Numerical analysis: numerical differentiation

Dr. Dmitry Batenkov

March 21, 2021

1 Approximating the derivative by interpolation polynomials

The main task is to approximate the derivative of a function $f(x)$ at some point $x = a$ using only values of f at some points $x_0, \ldots, x_n$ from the vicinity of a.

Consider the approximation of $f(x)$ by its interpolation polynomial in Newton form:

$$f(x) = P_n(x) + f[x_0, \ldots, x_n, x]\, q_{n+1}(x) = P_n(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} q_{n+1}(x). \tag{1}$$

We can now use this representation to compute approximation to *linear operators* acting on $f(x)$ such as $f'(x), \int f(x)\,dx$, etc. For the derivative we get

$$\begin{aligned} f'(x) &= P_n'(x) + \frac{d}{dx}\left\{f[x_0, \ldots, x_n, x]\, q_{n+1}(x)\right\} \\ &= P_n'(x) + \underbrace{q_{n+1}(x) \frac{d}{dx}\left\{f[x_0, \ldots, x_n, x]\right\} + f[x_0, \ldots, x_n, x]\, q_{n+1}'(x)}_{E(x)}. \end{aligned} \tag{2}$$

Claim 1. The divided differences satisfy the following properties:

1. $f[x_0, \ldots, x_n]$ does not depend on the order of the points, if identical points are ajacent in the list;

2. $f[x_0, \ldots, x_n, x]$ is a continuous function of x;

3. $\frac{d}{dx}\left\{f[x_0, \ldots, x_n, x]\right\} = f[x_0, \ldots, x_n, x, x]$.

Proof. Since the interpolation polynomial does not depend on the order of the points, so does its highest coefficient, proving 1). As long as f has sufficiently many derivatives, 2) can be proved by induction using the recursive definition of the divided differences. For 3), by definition of derivative, 1) and continuity of the divided differences we have

$$\begin{aligned} \frac{d}{dx}\left\{f[x_0, \ldots, x_n, x]\right\} &= \lim_{h\to 0} \frac{f[x_0, \ldots, x_n, x+h] - f[x_0, \ldots, x_n, x]}{h} \\ &= \lim_{h\to 0} \frac{f[x_0, \ldots, x_n, x+h] - f[x, x_0, \ldots, x_n]}{h} \\ &= \lim_{h\to 0} f[x, x_0, \ldots, x_n, x+h] \\ &= f[x, x_0, \ldots, x_n, x] \\ &= f[x, \ldots, x_n, x, x]. \end{aligned}$$

□

Recall that $f[x_0,\ldots,x_n] = \frac{f^{(n)}(c)}{n!}$ for some intermediate point $c \in [\min_k x_k, \max_k x_k]$. Combining the above with (2) we obtain the following result.

Corollary 1. *The error formula for the derivative approximation is given by*

$$E(x) = f'(x) - P_n'(x) = \frac{f^{(n+2)}(c)}{(n+2)!} q_{n+1}(x) + \frac{f^{(n+1)}(d)}{(n+1)!} q_{n+1}'(x), \tag{3}$$

for some intermediate points $c = c(x)$ and $d = d(x)$ in the interval containing $\{x_0, \ldots, x_n, x\}$.

The expression (3) can be evaluated easily if either

- **Case A:** $q_{n+1}(x) = 0$ (i.e. x is equal to one of the interpolation nodes $x = x_i$), in which case

$$\begin{aligned} E(x) &= \frac{f^{(n+1)}(d)}{(n+1)!} q_{n+1}'(x) \\ &= \frac{f^{(n+1)}(d)}{(n+1)!} \left\{ \sum_{k=0}^{n} \prod_{j\neq k, j=0,\ldots,n} (x - x_j) \right\} \\ &= \frac{f^{(n+1)}(d)}{(n+1)!} \prod_{j\neq i,, j=0,\ldots,n} (x_i - x_j); \end{aligned}$$

- **Case B:** $q_{n+1}'(x) = 0$, in which case

$$E(x) = \frac{f^{(n+2)}(c)}{(n+2)!} q_{n+1}(x).$$

Example 1. Approximate $f'(a)$ using the values of $f(x)$ at $x_0 = a, x_1 = a + h$, and estimate the error.

Solution. Here $n = 1$. We are in **Case A**.

$$\begin{aligned} P_1(x) &= f(a) + f[a, a+h](x - a) \\ P_1'(a) &= f[a, a+h] = \frac{f(a+h) - f(a)}{h} \\ E(a) &= \frac{f''(d)}{2!}(a - (a+h)) = -\frac{f''(c)}{2} h. \end{aligned}$$

Notice that we can easily obtain this from the Taylor expansion (more on this later):

$$\begin{aligned} f(a+h) &= f(a) + hf'(a) + \frac{h^2}{2} f''(c) \\ f'(a) &= \frac{f(a+h) - f(a)}{h} - \frac{h}{2} f''(c). \end{aligned}$$

This is called the ***2-point forward difference scheme.***

Which is better, Case A or Case B?

As mentioned above, we usually are interested in the case where all the interpolation points are taken from some small neighborhood $\mathcal{N}$ of the point $x = a$ of size $h \ll 1$. Then $|q_{n+1}(x)| \leq h^{n+1}$ and $\left|q'_{n+1}(x)\right| \leq C_n h^n$ for all $x \in \mathcal{N}$. If f has $n+2$ bounded derivatives, then

$$|E(x)| \leq C_1 h^{n+1} + C_2 h^n = O(h^n).$$

Definition 1 (Order of approximation/error)**.** The **approximation order** of a method is the largest integer p such that there exists a constant C (in general depending on f, n but not on h) such that

$$|E(a)| \leq Ch^p,\ h \to 0, \quad \min_{i \neq j} |x_i - x_j| \leq h \leq \max_{i \neq j} |x_i - x_j|.$$

The 2-point forward difference scheme is therefore of first order ($p = 1$).

Thus, in general **Case B** will provide higher approximation order than **Case A**.

Definition 2. The **algebraic degree of exactness** of a method is the highest possible degree r for which the method is exact (i.e. the error $E(x) = 0$) for all polynomials $f(x) = P(x) \in \Pi_r$ (and therefore there exists at least one polynomial of degree $= r+1$ for which $E(x) \neq 0$).

The 2-point forward difference scheme has algebraic degree of exactness $= 1$.

Example 2 (2-point central difference scheme)**.** Approximate $f'(a)$ using the values of f at $x_0 = a - h$ and $x_1 = a + h$ – so a itself is not an interpolation point.

Solution. As before, $n = 1$ but now we are in **Case** B because $q_2(x) = (x - a + h)(x - a - h)$ and $q'_2(x) = x - a + h + x - a - h = 2(x - a)$ and so $q_2(a) = -h^2$ and $q'_2(a) = 0$:

$$\begin{aligned} P_1(x) &= f(a-h) + f[a-h, a+h](x - (a-h)) \\ P'_1(a) &= f[a-h, a+h] = \frac{f(a+h) - f(a-h)}{2h} \\ E(a) &= -\frac{f^{(3)}(c)}{3!} h^2. \end{aligned}$$

We see that the method is of approximation order=2 and algebraic degree of exactness=2.

It is not possible that both $q_{n+1}(a) = 0$ and $q'_{n+1}(a) = 0$ (why?) If so, when would we have $q'_{n+1}(a) = 0$? The following fact is presented without proof.

Claim 2. Suppose that $a \notin \{x_0, \ldots, x_n\}$ but a is the center of symmetry for the nodes $x_0, \ldots, x_n$, in other words, for each $y \in \{x_0, \ldots, x_n\}$ it is true that $z = 2a - y \in \{x_0, \ldots, x_n\}$ (and so $a = \frac{y+z}{2}$). Then $q'_{n+1}(a) = 0$ and we are in **Case B.**

Example 3 (3-point forward difference scheme)**.** Approximate $f'(a)$ using the values of f at $x_0 = a$, $x_1 = a + h$ and $x_2 = a + 2h$.

Solution. Now $n=2$ and we are in **Case A**. Notice that $q_3'(a) = (a-x_1)(a-x_2) = 2h^2$.

$$\begin{aligned}
P_2(x) &= f[x_0] + f[x_0,x_1](x-x_0) + f[x_0,x_1,x_2](x-x_0)(x-x_1) \\
&= f(a) + \frac{f(a+h)-f(a)}{h}(x-a) + \frac{f(a+2h)-2f(a+h)+f(a)}{2h^2}(x-a)(x-a-h) \\
P_2'(x) &= \frac{f(a+h)-f(a)}{h} + \frac{f(a+2h)-2f(a+h)+f(a)}{2h^2}(2x-2a-h) \\
P_2'(a) &= \frac{f(a+h)-f(a)}{h} - \frac{f(a+2h)-2f(a+h)+f(a)}{2h} = \frac{-3f(a)+4f(a+h)-f(a+2h)}{2h} \\
E(a) &= \frac{f^{(3)}(d)}{3!}q_3'(a) = \frac{f^{(3)}(d)}{3!}2h^2.
\end{aligned}$$

Therefore the scheme is of approximation order=2 and degree of algebraic exactness=2 – same as in 2-point central difference scheme.

Remark 1. The same formulas can be obtained using the Lagrange form of $P_n(x)$:

$$\begin{aligned}
P_n(x) &= \sum_{i=0}^{n} f(x_i)\,\ell_i(x) \\
P_n'(a) &= \sum_{i=0}^{n} f(x_i)\underbrace{\ell_i'(a)}_{A_i},
\end{aligned}$$

i.e. the approximation is a linear combination of the values $\{f(x_i)\}$. The coefficients A_i can be found by Taylor expansion (below).

Remark 2. Another possibility is to require that a formula be exact for polynomials $\{1, x, x^2, \ldots, x^n\}$, i.e. have degree of algebraic exactness $r=n$.

Remark 3. When using the scheme $f'(a) \approx P_n'(a)$ with a certain n, then automatically we have that the degree of algebraic exactness is at least n. Indeed, if $f(x) \in \Pi_n$ then $P_n(x) = f(x)$ and therefore $E(x) = 0$. This argument also holds for other approximation operators such as high order derivatives, integrals etc.

2 Taylor series method for approximating derivatives

The general method

We seek approximation of the form $f'(a) \approx \sum_{i=0}^{n} A_i f(x_i)$ where $A_0, \dots, A_n$ do not depend on f.

$$\begin{aligned}
\sum_{i=0}^{n} A_i f(x_i) &= \sum_{i=0}^{n} A_i \underbrace{f\left(a + \underbrace{(x_i - a)}_{h_i}\right)}_{\text{expand into Taylor series around } a} \\
&= \sum_{i=0}^{n} A_i \left(\sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!} h_i^k + \frac{f^{(n+1)}(c_i)}{(n+1)!} h_i^{n+1} \right) \qquad (4) \\
&= \underbrace{\sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!} \left\{ \sum_{i=0}^{n} A_i h_i^k \right\}}_{D(a)} + \underbrace{\frac{1}{(n+1)!} \sum_{i=0}^{n} A_i f^{(n+1)}(c_i) h_i^{n+1}}_{-E(a)}.
\end{aligned}$$

We seek $A_0, \dots, A_n$ so that $D(a) \equiv f'(a)$. To do that, we compare coefficients of the derivatives $f^{(k)}(a)$ on both sides for $k = 0, 1, \dots, n$:

$$\begin{aligned}
0 &= \sum_{i=0}^{n} A_i \\
1 &= \sum_{i=0}^{n} A_i h_i \\
0 &= \sum_{i=0}^{n} A_i h_i^k, \quad k = 2, \dots, n.
\end{aligned}$$

This is a linear system of equations, from which $A_0, \dots, A_n$ can be found.

The error can be estimated as follows:

$$\begin{aligned}
E(a) &= f'(a) - \sum_{i=0}^{n} A_i f(x_i) \\
&= -\frac{1}{(n+1)!} \sum_{i=0}^{n} A_i f^{(n+1)}(c_i) h_i^{n+1}.
\end{aligned}$$

Example 4 (3-point forward difference)**.** As in Example 3, $n = 2$ and $x_0 = a, x_1 = a+h, x_2 = a+2h$, i.e. $h_0 = 0, h_1 = h, h_2 = 2h$. We get

$$\begin{aligned}
0 &= A_0 + A_1 + A_2 \\
1 &= A_1 h + 2A_2 h \\
0 &= A_1 h^2 + 4A_2 h^2
\end{aligned}$$

Rewriting this in matrix form

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \\ 0 & 1 & 4 \end{pmatrix} \begin{pmatrix} A_0 \\ A_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{1}{h} \\ 0 \end{pmatrix}.$$

So $A_1 = -4A_2 \Rightarrow -2A_2 = \frac{1}{h} \Rightarrow A_2 = -\frac{1}{2h}, A_1 = \frac{2}{h}, A_0 = -\frac{3}{2h}$ and the scheme is, as before:

$$\begin{aligned} f'(a) &\approx A_0 f(a) + A_1 f(a+h) + A_2 f(a+2h) \\ &= \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h}. \end{aligned}$$

The error is

$$\begin{aligned} E(a) &= -\frac{1}{3!}\left(A_1 f^{(3)}(c_1) h_1^3 + A_2 f^{(3)}(c_2) h_2^3\right) \\ &= -\frac{1}{6}\left(\frac{2}{h} f^{(3)}(c_1) h^3 - \frac{1}{2h} \cdot 8 f^{(3)}(c_2) h^3\right) \\ |E(a)| &\le \frac{1}{6}\left(2h^2 + 4h^2\right) \max_{x\in[a,a+2h]} \left|f^{(3)}(x)\right| \\ &= h^2 \max_{x\in[a,a+2h]} \left|f^{(3)}(x)\right|. \end{aligned}$$

Remark 4. If the linear system with respect to $\{A_0, \ldots, A_n\}$ does not have a unique solution, we may increase n and add another equation to the system (increasing the algebraic degree of exactness).

It may happen that once we solved for $\{A_0, \ldots, A_n\}$, additional terms ($\ge n+1$) in the Taylor series for $\sum_{i=0}^{n} A_i f(x_i)$ get cancelled, increasing the approximation order. In this case we need to add some terms to get a correct estimate of the order.

3 Approximating the second derivative

Returning to (1), let us differentiate twice:

$$\begin{aligned} f(x) &= P_n(x) + f[x_0, \ldots, x_n, x]\, q_{n+1}(x) \\ f'(x) &= P_n'(x) + q_{n+1}(x) f[x_0, \ldots, x_n, x, x] + f[x_0, \ldots, x_n, x]\, q_{n+1}'(x) \\ f''(x) &= P_n''(x) + q_{n+1}'(x) f[x_0, \ldots, x_n, x, x] + f[x_0, \ldots, x_n, x, x, x]\, q_{n+1}(x) \\ &\quad + f[x_0, \ldots, x_n, x, x]\, q_{n+1}'(x) + q_{n+1}''(x) f[x_0, \ldots, x_n, x] \\ &= P_n''(x) + 2f[x_0, \ldots, x_n, x, x]\, q_{n+1}'(x) + f[x_0, \ldots, x_n, x, x, x]\, q_{n+1}(x) + q_{n+1}''(x) f[x_0, \ldots, x_n, x] \\ &= P_n''(x) + \frac{f^{(n+3)}(\xi)}{(n+3)!} q_{n+1}(x) + 2\frac{f^{(n+2)}(\eta)}{(n+2)!} q_{n+1}'(x) + \frac{f^{(n+1)}(\zeta)}{(n+1)!} q_{n+1}''(x) \end{aligned}$$

Example 5. Find approximation to $f''(a)$ using $x_0 = a, x_1 = a+h, x_2 = a-h$.

Solution. Here $n = 2$. Using the general equation (4), we seek A_0, A_1, A_2 for which $D(a) \equiv f''(a)$, which leads to the system of equations (here $h_0 = 0, h_1 = h, h_2 = -h$)

$$\begin{aligned} 0 &= A_0 + A_1 + A_2 \\ 0 &= A_1 h - A_2 h \\ 1 &= \frac{1}{2}\left(A_1 h^2 + A_2 h^2\right) \end{aligned}$$

from which we have $A_1 = A_2 = \frac{1}{h^2}$ and $A_0 = -\frac{2}{h^2}$. Therefore the scheme is

$$f''(a) \approx \frac{f(a+h) - 2f(a) + f(a-h)}{h^2} = f[a, a+h, a-h].$$

We get an additional order of approximation for free:

$$\begin{aligned} f(a+h) - 2f(a) + f(a-h) &= f(a) + hf'(a) + \frac{h^2}{2} f''(a) + \frac{h^3}{3!} f^{(3)}(a) + \frac{h^4}{4!} f^{(4)}(\xi) \\ &\quad - 2f(a) \\ &\quad + f(a) - hf'(a) + \frac{h^2}{2} f''(a) - \frac{h^3}{3!} f^{(3)}(a) + \frac{h^4}{4!} f^{(4)}(\eta) \\ &= h^2 f''(a) + \frac{h^4}{4!} \left(f^{(4)}(\xi) + f^{(4)}(\eta) \right) \end{aligned}$$

The error can be estimated therefore by

$$\begin{aligned} E(a) &= f''(a) - \frac{f(a+h) - 2f(a) + f(a-h)}{h^2} \\ &= -\frac{h^2}{24} \left(f^{(4)}(\xi) + f^{(4)}(\eta) \right) \\ &= -\frac{h^2}{12} f^{(4)}(\zeta), \end{aligned}$$

thus the scheme has approximation order=2 and degree of algebraic order exactness=3.