Solving PDEs using Spectral Methods in the Chebyshev basis

by example of the Heat Equation

Special Topic on APPROXIMATION OF FUNCTIONS

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Abstract

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1 Introduction

Let $\mathbb{N}$ denote the nonnegative integers, so $0 \in \mathbb{N}$.

1.1 Definition: Chebyshev polynomial

Chebyshev[1] polynomials $T_k : \mathbb{R} \mapsto \mathbb{R}$ are functions satisfying

$$T_k(x) = T_k(\cos\theta) := \cos(k\theta) = \frac{1}{2}(z^k + z^{-k})$$
$$z := \mathrm{e}^{i\theta}, \quad x := \mathfrak{Re}(z) = \cos(\theta) = \frac{1}{2}(z + z^{-1})$$

for $k \in \mathbb{N}$. Then, $T_0(x) = 1$, $T_1(x) = x$, $T_2(x) = 2x^2 - 1$, and so on.

These relations between x, z and θ reveal fundamental connections between three famous basis sets (as we will confirm later): CHEBYSHEV, LEGENDRE and FOURIER.

1.1 Theorem: Chebyshev Recursion Formula

The Chebyshev polyomials satisfy the three-term recurrence relation

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)\,.$$

[1] named after Pafnuty Lvovich CHEBYSHEV, alternatively transliterated as Tchebycheff, Tchebyshev (French) or Tschebyschow (German)

Proof. Theorem 1.1 For $k > 1$,

$$\begin{aligned}
2xT_k(x) - T_{k-1}(x) &= 2x\frac{1}{2}(z^k + z^{-k}) - \frac{1}{2}(z^{k-1} + z^{-(k-1)}) \\
&= 2\frac{1}{2}(z + z^{-1})\frac{1}{2}(z^k + z^{-k}) - \frac{1}{2}(z^{k-1} + z^{-k+1}) \\
&= \frac{1}{2}(z^{k+1} + z^{k-1} + z^{-k+1} + z^{-k-1}) - \frac{1}{2}(z^{k-1} + z^{-k+1}) \\
&= \frac{1}{2}(z^{k+1} + z^{-(k+1)}) = T_{k+1}(x)
\end{aligned}$$

□

The Chebyshev polynomials also satisfy an *orthogonality relation*,

$$\langle T_m, T_n \rangle := \int_{-1}^{1} T_m(x)T_n(x)\frac{1}{\sqrt{1-x^2}}\mathrm{d}x = \int_{\pi}^{0} \cos(m\theta)\cos(n\theta)\frac{-\sin(\theta)}{\sqrt{1-\cos^2(\theta)}}\mathrm{d}\theta\,,$$

which becomes, with the fitting substitution $x = \cos(\theta)$ and $\mathrm{d}x = -\sin(\theta)\mathrm{d}\theta$,

$$\begin{aligned}
\langle T_m, T_n \rangle &= \int_0^{\pi} T_m(\cos\theta)T_n(\cos\theta)\frac{\sin\theta}{\sin\theta}\mathrm{d}\theta = \int_0^{\pi} \cos(m\theta)\cos(n\theta)\mathrm{d}\theta \\
&= \frac{1}{2}\int_0^{\pi} \Big(\underbrace{\cos((m+n)\theta)}_{=\cos(2m\theta)\text{ for }m=n} + \underbrace{\cos((m-n)\theta)}_{=1\text{ for }m=n} \Big)\mathrm{d}\theta
\end{aligned}$$

along with the knowledge that $\int_0^{\pi} \cos(k\theta)\mathrm{d}\theta = k^{-1}\left[\sin(k\theta)\right]_0^{\pi} = 0$ for $k \in \mathbb{Z}\backslash\{0\}$,

$$\langle T_m, T_n \rangle = \int_0^{\pi} T_m(\cos\theta)T_n(\cos\theta)\mathrm{d}\theta = \begin{cases} 0 & \text{for } m \neq n \\ \pi/2 & \text{for } m = n \neq 0 \\ \pi & \text{for } m = n = 0 \end{cases}$$

which can be effectively utilised to define a function space $(\mathcal{T}, +, \cdot)$ in the *orthogonal* basis of Chebyshev polynomials $\mathcal{T} := \{T_k\}_{k\in\mathbb{N}}$. Note that the operation $\langle\cdot,\cdot\rangle$ satisfies all axioms of an authentic inner product (linearity, etc.) over a function space due to the linearity of the integral.

In the following proceedings, we will restrict our view on functions over the interval $[-1, 1] \subset \mathbb{R}$. Any (real) Lipschitz-continuous function $f \in \mathcal{C}_L$, where $\mathcal{C}_L := \{g : [-1,1] \mapsto \mathbb{R} \mid \exists L \text{ s.t. } \forall x_1, x_2 \in \mathbb{R},\ |g(x_1) - g(x_2)| \leq L \cdot |x_1 - x_2|\}$ can be represented in the Chebyshev basis $\mathcal{T}$, as Lipschitz continuity is a sufficient condition for absolute and uniform convergence of the corresponding series representation

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x), \quad a_k \in \mathbb{R}, \quad k \in \mathbb{N}\,.$$

Utilising orthogonality, for any $f \in \mathcal{C}_L$, we find coefficients $a_l \in \mathbb{R}$ by 'right-multiplying' the equation $f = \sum_{k=0}^{\infty} a_k T_k$ with any one of the Chebyshev polynomials T_l.

$$\begin{aligned}
\langle f, T_l \rangle = \langle \sum_{k=0}^{\infty} a_k T_k, T_l \rangle &= \int_0^{\pi} a_k T_k(\cos\theta) T_l(\cos\theta) \mathrm{d}\theta \\
&= \sum_{k=0}^{\infty} a_k \langle T_k, T_l \rangle \quad \text{by linearity} \\
&= \begin{cases} a_0 \pi & \text{for } l = 0 \\ a_l \pi / 2 & \text{for } l \neq 0 \end{cases}
\end{aligned}$$

which can easily be rearranged to give explicit relations for a_0 and a_k

$$\begin{aligned}
a_0 &= \frac{1}{\pi} \langle f, T_0 \rangle = \frac{1}{\pi} \int_0^{\pi} f(\cos\theta) \mathrm{d}\theta \\
a_k &= \frac{2}{\pi} \langle f, T_k \rangle = \frac{2}{\pi} \int_0^{\pi} f(\cos\theta) \cos(k\theta) \mathrm{d}\theta, \quad k \neq 0 \,.
\end{aligned}$$

Dealing with a numerical problem, we shall approximate the above two integrals by the rectangular integral rule. Another proof for the explicit coefficient integrals can be found in Trefethen 2019.

1.2 Theorem: Rectangular integral rule

$$\int_a^b f(x) \mathrm{d}x = \lim_{N \to \infty} \frac{b-a}{N} \sum_{k=0}^{N} f(x_k), \quad x_k := a + \frac{b-a}{N} k$$

Bonthuis and Schachinger 2021, p. 128

Most importantly, this quadrature-style integral approximation is only one way of numerically determining the coefficients a_k. Another is to recognise the structure of the above integral for $k \neq 0$ as a cosine transform of the function $(f \circ \cos)$.

1.2 Definition: Cosine Transform

1.3 Definition: Discrete Cosine Transform

Most significantly, this approach via the Discrete Cosine Transform can be sped up by means of the *Fast Fourier Transform* (Cooley and Tukey 1965).

Numerically speaking, a significant improvement to these two approaches can be made by using the *Barycentric interpolation formula in Chebyshev points*.

1.4 Definition: Chebyshev points

From the equispaced points

$$\Theta := \{\theta_j := jN/\pi \mid j = 0, ..., N\} ,$$

we can further define the Chebyshev points as the corresponding $\cos(\theta_j)$,

$$X := \{x_j := \cos(\theta_j) \mid \theta_j \in \Theta\} .$$

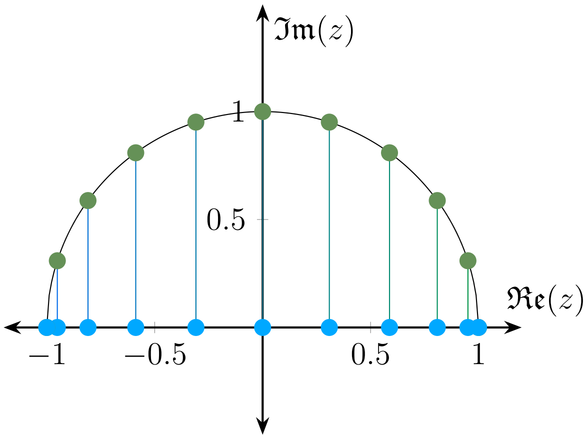

Figure 1: The Chebyshev points $\{x_j = \cos(\theta_j)\}$ are projections of the equispaced points $\{\theta_j\}$ on the unit circle onto the x-axis.

One way of forcing the boundary conditions, at least the first that came to my mind when thinking of this issue, is to pin down the two highest-order coefficients in the series representation.

2 The heat equation and its solution

3 Differentiation

4 Results

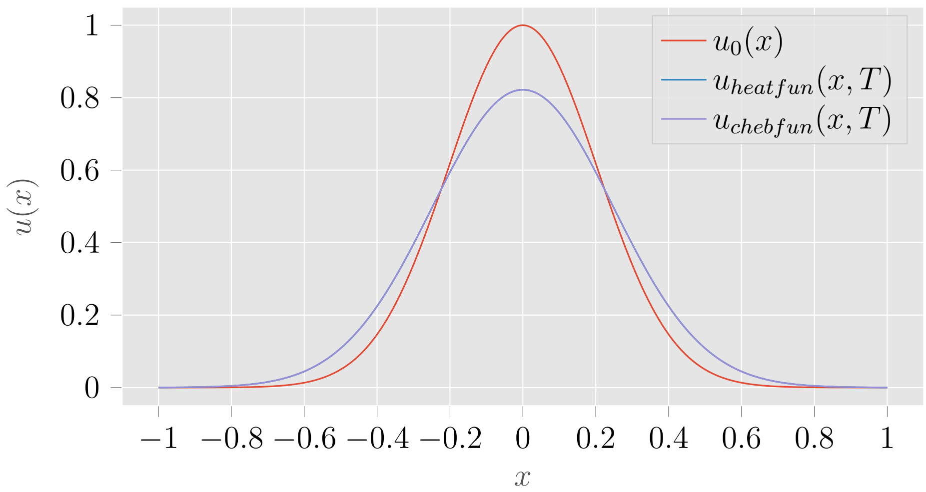

Figure 2: Comparison of heatfun and chebfun

5 Discussion

References

Bonthuis, Douwe and Ewald Schachinger (2021). *Lecture Notes in Computational Physics*. Institute of Theoretical and Computational Physics, Technical University of Graz.

Cooley, James W. and John W. Tukey (1965). 'An algorithm for the machine calculation of complex Fourier series'. In: *Mathematics of Computation* 19, pp. 297–301. DOI: 10.2307/2003354.

Trefethen, Lloyd N. (2019). *Approximation Theory and Approximation Practice, Extended Edition*. Philadelphia, PA: Society for Industrial and Applied Mathematics. DOI: 10.1137/1.9781611975949. eprint: https://epubs.siam.org/doi/pdf/10.1137/1.9781611975949.

A Title of Appendix

Appendices are definitely not necessary and assessors are not obliged to read them so only use them for non-vital text, figures or calculations.