Differentiation Matrices
for Fun and Profit

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• Some differentiation matrices are like finite differences, but different in that they provide derivatives at all mesh points at once
• Other differentiation matrices work on vectors of coefficients
• We’ll look mostly at this latter kind, so that the $n + 1$ by $n + 1$ differentiation matrix $D$ is exact for polynomials of degree at most $n$. 
Examples

The most familiar differentiation matrix is of course that of the monomial basis $\phi_k(x) = x^k$. The $4 \times 4$ differentiation matrix, for polynomials of degree at most 3 is, in this basis,

$$D_{\text{monomial}} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (1)$$

Applying this matrix to the vector $[a_0, a_1, a_2, a_3]^T$ gives $[a_1, 2a_2, 3a_3, 0]^T$ which are obviously the coefficients of the derivative of $p(x) = a_0 \phi_0(x) + a_1 \phi_1(x) + a_2 \phi_2(x) + a_3 \phi_3(x)$. 
A More Interesting Example, \( T_k(x) = \cos(k \arccos(x)) \)

Finite order differentiation matrices for Chebyshev polynomials are merely truncations of this. For a recent application of this matrix to the solution of pantograph equations, see [Yang, 2018].
Suppose nodes $\tau = [-1, -\frac{1}{2}, \frac{1}{2}, 1]$ are given. Then the differentiation matrix is

$$D_{\text{Lagrange}} = \frac{1}{6} \begin{bmatrix} -19 & 24 & -8 & 3 \\ -6 & 2 & 6 & -2 \\ 2 & -6 & -2 & 6 \\ -3 & 8 & -24 & 19 \end{bmatrix}.$$  \hspace{1cm} (3)

What this means is that given a vector of values $\rho = [\rho_0, \rho_1, \rho_2, \rho_3]^T$ taken by a polynomial of degree at most 3 on those nodes $\tau$, then applying the matrix to that vector gives a vector of derivative values at those nodes, $dp = [dp_0, dp_1, dp_2, dp_3]^T$. 
Why do this?

- Changing bases is usually ill-conditioned (exponential in degree)
- If you have a stable and convenient way to evaluate $p(x)$ in the basis you’re using, e.g. barycentric form for Lagrange polynomials, then you have a stable and convenient way to evaluate $p'(x)$ once its coefficients are known
- The pseudo-inverse of the differentiation matrix can be used for integration
- The differentiation matrix itself can be used in spectral semidiscretizations of PDE
- The differentiation matrix can be used in Levin-type methods for quadrature of highly-oscillatory integrals
Spectral methods for PDE

\[ D = \text{gallery('chebspec',n+2)}; \]
\[ x = \cos(\pi(0:n+1)/(n+1)); \]
\[ \text{function } dy = \text{mol}(t,y) \]
\[ \text{my} = [0; y; 0]; \]
\[ \text{tmp} = -aD*\text{my} + \nu D*D*\text{my}; \]
\[ dy = \text{tmp}(2:end-1); \]
\[ \text{end} \]

This forms the key piece of a Chebyshev spectral method-of-lines solution to an advection-diffusion equation \( u_t = -au_x + \nu u_{xx} \).

See [Trefethen, 2000] or [Corless and Fillion, 2013].
Levin-type methods for oscillatory integrals

This is joint work with Jeet Trivedi. Suppose we wish to evaluate

$$ I = \int_{-1}^{1} f(x)e^{i\omega x} \, dx $$

(4)

for large positive $\omega$, and that $f(x)$ is slowly varying in comparison. Normal quadrature methods are unaffordable, because the integral is ill-conditioned in a relative sense, with condition number $K$ given by

$$ K = \frac{\|f(x)\|_1}{|I|} = \frac{\int_{-1}^{1} |f(x)| \, dx}{|I|} $$

(5)

because then $|\Delta I/I| \leq K\|\Delta f \exp(i\omega x)\|_1/\|f\|_1$. 

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Levin methods are exact for polynomial $f$

If $f(x)$ is a polynomial of degree at most $n$ then we may look for a polynomial $F(x)$ such that $(F(x) \exp(i \omega x))' = f(x) \exp(i \omega x)$, in which case

$$I = F(1)e^{i \omega} - F(-1)e^{-i \omega}.$$  \hfill (6)

The product rule gives that $(F' + i \omega F) \exp(i \omega x) = f(x) \exp(i \omega x)$, or more simply

$$F'(x) + i \omega F(x) = f(x).$$  \hfill (7)

Replacing an integral with an ODE does not seem like progress, but remember that $f$ and $F$ are polynomials of degree at most $n$, so this is a finite-dimensional problem. We can thus work with vectors of coefficients.
If \( f(x) \) is not polynomial, then approximation theory comes to the rescue: \( f(x) = p^*(x) + \varepsilon(x) \) and we can replace \( I(f) \) with \( I(p^*) \) with much less consequence. Consider

\[
I_2 = \int_{-1}^{1} \left( \frac{1}{1 + x^2} \right) e^{i\omega x} \, dx .
\] (8)

Maple gets an analytical answer involving exponential integrals which it can expand in an asymptotic series:

\[
I_2 = \frac{\sin \omega}{\omega} - \frac{\cos \omega}{\omega^2} - \frac{\sin \omega}{\omega^3} - 6 \frac{\sin \omega}{\omega^5} + O \left( \frac{1}{\omega^6} \right) \] (9)
Figure: Absolute error multiplied by $\omega^2$ using the Levin-Lagrange method with 4 Chebyshev nodes, that is, interpolating $1/(1 + t^2)$ using a degree at most 3 polynomial.
How this works

We interpolate $f(t) = 1/(1 + t^2)$ at the four nodes $[-1, -\frac{1}{2}, \frac{1}{2}, 1]$ to get $f = [\frac{1}{2}, \frac{4}{5}, \frac{4}{5}, \frac{1}{2}]^T$. We write the equation $F'(x) + i\omega F(x) = f(x)$ as

$$DF + i\omega F = f,$$  \hspace{1cm} (10)

or

$$(D + i\omega I)F = f.$$  \hspace{1cm} (11)

We solve this four-by-four linear system numerically (given a numerical value for $\omega$). The resulting vector $F$ of values at the nodes are the coefficients in the Lagrange basis.
Formally,

\[
(D + i\omega I)^{-1} = \frac{1}{i\omega} \left( I - \frac{i}{\omega} D \right)^{-1}
\]

\[
= \frac{1}{i\omega} \left( I + \frac{i}{\omega} D + \frac{i^2}{\omega^2} D^2 + \cdots \right) .
\]

This suggests that powers of $D$ might be important.
D is nilpotent and nonderogatory in any basis

**Theorem:** D is nilpotent, and nonderogatory.

**Proof:** For $k = 0, 1, 2, \ldots, n$ let $v_k$ be the column vector of the coefficients of $x^k/k!$ expressed in the polynomial basis being used. Collect all these columns in an invertible matrix $V = [v_0, v_1, \ldots, v_n]$. Then $Dv_k = v_{k-1}$ for $k = 1, 2, \ldots, n$, and moreover $Dv_0 = 0$. The Jordan Canonical Form of $D$ is thus revealed by

$$DV = V \begin{bmatrix} 0 & 1 & & & \\ 0 & 1 & & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix}. \tag{12}$$
Pseudospectra (see [Trefethen and Embree, 2005]) are eigenvalues of nearby matrices, and likely to be surprising for nonnormal matrices such as these: \( DD^T \neq D^T D \).

\[
\begin{align*}
  n &= 3; \\
  D3 &= \text{gallery}('chebspec',n+1); \\
  \text{eigtool}(D3) \\
  n &= 13; \\
  D13 &= \text{gallery}('chebspec',n+1); \\
  \text{eigtool}(D13)
\end{align*}
\]
Figure: Pseudospectra of the four-by-four Chebyshev-Lagrange matrix
Figure: Pseudospectra of the fourteen-by-fourteen Chebyshev-Lagrange matrix
Pseudo-inverse

\[ D^+ V = V \]

\[
\begin{bmatrix}
0 & & & \\
1 & 0 & & \\
& 1 & \ddots & \\
& & \ddots & 0 \\
& & & 1 & 0
\end{bmatrix}
\]

(13)
Chebyshev \( n = 5 \)

If we ask Maple to compute the Moore-Penrose pseudo-inverse of the \( n = 5 \) truncation of the Chebyshev basis differentiation matrix we get

\[
D^\dagger = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -1/2 & 0 & 0 & 0 \\
0 & 1/4 & 0 & -1/4 & 0 & 0 \\
0 & 0 & 1/6 & 0 & -1/6 & 0 \\
0 & 0 & 0 & 1/8 & 0 & 0 \\
0 & 0 & 0 & 0 & 1/10 & 0
\end{bmatrix}
\] (14)

Lanczos used this in his \( \tau \) method for solving ODE.
Our construction is different

If we compute $V$ with columns $x^k/k!$ expressed in the Chebyshev basis and compute $D^+$ we get

$$D^+ = \begin{bmatrix}
0 & 1/4 & 0 & -3/8 & 0 & -5/8 \\
1 & 0 & -1/2 & 0 & 0 & 0 \\
0 & 1/4 & 0 & -1/4 & 0 & -5/4 \\
0 & 0 & 1/6 & 0 & -1/6 & 0 \\
0 & 0 & 0 & 1/8 & 0 & -5/8 \\
0 & 0 & 0 & 0 & 1/10 & 0
\end{bmatrix}. \quad (15)$$

But if the last entry of the vector $f$ is 0 (polynomial of degree at most $n - 1$) then $D^+f$ differs only by a constant from $D^f$. 
Explicit example

If \( p'(x) = a_1 T_0(x) + a_2 T_1(x) + a_3 T_2(x) + a_4 T_3(x) + a_5 T_4(x) \) then we form the coefficient vector \( b = \begin{bmatrix} a_1 & a_2 & a_3 & a_4 & a_5 & 0 \end{bmatrix}^T \).

Multiplying this by \( D^+ \) we get the vector of coefficients
\[
\begin{bmatrix} 0, & a_1 - a_3/2, & a_2/4 - a_4/4, & a_3/6 - a_5/6, & a_4/8, & a_5/10 \end{bmatrix}^T,
\]
which once we add the constant \( K \ T_0(x) \) corresponds to

\[
p(x) = K \ T_0(x) + \left( a_1 - \frac{a_3}{2} \right) T_1(x) + \left( \frac{a_2}{4} - \frac{a_4}{4} \right) T_2(x)
+ \left( \frac{a_3}{6} - \frac{a_5}{6} \right) T_3(x) + \frac{a_4}{8} T_4(x) + \frac{a_5}{10} T_5(x) .
\]

(16)

This gives the correct antiderivatives for \( p'(x) \). \( D^+ \) is equivalent, though it has a messier constant term.
Some families we know how to differentiate

We have explicit formulae and/or algorithms for differentiation matrices for all of the following:

1. Monomial, Taylor, Newton bases
2. Chebyshev, Legendre, all orthogonal polynomial bases
3. Lagrange interpolational bases
4. Hermite interpolational bases
5. Bernstein bases $B^n_k(x) = \binom{n}{k} x^k (1 - x)^{n-k}$
A Bernstein example

For polynomials of degree at most $n = 4$ expressed in the Bernstein basis, the matrix is explicitly

$$
\begin{bmatrix}
-4 & 4 & 0 & 0 & 0 \\
-1 & -2 & 3 & 0 & 0 \\
0 & -2 & 0 & 2 & 0 \\
0 & 0 & -3 & 2 & 1 \\
0 & 0 & 0 & -4 & 4 \\
\end{bmatrix}.
$$

(17)
Accuracy and Stability

- In general, differentiation is infinitely ill-conditioned. However, if both $f$ and the perturbation are restricted to be polynomial, then the ill-conditioning is finite, and the absolute condition number is bounded by $\|D\|$.

- For the Bernstein basis of dimension $n + 1$ we find experimentally that $\|D^n\|_\infty = 2^n n!$. $D^{n+1} = 0$ of course.

- As a corollary, from the results discussed in [Embree, 2013] the $\varepsilon$-pseudospectral radius of the $n + 1$-dimensional Bernstein matrix must then at least be $(2^n n!)^{1/(n+1)}\varepsilon^{1/(n+1)} \sim 2n\varepsilon^{1/(n+1)}/e$ as $n \to \infty$, for any $\varepsilon > 0$. This suggests instability for powers of $D$. 

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For some bases (e.g. the monomial basis, or the Lagrange interpolational basis when the nodes are roots of unity) that \( \| \mathbf{D} \| = n \), showing only linear growth. Moreover, we frequently use \( \mathbf{D} \) in the sense of a constraint that has to be solved (as in spectral methods for PDE and in quadrature) and in those cases we have smoothing. Of course this is familiar from functional analysis: the differentiation operator is unbounded, but integration operators are bounded.
Other kinds of differentiation

There are other kinds of differentiation matrix not in this class: compact finite difference matrices, for instance, which are best thought of as pairs $\mathbf{M}, \mathbf{B}$ where $\mathbf{M}f' = \mathbf{B}f$ is to be solved for $f'$. Typically $\mathbf{M}$ is banded (e.g. tridiagonal). In theory, $\mathbf{D} = \mathbf{M}^{-1}\mathbf{B}$ but of course we never form this (it would be full). Compact finite differentiation matrices are not nilpotent. Instead they have a $p$-fold 0 eigenvalue and a complicated nonzero eigenstructure. Looking at these is work in progress.
Concluding Remarks

Differentiation is a fundamental operation and it is helpful to be able to do so without changing bases.

Levin-type quadrature is *moment-free*. The current state-of-the-art is represented by [Olver and Townsend, 2013] and [Iserles, 2009] and citing works. We have refined some of their results to use Hermite interpolational bases and Bernstein bases and compact finite differences. More general problems, including ones with stationary points in the integrand, can be solved in this manner.

Differentiation matrices are well known in spectral methods for PDE, and in addition to the works already cited see [Weideman and Reddy, 2000].
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