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Application of Chebyshev collocation method to solving the heat equation

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Investigating various problems in mathematics and physics it is often necessary to solve a partial differential equation of the following form

$$\frac{\partial y(x,t)}{\partial t} = f\left(t, x, y, \frac{\partial y}{\partial x}, \ldots, \frac{\partial^n y}{\partial x^n}\right), \qquad -1 < x < 1, \qquad 0 < t < \infty \quad (1)$$

with rather complicated function f.

Problems on other finite interval $a < \xi < b$ may trivially be reduced onto the standard interval $-1 < x < 1$ by mapping

$$x = \frac{2\xi - a - b}{b - a}. \quad (2)$$

Equation (1) must be supplemented with an initial condition

$$y(x, 0) = y_0(x)$$

and appropriate boundary conditions.

Sometimes, in particular cases, a method of separation of variables may be used for solving equation (1). According to this method we look for a solution as a product

$$y(x,t) = a(t)\, b(x).$$

If a solution is parametrized by a natural number n, then

$$y(x,t) = \sum_{n=0}^{\infty} a_n(t)\, b_n(x).$$

In reality we cannot calculate an infinite series, hence calculations are done using a finite sum

$$y(x,t) = \sum_{n=0}^{M} a_n(t)\, b_n(x), \quad (3)$$

where a number M is determined by the demanding accuracy.

For example, let us consider the heat equation

$$\frac{\partial y(x,t)}{\partial t} = \frac{\partial^2 y(x,t)}{\partial x^2}, \qquad -1 < x < 1, \qquad 0 < t < \infty \tag{4}$$

with very simple boundary and initial conditions

$$x = -1: \qquad y = 1, \tag{5}$$

$$x = +1: \qquad y = 0, \tag{6}$$

$$t = 0: \qquad y = 0. \tag{7}$$

In this case

$$y(x,t) = \sum_{n=0}^{\infty} \exp\left(-\mu_n^2 t\right) (C_n \cos \mu_n x + D_n \sin \mu_n x),$$

where

$$\mu_n = n\pi.$$

It is convenient to separate a linear part of a solution. Thus, we finally obtain the solution of the heat equation (4) satisfying the boundary and initial conditions (5)–(7):

$$y - \frac{1}{2}(1-x) = -\sum_{n=1}^{M} \frac{2}{n\pi} \exp\left(-n^2\pi^2 t\right) \sin\left[\frac{n\pi}{2}(x+1)\right]. \tag{8}$$

When the right–hand side of equation (1) is complicated, this equation should be solved numerically. A Chebyshev collocation method [2] is very effective in this case. If we consider the complicated mathematical problem and use complicated numerical method to obtain its solution, at first we must consider the partial case, namely, the test problem which can be solved analytically. Thus, we can verify does this numerical method work, what is its accuracy and how much time does it need for its realization?

To illustrate the possibility of Chebyshev collocation method we shall solve the same boundary value problem for the heat equation using this method. The solutions (8) and (9) allow us to compare results obtained by two different methods and to answer the abovementioned questions.

Now we seek a solution in the form

$$y(x,t) = \sum_{n=0}^{N} a_n(t)\, T_n(x), \tag{9}$$

where $T_n(x)$ are the Chebyshev polynomials of the first kind. A difference between equations (3) and (9) is as follows. Equation (4) is satisfied by the whole sum (9), while every term of the sum (3) is a solution of this equation. In the first stage of solving the problem both the functions $a_n(t)$ and $b_n(x)$ in equation (3) are unknown, later on they are found from equation (4) which is satisfied at all times $t > 0$ and at all points of an interval $(-1, 1)$. In equation (9) functions $a_n(t)$ are unknown, but the Chebyshev polynomials $T_n(x)$ are set from the very beginning. Equation (1) must be satisfied by the sum (9) at all times $t > 0$, but only at some points of an interval $(-1, 1)$ called the collocation points. How many collocation points should be choosen and how should they be placed in the interval (-1,1)? As we consider a sum from $n = 0$ to $n = N$, we have $N + 1$ coefficients a_n. Two boundary conditions lead to two equations for a_n. Hence, there should be $N - 1$ collocation points. The best choice of collocation points is a choice of zeros of the corresponding Chebyshev polynomial.

Here we recall some results concerning the Chebyshev $T_n(x)$ and Gegenbauer $G_n^\lambda(x)$ polynomials which are used in the following.

The Chebyshev polynomials are orthogonal over the interval $(-1, 1)$ with respect to a weight function $w(x) = \dfrac{1}{\sqrt{1-x^2}}$ [3]:

$$\int_{-1}^{1} T_m(x)\, T_n(x)\, \frac{dx}{\sqrt{1-x^2}} = \begin{cases} 0 & m \neq n \\ \pi & m = n = 0 \\ \dfrac{\pi}{2} & m = n \neq 0 \end{cases}$$

The first two Chebyshev polynomials are

$$T_0(x) = 1, \qquad T_1(x) = x, \tag{10}$$

other can be obtained from the recurrence equation

$$T_{n+1}(x) = 2x T_n(x) - T_{n-1}(x). \tag{11}$$

We also need some properties of the Gegenbauer polynomials $G_n^\lambda(x)$ which are orthogonal over the interval $(-1, 1)$ with respect to a weight function depending on the parameter λ, i.e. $w(x) = (1 - x^2)^{\lambda - 1/2}$:

$$\int_{-1}^{1} G_m^\lambda(x)\, G_n^\lambda(x)\, (1-x^2)^{\lambda-1/2}\, dx =$$

$$= \begin{cases} 0 & m \neq n \\ \dfrac{\sqrt{\pi}\, \Gamma(\lambda + 1/2)\, \Gamma(2\lambda + n)}{(n+\lambda)\, n!\, \Gamma(\lambda)\, \Gamma(2\lambda)} & m = n \end{cases}$$

where $\Gamma(x)$ is the gamma function.

The recurrence equation

$$(n+1)\,G_{n+1}^{\lambda}(x) = 2(n+\lambda)x\,G_n^{\lambda}(x) - (n+2\lambda-1)\,G_{n-1}^{\lambda}(x) \tag{12}$$

is fulfilled with

$$G_0^{\lambda}(x) = 1, \qquad G_1^{\lambda}(x) = 2\lambda x. \tag{13}$$

The Gegenbauer polynomials allow us to calculate the derivatives of the Chebyshev polynomials according to the relation [1]

$$\frac{d^m T_n(x)}{dx^m} = 2^{m-1}(m-1)!\,n\,G_{n-m}^m, \qquad n \geq m. \tag{14}$$

Thus, using equations (12) and (14) we can obtain the recurrence equation for the mth derivative of the Chebyshev polynomials

$$\frac{d^m T_{n+m+1}}{dx^m} = 2x\frac{n+m+1}{n+1}\frac{d^m T_{n+m}}{dx^m} -$$

$$-\frac{(n+m+1)(n+2m-1)}{(n+m-1)(n+1)}\frac{d^m T_{n+m-1}}{dx^m}. \tag{15}$$

The following formulae are useful to satisfy the boundary conditions at $x = \pm 1$

$$T_n(\pm 1) = (\pm 1)^n, \tag{16}$$

$$T_n'(\pm 1) = (\pm 1)^{n+1} n^2, \tag{17}$$

$$T_n''(\pm 1) = (\pm 1)^n \frac{1}{3} n^2 (n^2-1), \tag{18}$$

$$T_n'''(\pm 1) = (\pm 1)^{n+1} \frac{1}{15} n^2 (n^2-1)(n^2-4), \tag{19}$$

and generally

$$\frac{d^m T_n(\pm 1)}{dx^m} = (\pm 1)^{n+m} 2^{m-1} n \frac{(n+m-1)!\,(m-1)!}{(n-m)!\,(2m-1)!}, \qquad n \geq m. \tag{20}$$

From the boundary conditions (5), (6) and formulae (9) and (16) we have two equations

$$\sum_{n=0}^{N} (-1)^n a_n = 1,$$

$$\sum_{n=0}^{N} a_n = 0$$

or after differentiation with respect to t

$$\sum_{n=0}^{N}(-1)^n \frac{da_n}{dt} = 0, \tag{21}$$

$$\sum_{n=0}^{N} \frac{da_n}{dt} = 0. \tag{22}$$

Next, we introduce equation (9) into the heat equation (4) and (as there are $N+1$ unknown coefficients a_n, $n = 0, 1, \ldots, N$) demand that this equation is satisfied at $N-1$ points ξ_j

$$\sum_{n=0}^{N} \frac{da_n}{dt} T_n(\xi_j) = \sum_{n=0}^{N} a_n\, T_n''(\xi_j), \qquad j = 1, 2, \ldots, N-1. \tag{23}$$

A particularly convenient choice for the collocation points ξ_j is

$$\xi_j = \cos\frac{\pi j}{N}, \qquad j = 1, 2, \ldots, N-1. \tag{24}$$

Considering $N-1$ equations (23) and two equations (21) and (22) we obtain a system of $N+1$ linear equations with $N+1$ unknown functions da_n/dt. Solving this system with respect to da_n/dt we arrive at a system of ordinary differential equations

$$\frac{da_n}{\mathrm{d}t} = F_n(t, a_0, a_1, a_2, \ldots, a_N), \qquad n = 0, 1, 2, \ldots, N \tag{25}$$

with initial conditions

$$t = 0: \qquad a_n = 0. \tag{26}$$

The coefficients a_n are obtained as a numerical solution of equations (25). Table 1 represents the results of such a solution for various values of N.

Table 1

$N=8$	$t=0.5$	$t=1.0$
n	a_n	a_n
0	0.412796124597	0.474632083693
1	-0.498657645514	-0.499990388494
2	0.092264100976	0.026840649208
3	-0.001572884367	-0.000011262142
4	-0.005168470998	-0.001504446775
5	0.000245876899	0.000001760523
6	0.000109378559	0.000032075147
7	-0.000015347018	-0.000000109887
8	-0.000001133133	-0.000000361273

$N = 14$	$t = 0.5$	$t = 1.0$
n	a_n	a_n
0	0.412545689816	0.474536953303
1	-0.498697819610	-0.499990640845
2	0.092529648555	0.026941304489
3	-0.001525648034	-0.000010965284
4	-0.005184082247	-0.001510088512
5	0.000238557511	0.000001714586
6	0.000109903616	0.000032189902
7	-0.000015648596	-0.000000112472
8	-0.000001163050	-0.000000361681
9	0.000000571894	0.000000004111
10	0.000000003108	0.000000002510
11	-0.000000013380	-0.000000000096
12	0.000000000211	-0.000000000012
13	0.000000000215	0.000000000002
14	-0.000000000008	0.000000000000

Table 2 contains comparison between results obtained from equations (8) and (9) for various times having used the values of coefficients a_n listed in Table 1.

Table 2

$t = 0.5$

x	Exact	Approximate $N = 8$	Approximate $N = 14$
-1.0	1.000000	1.000000	1.000000
-0.8	0.841362	0.841519	0.841397
-0.6	0.688849	0.689158	0.688915
-0.4	0.547836	0.548288	0.547926
-0.2	0.422338	0.422908	0.422443
0.0	0.314611	0.315253	0.314720
0.2	0.225029	0.225678	0.225132
0.4	0.152191	0.152774	0.152278
0.6	0.093203	0.093645	0.093266
0.8	0.044053	0.044290	0.044086
1.0	0.000000	0.000000	0.000000

$t = 1.0$

	Exact	Approximate	
x		$N = 8$	$N = 14$
-1.0	1.000000	1.000000	1.000000
-0.8	0.883307	0.883382	0.883320
-0.6	0.768250	0.768393	0.768275
-0.4	0.656307	0.656503	0.656340
-0.2	0.548644	0.548875	0.548684
0.0	0.446011	0.446255	0.446053
0.2	0.348664	0.348895	0.348703
0.4	0.256338	0.256535	0.256371
0.6	0.168282	0.168425	0.168306
0.8	0.083326	0.083402	0.083339
1.0	0.000000	0.000000	0.000000

Thus, the choice $N = 8$ ensures three accurate numbers, while the choice $N = 14$ ensures four accurate numbers.

Considering various physical problems (for example, phase transition – melting or solidification) it is often necessary to solve the heat equation

$$\frac{\partial y(\xi,t)}{\partial t} = \frac{\partial^2 y(\xi,t)}{\partial \xi^2}, \qquad 0 < t < \infty \tag{27}$$

in a domain with moving boundaries

$$a(t) < \xi < b(t). \tag{28}$$

Equations (27) and (28) must be supplemented with initial condition

$$y(\xi, 0) = y_0(\xi), \tag{29}$$

$$a(0) = a_0, \qquad b(0) = b_0 \tag{30}$$

and appropriate boundary conditions

$$y(a(t), t) = \varphi(t), \tag{31}$$

$$y(b(t), t) = \psi(t). \tag{32}$$

It is convenient to reduce the problem on the interval $a(t) < \xi < b(t)$ onto the standard interval $-1 < x < 1$ by mapping (compare equations (2) and (33))

$$x = \frac{2\xi - a(t) - b(t)}{b(t) - a(t)}, \tag{33}$$

but the heat equation (27) becomes more complicated

$$\frac{\partial y(x,t)}{\partial t} = \frac{4}{[b(t)-a(t)]^2}\frac{\partial^2 y(x,t)}{\partial x^2} -$$

$$-\frac{\partial y(x,t)}{\partial x}\left[\frac{b'(t)+a'(t)}{[b(t)-a(t)]^2} + x\frac{b'(t)-a'(t)}{b(t)-a(t)}\right], \tag{34}$$

$$-1 < x < +1 \qquad 0 < t < \infty.$$

For simplicity we consider a linearly expanding domain with

$$a(t) = -(1+vt), \qquad b(t) = 1+vt \tag{35}$$

and supplement the transformed heat equation (34) by the same simple boundary and initial conditions as in the previous problem with constant boundaries:

$$x = -1: \qquad y = 1, \tag{36}$$

$$x = +1: \qquad y = 0, \tag{37}$$

$$t = 0: \qquad y = 0. \tag{38}$$

The coefficients a_n of the Chebyshev sum (9) are obtained as a numerical solution of corresponding system of ordinary differential equations similar to the system (25) but with more complicated functions F_n.

Tables 3 represents the results of such a solution with $N = 16$ for various values of t and corresponds to the velocity $v = 5$.

Table 3

$N = 16$	$t = 0.1$	$t = 1.0$
n	a_n	a_n
0	0.304746800768	0.455985145231
1	-0.495629137273	-0.612872714879
2	0.245560188273	0.077222759271
3	-0.033553081825	0.151006409048
4	-0.049029440250	-0.052603118874
5	0.036163171329	-0.049873114893
6	-0.004675005264	0.028412230652
7	-0.007206358867	0.014630234545
8	0.004224405734	-0.012466451534
9	-0.000016098813	-0.003378723310
10	-0.000909251302	0.004555939254
11	0.000309554294	0.000503068237
12	0.000077377939	-0.001398454299
13	-0.000077705466	0.000016787663
14	0.000008807871	0.000393560915
15	0.000009656620	-0.000031946410
16	-0.000003883770	-0.000101610617

Table 4 shows the values of the function $y(x,t) = \sum_{n=0}^{N} a_n(t)T_n(x)$ for $v = 5$ and various values of time t.

Table 4

$t = 0.1$

x	ξ	y
-1.0	-1.5	1.0000000000
-0.8	-1.2	0.8382833986
-0.6	-0.9	0.5525618355
-0.4	-0.6	0.2654931598
-0.2	-0.3	0.0886136651
0.0	0.0	0.0200305208
0.2	0.3	0.0032220022
0.4	0.6	0.0007344405
0.6	0.9	0.0004725351
0.8	1.2	0.0002169918
1.0	1.5	0.0000000000

$t = 1.0$

x	ξ	y
-1.0	-6.0	1.0000000000
-0.8	-4.8	0.9987012753
-0.6	-3.6	0.9802912902
-0.4	-2.4	0.8770675672
-0.2	-1.2	0.6109958900
0.0	0.0	0.2788310198
0.2	1.2	0.0737838302
0.4	2.4	0.0105157857
0.6	3.6	0.0008418829
0.8	4.8	0.0000095677
1.0	6.0	0.0000000000

Previous experience testifies that the choice $N = 16$ ensures four of five accurate numbers of the solution.

References

[1] Bateman H., Erdélyi A., *Higher Transcendental Functions.* Vol. 2, McGraw–Hill, New York, 1953.

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