A THEORY OF EXPPLICIT FINITE-DIFFERENCE SCHEMES

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Abstract. Conventional finite-difference schemes for solving partial differential equations are based on approximating derivatives by finite-differences. In this work, an alternative theory is proposed which view finite-difference schemes as systematic ways of matching up to the operator solution of the partial differential equation. By completely abandon the idea of approximating derivatives directly, the theory provides a unified description of explicit finite-difference schemes for solving a general linear partial differential equation with constant coefficients to any time-marching order. As a result, the stability of the first-order algorithm for an entire class of linear equations can be determined all at once. Because the method is based on solution-matching, it can also be used to derive any order schemes for solving the general nonlinear advection equation.

Key words. Finite-difference schemes, higher order methods, Burgers’ equation.

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1. Introduction. The most fundamental aspect of devising numerical algorithms for solving partial differential equations is to derive finite-difference schemes for solving a general linear equation of the form

\[
\frac{\partial u}{\partial t} = \sum_{m=1}^{M} a_m \partial_x^m u,
\]

with constant coefficients \( a_m \). Conventionally, numerical schemes are obtained by approximating the temporal and spatial derivatives of the equation by finite-differences. Such a direct use of finite-difference approximations produces a large collection of seemingly unrelated and disparate finite-difference schemes which must be analyzed one by one for stability and efficiency. There does not appear to be a unifying theme that connects all such schemes. Moreover, if only explicit schemes are desired, then discretizing the equation can only produce first-order algorithms, since the required grid values at multiple time steps can only be obtained implicitly.

To go beyond first-order, instead of approximating the equation, one can approximate the formal operator solution to the equation. In the case of (1), the solution is

\[
u(x, \Delta t) = \exp \left( \Delta t \sum_{m=1}^{M} a_m \partial_x^m \right) u(x, 0).
\]

Since for constant coefficients \( [\partial_x^n, \partial_x^m] = 0 \), the solution factorizes to

\[
u(x, \Delta t) = \prod_{m=1}^{M} e^{\Delta t a_m \partial_x^m} u(x, 0),
\]

it is sufficient to study the effect of a single derivative operator at a time:

\[
u(x, \Delta t) = e^{\Delta t a_m \partial_x^m} u(x, 0).
\]

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Once numerical methods for solving (4) for any \( m \) are known, the general equation (1) can be solved by a sequential application of such schemes according to (3). Higher dimension algorithms then follow from dimensional splittings.

Conventionally, one expands out the RHS of (4) and again approximates the spatial derivatives by finite-differences[1, 2]. However, in such an approach, how each derivative is to be approximated by a finite-difference (to what order, use which grid points) remained arbitrary and must be decided by some extrinsic considerations. Moreover, the resulting collection of schemes are just as disjoint and unrelated.

This work proposes a theory of deriving explicit finite-difference schemes that is still based on approximating the operator solution, but abandons the practice of approximating derivatives directly by finite-differences. Instead, such approximations are automatically generated by matching the finite-difference scheme to the formal solution and are completely prescribed by the temporal order of the algorithm. From this theory, all explicit finite-difference schemes for solving (4) to any time-marching order are given by a single formula.

The key idea of this theory is to use an operator form of the finite-difference scheme so that it can be transparently matched to operator solution. This is described in the next section. Once this done, three fundamental theorems immediately follow that completely characterize all \( n \)th-order explicit time-marching algorithms for solving any \( m \)-order partial differential equation. In Section 3, the explicit form and the stability of the first-order time-marching algorithm are determined for all \( m \) simultaneously. In Section 4, many higher-order time-marching algorithms are given for \( m = 1 \) and \( m = 2 \). These examples serve to illustrate the three theorems in Section 2. The nonlinear advection case is described in Section 5. Some concluding remarks are given in Section 6.

2. Operator matching for linear equations. An explicit finite-difference scheme seeks to approximate the exact solution (4) via

\[
u(x, \Delta t) = \sum_{i=1}^{N} c_i u(x + k_i \Delta x, 0),
\]

where \( \{k_i\} \) is a set of \( N \) integers clustered around zero and \( \{c_i\} \) is a set of coefficients. In the conventional approach, \( \{k_i\} \) and \( \{c_i\} \) are by-products of the way spatial and temporal derivatives are approximated by finite-differences, and are therefore obtained concomitantly, mixed together. This obscures the underlying relationship among schemes of different time-marching order \( n \) for solving equations of different derivative order \( m \). In this work, we disentangle the two and determine \( \{k_i\} \) and \( \{c_i\} \) separately.

First, we will assume that \( \{k_i\} \) is given set of \( N \) integers, usually, a set of \( N \) consecutive integers containing zero. The power of our theory is that they need not be specified initially. They are a set of parameters that will ultimately be decided by the stability of the resulting numerical scheme.

Next, to determine \( \{c_i\} \) for a given set of \( \{k_i\} \), we make the following key observation: that each grid value can also be represented in an operator form:

\[
u(x + k_i \Delta x, 0) = e^{k_i \Delta x \partial_x} u(x, 0).
\]

The finite-difference approximation (5) then corresponds to

\[
u(x, \Delta t) = \sum_{i=1}^{N} c_i e^{k_i \Delta x \partial_x} u(x, 0).
\]
Comparing this to the exact solution (4), due to the linearity of the equation, the coefficients \( c_i \) can be determined by solving the operator equality

\[
e^{\Delta t a_m \partial_x^m} = \sum_{i=1}^{N} c_i e^{k_i \Delta x \partial_x}.
\]  

(8)

The simplest way to solve for \( c_i \) is to Taylor expand both sides of (8) and matches the powers of the derivative operator \( \partial_x \):

\[
1 + \Delta t a_m \partial_x^m + \frac{1}{2}(\Delta t a_m)^2 \partial_x^{2m} + \cdots = \sum_{i=1}^{N} c_i + \sum_{i=1}^{N} c_i(k_i \Delta x)\partial_x + \frac{1}{2} \sum_{i=1}^{N} c_i(k_i \Delta x)^2 \partial_x^2 + \cdots.
\]  

(9)

From this, one immediately sees that for a given \( m \), an \( n \)th-order time-marching algorithm on the right, must match up to the \( nm \)th power of \( \partial_x \) on the left. Thus \( \{c_i\} \) must satisfy \( N = nm + 1 \) linear order-conditions and therefore requires the same number of grid points. Thus we have proved the following fundamental theorem for explicit finite-difference schemes:

**Theorem 1 (Fundamental).** An \( n \)th-order time-marching finite-difference scheme of the form

\[
u(x, \Delta t) = \sum_{i=1}^{N} c_i u(x + k_i \Delta x, 0)
\]

for solving the equation

\[
\frac{\partial u}{\partial t} = a_m \partial_x^m u,
\]

where \( a_m \) is a real constant and \( m \) a whole number \( \geq 1 \), must have a minimum of \( N = nm + 1 \) grid points. The latter is any set of \( N \) integers \( \{k_i\} \) clustered around zero.

Note that this result is obtained without any prior knowledge of how derivatives are to be approximated by finite-differences. Such approximations are automatically generated by the order conditions in (9) for any set of \( \{k_i\} \). In this theory of explicit finite-difference schemes, everything follow from this set of order-conditions. One can easily check that all known low-order explicit schemes obey this theorem.

The set of order-conditions in (9) can be solved easily, and we have our central result:

**Theorem 2 (Central).** An \( n \)th-order time-marching scheme

\[
u(x, \Delta t) = \sum_{i=1}^{N} c_i u(x + k_i \Delta x, 0)
\]

with \( \{c_i\} \) satisfying \( N = nm + 1 \) order-conditions in (9) for solving the equation

\[
\frac{\partial u}{\partial t} = a_m \partial_x^m u,
\]

has the closed-form solution

\[
c_i = \sum_{j=0}^{n} \nu^j_m \frac{1}{j!} L^j_x(jm)(0)
\]  

(10)
where
\[
\nu_m = \frac{\Delta t_{am}}{\Delta x^m}
\]  
(11)
is the generalized Courant number and \(L_i^{(jm)}(0)\) are the \((jm)^{th}\)-order derivatives of Lagrange polynomials of degree \(N - 1 = nm\)

\[
L_i(x) = \prod_{j=1(\neq i)}^{N} \frac{(x - k_j)}{(k_i - k_j)}
\]
evaluated at the origin.

**Proof.** The order-condition (9) reads individually,

\[
\sum_{i=1}^{N} c_i = 1
\]
(12)
\[
\sum_{i=1}^{N} c_i k_i^m = m! \nu_m
\]
\[
\sum_{i=1}^{N} c_i k_i^{2m} = (2m)! \frac{\nu_m^2}{2!}
\]
\[
\ldots
\]
\[
\sum_{i=1}^{N} c_i k_i^{nm} = (nm)! \frac{\nu_m^n}{n!}
\]
(13)
where \(\nu_m\) is the generalized Courant number (11) and where all other powers of \(k_i\) less than \(nm\) sum to zero. We compare these order conditions to the Vandermonde equation satisfied by Lagrange polynomials of \(N - 1 = nm\) degree with grid points \(\{k_i\}\) (See Appendix):

\[
\begin{pmatrix}
1 & 1 & 1 & \ldots & 1 \\
k_1 & k_2 & k_3 & \ldots & k_N \\
k_1^2 & k_2^2 & k_3^2 & \ldots & k_N^2 \\
k_1^3 & k_2^3 & k_3^3 & \ldots & k_N^3 \\
\ldots & \ldots & \ldots & \ldots & \ldots \\
k_1^{(N-1)} & k_2^{(N-1)} & k_3^{(N-1)} & \ldots & k_N^{(N-1)}
\end{pmatrix}
\begin{pmatrix}
L_1(x) \\
L_2(x) \\
L_3(x) \\
L_N(x)
\end{pmatrix}
= 
\begin{pmatrix}
1 \\
x \\
x^2 \\
x^3 \\
\ldots \\
N^{(N-1)}
\end{pmatrix}
\]
(14)

If we take the \(\ell^{th}\) derivatives (including the zero-derivative) of this system of equations with respect to \(x\) and set \(x = 0\) afterward, we would have

\[
\sum_{i=1}^{N} k_i^{\ell} L_i^{(\ell)}(0) = \ell! \delta_{j,\ell}
\]
(15)

This means that when \(L_i^{(\ell)}(0)\) is summed over all powers of \(k_i\) from 0 to \(nm\), only the sum with \(k_i^{\ell}\) is non-vanishing. If \(c_i\) were a sum of \(L_i^{(\ell)}(0)\) terms, with \(\ell = 0, m, 2m, \ldots, nm\), then when \(c_i\) is summed over powers of \(k_i\), the sum will be non-vanishing only at the required order-conditions (12)-(13). Adjusting the coefficients of \(L_i^{(\ell)}(0)\) to exactly match the order conditions then yields the solution (10). □
Eq. (10) is the master formula for solving a general \( m \)-order partial differential equation to an arbitrary \( n \)th time-marching order. All explicit schemes are related by their use of Lagrange polynomials. \( L_i^{(\ell)}(0) \) is just \( \ell! \) times the coefficient of the monomial \( x^\ell \) in \( L_i(x) \).

For the next theorem, we need the sums of \( L_i(x) \) over \( k_i^N \) and \( k_i^{N+1} \), which are outside of (14). They are given by

\[
\sum_{i=1}^N k_i^N L_i(x) = P(x) \quad \text{and} \quad \sum_{i=1}^N k_i^{N+1} L_i(x) = Q(x),
\]

where

\[
P(x) = x^N - s(x), \quad Q(x) = x^{N+1} - \left( x + \sum_{i=1}^N k_i \right) s(x), \quad \text{and} \quad s(x) = \prod_{i=1}^N (x - k_i).
\]

Note that \( P(x) \) and \( Q(x) \) are just \( N-1 \) degree polynomials. Taking the \( \ell \)th derivative \( (0 \leq \ell \leq N-1) \) with respect to \( x \) and set \( x = 0 \) afterward yields,

\[
\sum_{i=1}^N k_i^N L_i^{(\ell)}(0) = P^{(\ell)}(0) \quad \text{and} \quad \sum_{i=1}^N k_i^{N+1} L_i^{(\ell)}(0) = Q^{(\ell)}(0)
\]

By the way these schemes are constructed, it is very easy to compute their errors with respect to the exact solution. Moreover, all such explicit finite-difference schemes are characterized by a uniformity property:

**Theorem 3.** An \( n \)th-order time-marching scheme

\[
u(x, \Delta t) = \sum_{i=1}^N c_i u(x + k_i \Delta x, 0)
\]

with \( N = nm + 1 \) and with \( \{c_i\} \) given by Theorem 2 for solving the equation

\[
\frac{\partial u}{\partial t} = a_m \partial_x^m u,
\]

approximates all spatial derivatives \( u^{(jm)}(x, 0) \) from \( j = 0 \) to \( j = n \) uniformly to order \( \Delta x^m \) and has an overall local error of

\[
E = \Delta x^N \left( \sum_{j=0}^n \frac{\nu_j^m}{j!} P^{(jm)}(0) \right) \frac{u^{(N)}(x, 0)}{N!} + \Delta x^{N+1} \left( \sum_{j=0}^n \frac{\nu_j^m}{j!} Q^{(jm)}(0) \right) \frac{u^{(N+1)}(x, 0)}{(N+1)!}
\]

\[
- \Delta t a_m (n+1) u^{((n+1)m)}(x, 0) \left( \frac{x}{(n+1)!} \right). \quad (19)
\]

The local truncation error is just \( E/\Delta t \).

**Proof.** Substitute in the solution for \( c_i \) from (10) gives

\[
\sum_{i=1}^N c_i u(x + k_i \Delta x, 0) = \sum_{i=1}^N \frac{\nu_j^m}{j!} \sum_{i=1}^N L_i^{(jm)}(0) u(x + k_i \Delta x, 0)
\]

\[
= \sum_{j=0}^n \frac{\nu_j^m}{j!} \sum_{i=1}^N L_i^{(jm)}(0) \left[ u(x, 0) + (k_i \Delta x) u^{(1)}(x, 0) + \frac{1}{2!} (k_i \Delta x)^2 u^{(2)}(x, 0) + \cdots \right]
\]

\[
+ \Delta x^N \sum_{j=0}^n \frac{\nu_j^m}{j!} \sum_{i=1}^N L_i^{(jm)}(0) \left[ u^{(N)}(x, 0) + \frac{(k_i \Delta x)^{N+1}}{(N+1)!} u^{(N+1)}(x, 0) + O(\Delta x^{N+2}) \right] \quad (20)
\]
By (15) and (18), we have

\[
\sum_{i=1}^{N} c_i u(x + k_i \Delta x, 0) = \sum_{j=0}^{n} \frac{\nu^j_m}{j!} \left[ (\Delta x)^j u^{(j)}(x, 0) + \frac{P^{(jm)}(0)}{N!} \Delta x^N u^{(N)}(x, 0) \right.
\]

\[
+ \left. \frac{Q^{(jm)}(0)}{(N + 1)!} \Delta x^{N+1} u^{(N+1)}(x, 0) + O(\Delta x^{N+2}) \right].
\]

(21)

All approximations of \(u^{(jm)}(x, 0)\) for \(0 \leq j \leq n\) are therefore uniformly correct to at least spatial order \(N - 1 = nm\). Subtracting the exact solution (4) from above gives the local error (19).

Note that \(P^{(jm)}(0)\) may vanish, if so, that derivative approximation will then be correct to one order higher. This is why we needed the \(Q^{(jm)}(0)\) term for the diffusion equation. Also, the \(j = 0\) case means that \(u(x, 0)\) is correctly approximated to order \(\Delta x^{nm}\), if \(\{k_i\}\) does not contain 0. See (26) below.

This theorem states that the error analysis can be done once for all explicit finite-differences schemes. There is no need to do Taylor expansions for each finite-difference scheme, one by one. Also, this theorem shows that there is no arbitrariness in specifying the order of the spatial derivatives approximations. At time-marching order \(n\), all spatial derivatives (including the initial function itself) must be uniformly approximated to order \(nm\). The spatial order of approximation is completely fixed by the temporal order of the algorithm. Examples illustrating these three theorems will be given in Section 4.

### 3. Complete characterization of first-order algorithms

From Theorem 2, all explicit numerical schemes are given by the master formula (10). However, for a given \((m, n)\), it is easy to show that for \((1, n)\) and \((m, 1)\), the coefficients \(c_i\) are particularly simple. We will discuss the first case in the next section. For the second case, the set of \(\{c_i\}\) has the following simple form:

**Theorem 4.** The \(m + 1\) first-order time marching finite-difference schemes

\[
u(x, \Delta t) = \sum_{k=-r}^{m-r} c_k u(x + k \Delta x, 0)
\]

characterized by \(r = 0, 1, 2, \ldots m\) for solving the equation

\[
\frac{\partial u}{\partial t} = a_m \partial_x^m u
\]

have explicit solutions

\[
c_0 = 1 + (-1)^m (-1)^r C^m_r \nu_m \quad \text{and} \quad c_k = (-1)^m (-1)^{r+k} C^m_{r+k} \nu_m
\]

(22)

given in terms of the generalized Courant number \(\nu_m = \Delta t a_m / \Delta x^m\) and binomial coefficients

\[
C^m_k = \frac{m!}{k!(m-k)!}
\]

(23)

**Proof.** For a first-order time-marching scheme, we have \(N = m + 1\) grid points, which we can take to be \(k_i = \{-r, -r + 1, \ldots, -1, 0, 1, \ldots s\}\), where \(s = m - r\) and
where each value of \( r = 0, 1, 2, \ldots m \) labels a distinct algorithm. The corresponding coefficients can then be denoted directly by their \( k_i \) values as \( c_{-r}, c_{-r+1}, \ldots, c_0, c_1, \ldots c_s \). From Theorem 3, since each Lagrangian polynomial is defined by

\[
L_i(x) = \prod_{j=1(\neq i)}^{m+1} \frac{(x - k_j)}{(k_i - k_j)},
\]

one has

\[
L_i^{(m)}(0) = \frac{m!}{\prod_{j=1(\neq i)}^{m+1}(k_i - k_j)}.
\]

We now eliminate the index “\( i \)” by replacing \( k_i \) by its actual value denoted by \( k \). One then sees that

\[
L_k(0) = \prod_{j=-r(\neq k)}^{s} \frac{(0 - j)}{(k - j)} = \delta_{k,0}
\]

and

\[
L_k^{(m)}(0) = \frac{(-1)^m m!}{(s - k)(s - k - 1)(-r - k + 1)(-r - k)}
= \frac{(-1)^m m!}{(s - k)!(-1)(-r - k + 1)(-r - k)}
= \frac{(-1)^m (-1)^{r+k} m!}{(s - k)!(r + k)!} = \frac{(-1)^m (-1)^{r+k} m!}{(m - r - k)!(r + k)!}
= (-1)^m (-1)^{r+k} C^m_{r+k},
\]

which produces the explicit solution (22). \( \square \)

To gain insights about this set of first-order algorithms for all \( m \), consider the generation function for the coefficients \( c_k \):

\[
g(x) = \sum_{k=-r}^{m-r} c_k x^k = 1 + \nu_m \sum_{k=-r}^{m-r} (-1)^m (-1)^{r+k} C^m_{r+k} x^k
= 1 + \nu_m x^{-r} \sum_{k=-r}^{m-r} (-1)^m (-1)^{r+k} C^m_{r+k} x^{r+k}
\]

Shifting the dummy variable \( k \to r + k \) gives

\[
g(x) = 1 + \nu_m x^{-r} \sum_{k=0}^{m} (-1)^k C^m_k x^k
= 1 + \nu_m x^{-r} (x - 1)^m.
\]

Thus the coefficients of the algorithm are just coefficients of \( (x - 1)^m \).

This generation function can now be used to determine the stability of this set of first-order algorithms for all \( m \) simultaneously via the following two theorems.

**Theorem 5.** If the first-order time marching finite-difference scheme described in Theorem 4 for solving the equation

\[
\frac{\partial u}{\partial t} = a_m \partial_x^m u
\]
is von-Neumann stable, then its range of stability is limited to

$$|\nu_m| \leq \frac{1}{2^{m-1}}.$$  

Proof. The generation function (29) gives the following amplification factor for a single Fourier mode $e^{ipx}$,

$$g = \sum_{k=-r}^{m-r} c_k (e^{i\theta})^k = 1 + \nu_m e^{-ir\theta} (e^{i\theta} - 1)^m,$$  \hspace{1cm} (30)

where we have denoted $\theta = p\Delta x$. Since

$$e^{i\theta} - 1 = e^{i\theta/2} 2i \sin(\theta/2) = e^{i(\theta/2 + \pi/2)} 2 \sin(\theta/2)$$  \hspace{1cm} (31)

we have

$$g = 1 + \nu_m e^{i(m(\theta + \pi)/2 - r\theta)} [2 \sin(\theta/2)]^m,$$  \hspace{1cm} (32)

and therefore

$$|g|^2 = 1 + 2 \cos(\Phi) \nu_m [2 \sin(\theta/2)]^m + \nu_m^2 [2 \sin(\theta/2)]^{2m}$$  \hspace{1cm} (33)

with

$$\Phi = \frac{\theta}{2}(m - 2r) + m \frac{\pi}{2}.$$  \hspace{1cm} (34)

The algorithm can be stable at small $|\nu_m|$ only if

$$\text{sgn}(\nu_m) \cos(\Phi) < 0$$  \hspace{1cm} (35)

for all $\theta \in [0, 2\pi]$. In this case, $|g|^2$ as a quadratic function of $|\nu_m|$ would first dip below one, reaching a minimum at $|\nu_m|_{\text{min}} = |\cos(\Phi)|/[2 \sin(\theta/2)]^m$, then back up to one at $2|\nu_m|_{\text{min}}$. Thus the stability range of $|\nu_m|$ is limited to

$$|\nu_m| \leq 2|\nu_m|_{\text{min}} = \frac{2|\cos(\Phi)|}{[2 \sin(\theta/2)]^m} \leq \frac{1}{2^{m-1}},$$  \hspace{1cm} (36)

since the growth of $|g|^2$ is the greatest along $\theta = \pi$ with $|\cos(\Phi)| = |\cos((m - r)\pi)| = |\cos(s\pi)| = 1$. \[\square\]

Theorem 5 “explains” why the upwind algorithm for solving the $m=1$ advection equation is stable only for $|\nu_1| \leq 1$ and that the $m=2$ diffusion algorithm is stable only for $|\nu_2| \leq 1/2$. These are not just isolated idiosyncrasies of individual algorithm; they are part of the pattern of stability mandated by Theorem 5. One can easily check that this theorem is true for other values of $m$. Thus with increasing $m$, the range of stability decreases geometrically.

We can now decide, among the $m+1$ first-order algorithms corresponding to $r = 0, 1, 2, \ldots m$ of Theorem 4, which one is von-Neumann stable. Surprisingly, there is at most one stable first-order algorithm for a given value of $m$ and the sign of $\nu_m$:

**Theorem 6.** Among the $m+1$ first-order time marching finite-difference schemes described in Theorem 4 for solving the equation

$$\frac{\partial u}{\partial t} = a_m \partial_x^{m} u,$$  \hspace{1cm} (37)
there is at most one stable algorithm for each value of $m$ and the sign of $a_m$. For $m = 2\ell$ the algorithm $r = \ell$ is stable only for $\text{sgn}(a_m) = (-1)^{\ell-1}$. For $\text{sgn}(a_m) = (-1)^{\ell}$, there are no stable algorithms. For $m = 2\ell - 1$, the algorithms $r = \ell$ and $r = \ell - 1$ are stable for $\text{sgn}(a_m) = (-1)^{\ell}$ and $\text{sgn}(a_m) = (-1)^{\ell-1}$ respectively.

Proof. Consider first the even case of $m = 2\ell$, with $\ell = 1, 2, 3, \ldots$. In this case

$$\cos(\Phi) = \cos(\theta(\ell - r) + \ell \pi) = (-1)^{\ell} \cos(\theta(\ell - r)).$$

(38)

If $(\ell - r) \neq 0$, then as $\theta$ ranges from 0 to $2\pi$, $\cos(\theta(\ell - r))$ must change sign and the stability condition (35) cannot hold for all values of $\theta$. The only possible stable algorithm is therefore the central-symmetric algorithm with $r = \ell$, which then places the following restriction on the sign of $\nu_m$:

$$\text{sgn}(\nu_m)(-1)^{\ell} = -1 \implies \text{sgn}(\nu_m) = (-1)^{m/2-1}.$$  

(39)

That is, a stable first-order algorithm is only possible for $a_2 > 0, a_4 < 0, a_6 > 0$, etc., and no stable algorithm otherwise.

For the odd case of $m = 2\ell - 1$, with $\ell = 1, 2, 3, \ldots$, we now have

$$\cos(\Phi) = \cos\left[ \theta(\ell - r) + \ell \pi - \frac{1}{2}(\theta + \pi) \right] = (-1)^{\ell} \cos\left[ \theta(\ell - r) - \frac{1}{2}(\theta + \pi) \right].$$

(40)

For $r = \ell$, $\cos\left[ -\frac{1}{2}(\theta + \pi) \right] < 0$ for $0 < \theta < 2\pi$. Thus this algorithm is stable for

$$\text{sgn}(\nu_m)(-1)^{\ell+1} = -1 \implies \text{sgn}(\nu_m) = (-1)^{\ell}.$$  

(41)

For $r = \ell - 1$, we have $\cos\left[ \frac{1}{2}(\theta - \pi) \right] > 0$ for $0 < \theta < 2\pi$ and this algorithm is stable for

$$\text{sgn}(\nu_m)(-1)^{\ell} = -1 \implies \text{sgn}(\nu_m) = (-1)^{\ell-1}.$$  

(42)

Other than these two values of $r$, $\cos\left[ \theta(\ell - r) - \frac{1}{2}(\theta + \pi) \right]$ will change sign as $\theta$ ranges over $2\pi$. For each sign of $a_{2\ell-1}$, there is only one stable algorithm. □

Theorems 1, 2, 4, 5, 6 completely characterize all minimum grid-point, first-order time-marching algorithms for solving (37). The pattern of stability proscribed by Theorem 6 is easily understood from the following plane wave solution to (37):

$$u(x, t) = A e^{ipx + a_mipt}.$$  

(43)

For $m = 1$, the wave propagates to the positive $x$-direction for $a_1 < 0$, therefore only the algorithm $r = 1$ is stable, corresponding to the upwind algorithm. For $a_1 > 0$, the wave propagates to the negative $x$-direction and $r = 0$ is the corresponding upwind algorithm.

For $m = 2$, the wave decays in time only for $a_2 > 0$ and $r = 1$ gives the well-known first-order diffusion algorithm. For $a_2 < 0$, there is no stable algorithm because the solution grows without bound with time.

For $m = 3$, the wave propagates to the positive $x$-direction with $a_3 > 0$; therefore only the $r = 2$ algorithm is stable, the analog of the $m = 1$ upwind algorithm. For $a_3 < 0$, the wave propagates to the negative $x$-direction and $r = 1$ is the analogous upwind algorithm. Note that the scheme with grid points $\{k_i\} = \{-2, -1, 1, 2\}$, excluding 0, is unstable.

For $m = 4$, the wave decays in time only for $a_4 < 0$ and pattern repeats as $i^m$ cycles through its four possible values.
4. Higher order time-marching algorithms. For the case of \((m, n) = (1, n)\), the algorithm for solving the advection equation to the \(n\)th time-marching order is given by

\[
c_i = \sum_{k=0}^{n} L_i^{(k)}(0) \frac{\mu_i^k}{k!} = L_i(\mu_1),
\]

which is the seminal case studied by Strang\cite{strang}, Iserles and Strang\cite{iserles-strang} and recounted in Ref.\cite{ref}. This is now just a special case of Theorem\cite{theorem}. Note that the last equality can be used to identify \(L_i^{(k)}(0)\) needed by other algorithms, see further discussion below.

For \(k_i = \{-r, -r + 1, \ldots -1, 0, 1, \ldots s\}\), as shown by Strang\cite{strang} and Iserles and Strang\cite{iserles-strang}, only three cases are stable for each sign of \(a_1\). For the conventional choice of \(a_1 < 0\), where the wave propagates from left to right, \(r = s + 1\) and \(r = s\) are stable for \(0 \leq |\nu_1| \leq 1\), and \(r = s + 2\) is stable for \(0 \leq |\nu_1| \leq 2\). Since \(r + s = n\), the order of each type of algorithm are \(n = 2s + 1\), \(n = 2s\) and \(n = 2s + 2\) respectively. Thus there is one stable algorithm at each odd-order and two stable algorithms at each even-order. The odd-order algorithms begin with the first-order upwind (UW) scheme with \(s = 0\) and the even-order schemes begin with the second-order Lax-Wendroff (LW) scheme with \(s = 1\) and the second-order Beam-Warming (BW) scheme with \(s = 0\), respectively. The even-order schemes can be distinguished as being of the LW-type \((n = 2s)\) or BW-type \((n = 2s + 2)\).

The local error in this case is particularly simple. From (19), for \(m = 1\) and \(N = n + 1\), we have (ignoring the \(Q_{jm}(0)\) term),

\[
E = \left[ \Delta x^{n+1} \left( \sum_{j=0}^{n} \frac{(\nu_1)^j}{j!} P^{(j)}(0) \right) - (\Delta t a_1)^{n+1} \right] \frac{u^{(n+1)}(x, 0)}{(n+1)!}
\]

(45)

Since \(P(x)\) is a polynomial of \(N - 1 = n\) degree, we have

\[
E = \left[ \Delta x^{n+1} P(\nu_1) - (\Delta t a_1)^{n+1} \right] \frac{u^{(n+1)}(x, 0)}{(n+1)!}
\]

\[
= \left[ \Delta x^{n+1} \left( \nu_1^{n+1} - \sum_{i=1}^{n+1} (\nu_1 - k_i) \right) - (\Delta t a_1)^{n+1} \right] \frac{u^{(n+1)}(x, 0)}{(n+1)!}
\]

\[
= -\Delta x^{n+1} \sum_{i=1}^{n+1} (\nu_1 - k_i) \frac{u^{(n+1)}(x, 0)}{(n+1)!}.
\]

(46)

The local truncation error is obtained by dividing the above by \(\Delta t\).

For later illustration purposes, we list below the third-order scheme corresponding to \(s = 1\) with \(\{k_i\} = \{-2, -1, 0, 1\}\). The coefficients directly from (44) are

\[
c_{-2} = -\frac{\nu_1^2}{6} (\nu_1^2 - 1) \quad c_{-1} = \frac{\nu_1}{2} (\nu_1 + 2)(\nu_1 - 1)
\]

\[
c_0 = \frac{1}{2} (\nu_1 + 2)(\nu_1^2 - 1) \quad c_1 = \frac{\nu_1}{6} (\nu_1 + 2)(\nu_1 + 1),
\]

(47)
and the algorithm can also be arranged as a sum over powers of $\nu_1$:

$$u_j^{k+1} = u_j^k + \nu_1 \left( \frac{1}{6} u_{j-2}^k - u_{j-1}^k + \frac{1}{2} u_j^k + \frac{1}{3} u_{j+1}^k \right)$$

$$+ \frac{\nu_1^2}{2!} \left( u_{j-1}^k - 2u_j^k + u_{j+1}^k \right)$$

$$+ \frac{\nu_1^3}{3!} \left( -u_{j-2}^k + 3u_{j-1}^k - 3u_j^k + u_{j+1}^k \right),$$

(49)

where we have denoted $u_j^k \equiv u(k\Delta t, j\Delta x)$. Similarly, the fourth-order LW-type algorithm corresponding to $\{k_i\} = \{-2, -1, 0, 1, 2\}$ can be arranged as

$$u_j^{k+1} = u_j^k + \nu_1 \left( \frac{1}{12} u_{j-2}^k - \frac{2}{3} u_{j-1}^k + \frac{2}{3} u_j^k - \frac{1}{12} u_{j+2}^k \right)$$

$$+ \frac{\nu_1^2}{2!} \left( \frac{1}{12} u_{j-2}^k + \frac{4}{3} u_{j-1}^k - \frac{5}{2} u_j^k + \frac{4}{3} u_{j+1}^k - \frac{1}{12} u_{j+2}^k \right)$$

$$+ \frac{\nu_1^3}{3!} \left( -\frac{1}{2} u_{j-2}^k + u_{j-1}^k - u_{j+1}^k + \frac{1}{2} u_{j+2}^k \right)$$

$$+ \frac{\nu_1^4}{4!} \left( 6u_j^k - 4u_{j+1}^k + 6u_j^k - 4u_{j+1}^k + u_{j+2}^k \right).$$

(50)

Each parenthese in (49) and (50) gives the corresponding third and fourth-order spatial discretization of derivatives respectively, as mandated by Theorem 2. The coefficients of the last term are just those of $(x - 1)^3$ and $(x - 1)^4$, in accordance with Theorem 4.

The above examples are for later illustrations only. In practice, it is absolutely unnecessary to write out the coefficients $c_i$ explicitly as in the above examples, or disentangle them into powers of $\nu_1$. It is only necessary to write a short routine to compute $c_i$ directly from (44) for a given set of $\{k_i\}$ and generate an algorithm of any order. This is illustrated below.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{The propagation of an initial triangular and a rectangular profile (in black) 50 times around a periodic box of [-5,5] with $\Delta x = 0.1$, $\Delta t = 0.08$, $v = 1$, and $\nu_1 = 0.8$, corresponding to 6250 iterations of each algorithm. The numbers label odd-order algorithms beginning with the first-order upwind (UW) scheme. The highest order is 29.}
\end{figure}

In solving the advection equation, it is well-known that low-order algorithms are plagued with unwanted damping and negative oscillations. In the following figures, we
examine how each type of algorithm converges toward the exact solution with increasing time-marching orders. Figs.1, 2 and 3 show results for the odd-order UW-type and the two even-order LW-type and BW-type algorithms respectively. In each case, the lowest order algorithm, UW, LW and BW are all damped and dispersed beyond recognition. At increasing order (at fixed $\Delta x$ and $\Delta t$), the convergence toward the undamped triangular profile is excellent. For the rectangular profile, the convergence is consistent with having Gibb’s oscillations. The odd-order algorithms preserve the left-right symmetry of the original profile despite oscillations, whereas the two even-order algorithms are marred by asymmetries and phase errors until very high orders. In this study, the order 5 scheme seemed optimal. Beyond order 5, the improvement is incremental. The 29th and 30th-order algorithms are of course not very practical. They are shown here just to illustrate the fact that very high order algorithms are possible.

For solving the diffusion equation with $m = 2$, it is natural to take $N = 2n + 1$ grid points to be $\{k_i\} = \{-n, ..., -1, 0, 1, 2, ..., n\}$ with $c_{-l} = c_l$. For $n = 1$ one obtains
the familiar first-order time-marching algorithm from Theorem 4:

\[ u^{k+1}_j = u^k_j + \nu_2(u^k_{j-1} - 2u^k_j + u^k_{j+1}) \]  

(51)

The coefficients multiplying \( \nu_2 \) are just those of \((x - 1)^2\). For time-marching order 2, one has

\[ c_0 = 1 - \frac{5}{2} \nu_2 + 3\nu_2^2 \quad c_1 = \frac{4}{3} \nu_2 - 2\nu_2^2 \quad c_2 = -\frac{1}{12} \nu_2 + \frac{1}{2} \nu_2^2 \]  

(52)

and the resulting algorithm is

\[ u^{k+1}_j = u^k_j + \nu_2(-\frac{1}{12}u^k_{j-2} + \frac{4}{3}u^k_{j-1} - \frac{5}{2}u^k_j + \frac{4}{3}u^k_{j+1} - \frac{1}{12}u^k_{j+2}) \]

\[ + \frac{\nu_2^2}{2!}(u^k_{j-2} - 4u^k_{j-1} + 6u^k_j - 4u^k_{j+1} + u^k_{j+2}). \]  

(53)

Comparing this to the fourth-order advection algorithm (50), one sees that the coefficients inside the parentheses are just those of the second and fourth order terms of (50). Thus the coefficients of the diffusion algorithm are simply those of the even order terms of the advection algorithm, with appropriate change of factors \( \nu_i^k/(2k)! \rightarrow \nu_i^k/k! \), provided that both are using the same set of \( \{k_i\} \). (Similarly, one can pick out the \( jm \)-order terms of the advection scheme to generate algorithms for solving the \( m \)-order equation.)

For order 3, one has

\[ c_0 = 1 - \frac{49}{18} \nu_2 + \frac{14}{3} \nu_2^2 - \frac{10}{3} \nu_2^3 \quad c_1 = \frac{3}{2} \nu_2 - \frac{13}{4} \nu_2^2 + \frac{5}{2} \nu_2^3 \]  

(54)

\[ c_2 = -\frac{3}{20} \nu_2 + \nu_2^2 - \nu_2^3 \quad c_3 = \frac{1}{90} \nu_2^2 - \frac{1}{12} \nu_2^3 + \frac{1}{6} \nu_2^3. \]  

(55)

Again, the coefficients of \( \nu_2^3 \) are now binomial coefficients of \((x - 1)^6\) multiplied by 1/3!. The coefficients of \( \nu_2 \) and \( \nu_2^2 \) are from Theorem 3. The algorithm is now correct to sixth order in spatial discretizations.

For order 4, one has

\[ c_0 = 1 - \frac{205}{72} \nu_2 + \frac{91}{16} \nu_2^2 - \frac{25}{4} \nu_2^3 + \frac{35}{12} \nu_2^4 \]  

(56)

\[ c_1 = \frac{8}{5} \nu_2 - \frac{61}{15} \nu_2^2 + \frac{29}{6} \nu_2^3 - \frac{7}{3} \nu_2^4 \quad c_2 = -\frac{1}{5} \nu_2 + \frac{169}{120} \nu_2^2 - \frac{13}{6} \nu_2^3 + \frac{7}{6} \nu_2^4 \]  

(57)

\[ c_3 = \frac{8}{315} \nu_2 - \frac{1}{5} \nu_2^2 + \frac{1}{2} \nu_2^3 - \frac{1}{3} \nu_2^4 \quad c_4 = -\frac{1}{560} \nu_2 + \frac{7}{480} \nu_2^2 - \frac{1}{24} \nu_2^3 + \frac{1}{24} \nu_2^4, \]  

(58)

which is correct to the eighth-order in spatial discretizations.

In all these cases, one can check that the local error is correctly given by (49), unfortunately, there does not seem to be a closed form for the sum over \( Q^{(jm)}(0) \), and hence no simple expression for the local error as in (49).

For these algorithms, the amplification factor for a single Fourier mode \( e^{i\nu x} \) is

\[ g = 1 - 4 \sum_{j=1}^{n} c_j \sin^2 \left( \frac{j}{2} \theta \right) \]  

(59)
where \( \theta = p\Delta x \). For \( n = 1, c_1 = \nu_2 \), one obtains the usual stability criterion of \( \nu_2 \leq \nu_c \), where the critical stability point is \( \nu_c = 1/2 \). If one simply increases the spatial order of discretizing \( \partial^2 w_i^j \) to fourth-order without increasing the temporal order, \( \nu_c \) decreases to \( 3/8 = 0.375 \). (This is algorithm \( \text{[53]} \) without the second-order \( \nu_2^2 \) term.) However, the full second-order time-marching algorithm \( \text{[53]} \) has increased stability, with \( \nu_c = 2/3 = 0.667 \). Similarly, the third and fourth-order time-marching algorithm have increased stability of \( \nu_c = 0.841 \) and \( \nu_c = 1.015 \) respectively, while keeping only the first-order term in \( \nu_2 \) have decreased stability of \( \nu_c = 45/136 = 0.331 \) and \( \nu_c = 315/1024 = 0.308 \). Thus the old notion that increasing the order of spatial discretization leads to greater instability is dispelled if the time-march order is increased commensurately. Also, this increase in stability range is surprisingly linear with increase in time-marching order. Each order gains \( \approx 0.17 \) in \( \nu_c \). Thus the stability range doubles in going from the first to the fourth-order.

5. Solving nonlinear equations. Nonlinear equations are difficult to solve in general. However, in the case of the general nonlinear advection equation,

\[
\partial_t u = f(u) \partial_x u, \tag{60}
\]

a simple formal solution exists and can be used to derive time-marching algorithms of any order. By Taylor's expansion, one has

\[
u(x, \Delta t) = u(x, 0) + \Delta t \partial_t u + \frac{1}{2} \Delta t^2 \partial_x^2 u + \frac{1}{3!} \Delta t^3 \partial_x^3 u + \cdots, \tag{61}\]

where all the time-derivatives are evaluated at \( t = 0 \). These derivatives can be obtained by multiply both sides of \( \text{(60)} \) by \( f^j(u) \),

\[
f^j(u) \partial_t u = f^{j+1}(u) \partial_x u,
\Rightarrow \quad \partial_t u_j(u) = \partial_x u_{j+1}(u), \tag{62}\]

where we have defined, for \( j \geq 0 \),

\[
u_j(u) = \int f^j(u) du, \tag{63}\]

with \( u_0(u) \equiv u(x, t) \). These are the conserved densities, since

\[
\partial_t \int_a^b u_j(u) dx = \int_a^b \partial_x u_{j+1}(u) dx = 0 \tag{64}\]

for periodic or Dirichlet boundary conditions. It follows from \( \text{(62)} \) that

\[
\partial_t u = \partial_x u_1
\]

\[
\partial_t^2 u = \partial_x (\partial_t u_1) = \partial_x^2 u_2
\]

\[
\cdots
\]

\[
\partial_t^j u = \partial_x^{j-1} (\partial_t u_{j-1}) = \partial_x^j u_j \tag{65}\]

and therefore the solution is simply

\[
u(x, \Delta t) = u(x, 0) + \Delta t \partial_x u_1 + \frac{1}{2} \Delta t^2 \partial_x^2 u_2 + \frac{1}{3!} \Delta t^3 \partial_x^3 u_3 + \cdots. \tag{66}\]
To see how this solution works, consider the inviscid Burgers’ equation with
\[ f(u) = -u. \]

In this case,
\[ u_n(x, t) = (-1)^n \frac{u_{n+1}(x, t)}{n+1}. \]  
(67)

For the initial profile
\[ u(x, 0) = u_0(x) \equiv \begin{cases} 
1 & \text{if } x < 0 \\
1-x & \text{if } 0 \leq x \leq 1 \\
0 & \text{if } x > 0,
\end{cases} \]  
(68)

\[ \partial_x^n u_n = n!(1 - x), \]  
(69)

and the solution (66) gives, for \( 1 \geq u(x, \Delta t) \geq 0, \)
\[ u(x, \Delta t) = (1 + \Delta t + \Delta t^2 + \Delta t^3 + \cdots)(1 - x), \]  
(70)

\[ = \frac{(1 - x)}{(1 - \Delta t)}. \]  
(71)

Thus the top edge of the wave at \( u(x, \Delta t) = 1 \) moves with unit speed, \( x = \Delta t, \) and the shock-front forms at \( \Delta t = 1. \) This formal solution is incapable of describing the motion of the shock-front beyond \( \Delta t = 1, \) but remarkably, as will be shown below, finite-difference schemes base on it can.

The solution (66) suggests that one should generalize the finite-difference scheme to
\[ u(x, \Delta t) = \sum_{i=1}^{N} c_0 e^{k_i \Delta x} u(x, 0) + \sum_{i=1}^{N} c_1 e^{k_i \Delta x} \partial_x u_1 + \sum_{i=1}^{N} c_2 e^{k_i \Delta x} \partial_x u_2 + \cdots. \]  
(72)

Comparing this to (66), one sees that an nth-order time-marching algorithm now requires, in addition to \( N = n + 1 \) grid points, also nonlinear functions of \( u(x, 0) \) up to \( u_N(x, 0). \) For each \( u_j(x, 0), \) the set of coefficients \( \{c_{ji}\} \) must have vanishing sums over all powers of \( \{k_i\} \) up to \( n \) except the following:
\[ \sum_{i=1}^{N} c_{0i} = 1, \quad \sum_{i=1}^{N} c_{1i} k_i = \nu, \quad \sum_{i=1}^{N} c_{2i} k_i^2 = \nu^2, \quad \text{etc.} \]  
(73)

where here \( \nu = \Delta t/\Delta x. \) Recalling (15), the solutions are just
\[ c_{0i} = L_i(0), \quad c_{1i} = \nu L_i^{(1)}(0), \quad c_{2i} = \frac{\nu^2}{2!} L_i^{(2)}(0), \quad \text{etc.} \]  
(74)

and therefore the finite-difference scheme for solving (60) is
\[ u(x, \Delta t) = \sum_{i=1}^{N} L_i(0) u(x + k_i \Delta x, 0) + \nu \sum_{i=1}^{N} L_i^{(1)}(0) u_1(x + k_i \Delta x, 0) \]
\[ + \frac{\nu^2}{2!} \sum_{i=1}^{N} L_i^{(2)}(0) u_2(x + k_i \Delta x, 0) + \frac{\nu^3}{3!} \sum_{i=1}^{N} L_i^{(3)}(0) u_3(x + k_i \Delta x, 0) + \cdots \]  
(75)
If one were to replace all \(u_n(x, 0)\) by \(u(x, 0)\), then the above is just the linear advection scheme (44) with \(a_1 = 1\). Conversely, any linear advection scheme can now be used to solve the nonlinear advection equation by replacing the \(u(x, 0)\) terms multiplying \(\nu_n^k\) by \(u_n(x, 0)\). For example, the third-order advection scheme (49) for solving the inviscid Burgers’ equation can now be applied here as

\[
\begin{align*}
\frac{u_j^{k+1}}{u_j^k} &= u_j^k + \nu \left( \frac{1}{6} (u_1)^{k}_{j-2} - (u_1)^{k}_{j-1} + \frac{1}{2} (u_1)^{k}_{j} + \frac{1}{3} (u_1)^{k}_{j+1} \right) \\
&\quad + \frac{\nu^2}{3!} ((u_2)^{k}_{j-1} - 2(u_2)^{k}_{j} + (u_2)^{k}_{j+1}) \\
&\quad + \frac{\nu^3}{3!} (-3(u_3)^{k}_{j-2} + 3(u_3)^{k}_{j-1} - 3(u_3)^{k}_{j} + 3(u_3)^{k}_{j+1})
\end{align*}
\]

(76)

with \((u_n)^{k}_{j} = (-1)^n (u^k_j)^{n+1}/(n + 1)\). Thus arbitrary order schemes for solving the nonlinear advection equation (60) can be obtained from (44).

To see how these schemes work, we compare their results when propagating the initial profile (68) from \(t = 0\) to \(t = 2\). Before the formation of the shock front at \(t = 1\), the top edge of the wave is traveling at unit speed and reaches \(x = 0.5\) and \(x = 1.0\) at \(t = 0.5\) and \(t = 1.0\) respectively. After the shock has formed, the shock front travels at half the initial speed and reaches \(x = 1.25\) at \(t = 1.5\) and \(x = 1.5\) at \(t = 2.0\). The upwind (UW) scheme is overly diffusive, the Lax-Wendroff (LW) and the Beam-Warming (BW) schemes have unwanted oscillations trailing and ahead of the shock front respectively. Algorithm 3 has reduced oscillations both before and
after the shock front. While algorithms of any order for solving the linear advection equation is easily generated, it remains difficult to produce arbitrary order algorithms for solving the nonlinear advection equation, because one must disentangle each power of \( \nu \) in \( c_i \) by hands.

This example shows that for solving nonlinear equations, one must also discretize suitable nonlinear functions of the propagating wave. For the nonlinear advection equation, the set of needed nonlinear functions are given by (63). Unfortunately, the solution to the nonlinear diffusion equation is not of the form of (66) and further study is needed to derive finite-difference schemes that can match its solution.

6. Conclusions and discussions. In this work, we have shown that by matching the operator form of the finite-difference scheme to the formal operator solution, one can systematically derive explicit finite-difference schemes for solving any linear partial differential equation with constant coefficients. This theory provided a unified description of all explicit finite-difference schemes through the use of Lagrange polynomials. In a way, this work showed that, not only are Lagrange polynomials important for doing interpolations, they are also cornerstones for deriving finite-difference schemes.

Because one has a unified description of all finite-difference schemes, there is no need to analyze each finite-difference scheme one by one. Theorem \( \mathbf{3} \) for example, gives the local error for all algorithms at once. Also, the stability of first-order algorithms for solving (37) can be determined for all \( m \) simultaneously. It would be of great interest if all second-order time-marching algorithms for solving the \( m \)-order linear equations can also be characterized the same way. The method used here for solving the operator equality (33) is just Taylor’s expansion, alternative methods of solving the equality without Taylor’s expansion would yield entirely new classes of finite-difference schemes.

Finally, this work focuses attention on obtaining the formal operator solution to the partial differential equation. To the extent that the formal solution embodies all the conservative properties of the equation, a sufficiently high-order approximation to the formal solution should yield increasing better conservative schemes. The method is surprisingly effective in deriving arbitrary order schemes for solving the general nonlinear advection equation (60). One is therefore encouraged to gain a deeper understanding of formal solutions so that better numerical schemes can be derived for solving nonlinear equations.

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Appendix. Lagrange interpolation polynomials. Consider the Lagrange interpolation at \( N \) points \( \{k_1, k_2, \ldots, k_N\} \) with values \( \{f_1, f_2, \ldots, f_N\} \). The interpolating \( N - 1 \) degree polynomial is given by

\[
f(x) = \sum_{i=1}^{N} f_i L_i(x),
\]

(77)

where \( L_i(x) \) are the Lagrange polynomials defined by

\[
L_i(x) = \prod_{j=1}^{N} \frac{(x - k_j)}{(k_i - k_j)}.
\]

(78)
Since by construction
\[ L_i(k_j) = \delta_{ij} \] (79)
one has the desired interpolation,
\[ f(k_j) = \sum_{i=1}^{n} f_i L_i(k_j) = \sum_{i=1}^{n} f_i \delta_{ij} = f_j. \] (80)

Now let \( f_i = k_i^m \) for \( 0 \leq m \leq N - 1 \), then the interpolating polynomial
\[ f(x) = \sum_{i=1}^{n} k_i^m L_i(x) \] (81)

and the function
\[ g(x) = x^m \] (82)

both interpolate the same set of points and therefore must agree. Hence
\[ \sum_{i=1}^{N} k_i^m L_i(x) = x^m, \] (83)

for \( 0 \leq m \leq N - 1 \). This is then (14).

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