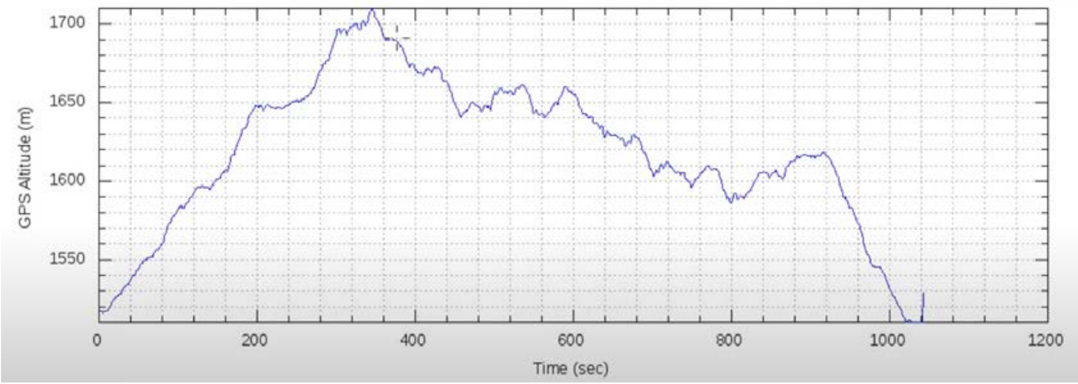
数值微分

1. 数值微分：前向和后向差分的推导



- 等间距数据
- 非等间距数据

导数的差商定义

$$f'(x) \triangleq \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} \tag{1.1}$$

泰勒级数-推导前向和后向差商：

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots \tag{1.2}$$

$$f(x_{i-1}) = f(x_i) + \frac{f'(x_i)}{1!}(x_{i-1}-x_i) + \frac{f''(x_i)}{2!}(x_{i-1}-x_i)^2 + \frac{f'''(x_i)}{3!}(x_{i-1}-x_i)^3 + \cdots \tag{1.3}$$

令$h = x_i - x_{i-1} (\rightarrow x_{i-1} = x_i - h)$

$$f(x_{i-1}) = f(x_i) - \frac{f'(x_i)}{1!}h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \cdots \tag{1.4}$$

$$\Rightarrow f'(x_i) = \frac{1}{h} f(x_i) - f(x_{i-1}) + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \cdots \tag{1.5}$$

舍去$\left[\frac{f''(x_i)}{2!}h^2-\frac{f'''(x_i)}{3!}h^3+\cdots\right]$得到

$$
\begin{aligned}
f'(x_i)&=\frac{f(x_i)-f(x_{i-1})}{h}+O(h)\\
f'(x_i)&=\frac{f(x_i)-f(x_i-h)}{h}+O(h)
\end{aligned}
\tag{1.6}
$$

以上是向后差商近似导数。前向差商使用x_{i+1}和h，同时$h=x_{i+1}-x_i$

$$
\begin{aligned}
f(x_{i+1})&=f(x_i)+\frac{f'(x_i)}{1!}h+\frac{f''(x_i)}{2!}h^2+\frac{f'''(x_i)}{3!}h^3+\cdots\\
\Rightarrow f'(x_i)&=\frac{1}{h}\left[-f(x_i)+f(x_{i+1})-\frac{f''(x_i)}{2!}h^2-\frac{f'''}{3!}(x_i)h^3-\cdots\right]\\
f'(x_i)&=-\frac{1}{h}f(x_i)+\frac{1}{h}f(x_{i+1})-\frac{f''(x_i)}{2!}h-\frac{f'''(x_i)}{3!}h^2-\cdots\\
f'(x_i)&=\frac{f(x_{i+1})-f(x_i)}{h}+O(h)
\end{aligned}
\tag{1.7}
$$

对比导数定义

$$
f'(x)\triangleq\lim_{\Delta x\to 0}\frac{f(x+\Delta x)-f(x)}{\Delta x}
\tag{1.8}
$$

2. 数值微分：中心差分法的推导

考虑对x_{i-1}和x_{i+1}的泰勒级数

$$
\begin{aligned}
f(x_{i-1})&=f(x_i)-\frac{f'(x_i)}{1!}h+\frac{f''(x_i)}{2!}h^2-\frac{f'''(x_i)}{3!}h^3+\cdots\\
f(x_{i+1})&=f(x_i)+\frac{f'(x_i)}{1!}h+\frac{f''(x_i)}{2!}h^2+\frac{f'''(x_i)}{3!}h^3+\cdots
\end{aligned}
\tag{1.9}
$$

对$f(x)$得到

$$
\begin{aligned}
-f(x_i)&=-f(x_{i-1})-\frac{f'(x_i)}{1!}h+\frac{f''(x_i)}{2!}h^2-\frac{f'''(x_i)}{3!}h^3+\cdots\\
-f(x_i)&=-f(x_{i+1})+\frac{f'(x_i)}{1!}h+\frac{f''(x_i)}{2!}h^2+\frac{f'''(x_i)}{3!}h^3+\cdots
\end{aligned}
\tag{1.10}
$$

令h相同，上式得到：

$$0=-f\left(x_{i+1}\right)+f\left(x_{i-1}\right)+2\frac{f^{'}\left(x_i\right)}{1!}h+2\frac{f^{'''}\left(x_i\right)}{3!}h^3+\cdots \tag{1.11}$$

$$\Rightarrow -f^{'}\left(x_i\right)=\frac{1}{2h}\left[f\left(x_{i-1}\right)-f\left(x_{i+1}\right)+2\frac{f^{'''}\left(x_i\right)}{3!}h^3+\cdots\right] \tag{1.12}$$

$$f^{'}\left(x_i\right)=\frac{f\left(x_{i+1}\right)-f\left(x_{i-1}\right)}{2h}-\frac{f^{'''}\left(x_i\right)}{3!}h^2+\cdots \tag{1.13}$$

$$f^{'}\left(x_i\right)-\frac{f\left(x_{i-1}\right)-f\left(x_{i+1}\right)}{2h}+O\left(h^2\right) \tag{1.14}$$

由上述几个公式可知，步长h越小，计算结果越准确。但从计算角度看，h越小，$f(x_0+h)$，$f(x_0)$与$f(x_0-h)$越接近，直接相减会造成有效数字的严重损失，因此，需要合理选取步长，至于步长的合理选取可参阅相关参考书。

3. 数值微分：高阶微分

我们可以接着往下做：

$$\begin{aligned}
f\left(x_{i-1}\right)&=f\left(x_i\right)-\frac{f^{'}\left(x_i\right)}{1!}h+\frac{f^{''}\left(x_i\right)}{2!}h^2-\frac{f^{'''}\left(x_i\right)}{3!}h^3+\cdots\\
f\left(x_{i+1}\right)&=f\left(x_i\right)+\frac{f^{'}\left(x_i\right)}{1!}h+\frac{f^{''}\left(x_i\right)}{2!}h^2+\frac{f^{''''}\left(x_i\right)}{3!}h^3+\cdots\\
f\left(x_{i-2}\right)&=f\left(x_i\right)-\frac{f^{'}\left(x_i\right)}{1!}2h\cdots\\
f\left(x_{i+2}\right)&=f\left(x_i\right)+\frac{f^{'}\left(x_i\right)}{1!}2h\cdots
\end{aligned} \tag{1.15}$$

考虑

$$f\left(x_{i+1}\right)=f\left(x_i\right)+f^{'}\left(x_i\right)h+\frac{f^{''}\left(x_i\right)}{2!}h^2+\cdots \tag{1.16}$$

$$f\left(x_{i+2}\right)=f\left(x_i\right)+f^{'}\left(x_i\right)(2h)+\frac{f^{''}\left(x_i\right)}{2!}(2h)^2+\cdots \tag{1.17}$$

得到

$$f\left(x_{i+2}\right)-2f\left(x_{i+1}\right)=-f\left(x_i\right)+f''\left(x_i\right)h^2+\cdots \tag{1.18}$$

变换得到：

$$f''\left(x_i\right)=\frac{f\left(x_{i+2}\right)-2f\left(x_{i+1}\right)+f\left(x_i\right)}{h^2}+O(h) \tag{1.19}$$

重新考虑

$$f\left(x_{i+1}\right)=f\left(x_i\right)+f'\left(x_i\right)h+\frac{f''\left(x_i\right)}{2}h^2+\cdots \tag{1.20}$$

得到

$$f'\left(x_i\right)=\frac{f\left(x_{i+1}\right)-f\left(x_i\right)}{h}-\frac{f''\left(x_i\right)}{2}h+O\left(h^2\right) \tag{1.21}$$

替换得到

$$f'\left(x_i\right)=\frac{f\left(x_{i+1}\right)-f\left(x_i\right)}{h}-\frac{f\left(x_{i+2}\right)-2f\left(x_{i+1}\right)+f\left(x_i\right)}{2h^2}h+O\left(h^2\right) \tag{1.22}$$

即

$$f'\left(x_i\right)=\frac{-f\left(x_{i+2}\right)+4f\left(x_{i+1}\right)-3f\left(x_i\right)}{2h}+O\left(h^2\right) \tag{1.23}$$

前向差分

First Derivative | Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} \qquad O(h)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} \qquad O(h^2)$$

Second Derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} \qquad O(h)$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} \qquad O(h^2)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3} \qquad O(h)$$

$$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3} \qquad O(h^2)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4} \qquad O(h)$$

$$f''''(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4} \qquad O(h^2)$$

后向差分

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

中心差分

First Derivative　　　　Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \qquad O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} \qquad O(h^4)$$

Second Derivative

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} \qquad O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} \qquad O(h^4)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3} \qquad O(h^2)$$

$$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3} \qquad O(h^4)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4} \qquad O(h^2)$$

$$f''''(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) - f(x_{i-3})}{6h^4} \qquad O(h^4)$$

切线、法线、梯度和法向量

考虑一元函数$f(x)$，导数为$f'(x)$，则对应的切线、法线、梯度和法向量为：

$$f_t(x) = f'(x_0)(x - x_0) + f(x_0) \tag{1.24}$$

$$f_n(x) = \frac{(x - x_0)}{-f'(x_0)} + f(x_0) \tag{1.25}$$

$$gradient(f(x)) \text{ at } x_0 = f'(x_0)\hat{x} \tag{1.26}$$

$$normal(f(x)) \text{ at } x_0 = \begin{pmatrix} f'(x_0) \\ -1 \end{pmatrix} \tag{1.27}$$

考虑二元函数$f(x,y)$，对x和对y的偏导数分别为$f_x(x,y) = \frac{\partial}{\partial x} f(x,y)$和$f_y(x,y) = \frac{\partial}{\partial y} f(x,y)$，则对应的切平面、法线、梯度和法向量为：

$$f_t(x,y) = f_x(x_0,y_0)(x - x_0) + f_y(x_0,y_0)(x - x_0) + f(x_0,y_0) \tag{1.28}$$

$$\ell_n(t) = \begin{cases} x = x_0 + at \\ y = y_0 + bt \\ z = f\left(x_0, y_0\right) - t \end{cases} \tag{1.29}$$

$$a = f_x\left(x_0, y_0\right) \quad \text{and} \quad b = f_y\left(x_0, y_0\right)$$

$$gradient(f(x,y)) \text{ at } (x_0, y_0) = f_x(x_0, y_0)\hat{x} + f_y(x_0, y_0)\hat{y} \tag{1.30}$$

$$normal(f(x,y)) \text{ at } (x_0, y_0) = \begin{pmatrix} f_x(x,y) \\ f_y(x,y) \\ -1 \end{pmatrix} \tag{1.31}$$