

# Scientific Computing

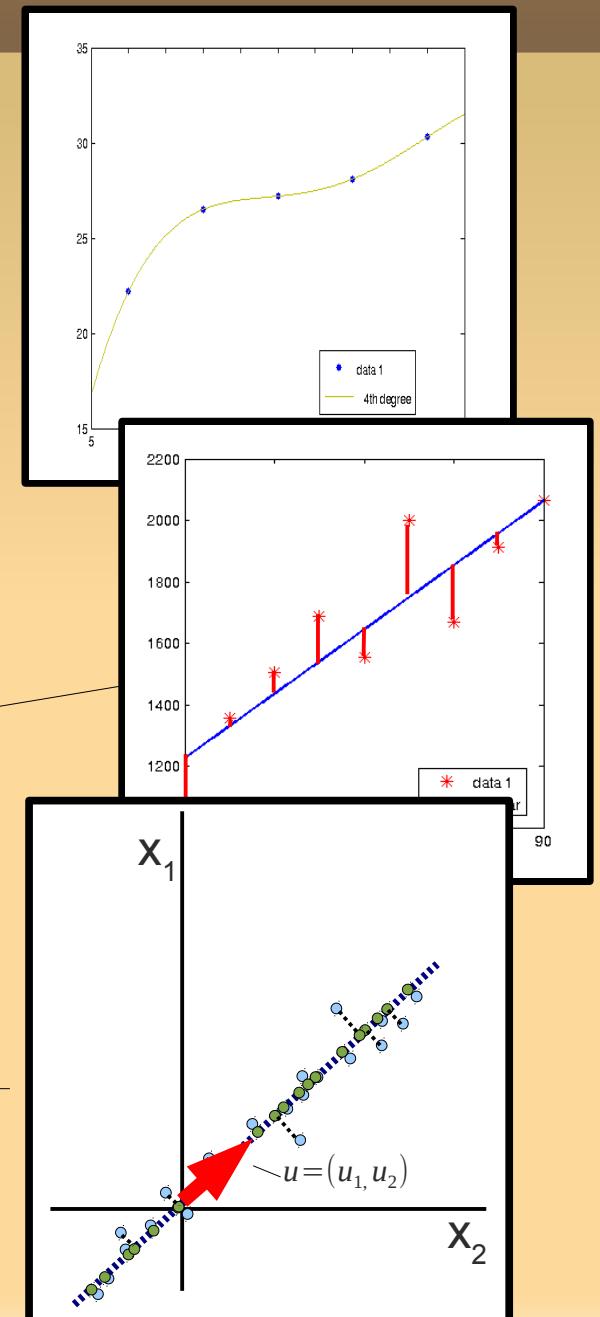
## Maastricht Science Program

### Week 4

Frans Oliehoek  
[<frans.oliehoek@maastrichtuniversity.nl>](mailto:frans.oliehoek@maastrichtuniversity.nl)

# Recap

- Matlab...!
- Supervised Learning
  - find  $f$  that maps  $\{x_1^{(j)}, \dots, x_D^{(j)}\} \rightarrow y^{(j)}$
  - Interpolation    ←
    - $f$  goes through the data points
  - linear regression
    - lossy fit, minimizes 'vertical' SSE
- Unsupervised Learning
  - PCA    ←
    - We just have data points  $\{x_1^{(j)}, \dots, x_D^{(j)}\}$



# Numerical Differentiation and Integration

# Numerical Differentiation and Integration

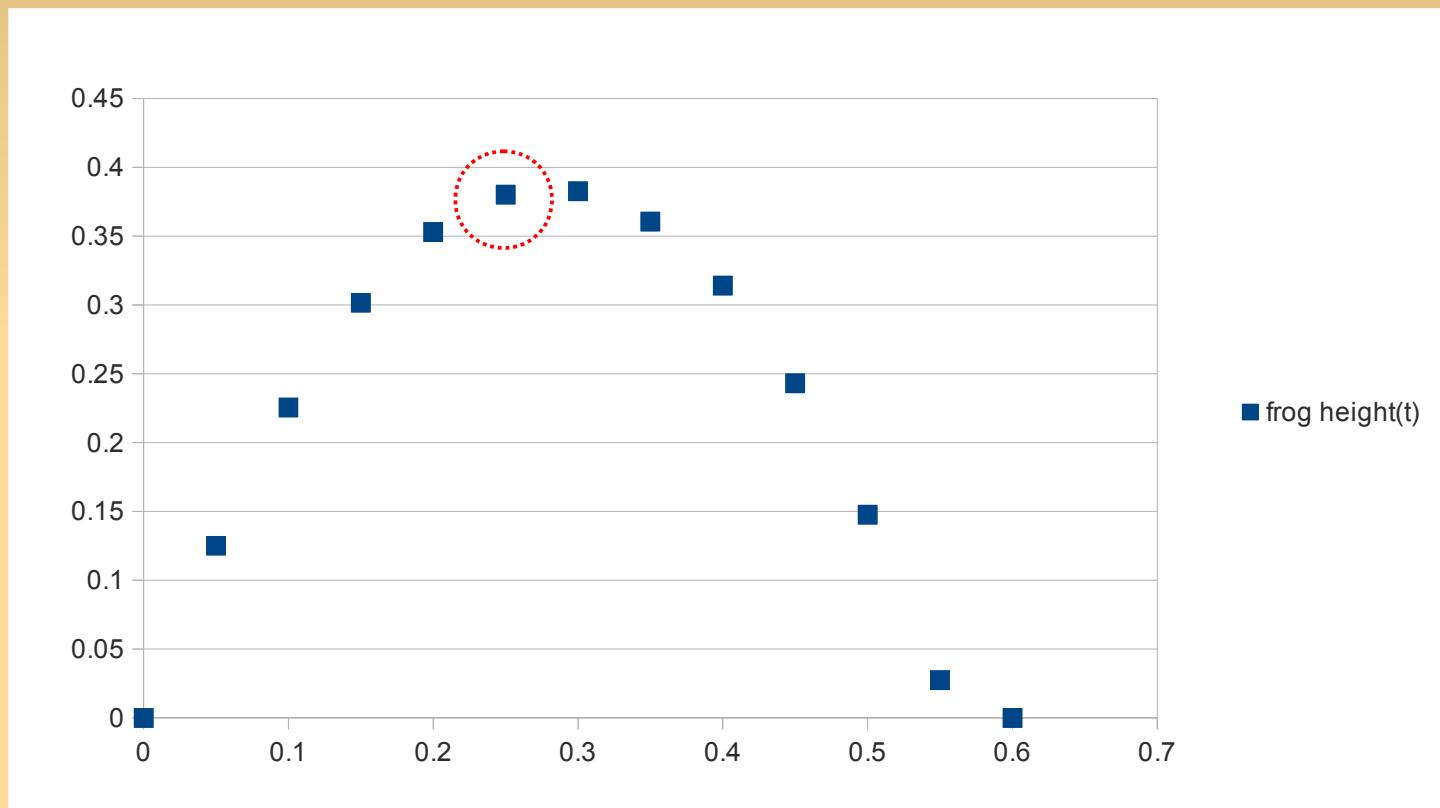
- Finding derivatives or primitives of a function  $f$
  - not always easy or possible....
    - no closed form solution exists
    - the solution is a very complex expression that is hard to evaluate
    - we may not know  $f$  (as before!)
- numerical methods

# Numerical Differentiation

- If we want to know the rate of change...
- E.g.:
  - fluid in a cylinder with a hole in the bottom, measured every 5 seconds.
  - High-speed camera images of animal movements, (jumping in frogs and insects, suction feeding in fish, and the strikes of mantis shrimp)
    - determine speed
    - and acceleration

# Numerical Differentiation

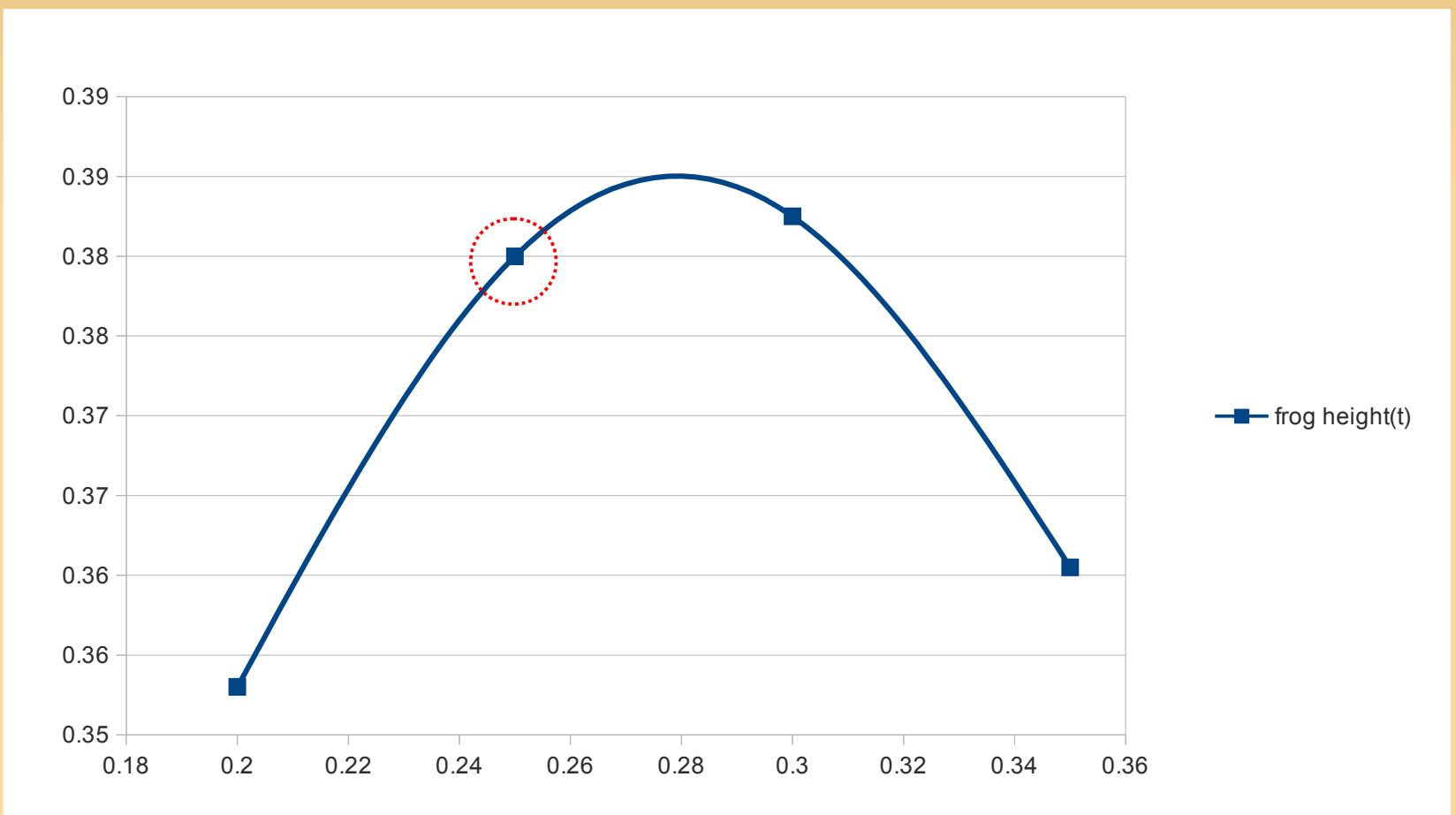
- Determine the vertical speed at  $t=0.25$



- what would you do?

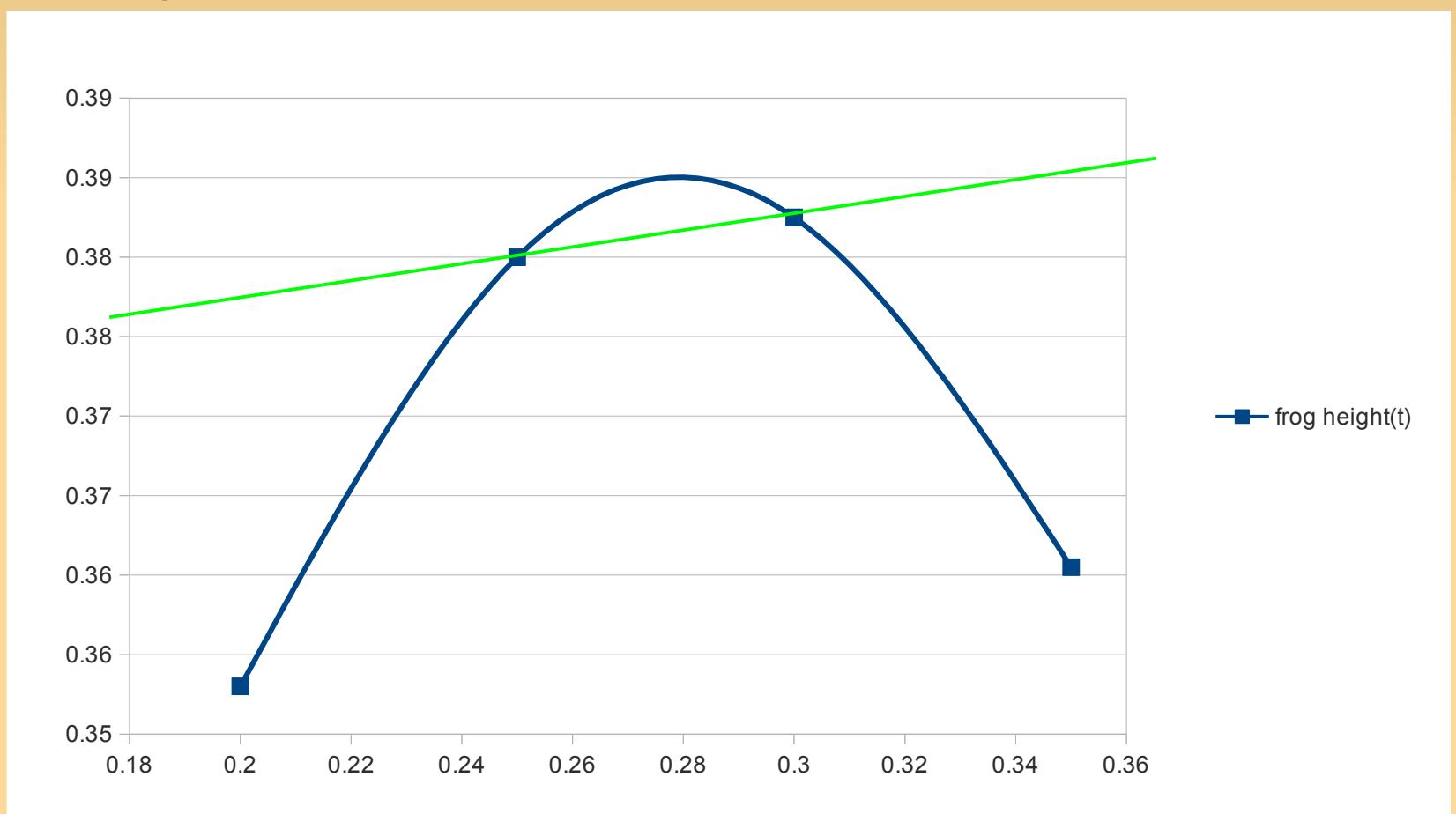
# Numerical Differentiation

- Determine the vertical speed at  $t=0.25\dots$ 
  - a few options...



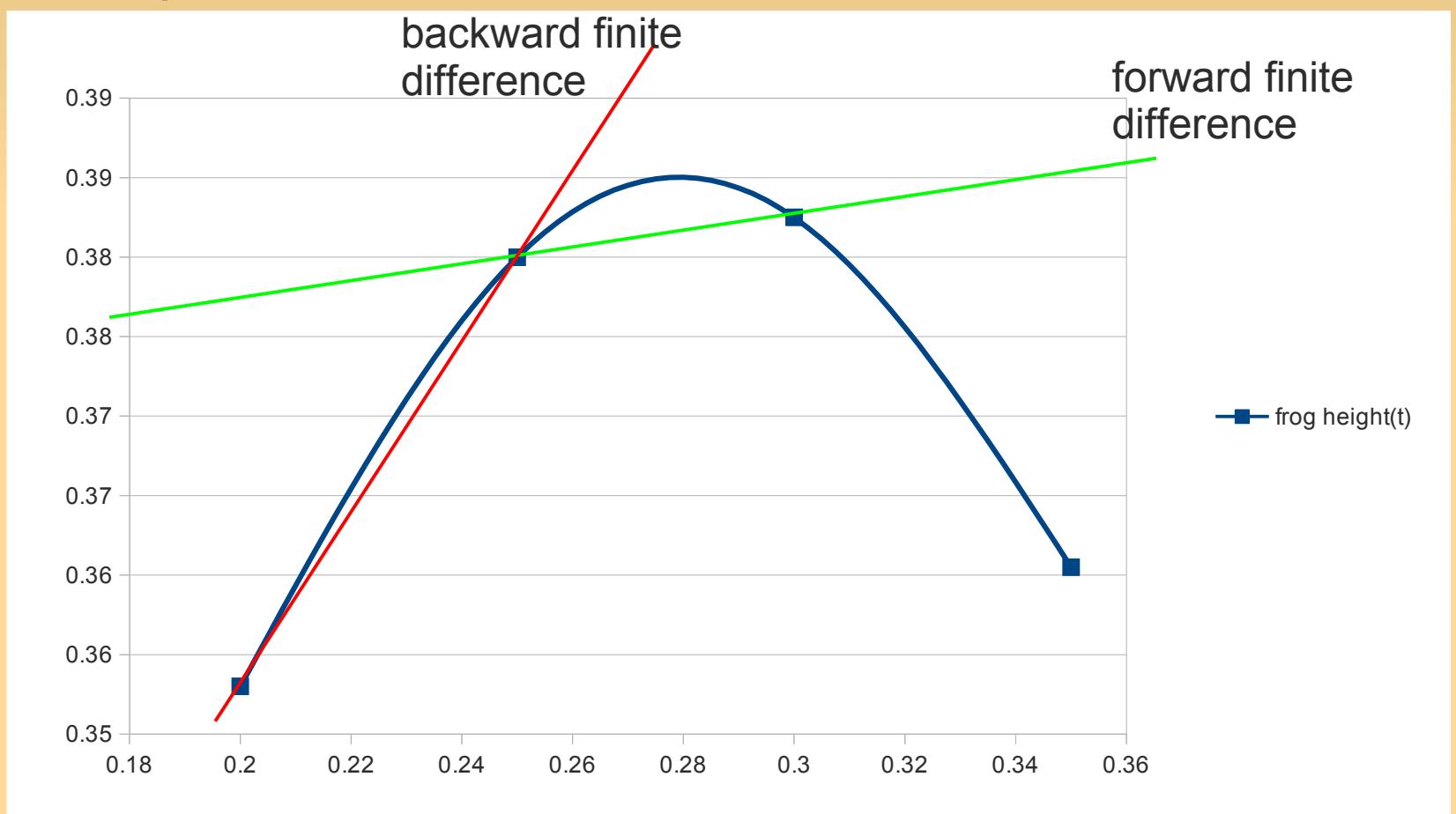
# Numerical Differentiation

- Determine the vertical speed at  $t=0.25\dots$ 
  - a few options...



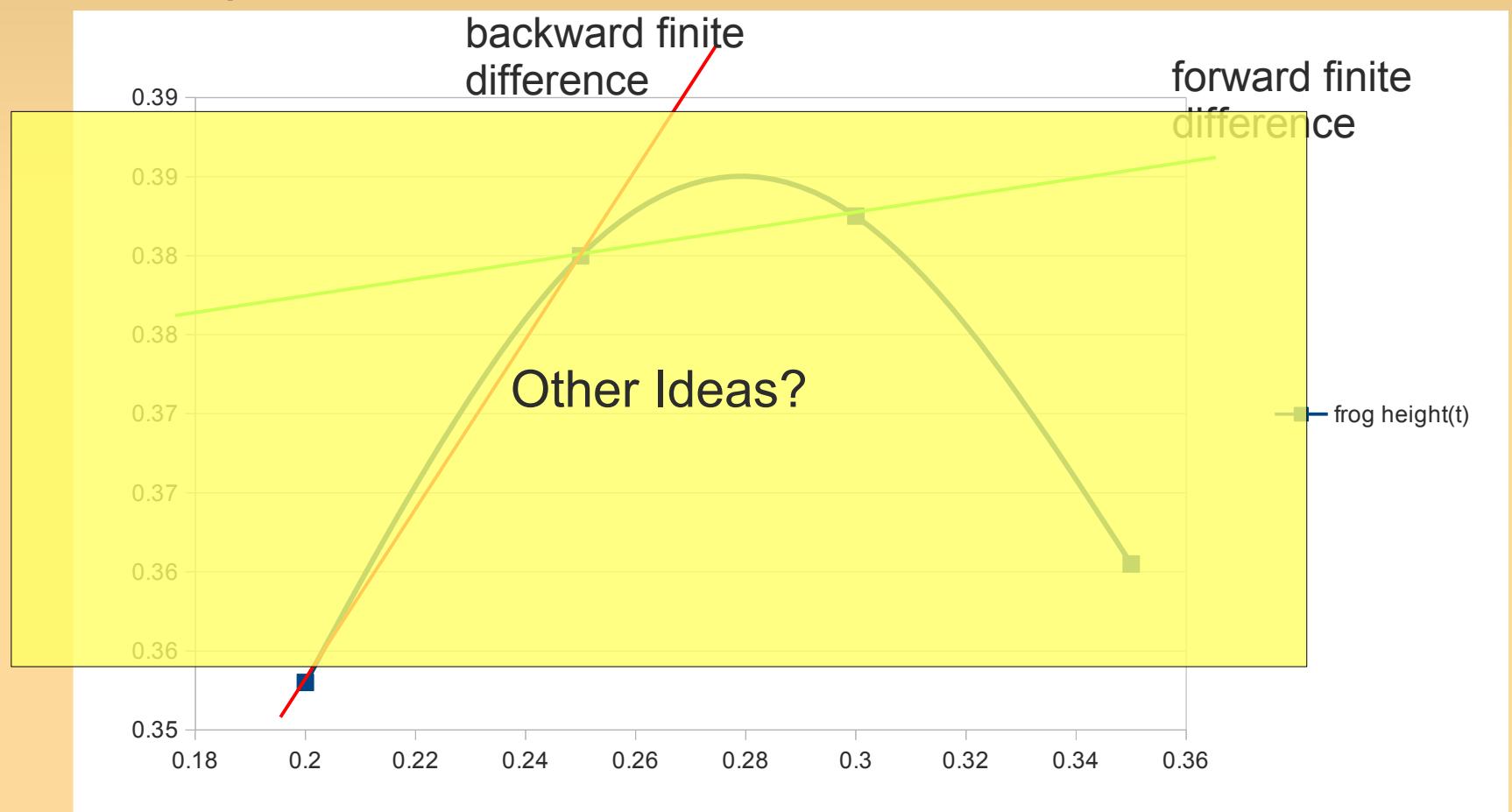
# Numerical Differentiation

- Determine the vertical speed at  $t=0.25\dots$ 
  - a few options...



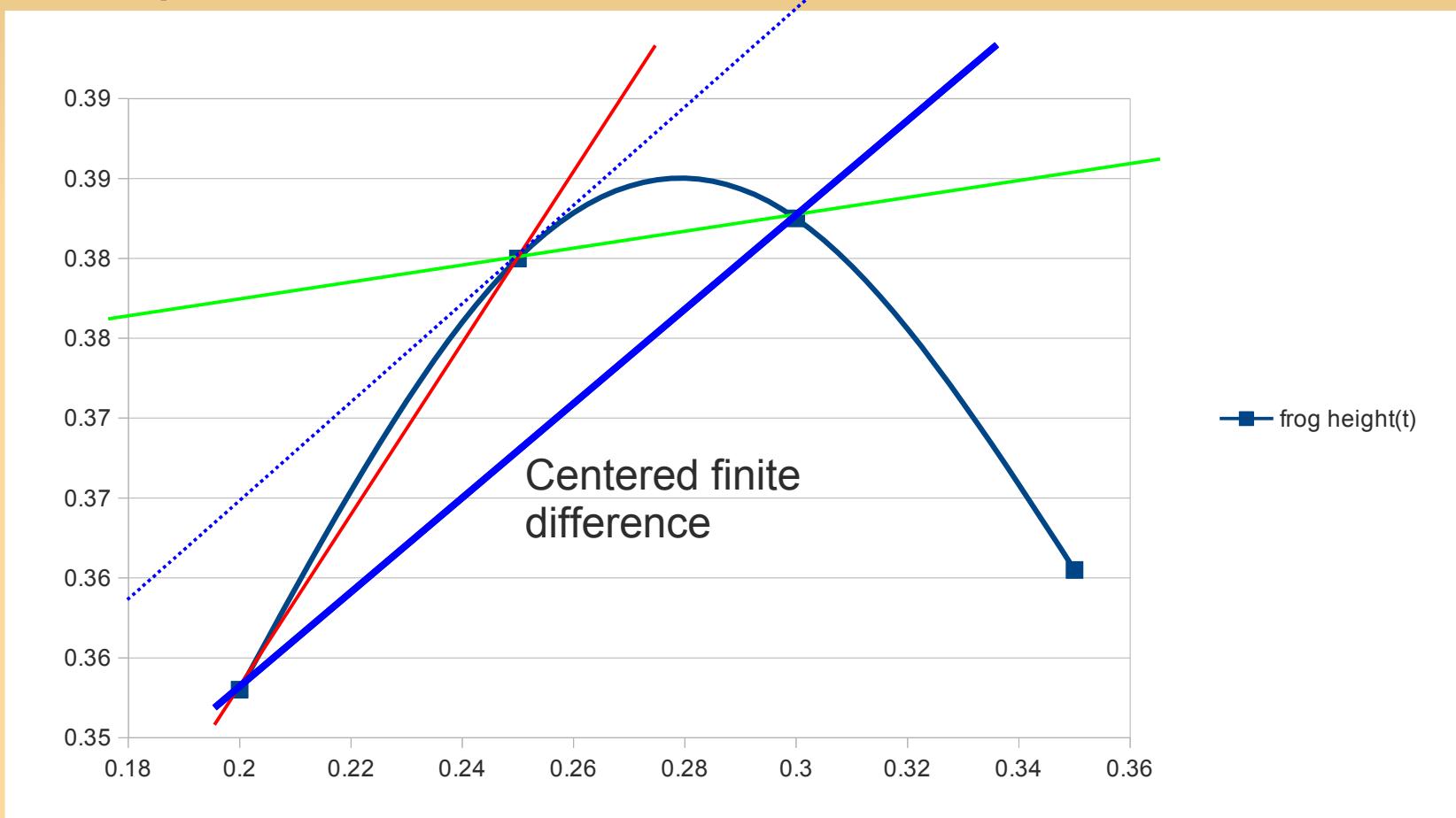
# Numerical Differentiation

- Determine the vertical speed at  $t=0.25\dots$ 
  - a few options...



# Numerical Differentiation

- Determine the vertical speed at  $t=0.25\dots$ 
  - a few options...



# Numerical Integration

- Integration: the reversed problem...
- Suppose we travel in a car with a broken odometer
- Speedometer is working...



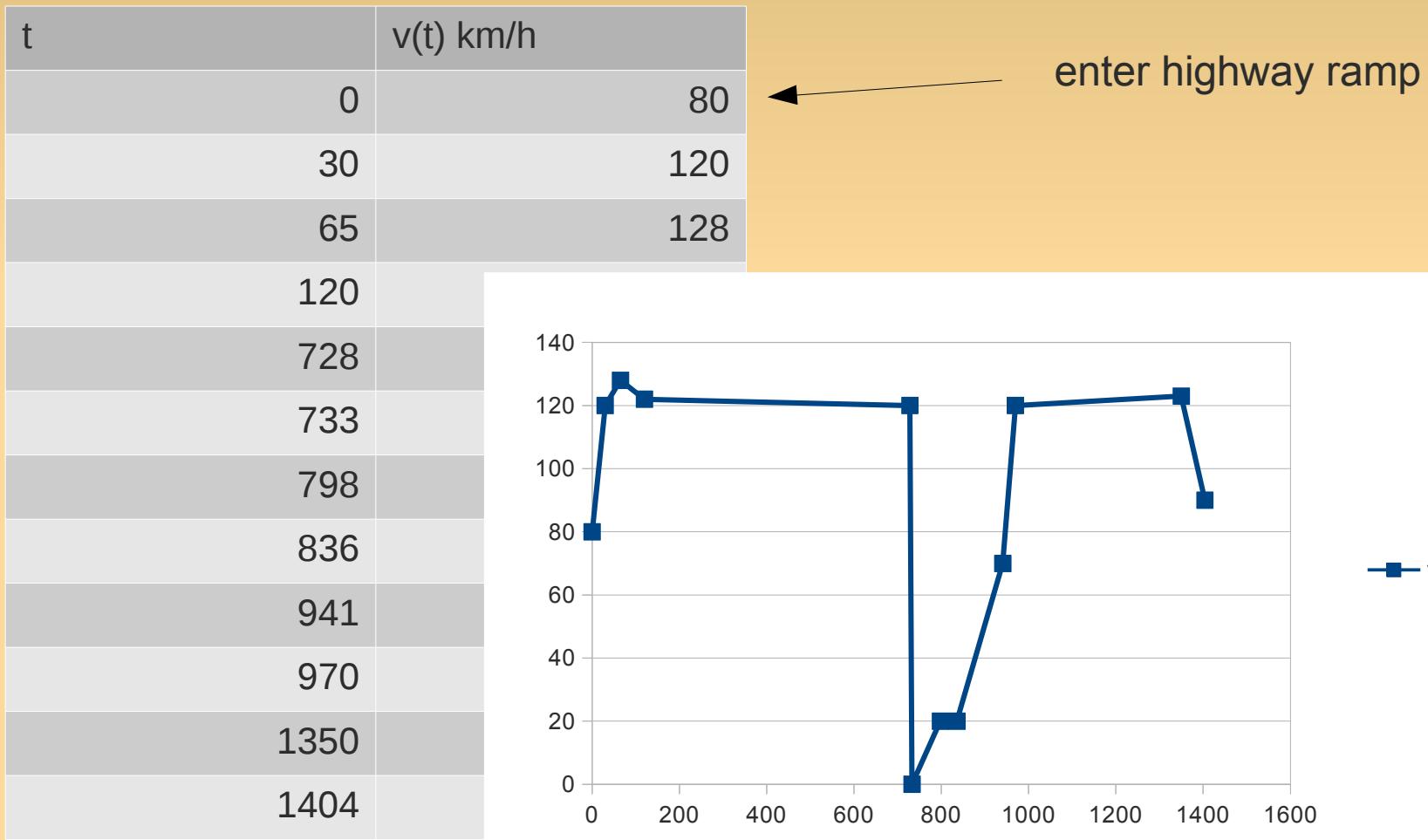
# Numerical Integration

- maintain speeds, to figure out traveled distance

t	v(t) km/h	
0	80	enter highway ramp
30	120	
65	128	
120	122	
728	120	
733	0	traffic jam
798	20	
836	20	
941	70	
970	120	
1350	123	
1404	90	exit highway ramp

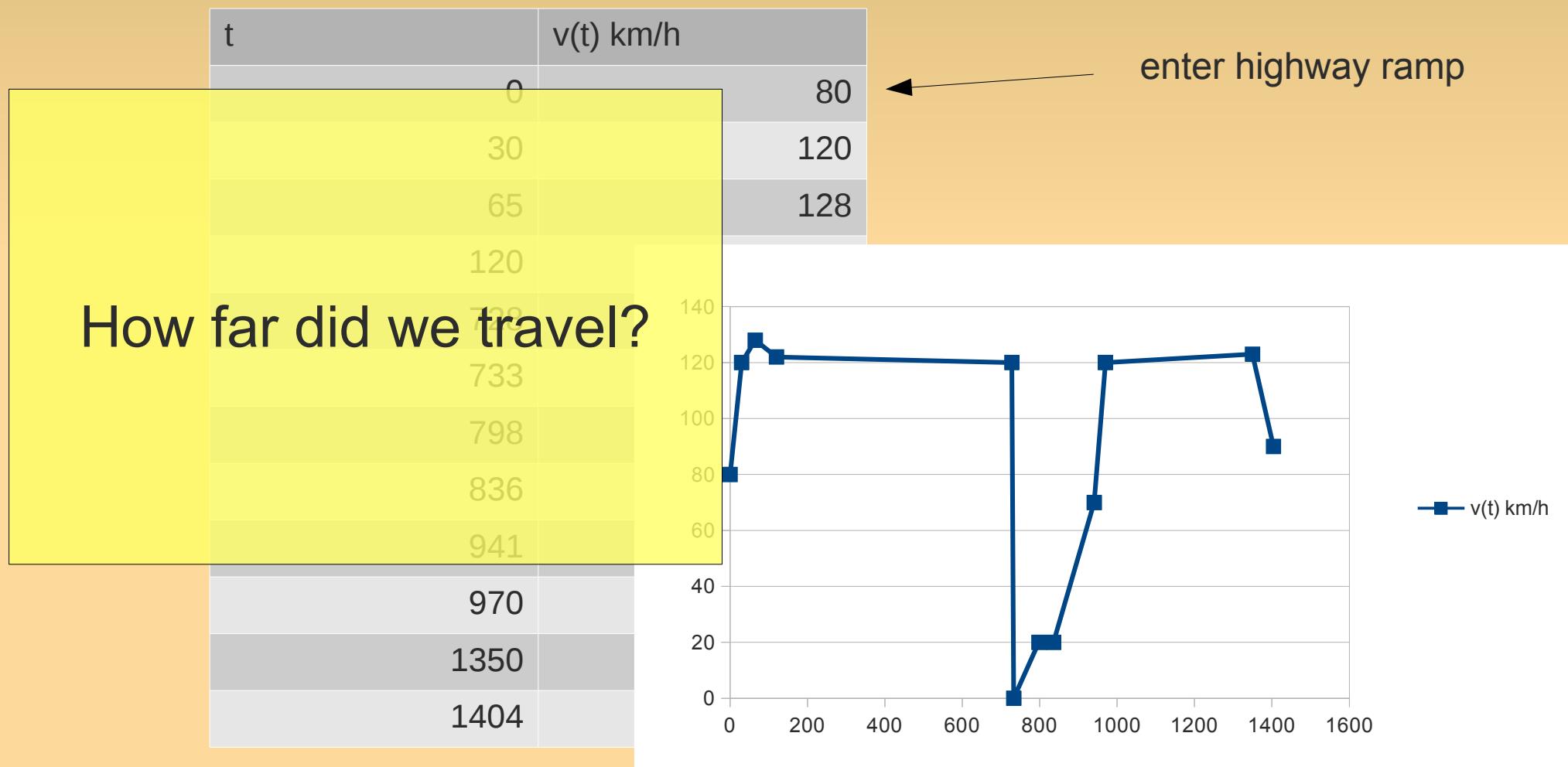
# Numerical Integration

- maintain speeds, to figure out traveled distance



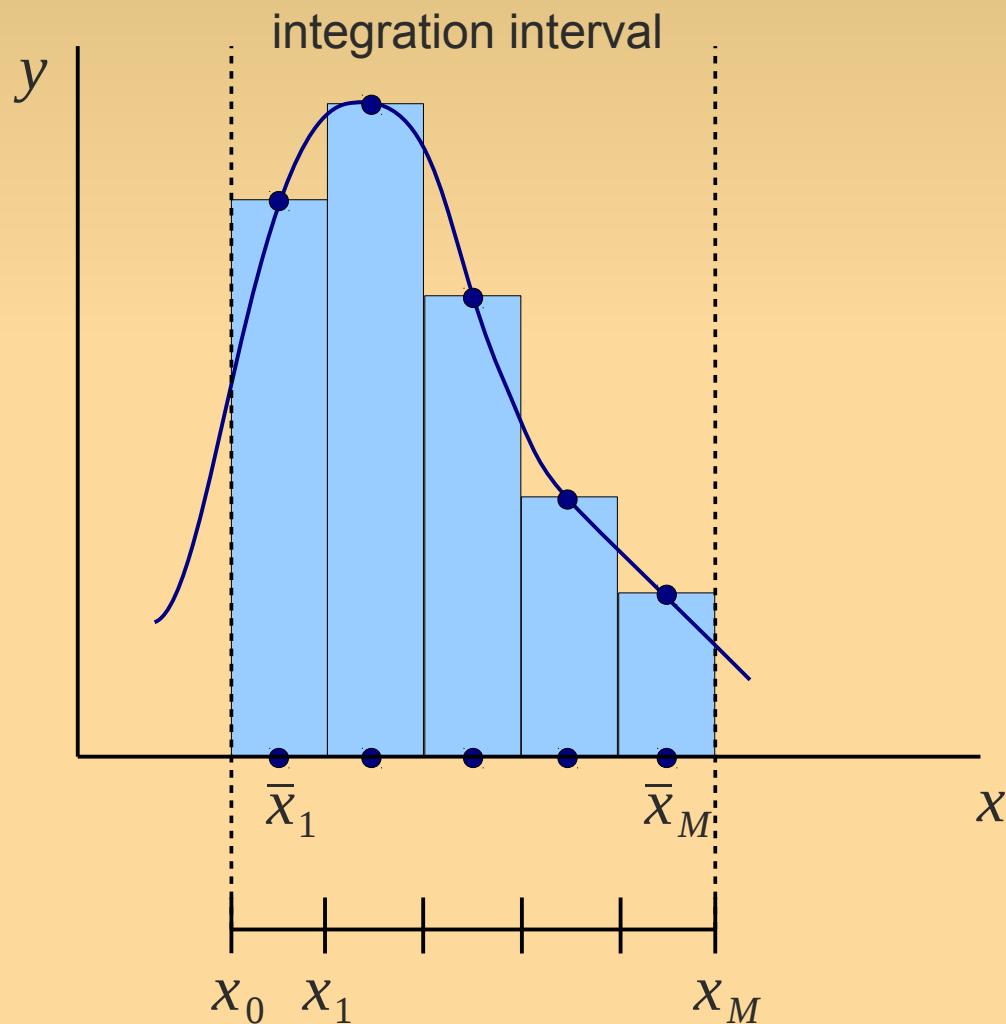
# Numerical Integration

- maintain speeds, to figure out traveled distance

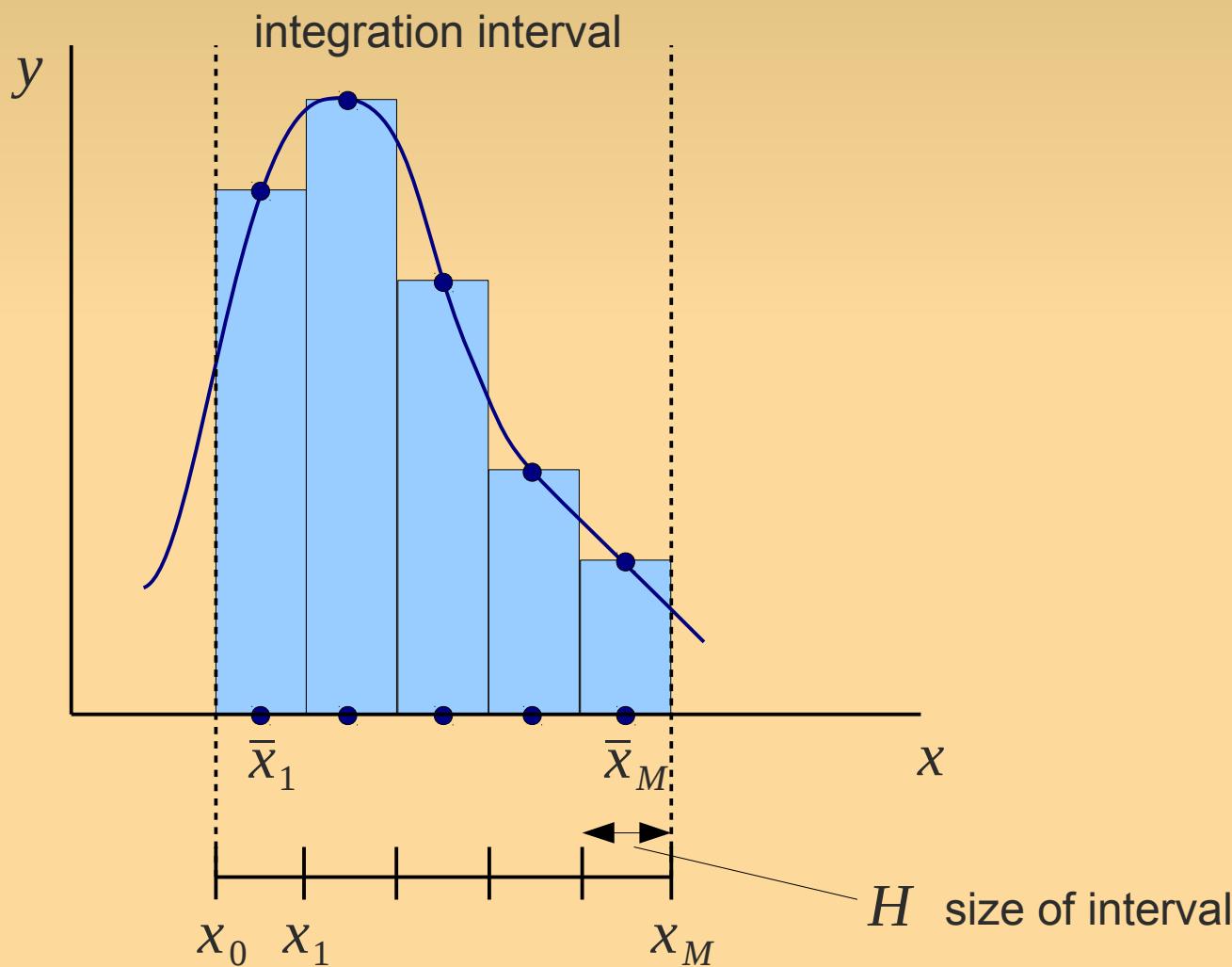


# Midpoint Formula

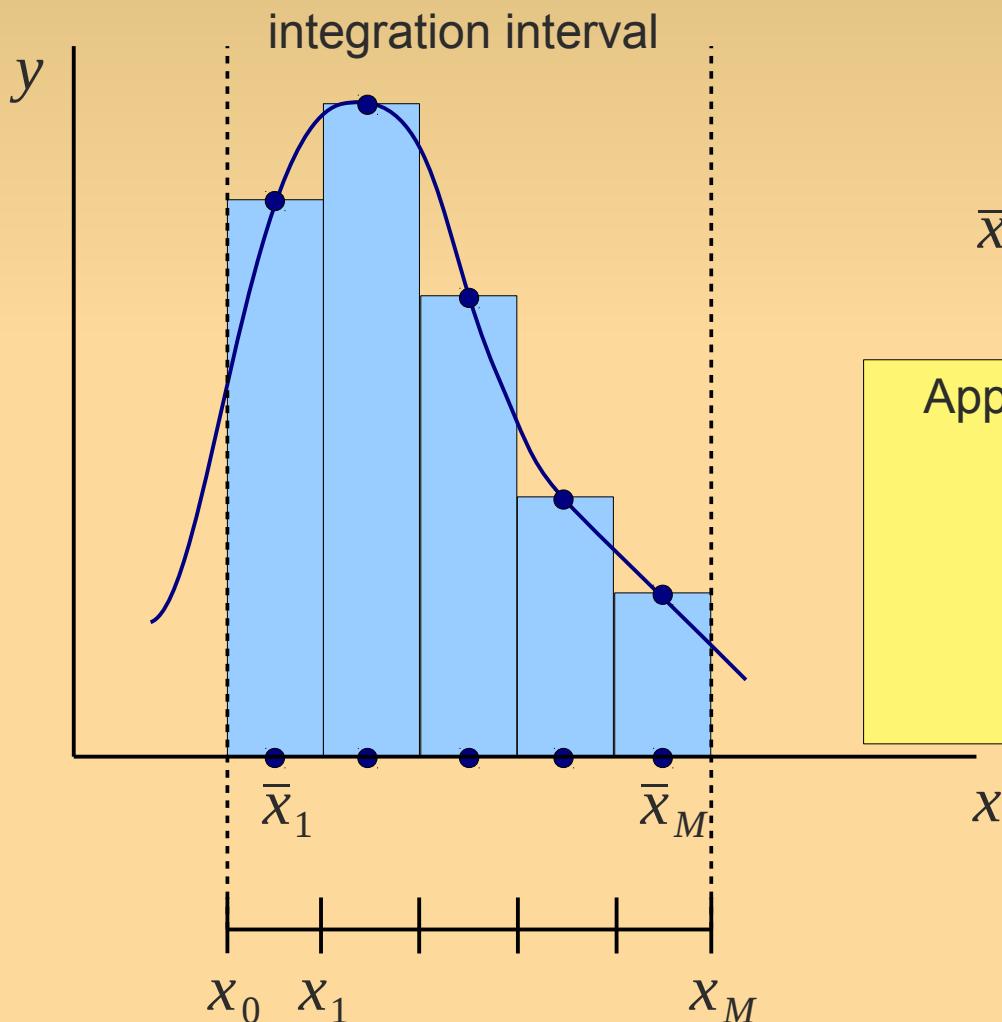
- Approximate the integral with a finite sum



# Midpoint Formula



# Midpoint Formula

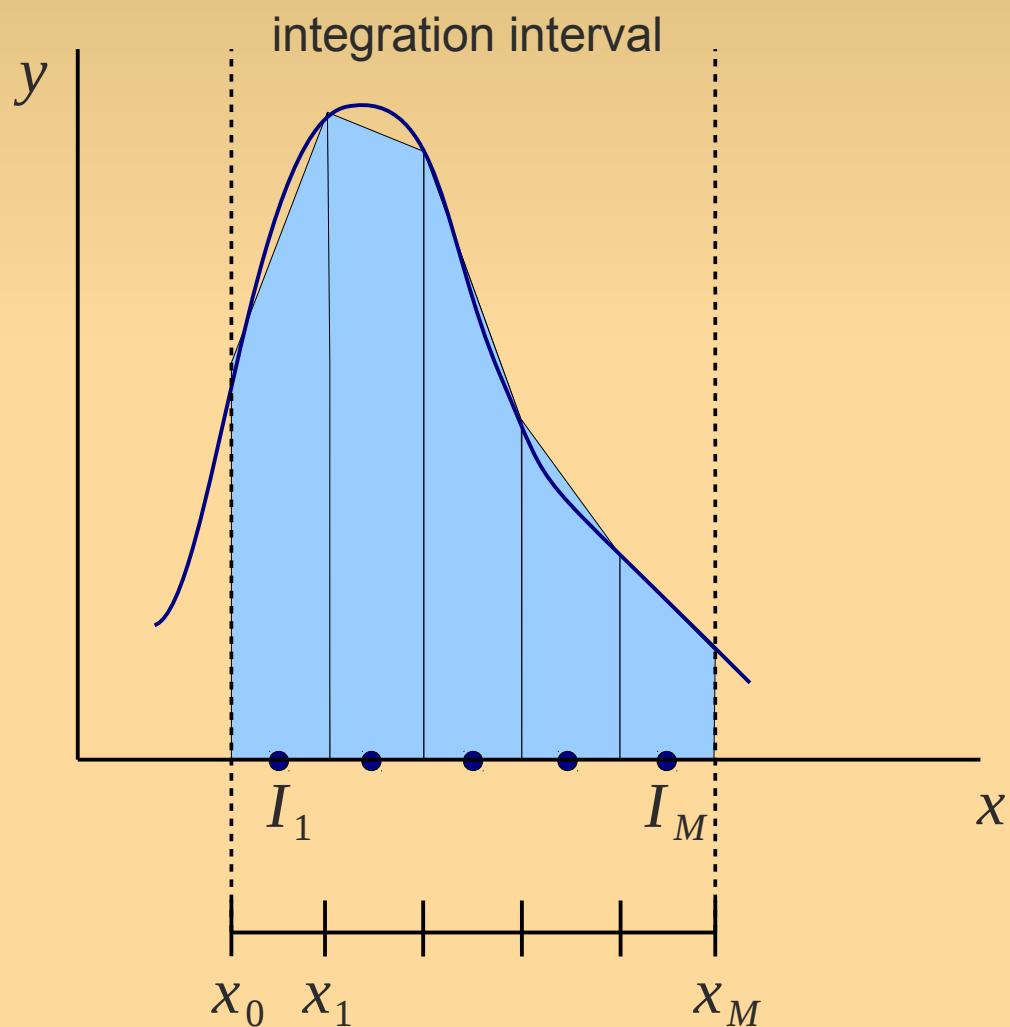


$$\bar{x}_k = \frac{x_{k-1} + x_k}{2}$$

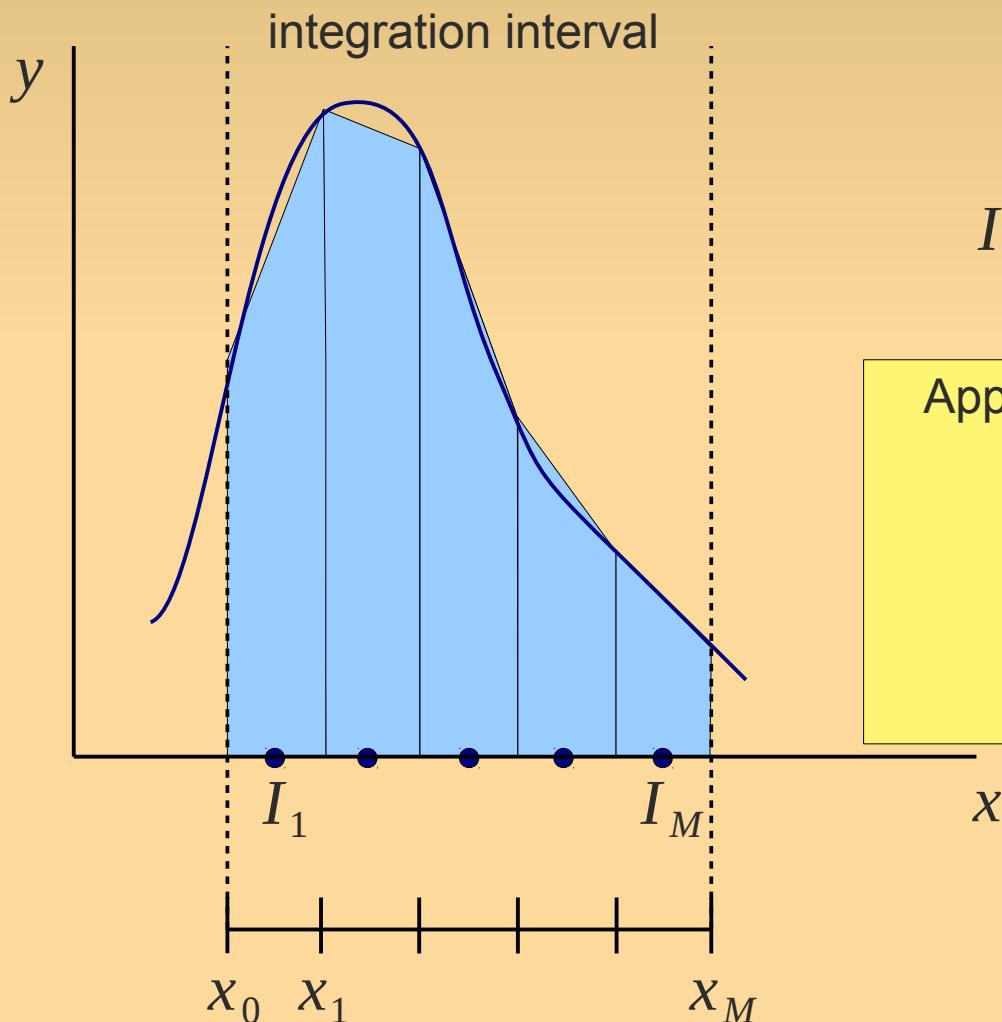
Approximation of the integral:

$$I_{MP}(f) = H \sum_{k=1}^M f(\bar{x}_k)$$

# Trapezoid Formula



# Trapezoid Formula



$$I_k = H \frac{f(x_{k-1}) + f(x_k)}{2}$$

Approximation of the integral:

$$I_{MP}(f) = \sum_{k=1}^M I_k$$

# Symbolic Integration

- Finally: when faced with a difficult integral...  
→ try 'symbolic' packages!

The screenshot shows a Mathematica notebook window with the title "symbolic-integration.nb \*". The menu bar includes File, Edit, Insert, Format, Cell, Graphics, Evaluation, Palettes, Window, and Help. The notebook contains the following content:

- An easy example :**

```
In[48]:= f[x_] = 3*x;
f[4]

Out[49]= 12
```
- A more complex example :**

```
In[50]:= Integrate[f[x], x]
Out[50]= 3 x^2
           2
```
- An example that has no closed form solution:**

```
In[51]:= g[x_] = Exp[x^2] * Cos[x]
          Integrate[g[x], x]

Out[51]= e^x^2 Cos[x]

Out[52]= 1/4 e^(1/4) Sqrt[π] (Erfi[(1/2) (-i + 2 x)] + Erfi[(1/2) (i + 2 x)])
```

■ An easy example :

```
In[48]:= f[x_] = 3*x;
```

```
f[4]
```

```
Out[49]= 12
```

```
In[50]:= Integrate[f[x], x]
```

```
Out[50]=  $\frac{3x^2}{2}$ 
```

■ A more complex example :

```
In[51]:= g[x_] = Exp[x^2]*Cos[x]
```

```
Integrate[g[x], x]
```

```
Out[51]=  $e^{x^2} \cos x$ 
```

```
Out[52]=  $\frac{1}{4} e^{1/4} \sqrt{\pi} \left( \text{Erfi}\left[\frac{1}{2} (-i + 2x)\right] + \text{Erfi}\left[\frac{1}{2} (i + 2x)\right] \right)$ 
```

■ An example that has no closed form solution:

```
In[53]:= h[x_] = x^(3*x)
```

```
Integrate[h[x], x]
```

```
N[Integrate[h[x], {x, 1, 2}]]
```

```
Out[53]=  $\{x^3 x\}$ 
```

```
Out[54]=  $\left\{ \int x^3 x \, dx \right\}$ 
```

```
Out[55]= {13.3445}
```