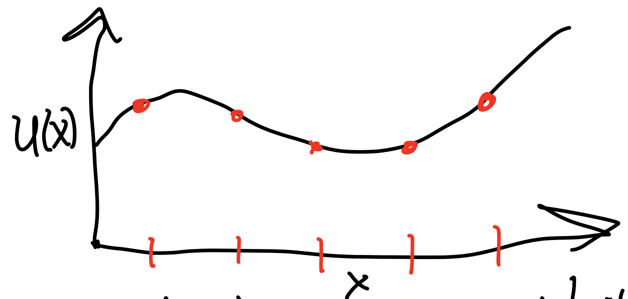
Given a function:



suppose that we only know some point values. How approximate the derivatives of u(x)?

Recall the definition of the derivative:

$$u'(x) = \lim_{h\to 0} \frac{u(x+h)-u(x)}{h}$$

This suggests the approximation:

$$u'(\bar{x}) \approx D_+ u(\bar{x}) = \frac{u(\bar{x}+h)-u(\bar{x})}{h} \qquad \text{forward difference}$$

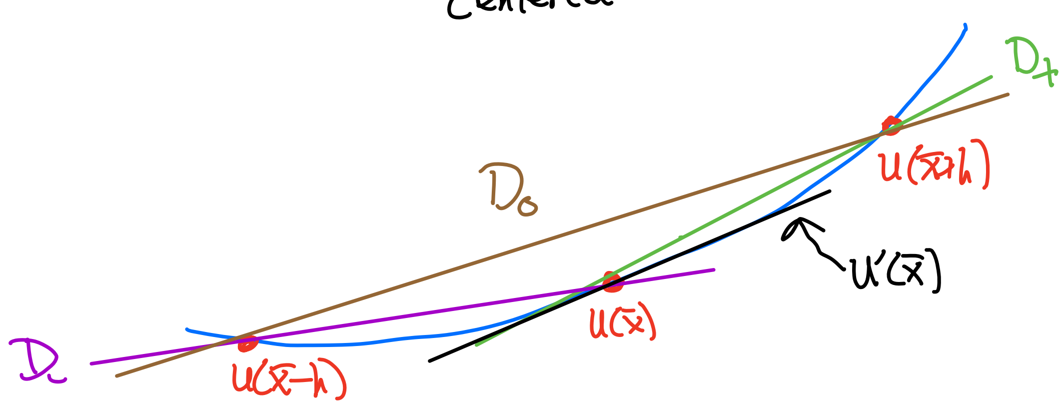
or

$$u'(x) \approx D_- u(\bar{x}) = \frac{u(\bar{x})-u(\bar{x}-h)}{h} \qquad \text{backward difference}$$

or their average:

$$u'(x) \approx D_0 u(\bar{x}) = \frac{1}{2}(D_+ + D_-)u(\bar{x}) = \frac{u(\bar{x}+h)-\bar{u}(\bar{x}-h)}{2h}$$

centered difference



The centered difference is the most accurate, for small h.

Recall Taylor's Theorem:

$$u(x) = \sum_{j=0}^{\infty} \frac{u^{(j)}(\bar{x}) \cdot (x-\bar{x})^j}{j!} = \sum_{j=0}^{p} \frac{u^{(j)}(\bar{x}) \cdot (x-\bar{x})^j}{j!} + \mathcal{O}((x-\bar{x})^{p+1})$$

Big-oh notation: $f(h) = \mathcal{O}(h^p)$ means $\exists\ C>0,\ h_0>0$ such that $|f(h)| < Ch^p$ for all $h \leq h_0$.

$$u(\bar{x}+h) = u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \frac{h^3}{6}u'''(\bar{x}) + \mathcal{O}(h^4)$$

$$u(\bar{x}-h) = u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) - \frac{h^3}{6}u'''(\bar{x}) + \mathcal{O}(h^4)$$

$$u(\bar{x}) = u(\bar{x})$$

$$D_+u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x})}{h} = \frac{\cancel{u(\bar{x})} + hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \mathcal{O}(h^3) - \cancel{u(\bar{x})}}{h}$$

$$= u'(\bar{x}) + \underbrace{\frac{h}{2}u''(\bar{x})}_{\text{Leading truncation error}} + \mathcal{O}(h^2)$$

This approximation is 1st-order accurate.

$$D_-u(\bar{x}) = \frac{u(\bar{x}) - u(\bar{x}-h)}{h} = \frac{\cancel{u(\bar{x})} - (\cancel{u(\bar{x})} - hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \mathcal{O}(h^3))}{h}$$

$$= u'(\bar{x}) - \frac{h}{2}u''(\bar{x}) + \mathcal{O}(h^2)$$

$$D_0u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h} = \frac{\cancel{u(\bar{x})} + hu'(\bar{x}) + \cancel{\frac{h^2}{2}u''(\bar{x})} - (\cancel{u(\bar{x})} - hu'(\bar{x}) + \cancel{\frac{h^2}{2}u''(\bar{x})}) + \mathcal{O}(h^3)}{2h}$$

$$= u'(\bar{x}) + \left(\frac{\frac{h^3}{6}u'''(\bar{x}) - (-\frac{h^3}{6}u'''(\bar{x}))}{2h}\right)$$

$$= u'(\bar{x}) + \frac{h^2}{6}u'''(\bar{x}) + O(h^4)$$ 2nd-order accurate

Deriving finite difference formulas

Suppose you are given

$$u(\bar{x}), \quad u(\bar{x}+h), \quad u(\bar{x}+2h)$$

and want to approximate $u''(\bar{x})$.

$$\longrightarrow a u(\bar{x}) + b u(\bar{x}+h) + c u(\bar{x}+2h) \approx u''(\bar{x})$$

We need the Taylor series

$$u(\bar{x}+2h) = u(\bar{x}) + 2hu'(\bar{x}) + 2h^2 u''(\bar{x}) + \frac{4h^3}{3}u'''(\bar{x}) + O(h^4)$$

Substitute to obtain:

$$a u(\bar{x}) + b\left(u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \frac{h^3}{6}u'''(\bar{x})\right)$$
$$+ c\left(u(\bar{x}) + 2hu'(\bar{x}) + 2h^2 u''(\bar{x}) + \frac{4h^3}{3}u'''(\bar{x})\right) \approx u''(\bar{x})$$

$$(a+b+c)u(\bar{x}) + (b+2c)hu'(\bar{x}) + \left(\frac{b}{2}+2c\right)h^2 u''(\bar{x})$$
$$+ \left(\frac{b}{6}+\frac{4c}{3}\right)h^3 u'''(\bar{x}) \approx u''(\bar{x})$$

This implies: $a+b+c=0$ $\quad \left(\frac{b}{2}+2c\right)h^2 = 1$

$$b+2c=0$$

$$\boxed{\cancel{\frac{b}{6}+\frac{4c}{3}=0}}$$

We find: $b = \frac{-2}{h^2}$ $\quad a = c = \frac{1}{h^2}$

So we have:

$$u''(\bar{x}) \approx \frac{u(\bar{x}) - 2u(\bar{x}+h) + u(\bar{x}+2h)}{h^2}$$ <u>Error is $O(h)$</u>

We could have obtained this formula by applying D_+ twice:

$$D_+(D_+(u(\bar{x}))) = D_+\left(\frac{u(\bar{x}+h) - u(\bar{x})}{h}\right)$$

$$= \frac{u(\bar{x}+2h) - u(\bar{x}+h)}{h^2} - \frac{u(\bar{x}+h) - u(\bar{x})}{h^2}$$

$$= \frac{u(\bar{x}+2h) - 2u(\bar{x}+h) + u(\bar{x})}{h^2}$$

$$D_+D_-u(\bar{x}) = \frac{u(\bar{x}+h) - 2u(\bar{x}) + u(\bar{x}-h)}{h^2} \approx u''(\bar{x})$$

centered formula $\rightarrow$ 2nd-order accurate

FD formulas can also be derived by constructing an interpolating polynomial and differentiating.

General method for finding FD formulas

Given values of u at $x_1, \ldots, x_n$, find the most accurate way to approximate $u^{(k)}(\bar{x})$.

$$u(x_j) = u(\bar{x}) + \underline{(x_j - \bar{x})} u'(\bar{x}) + \underline{\frac{(x_j-\bar{x})^2}{2}} u''(\bar{x}) + \cdots = \underline{\sum_{i=0}^{\infty} \frac{(x_j-\bar{x})^i}{i!} u^{(i)}(\bar{x})}$$

Our formula will be of the form:

$$c_1 u(x_1) + c_2 u(x_2) + \cdots + c_n u(x_n) = u^{(k)}(\bar{x}) + \mathcal{O}(h^p)$$

After substituting Taylor series for each $u(x_j)$, we collect terms:

$$\rightarrow \underline{(c_1 + c_2 + \cdots + c_n)} u(\bar{x})$$
$$+ \underline{\big(c_1(x_1-\bar{x}) + c_2(x_2-\bar{x}) + \cdots + c_n(x_n-\bar{x})\big)} u'(\bar{x})$$
$$+ \underline{\tfrac{1}{2}\big(c_1(x_1-\bar{x})^2 + \cdots + c_n(x_n-\bar{x})^2\big)} u''(\bar{x})$$
$$+ \cdots \qquad = u^{(k)}(\bar{x}) + \underline{\mathcal{O}(h^p)}$$

This yields a linear system of equations:

$$
\underbrace{\begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1-\bar{x} & x_2-\bar{x} & \cdots & x_n-\bar{x} \\ \frac{1}{2}(x_1-\bar{x})^2 & \cdots & & \frac{1}{2}(x_n-\bar{x})^2 \\ \vdots & & & \vdots \\ \frac{1}{(n-1)!}(x_1-\bar{x})^{n-1} & \cdots & & \frac{1}{(n-1)!}(x_n-\bar{x})^{n-1} \end{pmatrix}}_{\text{Vandermonde}} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \leftarrow k\text{th entry}
$$

The solution of this system will give us a FD formula $u^{(k)}(\bar{x})$.

What is the size of the error? $\mathcal{O}(h^{n-k})$

Homework: 1 Finite_differences.ipynb

Questions in bold

Due next Thursday.