Banded, skew-symmetric differentiation matrices of high order

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Abstract. This talk discusses the construction of skew-symmetric differentiation matrices of high order. Such matrices play an important role in the space discretization of partial differential equations. Recent results of [1] are presented, which permit to obtain differentiation matrices up to order 6 that are banded, stable, and skew symmetric.

Keywords: Differentiation matrices, space discretization of PDEs, skew-symmerty, order conditions
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INTRODUCTION

We consider the approximation of the first derivative $u'(\xi)$ on a grid over a finite interval

$$a = \xi_0 < \xi_1 < \cdots < \xi_n < \xi_{n+1} = b, \tag{1}$$

where we suppress the dependence of ξ_k on n. We always assume that the grid is dense in $[a,b]$, meaning that $\max_{k=0,\ldots,n} |\xi_{k+1} - \xi_k| = \mathscr{O}(n^{-1})$. In view of applications to the space discretisation of PDEs with Dirichlet boundary conditions, we restrict our considerations to functions $u(\xi)$ vanishing at both endpoints. The derivative approximation over the grid (1) is obtained by a linear combination of function values,

$$u'(\xi_m) \approx \sum_{k=1}^{n} \widehat{\mathscr{D}}_{m,k} u(\xi_k) \tag{2}$$

for $m = 1,\ldots,n$. The matrix $(\widehat{\mathscr{D}}_{m,k})$ is called a *differentiation matrix*. We follow [1] and focus our interest on such matrices that have the following properties:

- *banded*, i.e., there exists an integer $r \geq 1$ such that $\widehat{\mathscr{D}}_{m,k} = 0$ for $|m-k| \geq r+1$. This assumption brings an evident computational advantage, and guarantees that the derivative approximation is local.
- *stable*, i.e., the entries satisfy $|\widehat{\mathscr{D}}_{m,k}| = \mathscr{O}(n)$.
- *order* $P \geq 2$, i.e., for smooth functions $u(\xi)$ the defect in (2) is $\mathscr{O}(h^P)$, where $h = \max_{k=0}^{n} |\xi_{k+1} - \xi_k|$. For banded, stable formulas this is equivalent to requiring that (2) is exact for all polynomials of degree $\leq P$ that vanish at the endpoints.
- *skew-symmetric*. Since the first derivative is a skew-symmetric operator, this is a natural assumption in the spirit of geometric numerical integration. It has interesting implications for the discretization of PDEs (see [1, 2]).

For an equidistant grid $\{\xi_k = a + kh\}$ with $h = (b-a)/(n+1)$ the discretisation $u'(\xi) \approx \frac{1}{2h}\Big(u(\xi+h) - u(\xi-h)\Big)$ leads to a differentiation matrix that satisfies all four properties, but which is only of second order.

The fourth-order approximation

$$u'(\xi) \approx \frac{1}{12h}\Big(u(\xi-2h) - 8u(\xi-h) + 8u(\xi+h) - u(\xi+2h)\Big) \tag{3}$$

can be used at all points of an equidistant grid with the exception of ξ_1 and ξ_n. For these two grid points one-sided approximations can be used. This, however, destroys the skew-symmetry of the matrix.

For combining high order with skew-symmetry of a differentiation matrix, a "summation by parts rule" has been proposed in [3, 4, 5]). This approach consists in using an equidistant grid and a standard differentiation formula (like

(3)) in the interior of the interval. Close to the end points, one-sided finite difference approximations are considered such that the differentiation matrix becomes skew-symmetric with respect to a *modified scalar product*.

In the article [1] we propose an alternative to the "summation by parts" approach. We do not modify the inner product in the discrete summation by parts formula, but we consider instead a grid that is non-uniform near the endpoints of the interval.

STRUCTURE OF CONSIDERED DIFFERENTIATION MATRICES

The differentiation matrix based on a differentiation formula such as (3) is skew symmetric everywhere with the exception of its left upper and right lower corners. The study of [6, 2] motivates the use of non-equidistant grids.

The choice of the grid. We fix positive integers N and L and consider the symmetric grid

$$-a_L h, \dots, -a_1 h, 0, h, 2h, 3h, \dots, 1-h, 1, 1+a_1 h, \dots, 1+a_L h \tag{4}$$

where $h = 1/N$ and $a_1, \dots, a_L$ are parameters ($0 < a_1 < \cdots < a_L$), which may depend on h. This grid corresponds to the interval $[-a_L h, 1+a_L h]$ and has $n = N+2L-1$ interior grid points. It is equidistant except close to the endpoints.

The pattern of the differentiation matrix. Associated to the grid (4) we consider differentiation matrices $(\mathscr{D}_{m,k})$ yielding approximations

$$u'(x_m) \approx \sum_{k=-L+1}^{N+L-1} \mathscr{D}_{m,k} u(x_k) \tag{5}$$

for functions $u(x)$ vanishing at the endpoints x_{-L} and x_{N+L}. For the definition of the matrix $(\mathscr{D}_{m,k})$ we consider a basic differentiation rule

$$u'(x) \approx \sum_{k=-R}^{R} \delta_k u(x+kh) \tag{6}$$

satisfying $\delta_0 = 0$ and $\delta_{-k} = -\delta_k$. For example, the differentiation rule (3) has $R = 2$, $\delta_1 = 8/(12h)$ and $\delta_2 = -1/(12h)$.

We assume that

$$\mathscr{D}_{m,k} = \delta_{k-m} \tag{7}$$

for indices m,k satisfying $|k-m| \le R$, and $R \le m \le N-R$ or $R \le k \le N-R$. The remaining entries are zero, with the exception of the two $(R+L-1)\times(R+L-1)$ matrices on the upper left and lower right corners. We assume them to be skew symmetric. Moreover, we assume that the whole matrix is skew persymmetric, so that the lower right sub-matrix is determined by the upper left one. The whole situation is illustrated in Figure 1 for $L = 3$, $R = 2$, and $N = 7$. The symbol $\bullet$ indicates the entries given by (7), and $\times$ indicates non-zero entries of the two blocks.

$$\begin{bmatrix}
\circ & \times & \times & \times & & & & & & & & \\
\times & \circ & \times & \times & & & & & & & & \\
\times & \times & \circ & \times & \bullet & & & & & & & \\
\times & \times & \times & \circ & \bullet & \bullet & & & & & & \\
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 & & & & & & & & \times & \times & \circ & \times \\
 & & & & & & & & \times & \times & \times & \circ
\end{bmatrix}$$

FIGURE 1. Pattern of the differentiation matrix with $L = 3$, $R = 2$, and $N = 7$.

High order. In this talk we give necessary and sufficient conditions on the parameters $a_1, \dots, a_L$ of (4) that permit to obtain a differentiation matrix of a certain order P. The solution of the order conditions is discussed and skew-symmetric differentiation matrices of order up to 6 are presented.

APPLICATIONS TO PARTIAL DIFFERENTIAL EQUATIONS

A standard approach to high order space discretizations is to consider an equidistant grid $\xi_j = jh$ ($j = 0,1,\ldots,n+1$) with $h = 1/(n+1)$, and to use a standard differentiation formula like the one of (3). Obviously, this formula can be used only for $j = 2,\ldots,n-1$. The the left end point one can consider a one-sided formula (for $j = 1$)

$$u'(\xi) \approx \frac{1}{6h}\Big(-2u(\xi-h) - 3u(\xi) + 6u(\xi+h) - u(\xi+2h)\Big)$$

and for $j = n$ the reflected formula. This yields a banded, 3rd order differentiation matrix, which however is not skew-symmetric at the upper left and lower right corners. For later reference we call it Method (N). For comparison we consider the also a skew-symmetric differentiation matrix of order 3, and we call it Method (S).

The following examples demonstrate the advantage of using skew-symmetric differentiation matrices.

Advection equation. For $t \geq 0$ and $x \in [0,1]$ we consider the one-dimensional advection equation

$$\partial_t u + c(x)\partial_x u = 0 \tag{8}$$

where the wave speed $c(x)$ depends on the spatial coordinate. We assume $c(x) > 0$ for $0 < x < 1$, and zero speed at the boundary, $c(0) = c(1) = 0$, so that homogeneous Dirichlet boundary conditions, $u(t,0) = u(t,1) = 0$ for all $t \geq 0$, make sense. The initial condition $u(0,x) = u_0(x)$ is assumed to be compatible with the boundary conditions.

Under these assumptions the advection equation has for all sufficiently smooth functions $F(u)$ the expression

$$I_F(t) = \int_0^1 \frac{F\big(u(t,x)\big)}{c(x)}\,\mathrm{d}x \tag{9}$$

as a conserved quantity. This follows from differentiation with respect to time t. In particular, this is the case for $F(u) = |u|^2$. For a grid (1) we consider the following space discretisation of (8),

$$\dot{U} + \mathscr{C}\widehat{\mathscr{D}}U = 0, \qquad U(0) = U_0. \tag{10}$$

The elements of the vector $U(t) = \big(U_1(t),\ldots,U_n(t)\big)^\mathsf{T}$ are approximations to $u(t,\xi_j)$ (for $j = 1,\ldots,n$), $\mathscr{C}$ is a diagonal matrix with entries $c(\xi_j)$, and $\widehat{\mathscr{D}}$ is a differentiation matrix as introduced in the beginning of this abstract. If the differentiation matrix $\widehat{\mathscr{D}}$ is skew-symmetric, the expression

$$\mathscr{I}_2(t) = \frac{1}{n+1}\sum_{j=1}^{n}\frac{1}{c(\xi_j)}|U_j(t)|^2$$

is preserved along solutions of (10). Moreover, the differential equation (10) is stable and all the eigenvalues of $\mathscr{C}\widehat{\mathscr{D}}$ reside on the imaginary axis. This is not guaranteed with the use of non-skew-symmetric differentiation matrices.

We apply both discretisations (Method (N) and Method (S)) to the advection equation (8) with wave speed $c(x) = x(1-x)^2$ and initial condition $u_0(x) = 3x(1-x)$. We use $N = 100$ for method (S) and $n = 105$ for method (N), so that both methods have 105 grid points in the interior of the interval $(0,1)$. The corresponding ordinary differential

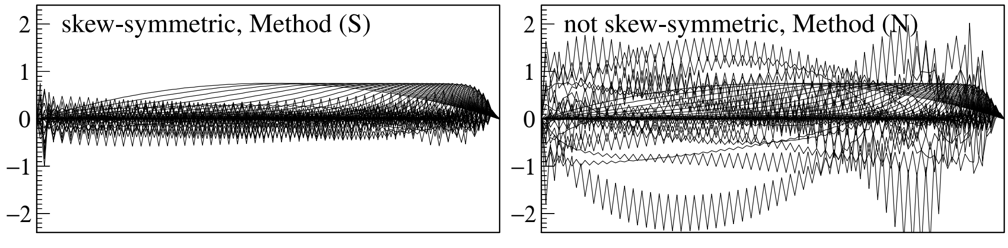

FIGURE 2. Solution $U_j(t)$ of the semi-discretised differential equation (10) as a function of $\xi_j \in [0,1]$, for various values of t ranging from $t = 0$ to $t = 100$.

equation (10) is solved with high precision by an explicit Runge-Kutta code. The result is shown in Figure 2. For many different time instances ranging from $t = 0$ to $t = 100$ we plot the solution $U_j(t)$ as a function of ξ_j (for better visibility the values are connected by a polygon). For values of t between 0 and 30, the functions are nearly the same for both methods. For larger values of t, spurious oscillations can be observed. Whereas they remain bounded and of moderate size for the skew-symmetric Method (S), they grow exponentially fast for Method (N). This can be explained by computing the eigenvalues of the matrix $\mathscr{C}\widehat{\mathscr{D}}$ of (10). They lie exactly on the imaginary axis for Method (S). For Method (N), numerical computations show that the matrix has eigenvalues with positive real part up to a size of ≈ 0.025.

Diffusion equation. As a further application we consider the diffusion equation

$$\partial_t u = \partial_x\big(c(x)\partial_x u\big), \tag{11}$$

where $c(x) > 0$ in $(0,1)$. We assume homogeneous Dirichlet boundary conditions $u(t,0) = u(t,1) = 0$ for all $t \geq 0$, and an initial condition $u(0,x) = u_0(x)$. Moreover, we let $c(0) = c(1) = 0$ so that not only $u(t,x)$, but also $c(x)\partial_x u(t,x)$ vanish at the endpoints of $[0,1]$. As before, an approximation of the space derivatives by finite differences leads to an ordinary differential equation

$$\dot{U} = \widehat{\mathscr{D}}\mathscr{C}\widehat{\mathscr{D}}U, \qquad U(0) = U_0. \tag{12}$$

If the differentiation matrix $\widehat{\mathscr{D}}$ is skew-symmetric, then the matrix of the linear system (12) is symmetric and negative semi-definite. As a consequence, the linear differential equation (12) and also its inhomogeneous analogue can be numerically solved by any integrator that has the negative real axis (or a large part thereof) in its stability region.

If $\widehat{\mathscr{D}}$ is not skew symmetric, the eigenvalues of $\widehat{\mathscr{D}}\mathscr{C}\widehat{\mathscr{D}}$ are in general not on the negative real axis. This happens with Method (N), when applied to the diffusion equation (11). Figure 3 shows the eigenvalues of $\widehat{\mathscr{D}}\mathscr{C}\widehat{\mathscr{D}}$ for $n = 50$ and for the choice $c(x) = x(1-x)\big((3x-1)^2 + 0.001\big)$. Only a few of the eigenvalues lie on the real axis. For numerical integrators that have only a narrow band around the negative real axis in the stability region (e.g., Runge–Kutta–Chebyshev methods, see [7, Section IV.2]), this may lead to severe step-size restrictions.

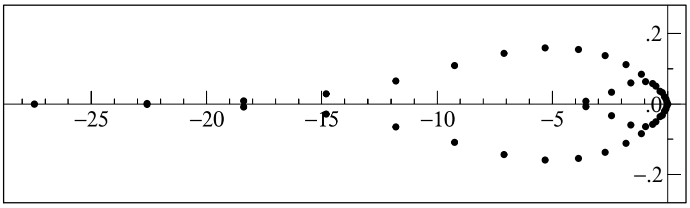

FIGURE 3. Eigenvalues of $\widehat{\mathscr{D}}\mathscr{C}\widehat{\mathscr{D}}$, where $\mathscr{D}$ is the differentiation matrix of Method (N) with $n = 50$, and $\mathscr{C}$ is given by $c(x) = x(1-x)\big((3x-1)^2 + 0.001\big)$.

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