6} = 0$$

, i.e. $\mu = 1/2$ when the order is 4.

(iv) The 3rd scheme is the most suitable. Since Scheme 2 is unstable, we exclude it first. The order of scheme 1 and 3 are the same but 3 has better stability with specific parameters. Therefore, we choose scheme 3 with appropriate parameters. The Courant number should be large enough that the time step is not too small, and such that a large time can be reached within a manageable number of iterations. Therefore, we choose v = 100 and thus $\rho = \frac{1}{2}*(1 - \frac{1}{6}*0.01)$ to maximize the order. The choice of N is relevant to the cost of computation. The computational cost is of order $\mathcal{O}((M-1)*(N-1))$. In each iteration, we solve the linear system

$$Lu^{m+1} = R(u^m + c)$$

with L being a band matrix of bandwidth 1. Therefore the computational cost is $\mathcal{O}(N-1)$. Therefore, we obtain the order of cost as claimed. Then, if we choose t=100 and N=100. The total operation count is of order $\mathcal{O}(10^4)$, which is manageable by the computer.

We can see in the final figure that the error is indeed small as expected.

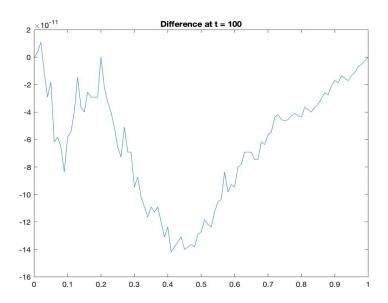


Figure 2.7: Difference between the numerical solution of scheme 3 with parameters as suggested at t=100

A Codes

A.1 P1

```
t = input('Enter_a_time_t');
N = input('Enter_a_truncation_number_N');
h = input('Enter_a_space_interval_size_h');
x = 0.0:h:1;

for i = 1:length(t)
    y = Theta(x,t(i),N);
    plot(x,y)
    hold on
end
legend('t_=0.1','t_=2/3', 't_=1')
xlabel position(x)
ylabel Temperature(\theta)
function phi = phi(x,t,N)
```

```
\begin{split} &g = @(n,x,t) \ 4*(1-3*t)*(n^3*\textbf{pi}^3)^-1+12*(n^5*\textbf{pi}^5)^-1 \ \dots \\ &-(4*(1+3*(n^2*\textbf{pi}^2)^-1)*(n^3*\textbf{pi}^3)^-1)*\textbf{exp}(-n^2*\textbf{pi}^2*t); \\ &\textbf{sum} = 0; \\ &\textbf{for} \ i = 1:N \\ & \textbf{sum} = \textbf{sum} + g(i,x,t)*\textbf{sin}(i*\textbf{pi}*x); \\ &\textbf{end} \\ &phi = \textbf{sum}; \\ &\textbf{end} \\ \end{split}  & \textbf{function} \ Theta = Theta(x,t,N) \\ & theta = @(x,t,N) \ phi(x,t,N)+(3*t-2)*t*(1-x); \\ & Theta = \textbf{zeros}(1,\textbf{length}(x)); \\ & \textbf{for} \ j = 1:\textbf{length}(x) \\ & Theta(j) = theta(x(j),t,N); \\ & \textbf{end} \\ & \textbf{end} \\ \end{split}
```

A.2 P2

```
xmax = 1;
N = input('Enter_a_value_for_N');
h = xmax/N;
x = 0:h:xmax;
v = input('Enter_a_value_for_the_Courant_number');
k = v*h^2;
tmax = input('Enter_a_representative_time');
choice = input('Choose_a_scheme');
t = 0:k:tmax;
I = input('Draw_the_asymptotic_limit?_If_yes_enter_0');
theta0 = zeros(N-1,1);
thetaL = @(t) t*(3*t-2);
thetaR = 0;
A = \mathbf{zeros}(N-1);
A(1,1) = -2; A(N-1,N-1) = -2;
A(1,2) = 1; A(N-1,N-2) = 1;
\mathbf{for} \quad i = 2:N-2
    A(i, i-1) = 1;
    A(i,i) = -2;
    A(i, i+1) = 1;
end
A = \mathbf{sparse}(A);
H1 = \mathbf{sparse}(\mathbf{eye}(N-1)+v*A);
U1 = iter1(H1, v, theta0, thetaL, thetaR, N, tmax, k);
U2 = iter 2 (A, v, theta0, thetaL, thetaR, N, tmax, k);
rho = input('enter_a_value_for_rho');
L = \mathbf{sparse}(\mathbf{eye}(N-1)-\mathbf{rho}*\mathbf{v}*A);
R = \mathbf{sparse}(\mathbf{eye}(N-1)+(1-\mathbf{rho})*\mathbf{v}*A);
U3 = iter3 (L,R,v,rho,theta0,thetaL,thetaR,N,tmax,k);
l = length(U1(1,:));
a = thetaL(tmax);
u1 = [a; U1(:, 1); 0];
u2 = [a; U2(:, 1); 0];
u3 = [a; U3(:,1); 0];
f = \lim(x, tmax);
```

```
if choice = 1
    plot(x, u1, 'LineStyle', '---')
    hold on
else
    if choice == 2
         plot(x, u2, 'LineStyle', '---')
         hold on
    else
         plot(x, u3, 'LineStyle', '---')
         hold on
    end
end
xlabel x
ylabel \theta
if I = 0
    \mathbf{plot}(x, f);
end
function U = iter1 (H, v, theta0, thetaL, thetaR, N, tmax, k)
 M = \mathbf{round}(tmax/k+1);
  U = zeros(N-1,M);
  b = zeros(N-1,M);
  U(:,1) = theta0;
  for m = 1:M-1
      b(1,m) = thetaL((m-1)*k);
      b(N-1,m) = thetaR;
      U(:,m+1) = H*U(:,m) + v*b(:,m);
  end
end
\textbf{function} \ U = iter2\left(A, v, theta0, thetaL, thetaR, N, tmax, k\right)
 M = round(tmax/k+1);
  U = zeros(N-1,M);
  b = zeros(N-1,M);
  U(:,1) = theta0;
  U(:,2) = U(:,1) + v*A*U(:,1) + v*b(:,1);
  b(1,1) = thetaL(0);
  b(N-1,1) = thetaR;
  for m = 2:M-1
      b(1,m) = thetaL((m-1)*k);
```

```
b(N-1,m) = thetaR;
  end
  for m = 2:M-1
      U(:,m+1) = 2*v*A*U(:,m) + U(:,m-1) + 2*v*b(:,m);
  end
end
function U = iter3(L,R,v,rho,theta0,thetaL,thetaR,N,tmax,k)
 M = round(tmax/k+1);
  U = zeros(N-1,M);
  b = zeros(N-1,M);
  U(:,1) = theta0;
  for m = 1:M
      b(1,m) = thetaL((m-1)*k);
      b(N-1,m) = thetaR;
  end
  for m = 1:M-1
      U(:,m+1) = L \setminus (R*U(:,m) + (1-rho)*v*b(:,m) + rho*v*b(:,m+1));
  end
\mathbf{end}
function f = \lim(x, \max)
  alpha = @(x) -x*(x-2)*(x-1);
  beta = @(x) -0.05*x*(x-1)*(x-2)*(x+2)*(x-4);
  f = zeros(1, length(x));
  for i = 1: length(x)
     f(i) = (3*tmax-2)*tmax*(1-x(i))+alpha(x(i))*tmax+beta(x(i));
  end
end
```