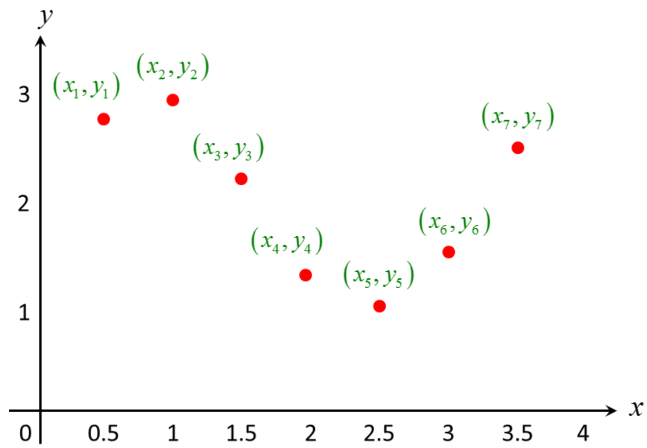
University of Washington
AMATH 301 Spring 2017
Instructor: Dr. King-Fai Li

Lecture Notes
Week 6
Numerical Calculus with Discrete Datasets

Given the following data set:

x	y
0.5	2.84
1	2.91
1.5	2.14
2	1.24
2.5	1.04
3	1.72
3.5	2.66



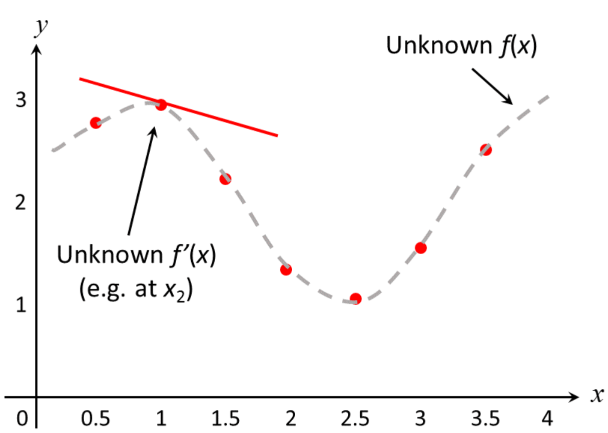

```
x = [.5    1     1.5   2     2.5   3     3.5];
y = [2.84  2.91  2.14  1.24  1.04  1.72  2.66];
```

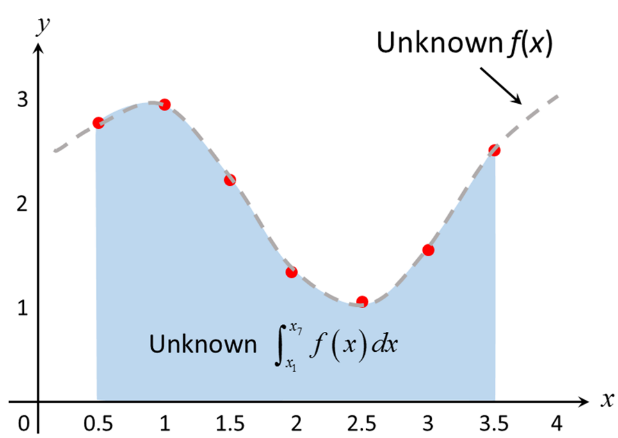
Statements of Problem:

1. The underlying function $f(x)$ is not known; only $y_k = f(x_k)$ are known.

2. How can we estimate the derivative $f'(x) = \dfrac{df(x)}{dx}$, say at x_2, based on the discrete data set?

3. How can we estimate the integral $\int_{x_1}^{x_7} f(x)\,dx$ based on the discrete data set?





Numerical Differentiation — First-order Accuracy

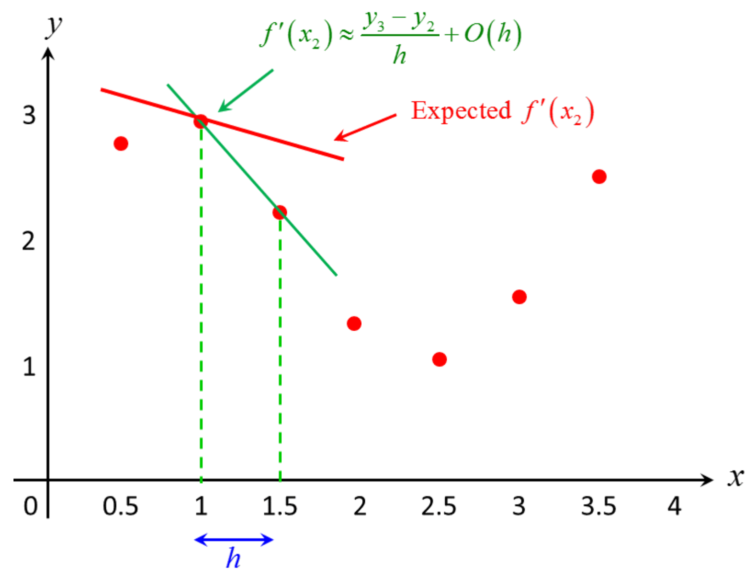
Let's calculate the derivative at x_2 (and later to other data points).

Newton's Quotient as a Forward Difference

$$f'(x_2) = \lim_{\Delta x \to 0} \frac{f(x_2+\Delta x) - f(x_2)}{\Delta x} \approx \frac{f(x_2+\Delta x) - f(x_2)}{\Delta x} + O(\Delta x)$$

Not known for arbitrary Δx

Choose Δx so that we can make use $y_k = f(x_k)$



Choose $\Delta x = h$,

$$f'(x_2) \approx \frac{f(x_2+h) - f(x_2)}{h} = \frac{y_3 - y_2}{h}$$

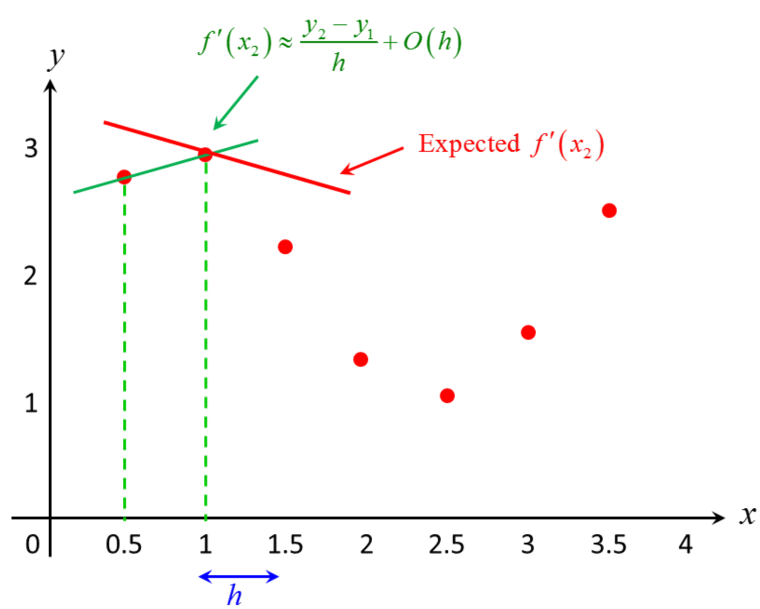
Applicable to all data points except the last point (i.e. x_7).

In Matlab,

```
dydx=zeros(1,7); h=x(2)-x(1);
dydx(1:end-1)=(y(2:end) - y(1:end-1))./h;  dydx(end)=dydx(end-1);
>> dydx=[0.14 -1.54 -1.80 -0.40  1.36  1.88  1.88]
```

Backward difference

$$f'(x_2) = \lim_{\Delta x \to 0} \frac{f(x_2) - f(x_2-\Delta x)}{\Delta x}$$
$$\approx \frac{f(x_2) - f(x_2-h)}{h} + O(h)$$
$$= \frac{y_2 - y_1}{h}$$

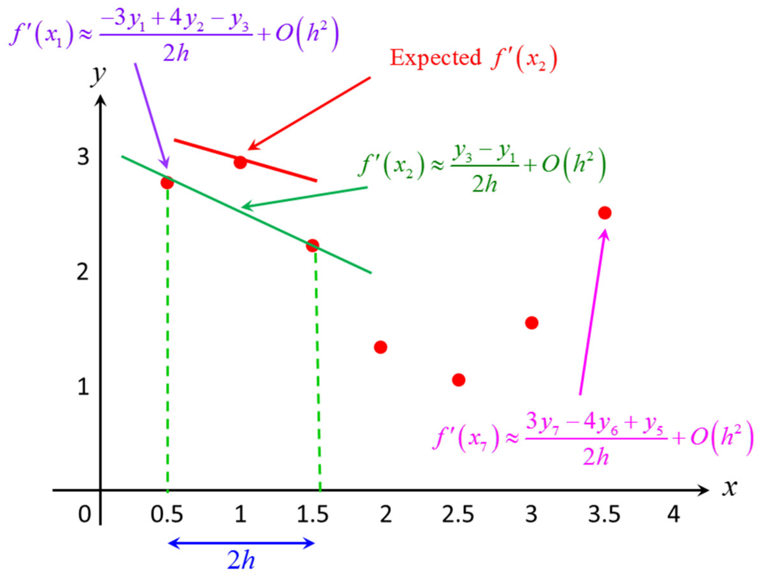


Applicable to all data points except the first point (i.e. x_1).

In Matlab,

```
dydx(2:end)=(y(2:end) - y(1:end-1))./h; dydx(1)=dydx(2);
>> dydx=[0.14   0.14 -1.54 -1.80 -0.40  1.36  1.88]
```

Numerical Differentiation — Second-order Accuracy



Central difference

$$f'(x_2)=\lim_{\Delta x\to 0}\frac{f(x_2+\Delta x)-f(x_2-\Delta x)}{2\Delta x}$$

$$\approx \frac{f(x_2+h)-f(x_2-h)}{2h}+O(h^2)$$

$$=\frac{y_3-y_1}{2h}$$

Applicable to all data points except the end-points (i.e. x_1 and x_7).

In Matlab,

```
dydx(2:end-1)= (y(3:end) - y(1:end-2))./(2.*h);
```

At the first point

From forward difference $f'(x_1)\equiv D(h)=\frac{f(x_1+h)-f(x_1)}{h}+\underbrace{O(h)}_{\text{Call this } e_1h}$.

Richardson extrapolation: Try two h's

$$f'(x_1)=D(h)\ +\ e_1h$$

$$f'(x_1)=D(2h)+2e_1h$$

$$2f'(x_1)=2D(h)\ +2e_1h$$

$$-)\quad f'(x_1)=D(2h)\ +2e_1h$$

$$\Rightarrow \quad f'(x_1)=2D(h)-D(2h)$$

$$=\frac{-3f(x_1)+4f(x_1+h)-f(x_1+2h)}{2h}+O(h^2)$$

In Matlab, `dydx(1)=( -3*y(1) +4*y(2) -y(3) )./(2.*h);`

At the end point

Richardson extrapolation using backward difference

$$f'(x_7)=\frac{3f(x_7)-4f(x_7-h)+f(x_7-2h)}{2h}+O(h^2)$$

In Matlab, `dydx(end) = ( 3.*y(end) -4.*y(end-1) +y(end-2) )./(2.*h);`

```
>> dydx = [0.98 -0.70 -1.67 -1.10  0.48  1.62  2.14]
```

Numerical Integration

Not known for arbitrary Δx

Choose Δx so that we can make use $y_k = f(x_k)$

<u>Riemann Sum</u>

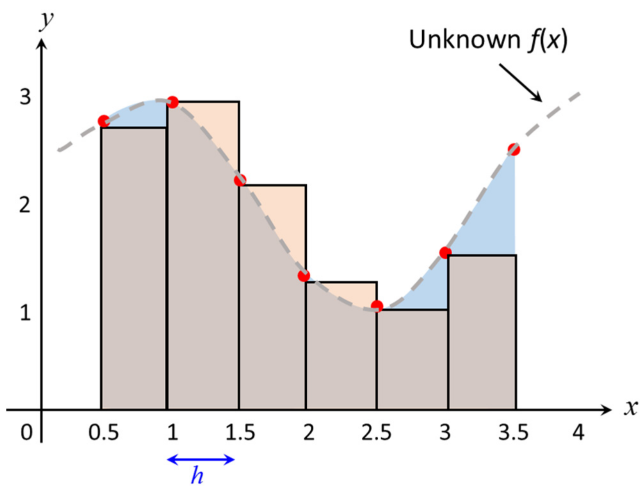
$$\int_{x_1}^{x_7} f(x)\,dx = \lim_{\substack{n\to\infty \\ \Delta x\to 0}} \sum_{k=1}^{n} f(x_k)\,\Delta x \approx \sum_{k=1}^{n} f(x_k)\,\Delta x$$

<u>Right/Left Sums</u>

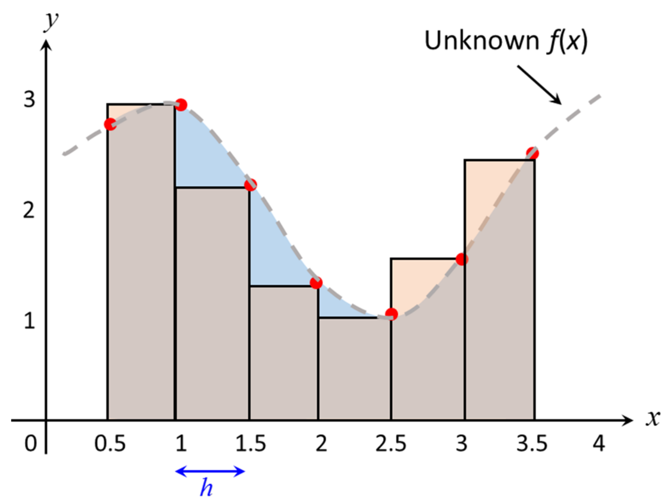
$$\int_{x_1}^{x_7} f(x)\,dx \approx \sum f(x)\,h + O(h)$$

$$\text{Left sum} = \sum_{j=1}^{6} f(x_j)\,h = y_1 h + y_2 h + \cdots + y_6 h \quad = \texttt{h.*sum(y(1:end-1))} = 5.945$$

$$\text{Right sum} = \sum_{j=2}^{7} f(x_j)\,h = y_2 h + y_3 h + \cdots + y_7 h = \texttt{h.*sum(y(2:end))} \quad = 5.855$$



Left sum



Right sum

Trapezoidal Rule

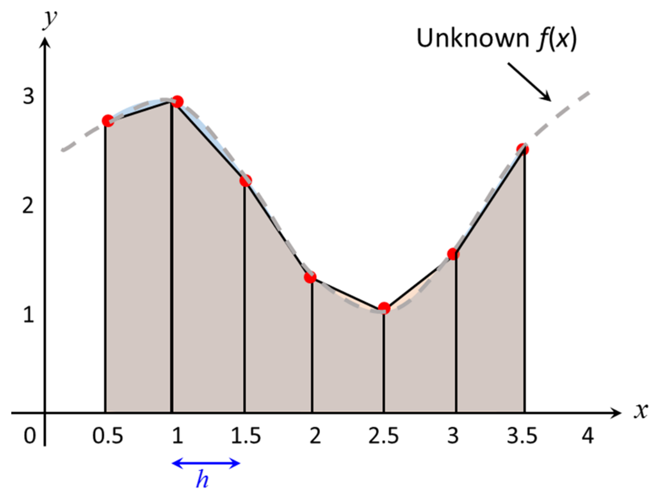
$$\int_{x_1}^{x_7} f(x)\,dx \approx \sum_{j=1}^{6} \frac{f(x_j)+f(x_{j+1})}{2} h + O(h^2)$$

$= \texttt{h./2.*sum(y(1:end-1)+y(2:end))}$

$= \texttt{trapz(x,y)}$

= Average of right and left sums

$= 5.900$

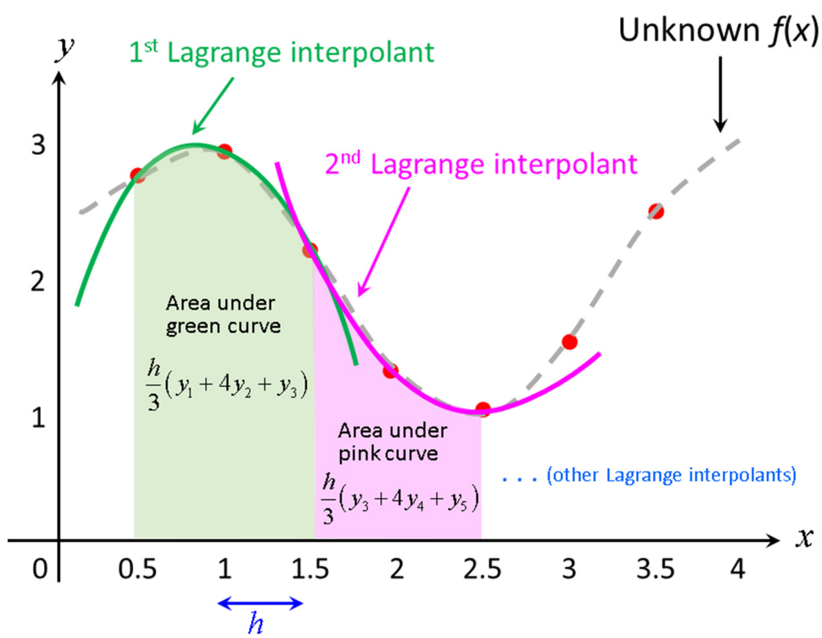


Simpson's rule

1. Make a continuous curve between every three points using Lagrange interpolation.
2. Integrate the area under the Lagrange interpolant.

$$\int_{x_1}^{x_3} f(x)\,dx \approx \frac{h}{3}\left[f(x_1)+4f(x_2)+f(x_3)\right] = \frac{h}{3}(y_1+4y_2+y_3)+O(h^4)$$

3. Do the same for all triplets.
4. Sum the areas under all triplets.



$$\int_{x_1}^{x_n} f(x)\,dx = \left(\int_{x_1}^{x_3}+\int_{x_3}^{x_5}+\cdots+\int_{x_{n-2}}^{x_n}\right) f(x)\,dx \quad + O(h^4)$$

$$= \sum_{j=1,3,\ldots,n-2} \frac{h}{3}\left[f(x_j)+4f(x_{j+1})+f(x_{j+2})\right]$$

n must be odd

$= \texttt{h./3.*sum(y(1:2:end-2)+4.*y(2:2:end-1)+y(3:2:end))}$

$= 5.890$

Numerical Calculus for Known Functions

The above dataset was actually generated using $f(x) = 2 + \sin(2x)$.

1. At any x, e.g. $x = x_2$, the derivative can be calculated directly by

$$f'(x_2) = \frac{f(x_2 + \delta) - f(x_2 - \delta)}{2\delta}$$

with a "sufficiently" small δ. In the video lectures, Prof. Brunton explained that

$$\delta \geq \sqrt[3]{\frac{3\varepsilon}{\max|f'''|}}, \quad \varepsilon = \text{machine precision} = 10^{-16}.$$

For this example,

$$|f'''(x)| = |-8\cos(2x)| \leq 8 \quad \rightarrow \quad \delta \geq \sqrt[3]{\frac{3\varepsilon}{\max|f'''|}} = 3.3\times 10^{-6}.$$

```
f = @(x) 2 + sin(2*x)
x = 0.5:.5:3.5;
del = 3.3e-6;
dydx = (f(x+del)-f(x-del))/(2*del);

>> dydx = 1.0806 -0.8323 -1.9800 -1.3073 0.5673 1.9203 1.5078
```

2. The integral can be calculated using Matlab's **quad** function (e.g. up to an accuracy of 10^{-4}):

$$\int_{0.5}^{3.5} f(x)\,dx = \texttt{quad}(@(x)\ 2+\sin(2.*x),\ 0.5,\ 3.5,\ 1e-4)$$
$$= 5.893$$

Second derivatives at the interior points (See Prof. Brunton's video)

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

$$+)\quad f(x-h)=f(x)-hf'(x)+\frac{h^2}{2}f''(x)-\frac{h^3}{3!}f'''(x)+O(h^4)$$

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

```
d2ydx2(2:end-1)  =  ( y(1:end-2)-2.*y(2:end-1)+y(3:end))./(h.^2);
```

```
>> d2ydx2(2:end-1) = [-3.64 -0.56  3.03  3.84  1.12]
```

Second derivatives at the end-points

Assume

$$\begin{aligned}
h^2 f''(x) &= a_1 f(x)+a_2 f(x+h)+a_3 f(x+2h)+a_4 f(x+3h)\\
&= a_1 f(x)\\
&\quad +a_2 f(x)+a_2 hf'(x)+a_2\frac{h^2}{2!}f''(x)+a_2\frac{h^3}{3!}f'''(x)\\
&\quad +a_3 f(x)+2a_3 hf'(x)+a_3\frac{(2h)^2}{2!}f''(x)+a_3\frac{(2h)^3}{3!}f'''(x)\\
&\quad +a_4 f(x)+3a_4 hf'(x)+a_4\frac{(3h)^2}{2!}f''(x)+a_4\frac{(3h)^3}{3!}f'''(x)\\
&\quad +O(h^4)
\end{aligned}$$

$$\begin{pmatrix}1 & 1 & 2^0 & 3^0\\ 0 & 1 & 2^1 & 3^1\\ 0 & 1 & 2^2 & 3^2\\ 0 & 1 & 2^3 & 3^3\end{pmatrix}\begin{pmatrix}a_1\\ a_2\\ a_3\\ a_4\end{pmatrix}=\begin{pmatrix}0\\ 0\\ 2\\ 0\end{pmatrix}\quad\Rightarrow\quad\begin{pmatrix}a_1\\ a_2\\ a_3\\ a_4\end{pmatrix}=\begin{pmatrix}2\\ -5\\ 4\\ -1\end{pmatrix}$$

$$\begin{aligned}
f''(x)&=\frac{2f(x)-5f(x+h)+4f(x+2h)-f(x+3h)}{h^2}+O(h^2)\\
&=\frac{2f(x)-5f(x-h)+4f(x-2h)-f(x-3h)}{h^2}+O(h^2)
\end{aligned}$$

In Matlab,

```
d2ydx2(1)    = (2.*y(1)  -5.*y(2)    +4.*y(3)    -y(4)    )./(h.^2);
d2ydx2(end)  = (2.*y(end)-5.*y(end-1)+4.*y(end-2)-y(end-3))./(h.^2);
```