The tau-method

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Abstract

The tau-method is an extensive technique for enforcing very general boundary conditions as well as continuity across cells in numerical methods. It is the technique employed by `Dedalus`, a parallelised software for spectral methods, and is implicitly utilized in the ultraspherical method of Olver and Townsend. In these notes we give a numerical linear algebra perspective on how to implement a tau-method which may be helpful for beginners to build an intuition.

This is a memo, i.e. notes on a mathematical topic that the author has encountered. These notes are not peer-reviewed and may contain errors. If you find any, please let me know!

1 Introduction

Discretizing a linear partial differential equation (PDE) with a spectral method typically leads to a square linear system. The boundary conditions of the original PDE are then added as additional constraints: one per boundary condition. Hence, one arrives at an overdetermined (more rows than columns) system. The tau-method remedies this issue by introducing as many new unknowns as equations. Hence, the discretization matrix gains new columns and the linear system becomes square once more.

The tau-method is dated back to Lanczos [3] and Ortiz [5]. More modern techniques, often referred to as *generalized* tau-methods [1], are an area of active research. There is no systematic methodology of choosing the τ-functions for enforcing the boundary conditions; this fact is reflected in the implementation setup of `Dedalus`, where it is the responsibility of the user to specify a choice [2].

Given a linear PDE, the tau-method appends the PDE with τ-functions which are polynomials. By doing so, one ensures that the augmented equation has polynomial solutions. The purpose of these notes is not to delve into the technical aspects of how tau-methods work, their conditioning, or attempt any unifying theory. Moreover, we emphasize that none of what follows is novel. The goal is to give a numerical linear algebra flavour that may be useful to any reader who is coding their first tau-method.

In these notes we solely focus on coefficient-based spectral methods. For linear ODEs/PDEs with (potentially spatially-varying) coefficients possessing high regularity, such methods typically lead to very *sparse* and almost-banded systems [2, 4].

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2 A simple Poisson problem

In this section, we assume that the reader has some familiarity with the ultraspherical method [4] and quasimatrices. Suppose we wish to solve the following Poisson's equation on the interval $[-1, 1]$:

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x) = f(x), \quad u(\pm 1) = 0. \tag{2.1}$$

We discretize (2.1) via the ultraspherical method. Consider the expansion of $u(x)$ in the Chebyshev polynomials of the first kind , $T_n(x)$, $n \in \mathbb{N}_0$, as well as an expansion of $f(x)$ in ultraspherical(2) polynomials, $C_n^{(2)}(x)$, $n \in \mathbb{N}_0$ [4, Sec. 3]:

$$u(x) = \mathbf{T}(x)\mathbf{u} \;\text{ and }\; f(x) = \mathbf{C}^{(2)}(x)\mathbf{f}. \tag{2.2}$$

Consider the truncation of the expansion at degree $N-1$. Let $\mathbf{T}_N(x)$ and $\mathbf{u}_N$ denote the truncation of the infinite-dimensional quasimatrix and vector at column and row N, respectively, i.e.

$$\mathbf{T}_N(x) \coloneqq \begin{pmatrix} T_0(x) & T_1(x) & \cdots & T_{N-1}(x) \end{pmatrix}, \tag{2.3}$$

$$\mathbf{u}_N \coloneqq \begin{pmatrix} u_0 & u_1 & \cdots & u_{N-1} \end{pmatrix}^\top. \tag{2.4}$$

Then the discretization of (2.1) may be rewritten in quasimatrix notation as

$$\mathcal{D}_N \mathbf{u}_N = \mathbf{f}_N, \quad \mathbf{T}_N(\pm 1)\mathbf{u}_N = 0, \tag{2.5}$$

where $\mathcal{D}_N \in \mathbb{R}^{N\times N}$ is [4, Sec. 3]

$$\mathcal{D}_N = \begin{pmatrix} 0 & 0 & 4 & & & & \\ & & & 6 & & & \\ & & & & 8 & & \\ & & & & & \ddots & \\ & & & & & & 2N+2 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}. \tag{2.6}$$

D_N is square (albeit singular) but only enforces the discretized PDE on the coefficients of the expansion but not the boundary conditions. Hence, the boundary conditions must be included as two additional constraints. We concatenate these two additional constraints as two rows at the top of the $\mathcal{D}_N$ leading to the rectangular system (two more rows than columns)

$$A_N \mathbf{u}_N = (0\; 0\; \mathbf{f}_N^\top)^\top, \quad A_N \coloneqq \begin{pmatrix} -1 & 1 & -1 & 1 & \cdots & (-1)^N \\ 1 & 1 & 1 & 1 & \cdots & 1 \\ & & \mathcal{D}_N & & & \end{pmatrix}. \tag{2.7}$$

In the ultraspherical method one truncates the final two rows of zeroes in A_N to form a square system once more and solves for $\mathbf{u}_N$. The spy plot of the truncated A_N is given in Fig. 1. This truncation has provably controllable conditioning [4, Thm. 4.5]. Note that for more general

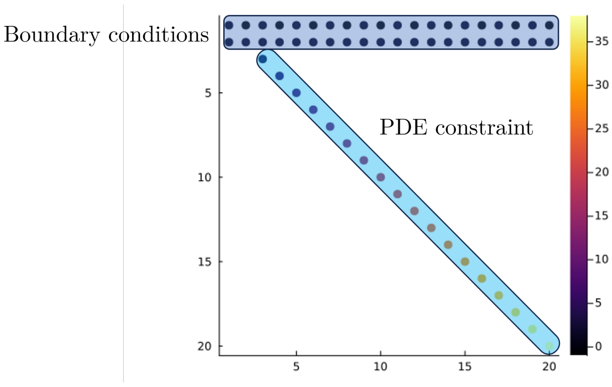


Figure 1: Spy plot of the truncated A_N as implemented in the ultraspherical method, $N = 19$.

ODEs, the last two rows will not necessarily have zero entries. It happens that the truncation of these final two rows is equivalent to using a tau-method to enforce the boundary condition where the two τ-functions (one for each boundary condition) are the polynomials $\tau_1(x) = C^{(2)}_{N-2}(x)$ and $\tau_2(x) = C^{(2)}_{N-1}(x)$.

The tau-method augments the equation in (2.1) with two polynomials multiplied by the unknown constants c_1 and c_2 forming the equation

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x) + c_1\tau_1(x) + c_2\tau_2(x) = f(x), \quad u(\pm 1) = 0. \tag{2.8}$$

By truncating the expansions of u and f at degree $N-1$ and picking the aforementioned τ-functions, the discretized problem now becomes to find the solution $(\mathbf{u}_N^\top \;\; c_1 \;\; c_2)^\top$ to the problem:

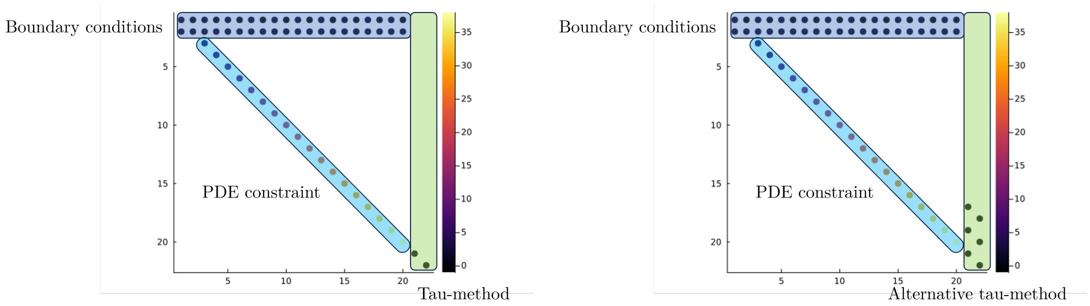
$$\begin{pmatrix} -1 & 1 & -1 & 1 & \cdots & (-1)^N & 0 & 0 \\ 1 & 1 & 1 & 1 & \cdots & 1 & 0 & 0 \\ & & & & & & \vdots & \vdots \\ & & \mathcal{D}_N & & & & 1 & 0 \\ & & & & & & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{u}_N \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \mathbf{f}_N \end{pmatrix}. \tag{2.9}$$

The spy plot of the linear system matrix is given in Fig. 2a. Since the final two rows of $\mathcal{D}_N$ are zero, it immediately follows that $c_1 = f_{N-2}$ and $c_2 = f_{N-1}$. Thus one may eliminate c_1 and c_2 from the linear system matrix. This results in removing the last two columns and rows and thus recovering the usual ultraspherical method linear system.

Suppose we picked different τ-functions, then we would have not been able to eliminate the final two rows and columns. For example, suppose that $\tau_1(x) = T_{N-2}(x)$ and $\tau_2(x) = T_{N-1}(x)$. Consider the connection matrix R such that $\mathbf{T}(x) = \mathbf{C}^{(2)}(x)R$. Then the discretization becomes

$$\begin{pmatrix} -1 & 1 & -1 & 1 & \cdots & (-1)^N & 0 & 0 \\ 1 & 1 & 1 & 1 & \cdots & 1 & 0 & 0 \\ & & \mathcal{D}_N & & & & (R\mathbf{e}^{N-1})_N & (R\mathbf{e}^N)_N. \end{pmatrix} \begin{pmatrix} \mathbf{u}_N \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \mathbf{f}_N \end{pmatrix}, \tag{2.10}$$

where $\mathbf{e}^n$ denotes the infinitely long vector of zeroes with a single one in the position n. The spy plot of the linear system matrix is given in Fig. 2b. Here the values of c_1 and c_2 cannot immediately deduced and one must solve the whole system (2.10) for the unknowns $\mathbf{u}_N$.



(a) τ-functions: $C^{(2)}_{N-2}(x)$ and $C^{(2)}_{N-1}(x)$.

(b) τ-functions: $T_{N-2}(x)$ and $T_{N-1}(x)$.

Figure 2: Spy plots of the tau-method column-augmented A_N, $N = 19$.

Remark 2.1 (Why not solve for the least-squares solution?)**.** *Indeed - why not? One may disperse with tau-methods entirely and simply find a least-squares solution to the overdetermined system. For this particular example, the least-squares solution is, in fact, equal to the normal ultraspherical solution.*

For more general problems, provided $N \gg 0$ is sufficiently large, then often the least-squares solutions are vanishingly close to the solution of discretization coupled with a working tau-method. For finite N, the least-squares solution is allowed to violate the boundary conditions. However, in general this violation tends quickly tends to machine precision for increasing N.

Nevertheless, there are disadvantages. Good choices of tau-methods allow one to recover banded and sparse systems (perhaps after utilizing a Schur complement factorization). Hence, one may develop optimal complexity solvers with significantly more ease. Furthermore, there are no guarantees for the behavior of the least-squares solution and the conditioning of the problem may be deteriorate quickly as $N \to \infty$.

3 The column nullspace

The correct choice of τ-functions may be elusive. This is particularly the case when one is enforcing continuity conditions across cells in a spectral element method in non-standard bases. A certainty is that there should always be as many τ-functions as boundary conditions. Hence we are required to add as many new columns as there are rows enforcing the boundary conditions. One desires to concatenate new columns that do not negatively impact the conditioning of the system as $N \to \infty$.

Thus a good proxy is to compute new columns that are orthonormal to the rest, e.g. by computing nullspace of the transpose of the rectangular system. In the case of (2.7) we (unsurprisingly) find that

$$\texttt{nullspace}\left[\begin{pmatrix} -1 & 1 & -1 & 1 & \cdots & (-1)^N \\ 1 & 1 & 1 & 1 & \cdots & 1 \\ & & \mathcal{D}_N & & & \end{pmatrix}^\top\right] = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.1}$$

Hence, we may deduce from the column nullspace that a good choice of τ-functions are $C^{(2)}_{N-2}(x)$ and $C^{(2)}_{N-1}(x)$.

For more general problems, by examining the columns of the nullspace, then with some luck all the entries of each nullspace column will be close to machine precision. Those which are not close to machine precision informs us of a good choice for the columns we concatenate to the least-squares system and implicitly the choice of the τ-functions. In particular, one may deduce for the τ-functions for a small value of N and thus deduce what they are as $N \to \infty$.

3.1 A screened-Poisson example

We provide an example where we utilize the column nullspace trick to deduce a a good choice of τ-functions for a screened Poisson equation:

$$-\frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x) + u(x) = f(x), \quad u(\pm 1) = 0. \tag{3.2}$$

After truncating at degree polynomial $N-1$ we recover the overdetermined system

$$B_N \mathbf{u}_N = (0\; 0\; \mathbf{f}_N^\top)^\top, \quad B_N \coloneqq \begin{pmatrix} -1 & 1 & -1 & 1 & \cdots & (-1)^N \\ 1 & 1 & 1 & 1 & \cdots & 1 \\ & & -\mathcal{D}_N + R_N & & & \end{pmatrix}. \tag{3.3}$$

We give the spy plot of the matrix B_N defined in (3.3) in Fig. 3. The ultraspherical method would truncate the last two rows of B_N. But unlike the Poisson example, these two rows are not identically zero. Thus it is not clear that this is the optimal choice.

By examining the column nullspace of $B_N^\top$, we recover a two-dimensional nullspace. In Fig. 4 we plot the magnitude of the 22 entries of each column (where we have chosen the truncation degree $N = 19$). We see that almost all entries are close to machine precision except one for each column. Upon further examination, those entries correspond to the τ-functions $\tau_1(x) = C^{(2)}_{N-2}(x)$ and $\tau_2(x) = C^{(2)}_{N-1}(x)$: the same τ-functions as in the Poisson example.

4 Code

Checkout `tau-method.jl` for a supplementary `Julia` script to these notes.

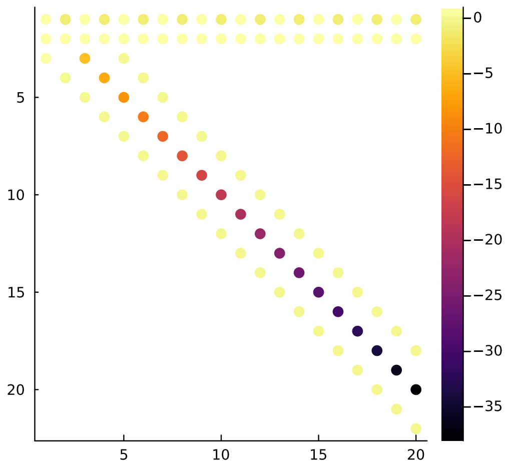


Figure 3: Spy plot of the matrix B_N defined in (3.3), $N = 19$.

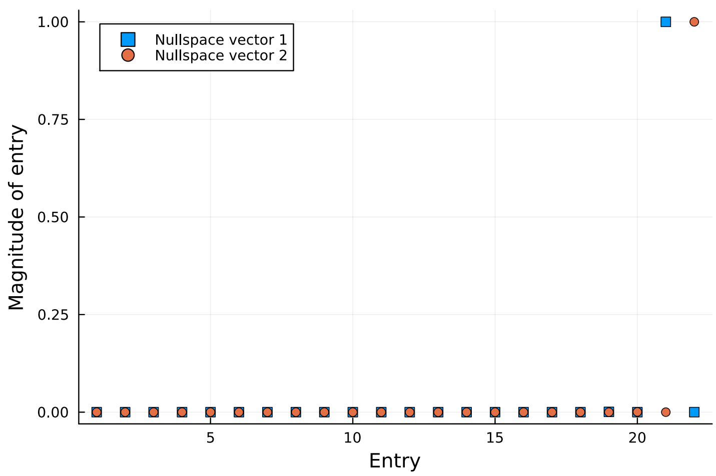


Figure 4: Magnitude of the entries of the two column vectors of `nullspace`$(B_N^\top)$ when $N = 19$. Upon further examination, the two nonzero entries correspond to the τ-functions $\tau_1(x) = C^{(2)}_{N-2}(x)$ and $\tau_2(x) = C^{(2)}_{N-1}(x)$: the same τ-functions as in the Poisson example.

References

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