第四章 （数值积分和）数值微分

内容提要

4.6 数值微分

知识结构图

数值微分
- 中点方法（Taylor展开型方法）
- 插值型求导公式

数值微分

如果函数$f(x)$以离散点列给出,或函数$f(x)$过于复杂,而要求我们给出导数值时，这两种情况都要求我们用数值的方法求函数的导数值.

微积分中，关于导数的定义如下：

$$f'(x)=\lim_{h\to 0}\frac{f(x+h)-f(x)}{h}=\lim_{h\to 0}\frac{f(x)-f(x-h)}{h}=\lim_{h\to 0}\frac{f(x+h)-f(x-h)}{2h}$$

自然，而又简单的方法就是，取极限的近似值，即差商.

1、差商型求导公式

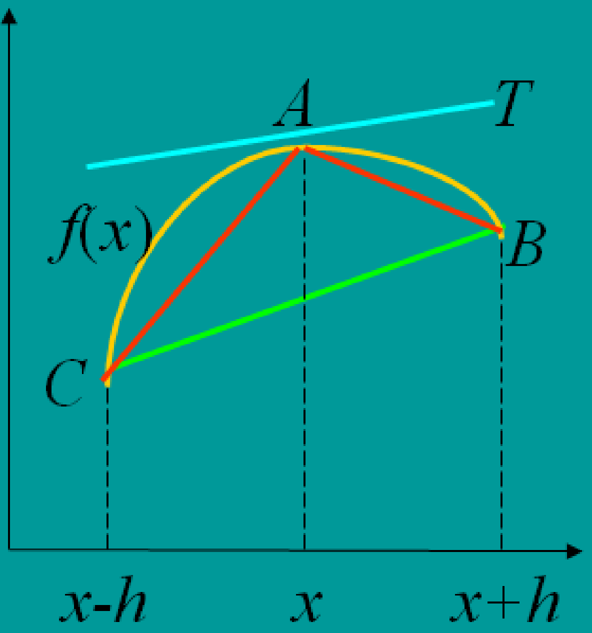
由导数定义 $f'(x)=\lim\limits_{h\to 0}\dfrac{f(x+h)-f(x)}{h}$

（1）向前差商公式

$$f'(x)\approx\frac{f(x+h)-f(x)}{h}$$

（2）向后差商公式

$$f'(x)\approx\frac{f(x)-f(x-h)}{h}$$



（3）中心差商公式（中点方法）

$$f'(x)\approx\frac{f(x+h)-f(x-h)}{2h}$$

4.6 数值微分

4.6.1 中点方法与误差分析

数值微分就是要用函数值的线性组合近似函数在某点的导数值。由导数定义差商来近似导数，得到数值微分公式。

$$f'(a) \approx \frac{f(a+h)-f(a)}{h},$$

$$f'(a) \approx \frac{f(a)-f(a-h)}{h},$$

$$f'(a) \approx \frac{f(a+h)-f(a-h)}{2h} \qquad \text{（中点公式）}$$

差商型数值微分

（1）向前差商数值微分公式

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$$

由Taylor展开式

$$f(x_0+h)=f(x_0)+f'(x_0)h+\frac{h^2}{2}f''(x_0+\theta h) \quad ,0\le\theta\le 1$$

可得误差

$$f'(x_0)-\frac{f(x_0+h)-f(x_0)}{h}=-\frac{h}{2}f''(x_0+\theta h) \qquad 0\le\theta\le 1$$

拉格朗日（Lagrange）余项形式

Truncation Errors

- **Uniform grid spacing**

$$\begin{cases} f(x_{i+1}) = f(x_i + h) = f(x_i) + hf'(x_i) + \dfrac{h^2}{2!} f''(x_i) + \dfrac{h^3}{3!} f'''(x_i) + \cdots \\ f(x_{i-1}) = f(x_i - h) = f(x_i) - hf'(x_i) + \dfrac{h^2}{2!} f''(x_i) - \dfrac{h^3}{3!} f'''(x_i) + \cdots \end{cases}$$

$$\begin{cases} forward: \ f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h} - \dfrac{h}{2} f''(\xi_1) \qquad O(h) \\ backward: \ f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h} + \dfrac{h}{2} f''(\xi_2) \qquad O(h) \\ central: \ f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h} - \dfrac{h^2}{6} f'''(\xi_3) \qquad O(h^2) \end{cases}$$

再学习，另一个写法

用中心差商近似导数得

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0-h)}{2h}$$

由*Taylor*展开

$$f(x_0+h)=f(x_0)+hf'(x_0)+\frac{h^2}{2!}f''(x_0)+\frac{h^3}{3!}f'''(\xi_1), x_0 \le \xi_1 \le x_0+h$$

$$f(x_0-h)=f(x_0)-hf'(x_0)+\frac{h^2}{2!}f''(x_0)-\frac{h^3}{3!}f'''(\xi_2), x_0-h \le \xi_2 \le x_0$$

因此，有误差

$$R(x)=f'(x_0)-\frac{f(x_0+h)-f(x_0-h)}{2h}$$

介值定理

$$=\frac{h^2}{12}[f'''(\xi_1)+f'''(\xi_2)]=\frac{h^2}{6}f'''(\xi)=O(h^2)$$

Example: First Derivatives

- **Use forward and backward difference approximations to estimate the first derivative of**

$$\boxed{f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2}$$

at x = 0.5 with h = 0.5 and 0.25 (exact solution = -0.9125)

- **Forward Difference**

$$\begin{cases} h = 0.5, \quad f'(0.5) \approx \dfrac{f(1) - f(0.5)}{1 - 0.5} = \dfrac{0.2 - 0.925}{0.5} = -1.45, \qquad |\varepsilon_t| = 58.9\% \\ h = 0.25, \quad f'(0.5) \approx \dfrac{f(0.75) - f(0.5)}{0.75 - 0.5} = \dfrac{0.63632813 - 0.925}{0.25} = -1.155, \quad |\varepsilon_t| = 26.5\% \end{cases}$$

- **Backward Difference**

$$\begin{cases} h = 0.5, \quad f'(0.5) \approx \dfrac{f(0.5) - f(0)}{0.5 - 0} = \dfrac{0.925 - 1.2}{0.5} = -0.55, \qquad |\varepsilon_t| = 39.7\% \\ h = 0.25, \quad f'(0.5) \approx \dfrac{f(0.5) - f(0.25)}{0.5 - 0.25} = \dfrac{0.925 - 1.10351563}{0.25} = -0.714, \quad |\varepsilon_t| = 21.7\% \end{cases}$$

Example: First Derivative

- **Use central difference approximation to estimate the first derivative of**

$$\boxed{f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2}$$

at x = 0.5 with h = 0.5 and 0.25 (exact solution = -0.9125)

- **<u>Central Difference</u>**

$$h = 0.5,\quad f'(0.5) \approx \frac{f(1) - f(0)}{1 - 0} = \frac{0.2 - 1.2}{1} = -1.0, \qquad |\varepsilon_t| = 9.6\%$$

$$h = 0.25,\quad f'(0.5) \approx \frac{f(0.75) - f(0.25)}{0.75 - 0.25}$$

$$= \frac{0.63632813 - 1.10351563}{0.5} = -0.934, \quad |\varepsilon_t| = 2.4\%$$

$$f(a\pm h)=f(a)\pm hf'(a)+\frac{h^2}{2!}f''(a)\pm\frac{h^3}{3!}f'''(a)+\frac{h^4}{4!}f^{(4)}(a)$$

$$\pm\frac{h^5}{5!}f^{(5)}(a)+\cdots,$$

$$G(h)\stackrel{\Delta}{=}\frac{f(a+h)-f(a-h)}{2h}=f'(a)+\frac{h^2}{3!}f'''(a)+\frac{h^4}{5!}f^{(5)}(a)+\cdots.$$

误差估计 $$\left|G(h)-f'(a)\right|\le\frac{h^2}{6}M,$$

其中 $M\ge\max\limits_{|x-a|\le h}\left|f'''(x)\right|.$

表面上看 h 越小越好，但从舍入误差角度考虑，h 不能太小。例如

$f(x)=\sqrt{x}$, 在$x=2$处的一阶导数（1/2*1/sqrt(2)=0.353553390593274）

$$G(h)=\frac{\sqrt{2+h}-\sqrt{2-h}}{2h},$$ 设取4位数字计算。

h	*G(h)*	*h*	*G(h)*	*h*	*G(h)*
1	0.3660	0.05	0.3530	0.001	0.3500
0.5	0.3564	0.01	0.3500	0.0005	0.3000
0.1	0.3535	0.005	0.3500	0.0001	0.3000

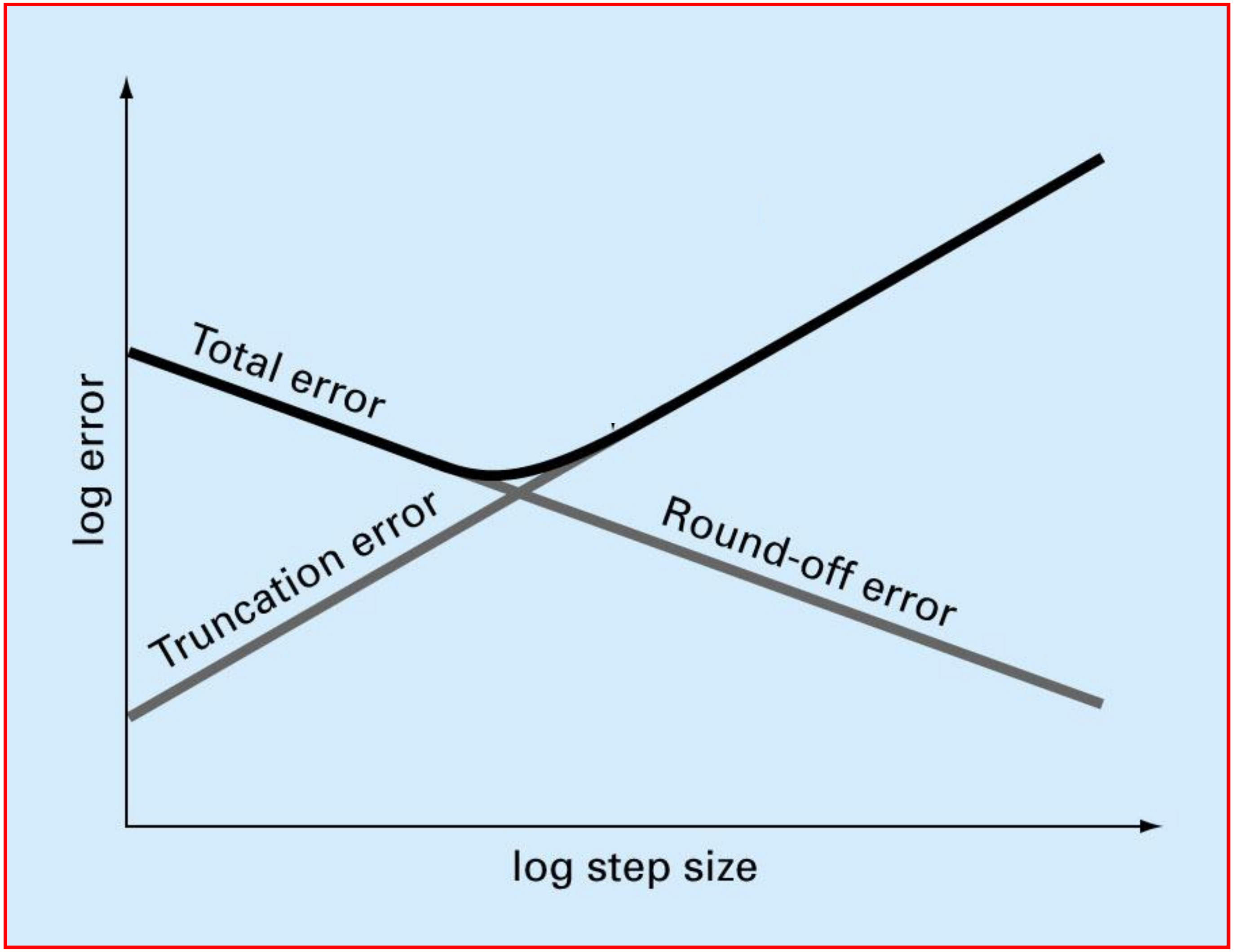
从表中看到h=0.1 的逼近效果最好，如果进一步缩小步长，则逼近效果反而越差。这是因为当$f(a+h)$ 及$f(a-h)$ 分别有舍入误差ε_1及ε_2。令$\varepsilon=\max\{|\varepsilon_1|,|\varepsilon_2|\}$，则计算$f'(a)$ 的舍入误差上界为

$$\delta(f'(a))=|f'(a)-G(a)|\le\frac{|\varepsilon_1|+|\varepsilon_2|}{2h}\le\frac{\varepsilon}{h}$$

表明h 越小，舍入误差$\delta(f'(a))$ 越大，故它是病态的。

见书129页最后一段

Total Numerical Error



Trade-off between truncation and round-off errors

再给一个例子

Round-off errors

Table 6.1 Finding the Difference Quotients $D_k = (e^{1+h_k} - e)/h_k$

h_k	$f_k = f(1+h_k)$	$f_k - e$	$D_k = (f_k - e)/h_k$
$h_1 = 0.1$	3.004166024	0.285884196	2.858841960
$h_2 = 0.01$	2.745601015	0.027319187	2.731918700
$h_3 = 0.001$	2.721001470	0.002719642	2.719642000
$h_4 = 0.0001$	2.718553670	0.000271842	2.718420000
$h_5 = 0.00001$	2.718309011	0.000027183	2.718300000
$h_6 = 10^{-6}$	2.718284547	0.000002719	2.719000000
$h_7 = 10^{-7}$	2.718282100	0.000000272	2.720000000
$h_8 = 10^{-8}$	2.718281856	0.000000028	2.800000000
$h_9 = 10^{-9}$	2.718281831	0.000000003	3.000000000
$h_{10} = 10^{-10}$	2.718281828	0.000000000	0.000000000

4.6.2 插值型的求导公式

已知函数 $y=f(x)$ 的节点上的函数值 $y_i=f(x_i)\ (i=0,1,\cdots,n)$,

建立插值多项式 $P(x)$

取 $$f'(x)\approx P'(x),$$

统称为**插值型求导公式.**

点数阶导

函数插值误差余项为 $f(x)-P_n(x)=\dfrac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}(x)$

点数阶乘

导数误差余项为

$$f'(x)-P_n'(x)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}'(x)+\frac{\omega_{n+1}(x)}{(n+1)!}\frac{\mathrm{d}}{\mathrm{d}x}f^{(n+1)}(\xi),$$

其中 $\xi\in(a,b)$, $\omega_{n+1}(x)=\prod_{j=0}^{n}(x-x_j)$.

$$\Rightarrow\qquad f'(x_k)-P_n'(x_k)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}'(x_k).$$

重要：不同表述再看一遍

插值型求导公式

利用插值原理,建立插值多项式$y=L_n(x)$作为$f(x)$的近似.由于多项式求导比较容易,取

$$f'(x) \approx L_n'(x)$$

但是,需要注意误差分析

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_n(x) = f(x) - L_n(x)$$

$$f'(x) - L_n'(x) = \frac{d}{dx}\left[\frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}(x)\right]$$

$$= \underline{\frac{d}{dx}\left[\frac{f^{(n+1)}(\xi)}{(n+1)!}\right]}\omega_{n+1}(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!}\frac{d}{dx}[\omega_{n+1}(x)]$$

ξ是x的函数,此项无法估计.

所以,对于任意给出的点x,误差无法预估的.

但是,如果限定求某个节点处的导数值时,上述第一项为零,这时余项公式为

$$\frac{f^{(n+1)}(\xi)}{(n+1)!}\left[\omega'_{n+1}(x)\right]$$

下面考虑在等距节点时节点上的导数值.

两点公式

$$P_1(x)=\frac{x-x_1}{x_0-x_1}f(x_0)+\frac{x-x_0}{x_1-x_0}f(x_1),$$

课堂推导

$$P_1'(x)=\frac{1}{h}\left[-f(x_0)+f(x_1)\right],$$

$$P_1'(x_0)=\frac{1}{h}\left[f(x_1)-f(x_0)\right],\quad P_1'(x_1)=\frac{1}{h}\left[f(x_1)-f(x_0)\right].$$

$$f'(x_0)=\frac{1}{h}\left[f(x_1)-f(x_0)\right]-\frac{h}{2}f''(\xi),$$

$$f'(x_1)=\frac{1}{h}\left[f(x_1)-f(x_0)\right]+\frac{h}{2}f''(\xi).$$

取n=2的等距节点($x_2-x_1=x_1-x_0=h$)抛物线插值:

$L_2(x)=[(x-x_1)(x-x_2)f(x_0)-2(x-x_0)(x-x_2)f(x_1)+(x-x_0)(x-x_1)f(x_2)]/2h^2$

则有 $L_2'(x)=[(2x-x_1-x_2)f(x_0)-2(2x-x_0-x_2)f(x_1)+(2x-x_0-x_1)f(x_2)]/2h^2$

$L_2''(x)=[2f(x_0)-4f(x_1)+2f(x_2)]/2h^2$

可得数值微分的三点公式:

$$\begin{cases} f'(x_0)=\dfrac{1}{2h}[-3f(x_0)+4f(x_1)-f(x_2)]+\dfrac{h^2}{3}f'''(\xi) \\ f'(x_1)=\dfrac{1}{2h}[-f(x_0)+f(x_2)]-\dfrac{h^2}{6}f'''(\xi) \\ f'(x_2)=\dfrac{1}{2h}[f(x_0)-4f(x_1)+3f(x_2)]+\dfrac{h^2}{3}f'''(\xi) \\ f''(x_0)=\dfrac{1}{h^2}[f(x_0)-2f(x_1)+f(x_2)]+[-hf'''(\xi_1)+\dfrac{h^2}{6}f^{(4)}(\xi_2)] \\ f''(x_1)=\dfrac{1}{h^2}[f(x_0)-2f(x_1)+f(x_2)]-\dfrac{h^2}{12}f^{(4)}(\xi) \\ f''(x_2)=\dfrac{1}{h^2}[f(x_0)-2f(x_1)+f(x_2)]+[hf'''(\xi_1)-\dfrac{h^2}{6}f^{(4)}(\xi_2)] \end{cases}$$

误差次项对否？

课堂推导

General Three-Point Formula

- **Lagrange interpolation polynomial for unequally spaced data**

部分答案

$$f(x) \approx l_{i-1}(x) f(x_{i-1}) + l_i(x) f(x_i) + l_{i+1}(x) f(x_{i+1})$$
$$= f(x_{i-1}) \frac{(x - x_i)(x - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f(x_i) \frac{(x - x_{i-1})(x - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})}$$
$$+ f(x_{i+1}) \frac{(x - x_{i-1})(x - x_i)}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)}$$

- **First derivative**

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

Three-point formula (Uniform Grid)

$$f'(x) \approx f(x_{i-1})\frac{2x - x_i - x_{i+1}}{2h^2} + f(x_i)\frac{2x - x_{i-1} - x_{i+1}}{-h^2} + f(x_{i+1})\frac{2x - x_{i-1} - x_i}{2h^2}$$

- **Forward difference**

$$\boxed{\begin{aligned} f'(x_{i-1}) &\approx f(x_{i-1})\frac{2x_{i-1} - x_i - x_{i+1}}{2h^2} + f(x_i)\frac{2x_{i-1} - x_{i-1} - x_{i+1}}{-h^2} + f(x_{i+1})\frac{2x_{i-1} - x_{i-1} - x_i}{2h^2} \\ &= \frac{-3h}{2h^2} f(x_{i-1}) + \frac{-2h}{-h^2} f(x_i) + \frac{-h}{2h^2} f(x_{i+1}) = \frac{-3f(x_{i-1}) + 4f(x_i) - f(x_{i+1})}{2h} \end{aligned}}$$

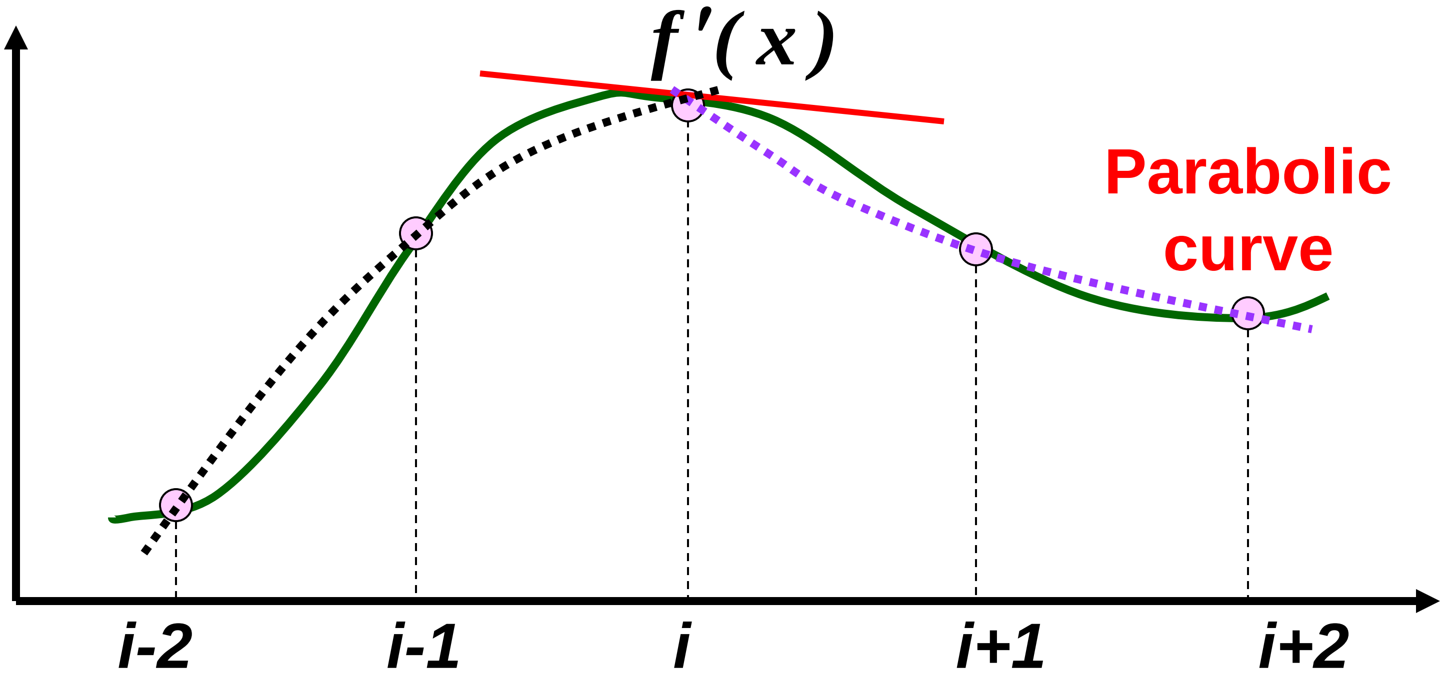
- **Centered difference**

$$\boxed{\begin{aligned} f'(x_i) &\approx f(x_{i-1})\frac{2x_i - x_i - x_{i+1}}{2h^2} + f(x_i)\frac{2x_i - x_{i-1} - x_{i+1}}{-h^2} + f(x_{i+1})\frac{2x_i - x_{i-1} - x_i}{2h^2} \\ &= \frac{-h}{2h^2} f(x_{i-1}) + \frac{h}{2h^2} f(x_{i+1}) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \end{aligned}}$$

- **Backward difference**

$$\boxed{\begin{aligned} f'(x_{i+1}) &\approx f(x_{i-1})\frac{2x_3 - x_2 - x_3}{2h^2} + f(x_i)\frac{2x_3 - x_1 - x_3}{-h^2} + f(x_{i+1})\frac{2x_3 - x_1 - x_2}{2h^2} \\ &= \frac{h}{2h^2} f(x_{i-1}) + \frac{2h}{-h^2} f(x_i) + \frac{3h}{2h^2} f(x_{i+1}) = \frac{f(x_{i-1}) - 4f(x_i) + 3f(x_{i+1})}{2h} \end{aligned}}$$

First Derivatives



- **3 -point Forward difference**

$$f'(x_i) \approx \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{x_{i+2} - x_i}$$

- **3 -point Backward difference**

$$f'(x_i) \approx \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{x_i - x_{i-2}}$$

Example: First Derivatives

- **Use forward and backward difference approximations of $O(h^2)$ to estimate the first derivative of**

$$\boxed{f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2}$$

at x = 0.5 with h = 0.25 (exact solution = -0.9125)

- **Forward Difference**

$$f'(0.5) \approx \frac{-f(1) + 4f(0.75) - 3f(0.5)}{2(0.25)}$$

$$= \frac{-0.2 + 4(0.6363281) - 3(0.925)}{0.5} = -0.859375, \quad |\varepsilon_t| = 5.82\%$$

- **Backward Difference**

$$f'(0.5) \approx \frac{3f(0.5) - 4f(0.25) + f(0)}{2(0.25)}$$

$$= \frac{3(0.925) - 4(1.035156) + 1.2}{0.5} = -0.878125, \quad |\varepsilon_t| = 3.77\%$$

习题(需提交)

P135: 17, 18

Centered Finite-Divided Differences

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \dfrac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4}$	$O(h^4)$

Forward Finite-Divided Differences

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Backward Finite-Divided Differences

First Derivative	Error
$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$	$O(h^2)$