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ON THE ACCURACY OF PSEUDOSPECTRAL DIFFERENTIATION

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Abstract For various grids on a finite interval we measure the accuracy of pseudospectral (collocation) differentiation matrices using two parameters. The first one is the the rank defficiency of the differentiation matrices. The second one quantifies the extent at which such matrices transform a constant vector into the null vector.

Keywords: pseudospectral differentiation; Chebyshev-Gauss-Lobatto grid; Legendre grid; equidistant grid; accuracy; floating-point arithmetic.

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1. INTRODUCTION

Fundamental results from approximation theory refers to the best uniform approximation of a smooth function by polynomials and the uniform approximation of a smooth 2π periodic function by trigonometric polynomials. These results are reviewed for instance in the monograph [1], Ch. 3. Thus, the Chebyshev equioscillation theorem states that a best approximation is unique for important classes of approximating functions but the set of nodes on which this approximation is realized is not necessarily unique. On the other hand, the spectral collocation methods essentially depend on the set of nodes on which the differential equation is collocated. In order to implement these methods one needs very accurate differentiation matrices of various orders.

Consequently, the accuracy at which the pseudospectral (collocation) differentiation matrices operate is of utmost importance in numerical analysis. In this note we will address the issue of the dependence of the accuracy of differentiation process on the node distribution in a grid covering a finite interval. We will consider an equispaced grid, an arbitrary one and then Legendre and Chebyshev grids. For non algebraic polynomials we will consider the Fourier interpolate.

2. ARBITRARY AND EQUIDISTANT GRIDS

It is well established that *spectral collocation methods* for solving differential equations is based on weighted interpolants of the form

$$u(x) \approx p_{N-1}(x) := \sum_{j=1}^{N} \frac{\alpha(x)}{\alpha\left(x_j\right)} \phi_j(x)\, u_j, \tag{1}$$

where $u_j := u\left(x_j\right)$, $u : [a,b] \to \mathbb{R}$, the set of interpolating functions $\phi_j(x),\ j = 1,\ldots,N$ satisfy $\phi_j(x_k) := \delta_{jk}$ (the Kronecker delta), the set of nodes $x_j,\ j = 1,\ldots,N$ in $[a,\ b] \subset \mathbb{R}$ is distinct but otherwise arbitrary and the weight $\alpha(x)$ is an arbitrary continuously differentiable positive function (see for instance our contribution [3]). Typically, $u(x)$ is the solution of an initial/boundary value problem.

The *baricentric form* of interpolation polynomial writes (see for instance the seminal paper [7])

$$p_{N-1}(x) = \frac{\alpha(x) \sum_{j=1}^{N} \frac{w_j}{x-x_j} \frac{u_j}{\alpha(x_j)}}{\sum_{j=1}^{N} \frac{w_j}{x-x_j}},$$

where $w_j^{-1} := \prod_{m=1,\ m\neq j}^{N} \left(x_j - x_m\right)$. This means that $p_{N-1}(x)$ defined above is an interpolant of the function $u(x)$ in the sense that

$$u(x_k) = p_{N-1}(x_k),\ k = 1,\ldots,N.$$

The *collocation derivative operators* are generated by taking various order derivatives of (1) and evaluating them at nodes $x_k,\ k = 1,\ldots,N$, i.e.,

$$u^{(l)}(x_k) \approx \sum_{j=1}^{N} \frac{d^l}{dx^l} \left[\frac{\alpha(x)}{\alpha\left(x_j\right)} \phi_j(x) \right]_{x=x_k} u_k,\ k = 1,\ldots,N.$$

Consequently, the $l-th$ order differentiation matrices associated to this operator are computed by

$$D_{k,j}^{(l)} = \frac{d^l}{dx^l} \left[\frac{\alpha(x)}{\alpha\left(x_j\right)} \phi_j(x) \right]_{x=x_k},\ k,j = 1,\ldots,N,\ l \in \mathbb{N}, \tag{2}$$

where $\phi_j(x)$ are given by Lagrange's formula

$$\phi_j(x) := \prod_{m=1,\ m\neq j}^{N} \left(\frac{x - x_m}{x_j - x_m} \right),\ j = 1,\ldots,N.$$

The approximation theory dictates that the set of nodes $x_j,\ j = 1, \ldots, N$ cannot be just any set of nodes. The main aim of this note is to make this statement more clear. Thus we use the MATLAB code `poldif.m` from [7] in order to perform the differentiation in (2).

In order to quantify the performances of every set of nodes we compute two specific parameters, namely:

- the norm of the *error* in approximating the zero vector, i.e., $\left\| D^{(1)} \cdot \mathbf{1}_N \right\|$ where $\mathbf{1}_N := ones(N, 1)$;
- the $rank\left(D^{(1)}\right)$ for various values of approximation parameter N.

Instead of the first parameter we could use another one reflecting the fact that the matrix $D^{(1)}$ has to satisfy

$$\sum_{j=1}^{N} D_{ij}^{(1)} = 0,\ \ 1 \le i \le N,$$

i.e., the derivative of a constant vanishes.

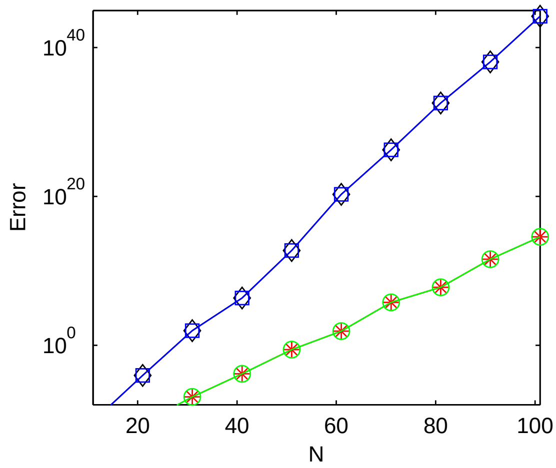

Fig. 1.: The accuracy of equidistant differentiation (starred line Euclidean norm, circled line inf norm) vs N and the accuracy of differentiation on grid (4) (diamonded line Euclidean norm, squared line inf norm) vs N.

Let's consider a set of equidistant nodes

$$x_j := \frac{j-1}{N-1},\ \ j = 1, \ldots, N, \tag{3}$$

where N takes in turn the value from the first row of Table 3.1. Thus the interval $[0,\ 1]$ is successively divided in $N - 1$ subintervals each of length $1/(N - 1)$.

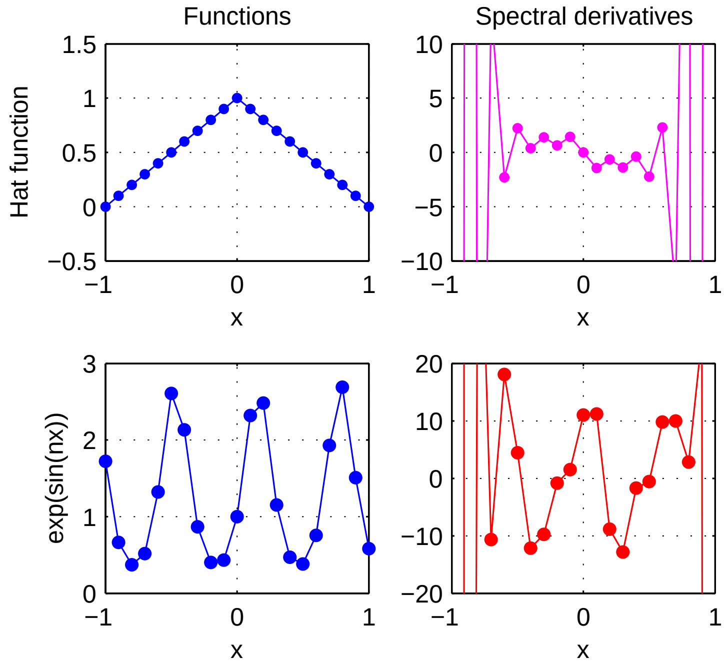

Fig. 2.: The collocation derivative of hat function and $\exp(\sin(nx))$, $n = 10$ on 20 equispaced nodes.

Along with the equidistant grid (3) we consider first an arbitrary one, namely

$$\widetilde{x}_j := \left(\frac{j-1}{N-1}\right)^2, \; j = 1, \ldots, N. \tag{4}$$

It is fairly clear that this new grid is a non uniform one with nodes clustering to the left margin 0. The extent at which the differentiation matrices perform on both grids is depicted in Fig. 1. The *error* in approximating the zero vector takes huge values. The collocation derivatives of the hat function and of a highly oscillatory but fairly smooth function, i.e., $\exp(\sin(nx))$, with $n = 10$ on 20 equispaced nodes are depicted in Fig. 2. They show large oscillations which cluster to the ends of the interval $[-1, \; 1]$.They are the direct consequence of the numerical instability of the differentiation process.

It is well known that given N nodes each of the differentiating matrices should be rank $N - 1$, a differentiating has the constant vector as its null space. Thus, it is important to point out that this equispaced approach works accurately for a very small number of nodes. As differentiating matrix $D^{(1)}$ should be rank one deficient, this simple test shows that even for a very rough approximation $D^{(1)}$ has additional null-spaces. Moreover, in case of quadratically spaced grid $\widetilde{x}_j$, the differentiation matrices

N	**11**	**21**	**31**	**41**	**51**	**61**	**71**	**81**	**91**	**101**
rank($D^{(1)}$)-(3)	10	20	30	37	42	9	8	8	7	7
rank($D^{(1)}$)-(4)	10	19	6	4	4	3	3	3	3	3

Table 1: The evolution of rank deficiency of differentiation matrices for equidistant grid (3) and squared grid. (4)

become much more degenerated. Table 3.1 shows that the situation dramatically deteriorates as N increases.

3. CONSECRATED GRIDS

In this section we will analyze some well known grids such as Legendre, Chebyshev and Fourier applied to a finite interval. First, let's reconsider two illustrative examples, the Chebyshev and Legendre derivatives of the hat function $h(x) := max(0, 1-abs(x))$ and of the smooth but fairly oscillatory function $\exp(\sin(nx))$, $n > 2$.

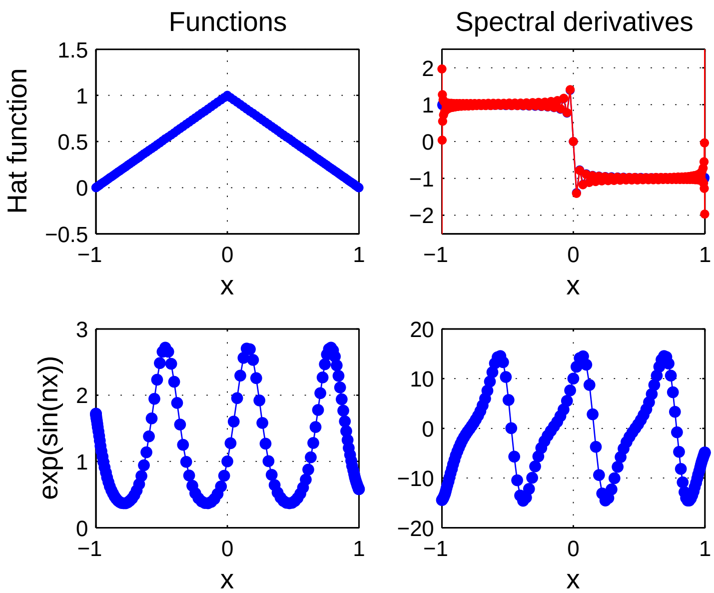

Fig. 3.: Chebyshev and Legendre derivatives of hat function and $\exp(\sin(nx))$, $n = 10$. The order of approximations equals 128.

The differentiation on the roots of Legendre polynomials presents an intermediate situation. As it is apparent from Fig. 4 the differentiation matrices for $N \leq 700$

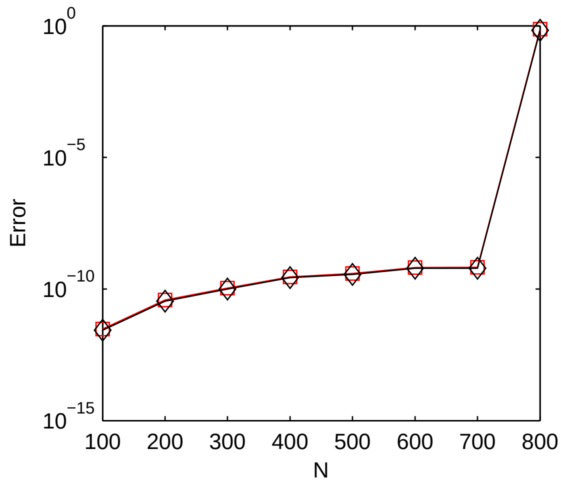

Fig. 4.: Semilogy plot of the accuracy of Legendre differentiation (squared line for Euclidian norm and diamonded line for inf norm) vs N.

perform satisfactorily well. Our numerical experiments have showed that all differentiation matrices keep a rank of order $N-1$. Most notably, for N larger than 700 the Legendre differentiation process rapidly becomes unstable.

The best situation with polynomial differentiation is encountered when Chebyshev nodes of second kind

$$x_k := \cos\left(\frac{(k-1)\,\pi}{N-1}\right),\ k = 1,\ldots,N, \tag{5}$$

or equivalently *Chebyshev-Gauss-Lobatto quadrature nodes* (see for instance [5] or our contribution [4] p. 11) are used. The corresponding differentiation matrix has the entries (see for instance [2], p. 69)

$$D_{kj}^{(1)} = \begin{cases} \frac{c_k(-1)^{j+k}}{c_j\left(x_k-x_j\right)},\ j \neq k,\ j,k = 1,2,...,N, \\ -\frac{x_k}{2\left(1-x_k^2\right)},\ j = k \neq 1,N, \\ \frac{2(N-1)^2+1}{6},\ j = k = 1, \\ -\frac{2(N-1)^2+1}{6},\ j = k = N. \end{cases}$$

The above differences $\left(x_k - x_j\right)$ may be subject to floating-point cancellation errors for large N. Various tricks based on simple trigonometric identities have been used in [7] in order to avoid such errors in floating-point arithmetic. Thus, the MATLAB code `chebdif.m` has been fairly stable algorithm in computing these matrices.

The upper curve in Fig 5 correspond to this situation.

Beyond this polynomial differentiation we will pay a particular attention to the Fourier differentiation matrices (see [7]). The Fourier interpolate reads

$$t_N(x) := \sum_{j=1}^{N} \phi_j(x)\, u_j,$$

where

$$\phi_j(x) := \tfrac{1}{N} \sin \tfrac{N}{2}\left(x - x_j\right) \cot \tfrac{1}{2}\left(x - x_j\right),\ N\ even,$$
$$\phi_j(x) := \tfrac{1}{N} \sin \tfrac{N}{2}\left(x - x_j\right) \csc \tfrac{1}{2}\left(x - x_j\right),\ N\ odd,\ j = 1, 2, ..., N.$$

Using the baricentric form of the interpolate (see [6] Sect. 13.6) the MATLAB code `fourdif.m` from [7] provides the Fourier differentiation matrices on the nodes

$$x_k := (k-1)\,h,\ h = \frac{2\pi}{N},\ k = 1, \ldots, N.$$

Their performances are the best as it is apparent from Fig. 5 (see the lower curve). For $N = O\left(2^6\right)$ it is of utmost importance to underline that Fourier and even Chebyshev differentiation matrices work fairly close to the *machine precision*. Excellent approximations are also attained when the cut off parameter ranges up to 2^{11}. It is also important to notice that all differentiation matrices conserve a correct rank. It is a practical illustration of the *spectral accuracy*.

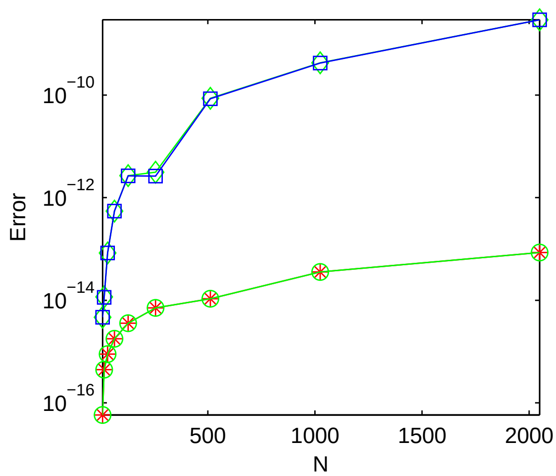

Fig. 5.: Semilogy plots of the accuracy of Fourier differentiation (starred line Euclidean norm, circled line inf norm) vs N and of the accuracy of Chebyshev differentiation (diamonded line Euclidean norm, squared line inf norm) vs N.

4. CONCLUDING REMARKS

In ([7]) p.478 the authors state that no general error analysis applicable to differentiation process on arbitrary grids has been undertaken. We hope that the present note fills this gap at least partially. Fourier and Chebyshev differentiation matrices have proved to be fairly reliable. This facts explain to some extent the success of the collocation spectral methods based on them.

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