Lecture 26: Numerical Differentiation using polynomial approximations

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NUMERICAL DIFFERENTIATION

- Till the last class, we have studied how you can use polynomials to approximate any functional relationships if you are given a set of data points $(x, f(x))$.
- You also used these polynomial approximations to the functions (whether exact fit or approximate fit) to interpolate any values of the function that are not given in the discrete data set.
- In this chapter, we will see how these polynomial approximations are also used to differentiate a set of discrete data or find derivatives from a set of discrete data.

x	$f(x)$
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_n	f_n

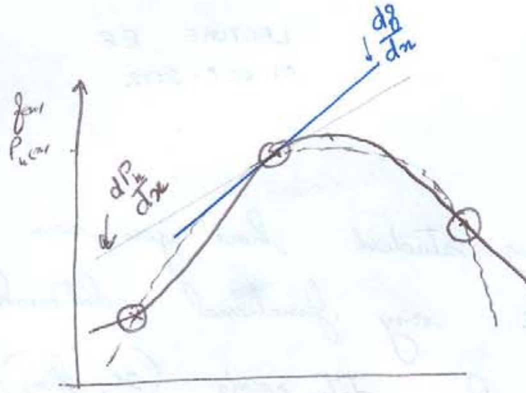
If you have approximated

$$f(x) \approx P_k(x)$$

(i.e a k^{th} order polynomial)

Then $f'(x) \approx P_k'(x)$.

i.e $\frac{d}{dx} f(x) \approx \frac{d}{dx}\left[P_k(x)\right]$



If you see the figure, although $f(x) \approx P_k(x)$ passes through the given data points, the derivative (or slope) of $f(x)$ and $P_k(x)$ may not match. Therefore, we cannot always say that the derivatives are also well matched by a given approximation.

The Polynomial Approx. to Function

Recall from the last chapter.

* We had provided polynomial approximations to the function of discrete data set by
  - → Direct-fit method
  - → Lagrange polynomials
  - → Divided difference polynomials
  - → Newton's forward & backward difference polynomials.
  - → Curve fitting using method of least squares, etc.

Among these

→ Direct-fit
→ Lagrange
→ Divided difference
→ Curve fitting

} can be used for both equally and unequally spaced data sets.

If we are fitting the highest degree of polynomial for a given $(n+1)$ data points, then we can find derivatives by:

The Direct Method

$$f(x) \approx P_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

$$f'(x) \approx \frac{d}{dx}\left[P_n(x)\right] = P_n'(x) = a_1 + 2a_2 x + \cdots + n a_n x^{n-1}$$

$$f''(x) \approx P_n''(x) = 2a_2 + 6a_3 x + \cdots + n(n-1) a_n x^{n-2}$$

The Lagrange Polynomials

Say
$$f(x) \approx P_2(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} f(x_i)$$
$$+ \frac{(x - x_i)(x - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} f(x_{i+1})$$
$$+ \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} f(x_{i+2})$$

$$\therefore f'(x) \approx P_2'(x) = \frac{2x - (x_{i+1} + x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} f(x_i) + \frac{2x - (x_i + x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} f(x_{i+1})$$
$$+ \frac{2x - (x_{i+1} + x_i)}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} f(x_{i+2})$$

and
$$f''(x) = P_2''(x) = \frac{2 f(x_i)}{(x_i - x_{i+1})(x_i - x_{i+2})} + \frac{2 f(x_{i+1})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}$$
$$+ \frac{2 f(x_{i+2})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}$$

The Divided Difference Polynomial

x	$f^{(0)}$	$f_i^{(1)}$	$f_i^{(2)}$
x_0	f_0		
x_1	f_1	$f_0^{(1)}$	$f_0^{(2)}$
x_2	f_2	$f_1^{(1)}$	
$\vdots$	$\vdots$		
x_n	f_n	$f_{n-1}^{(1)}$	

where

$$f_i^{(1)} = f[x_i, x_{i+1}] = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

$$f_i^{(2)} = f[x_i, x_{i+1}, x_{i+2}]$$

The divided difference polynomial

$$f(x) \approx P_n(x) = f_i^{(0)} + (x - x_0) f_i^{(1)} + (x - x_0)(x - x_1) f_i^{(2)} + \cdots$$

$$\cdots + (x - x_0)(x - x_1) \cdots (x - x_{n-1}) f_i^{(n)}$$

∴ Differentiating

$$f'(x) \approx P_n'(x) = f_i^{(1)} + (2x - (x_0 + x_1)) f_i^{(2)} + \cdots$$

Ily $f''(x)$ find it out.

I think, there is no need to give examples for these three cases as they are self explanatory.

⇒ If the data is equally spaced; we may go for Newton's forward or Backward difference polynomials:

Newton's forward difference polynomial

x	f	Δf	$\Delta^2 f$
x_0	f_0		
x_1	f_1	Δf_0	$\Delta^2 f_0$
x_2	f_2	Δf_1	$\Delta^2 f_1$
x_3	f_3	Δf_2	

$$\Delta f_i = f_{i+1} - f_i$$

$$\Delta^2 f_i = \Delta f_{i+1} - \Delta f_i$$

Recall the method by which forward-difference Newton's polynomials were formed.

$$P_n(x) = f_0 + s\,\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{6}\Delta^3 f_0 + \cdots\cdots + \frac{s(s-1)(s-2)\cdots(s-(n-1))}{n!}\Delta^n f_0$$

where $s = \dfrac{x - x_0}{\Delta x}$ or $x = x_0 + s\,\Delta x$

$\Delta x = x_1 - x_0$ or $x_2 - x_1 = x_3 - x_2$ - - -

The error using this polynomial was given as

$$\text{Error} = \frac{s(s-1)(s-2)(s-3)\cdots(s-n)}{(n+1)!}(\Delta x)^{n+1} f^{(n+1)}(\xi)$$

where $x_0 \le \xi \le x_n$

$$\therefore f'(x) = \frac{d}{dx}\left[P_n(x)\right] + \frac{d}{dx}(\text{Error})$$

We can write $x = x(s)$

$$\therefore \frac{d}{dx}f = \frac{d f}{ds}\cdot\frac{ds}{dx}$$

$$\therefore f'(x) \cong \frac{d}{dx}\left[P_n(x)\right] = \frac{d}{ds}\left(P_n(s)\right)\frac{ds}{dx}$$

Now what is $\dfrac{ds}{dx}$?

$$\frac{ds}{dx} = \frac{1}{\Delta x} = (\text{A constant}).$$

$$\therefore f'(x) \approx P_n'(x) = \frac{1}{\Delta x}\frac{d}{ds}\left[P_n(s)\right]$$

$$\therefore \quad P_n'(x) = \frac{1}{\Delta x}\Big[\Delta y_0 + \tfrac{1}{2}(s-1+s)\Delta^2 y_0 + \tfrac{1}{6}\big((s-1)(s-2) + s(s-2) + s(s-1)\big)\Delta^3 y_0 + \cdots\Big]$$

$$\text{i.e.} \quad P_n'(x) = \frac{1}{\Delta x}\Big[\Delta y_0 + \frac{2s-1}{2}\Delta^2 y_0 + \frac{3s^2-6s+2}{6}\Delta^3 y_0 + \cdots\Big]$$

The second derivative is also obtained by the same method

$$y''(x) \approx \frac{d}{dx}\big[P_n'(x)\big] = \frac{d}{ds}\big[P_n'(s)\big]\frac{ds}{dx} = \frac{1}{\Delta x}\big[P_n''(s)\big]$$

$$\text{i.e.} \quad P_n''(x) = \frac{1}{(\Delta x)^2}\Big[\Delta^2 y_0 + (s-1)\Delta^3 y_0 + \frac{6s^2-18s+11}{12}\Delta^4 y_0 + \cdots\Big]$$

→ As you have seen the base point is x_0.

→ Now what happens if $x = x_0$, then $s = 0$

$$\boxed{\begin{aligned} \therefore \quad P_n'(x_0) &= \frac{1}{\Delta x}\Big[\Delta y_0 - \tfrac{1}{2}\Delta^2 y_0 + \tfrac{1}{3}\Delta^3 y_0 - \tfrac{1}{4}\Delta^4 y_0 + \cdots\Big] \\ \text{and} \quad P_n''(x_0) &= \frac{1}{(\Delta x)^2}\Big[\Delta^2 y_0 - \Delta^3 y_0 + \tfrac{1}{2}\Delta^4 y_0 + \cdots\Big] \end{aligned}}$$

The equations for $P_n'(x_0)$ and $P_n''(x_0)$ are one-sided forward difference formulas to approximate derivatives.

→ Coming back into the error associated with forward difference polynomial.

$$Error = \frac{s(s-1)(s-2)\cdots(s-n)}{(n+1)!}(\Delta x)^{n+1} f^{(n+1)}(\xi)$$

$$\therefore \frac{d}{dx}(Error) = \frac{d}{ds}\left[\left(\qquad \right)\right]\frac{ds}{dx}$$

$$= \frac{1}{\Delta x}\frac{d}{ds}\left(\quad " \quad \right)$$

i.e. $$\frac{d}{dx}(Error) = \frac{(\Delta x)^n f^{(n+1)}(\xi)}{(n+1)!}\Big[(s-1)(s-2)\cdots(s-n) + s(s-2)\cdots(s-n) + \cdots + s(s-1)(s-2)\cdots(s-(n-1))\Big]$$

At $x = x_0$, we have $s = 0.0$

$$\therefore \frac{d}{dx}\left(Error(x_0)\right) = \frac{(-1)^n}{(n+1)}(\Delta x)^n f^{(n+1)}(\xi)$$

The error is of the order of $(\Delta x)^n$ as $\Delta x \to 0$.

i.e Even if $P_n(x_0)$ has no error, there can be error in $P_n'(x_0)$ of the order $O(\Delta x^n)$.

$\therefore$ We can interpret the one-sided forward differences:

$$P_1'(x_0) \rightarrow O(\Delta x)$$
$$P_2'(x_0) \rightarrow O(\Delta x^2)$$
$$P_3'(x_0) \rightarrow O(\Delta x^3)$$

As the order of Δx increases, more accurate is your approximation.

$\rightarrow$ However when you differentiate, you might have seen that (or inferred)

$$P_n''(x_0) \rightarrow O(\Delta x^{n-1})$$

eg $P_1''(x_0) \rightarrow$ Not possible

$$P_2''(x_0) \rightarrow O(\Delta x)$$

$$P_3''(x_0) \rightarrow O(\Delta x^2), \text{ etc.}$$

So accuracy decreases on further differentiating the polynomial.

→ Now we have developed the one-sided forward difference formula for $P_n'(x_0)$ and $P_n''(x_0)$

⇒ Suppose in Newton's forward difference polynomial if we had taken base point as x_0 and evaluated at $x = x_1$. Then $s = 1.0$

$$\boxed{\begin{aligned} P_n'(x_1) &= \frac{1}{\Delta x}\left[\Delta f_0 + \frac{1}{2}\Delta^2 f_0 - \frac{1}{6}\Delta^3 f_0 + \cdots\right] \\ P_n''(x_1) &= \frac{1}{(\Delta x)^2}\left[\Delta^2 f_0 - \frac{1}{12}\Delta^4 f_0 + \cdots\right] \end{aligned}}$$

These are centered-difference formulas for Newton's polynomials for first and second derivatives.

→ By inspection $P_1'(x_1) \rightarrow O(\Delta x)$

$$P_2'(x_1) \rightarrow O(\Delta x^2)$$

Also $P_2''(x_1) \rightarrow O(\Delta x^2)$ (Why?)