# Numeric Differentiation

**CH EN 2450**
**Numerical Methods**
**Fall 2020**

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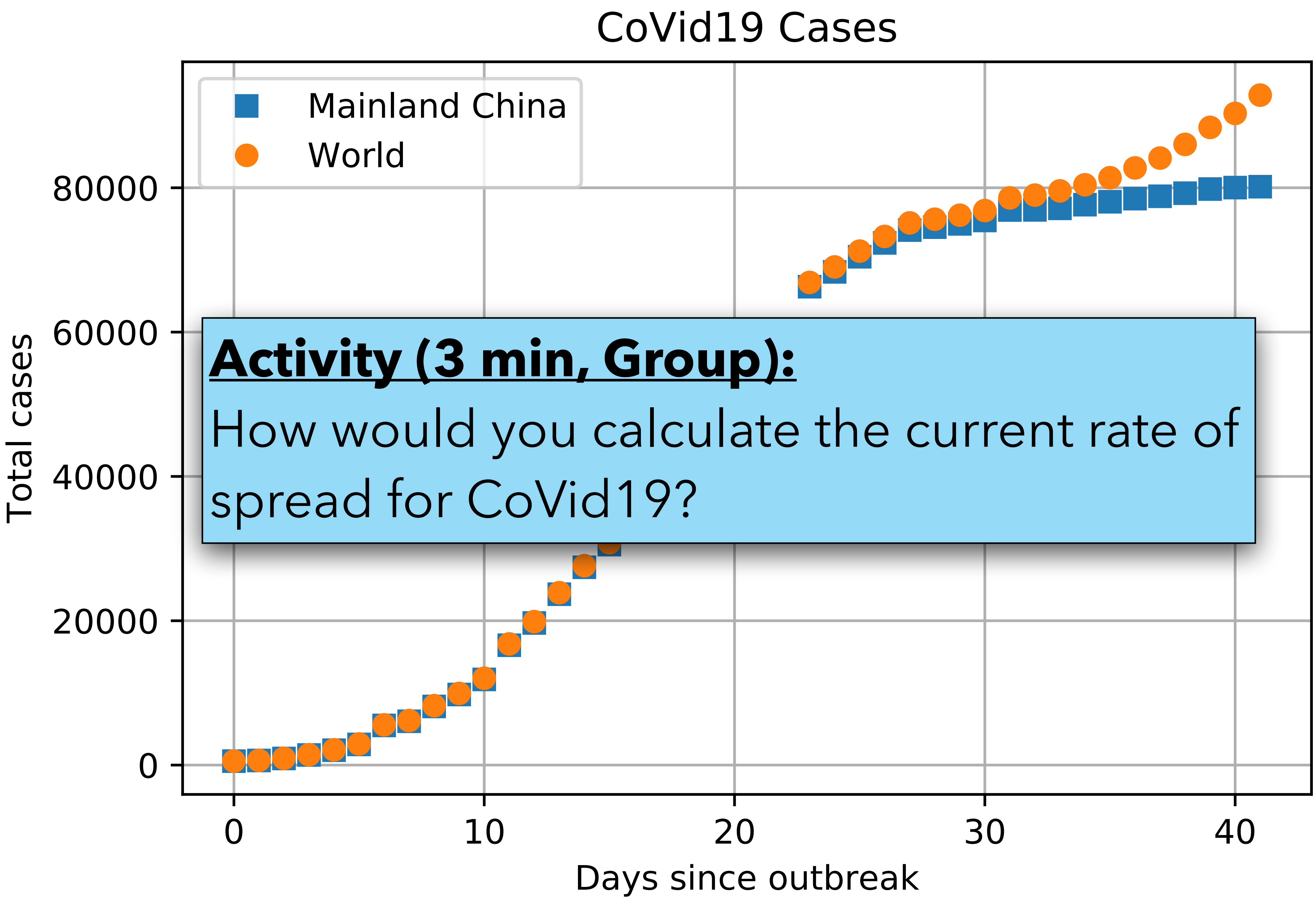
# Learning Objectives

At the end of this chapter, you should be able to do the following:

- Define the finite difference method
- Numerically compute the first and second derivatives for discrete data and continuous functions
- Define and estimate the convergence rate of finite difference schemes
- Define what is meant by order of accuracy of a given finite difference scheme
- Use the Taylor series to derive finite difference schemes




**Activity (3 min, Group):**

How would you calculate the current rate of spread for CoVid19?

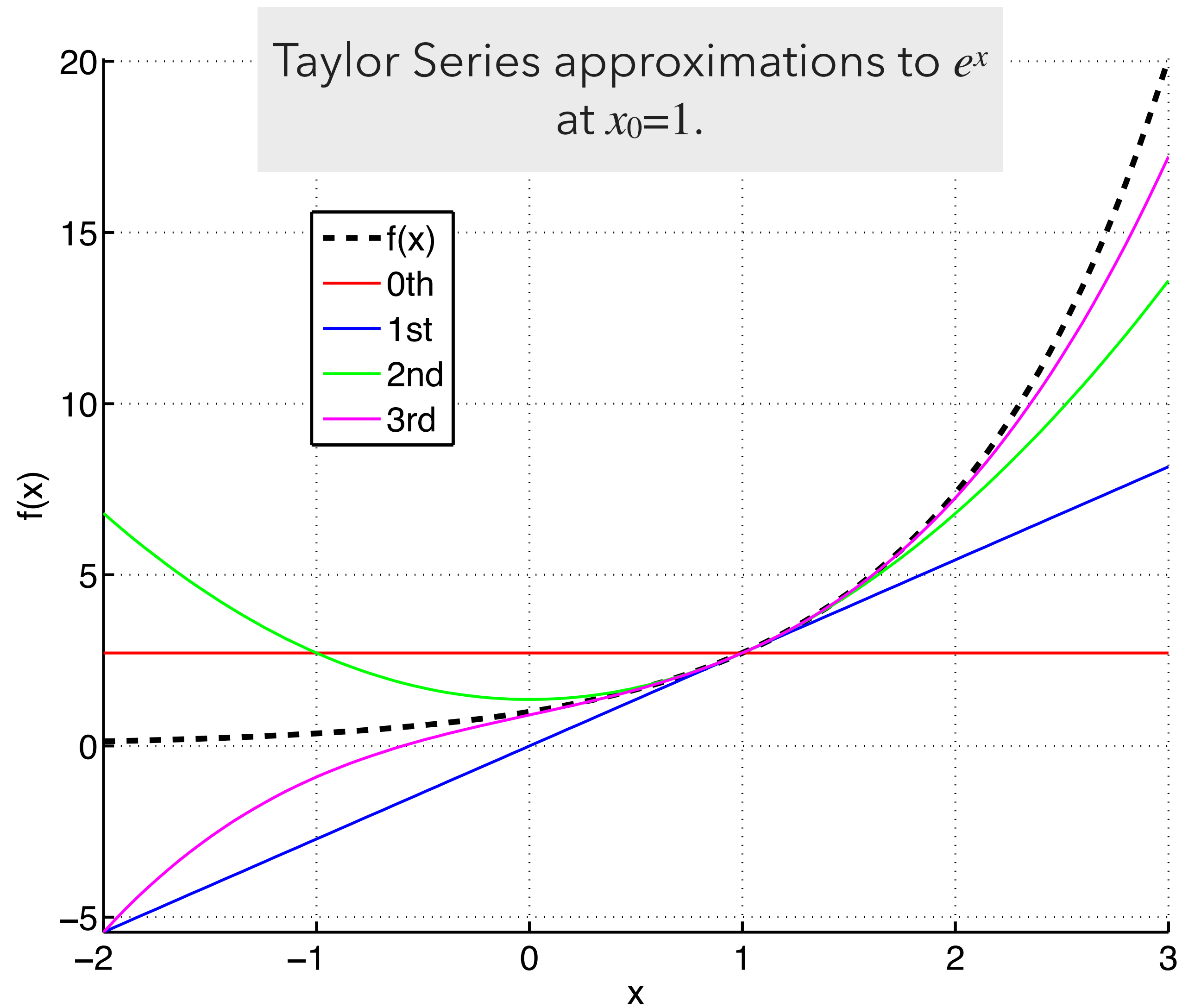
# Ideas

- Fit a polynomial and differentiate polynomial
- Fit a local polynomial and differentiate that local polynomial
- Use Taylor Series

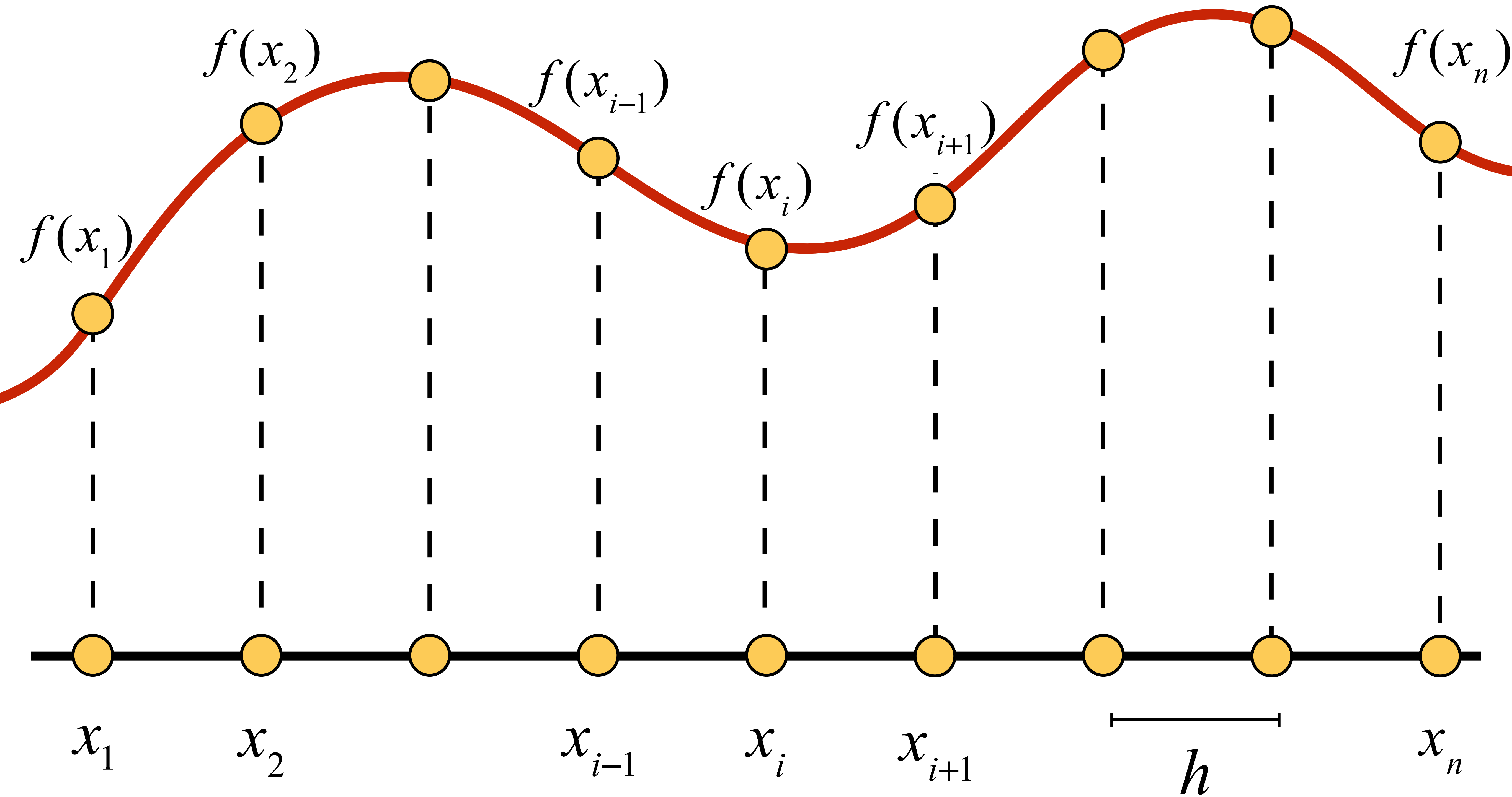
# Taylor Series

The Taylor series expansion of $f(x)$ about $x_0$:

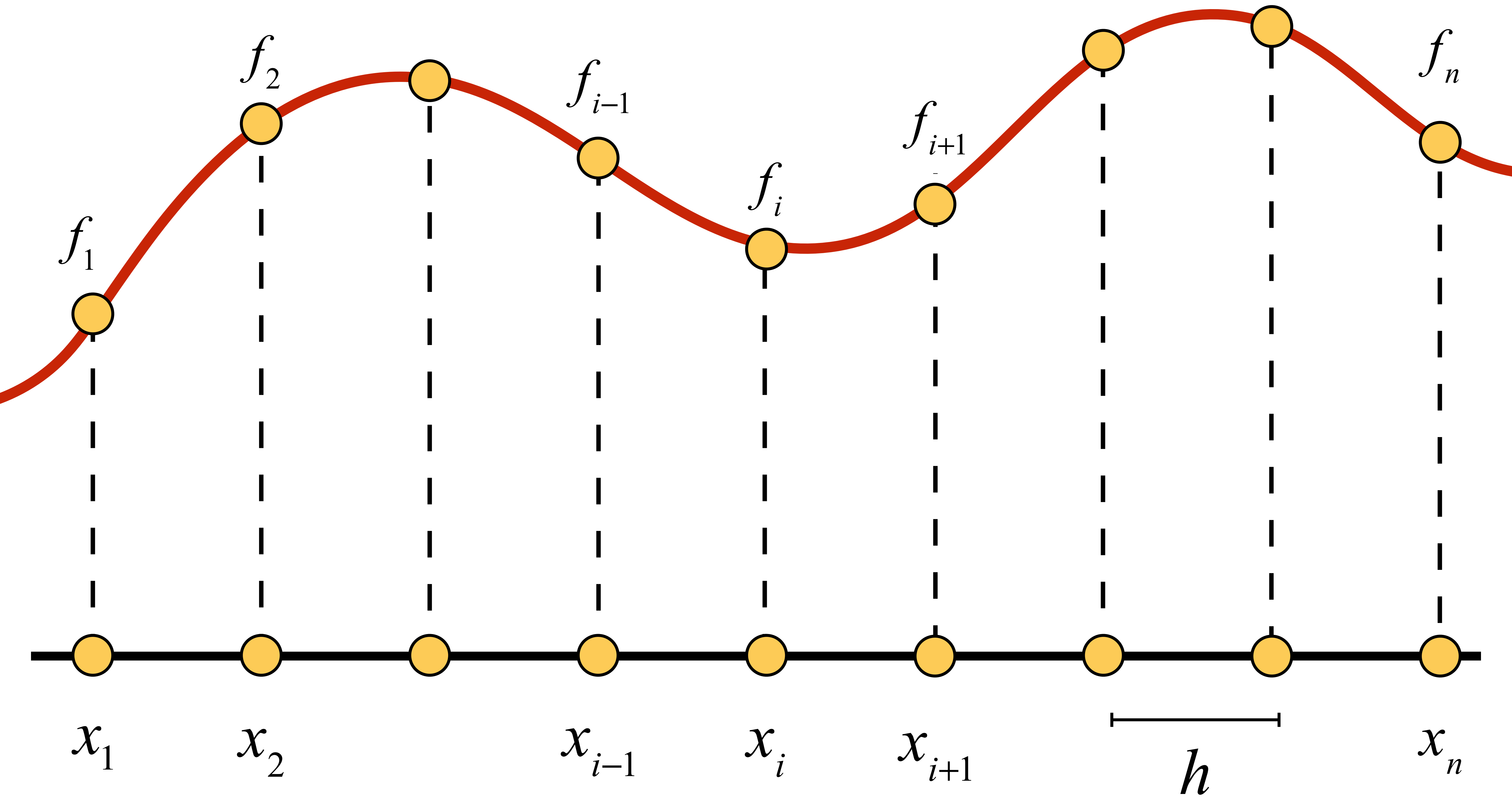
$$
\begin{aligned}
f(x) = f(x_0) \\
+ \frac{1}{1!} f'(x_0)(x - x_0) \\
+ \frac{1}{2!} f''(x_0)(x - x_0)^2 + \ldots \\
+ \frac{1}{n!} f^{(n)}(x_0)(x - x_0)^n
\end{aligned}
$$



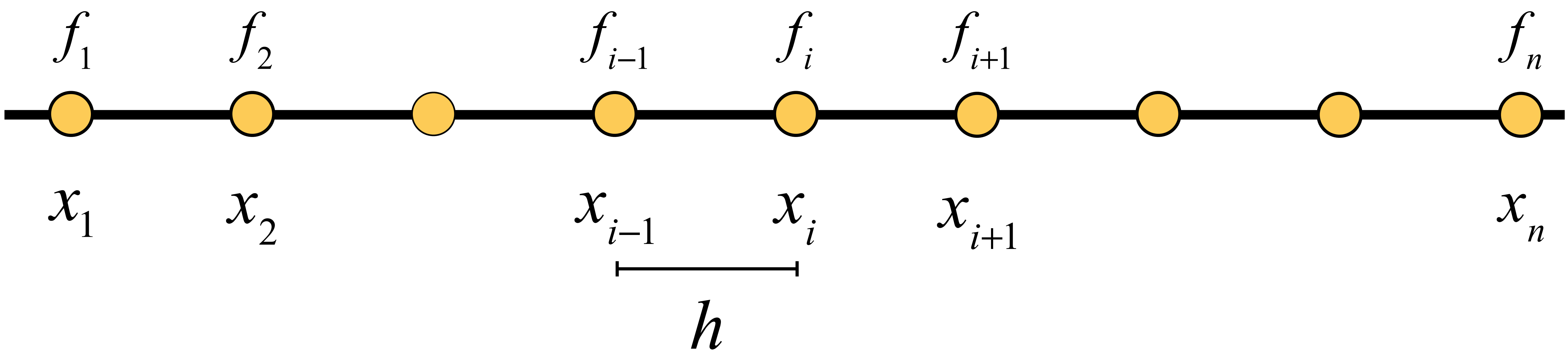
# Taylor Series Derivation - First Derivatives



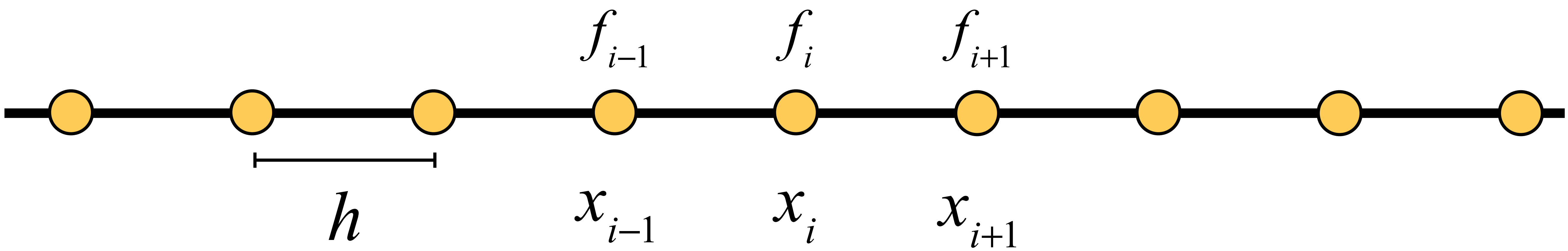
$$f(x_i) \to f_i$$



Given function values, the Taylor series is useful in finding the derivatives of that function




Find $f'(x_i)\ \forall\ i = 1,2,\ldots,n$



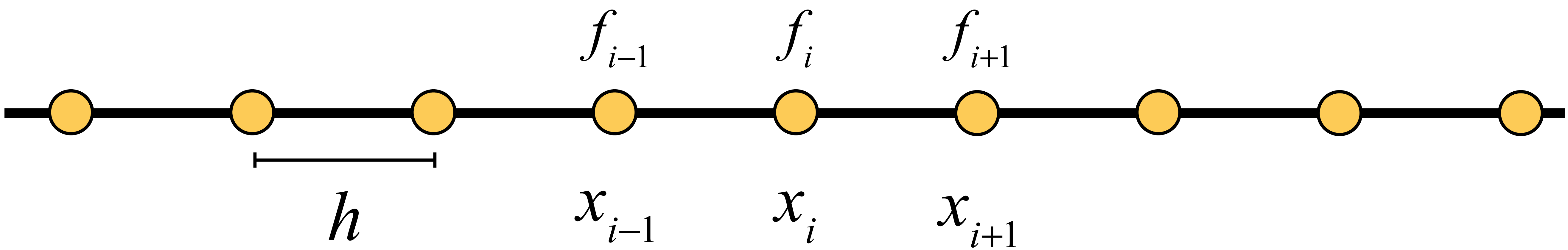

**Activity (3 min, Group):**

write the Taylor series of $f(x_{i+1})$ around $x_i$.

Carry terms up to the second derivative.

Recall, the Taylor series:

$$f(x) = f(x_0) + \frac{1}{1!}f'(x_0)(x - x_0) + \frac{1}{2!}f''(x_0)(x - x_0)^2 + \ldots + \frac{1}{n!}f^{(n)}(x_0)(x - x_0)^n$$




Recall, the Taylor series:

$$f(x) = f(x_0) + \frac{1}{1!}f'(x_0)(x-x_0) + \frac{1}{2!}f''(x_0)(x-x_0)^2 + \ldots + \frac{1}{n!}f^{(n)}(x_0)(x-x_0)^n$$

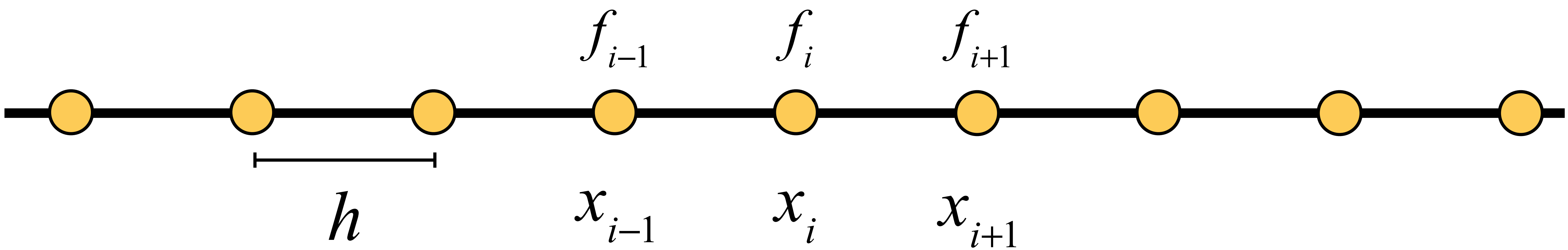
Set: $x = x_{i+1}$ and $x_0 = x_i$

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

$$f_{i+1} = f_i + (x_{i+1}-x_i)f_i' + \frac{1}{2}(x_{i+1}-x_i)^2 f_i'' + \ldots$$

or, using the fact that $(x_{i+1}-x_i) = h$

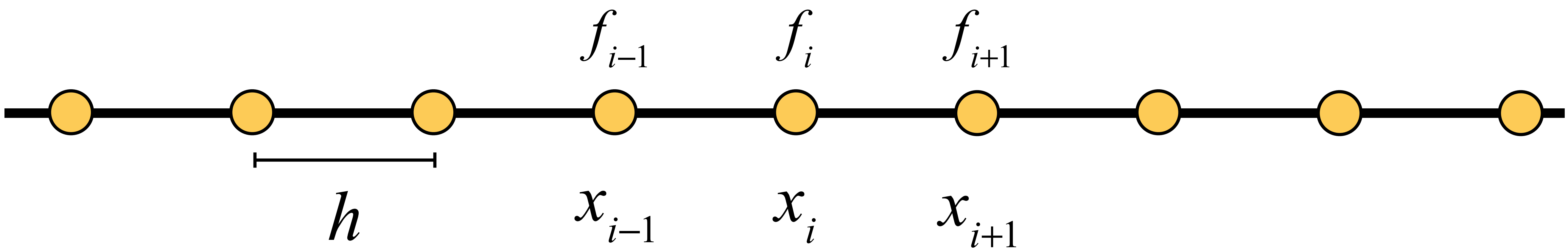
$$f_{i+1} = f_i + hf_i' + \frac{1}{2}h^2 f_i'' + \ldots$$




$$f_{i+1} = f_i + hf_i' + \frac{1}{2}h^2 f_i'' + \ldots$$

**Activity (1 min, Group):**

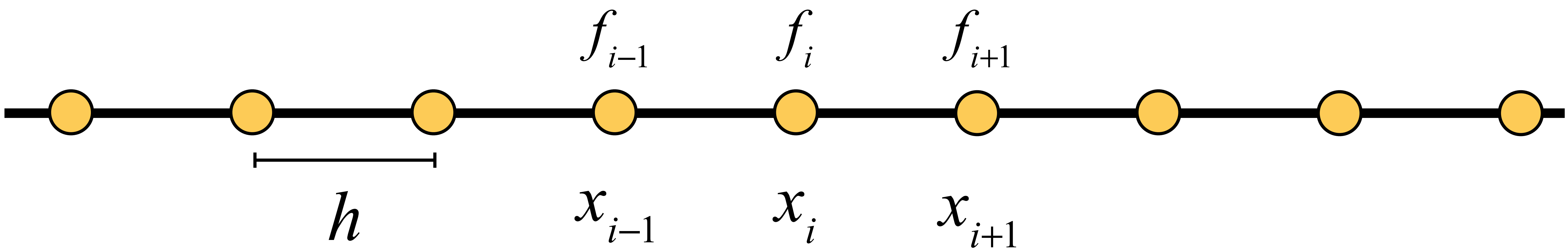
Now solve for $f_i'$.




$$f_{i+1} = f_i + h f_i' + \frac{1}{2} h^2 f_i'' + \ldots$$

Solve for $f_i'$

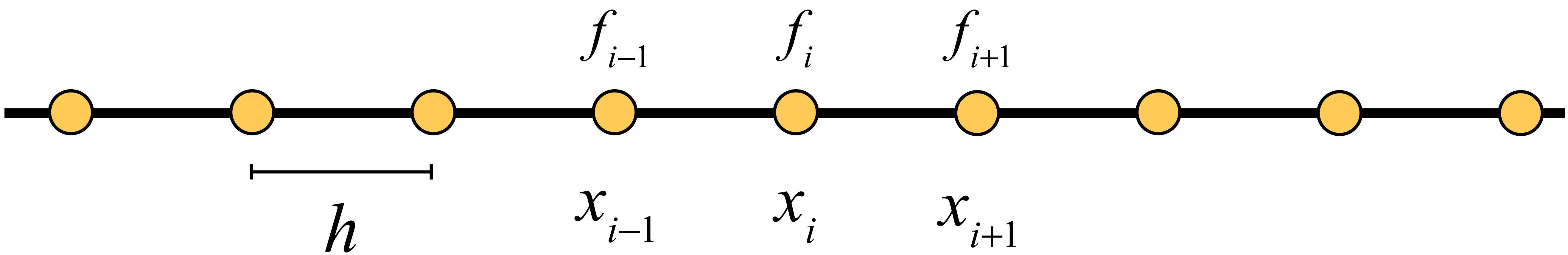
$$f_i' = \frac{f_{i+1} - f_i}{h} + \frac{1}{2} h f_i'' + \ldots$$




$$f_i' = \frac{f_{i+1} - f_i}{h} + \boxed{\frac{1}{2} h f_i'' + \ldots}$$

**Neglect all "unknown" terms**

$$f_i' \approx \frac{f_{i+1} - f_i}{h} \qquad \text{Error} = \frac{1}{2} h f_i'' + \ldots$$

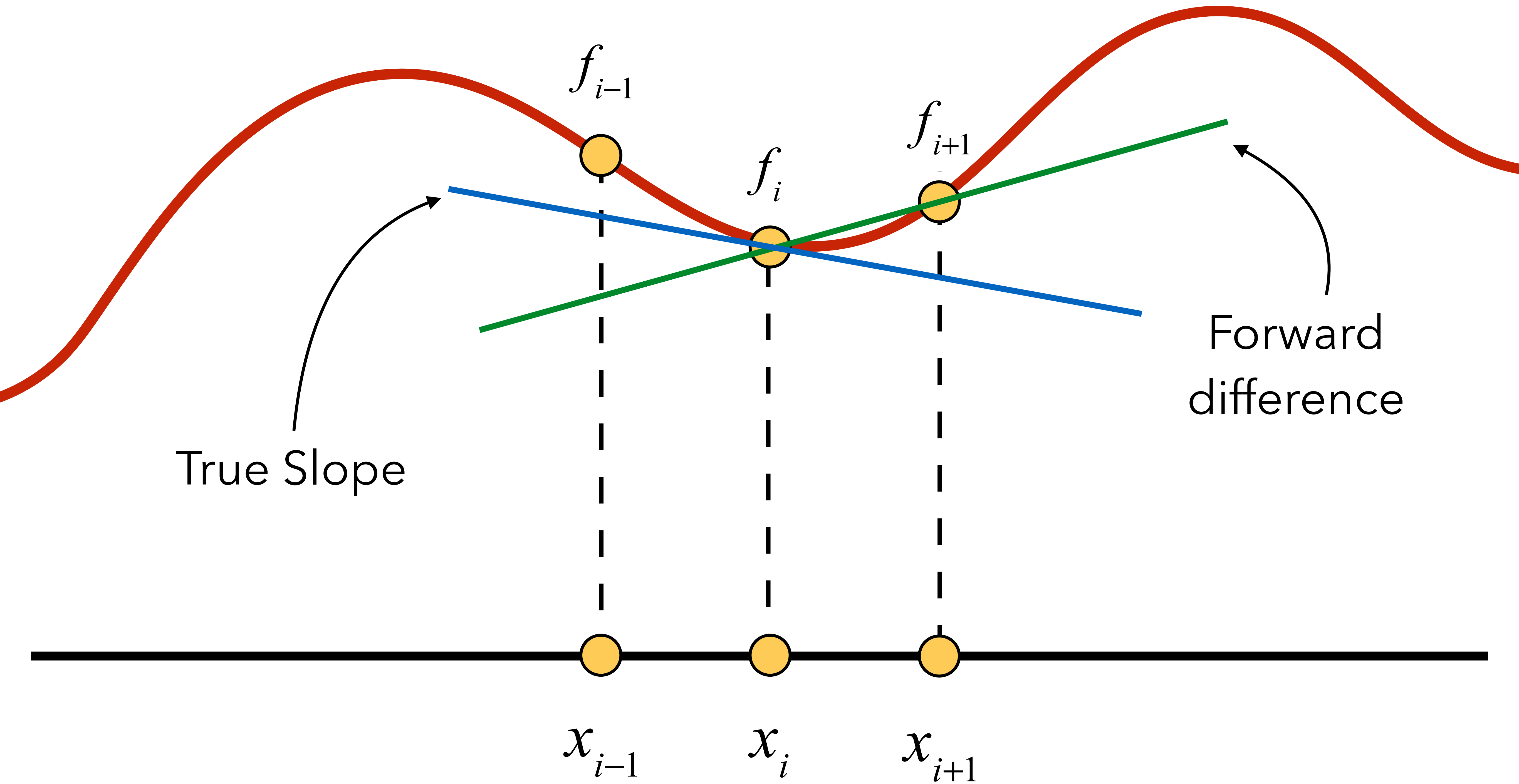



$$f_i' = \frac{f_{i+1} - f_i}{h} + \frac{1}{2} h f_i'' + \ldots \qquad f_i' \approx \frac{f_{i+1} - f_i}{h}$$

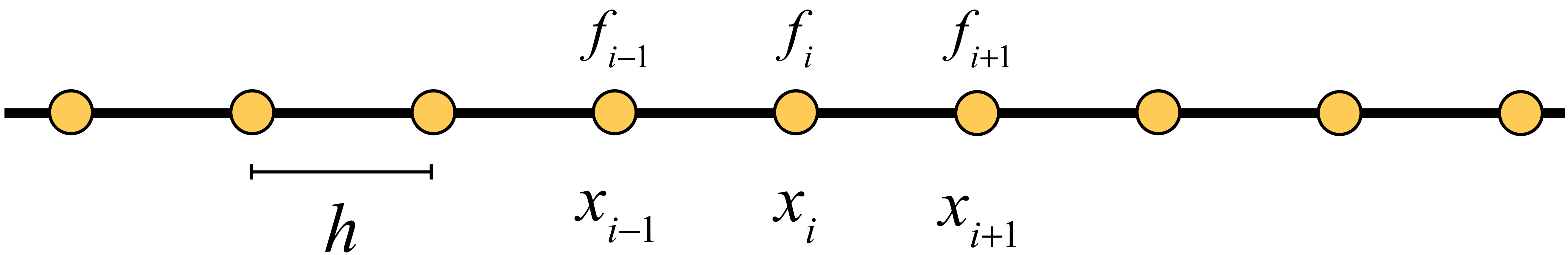
$$\text{Error} = \frac{1}{2} h f_i'' + \ldots \leq Ch = \mathcal{O}(h)$$

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

Forward difference formula



$f_{i-1}$
$f_i$
$f_{i+1}$
True Slope
Forward difference
$x_{i-1}$
$x_i$
$x_{i+1}$




$$\text{Error} = \frac{1}{2} h f_i'' + \ldots \leq Ch = \mathcal{O}(h) \qquad f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + \mathcal{O}(h)$$

We say that the error is "Order $h$"

This means that, if $h$ is cut in half, the error will also be cut in half

$$E_h = Ch$$

$$E_{h/2} = C\frac{h}{2} = \frac{E_h}{2}$$

$$E_{h/4} = C\frac{h}{4} = \frac{E_{h/2}}{2}$$

$$\ldots$$

**In general**, an approximation is said to be of order $p$ if the truncation error is $\mathcal{O}(h^p)$ or $E \le Ch^p$

**Activity (2 min, Group):**

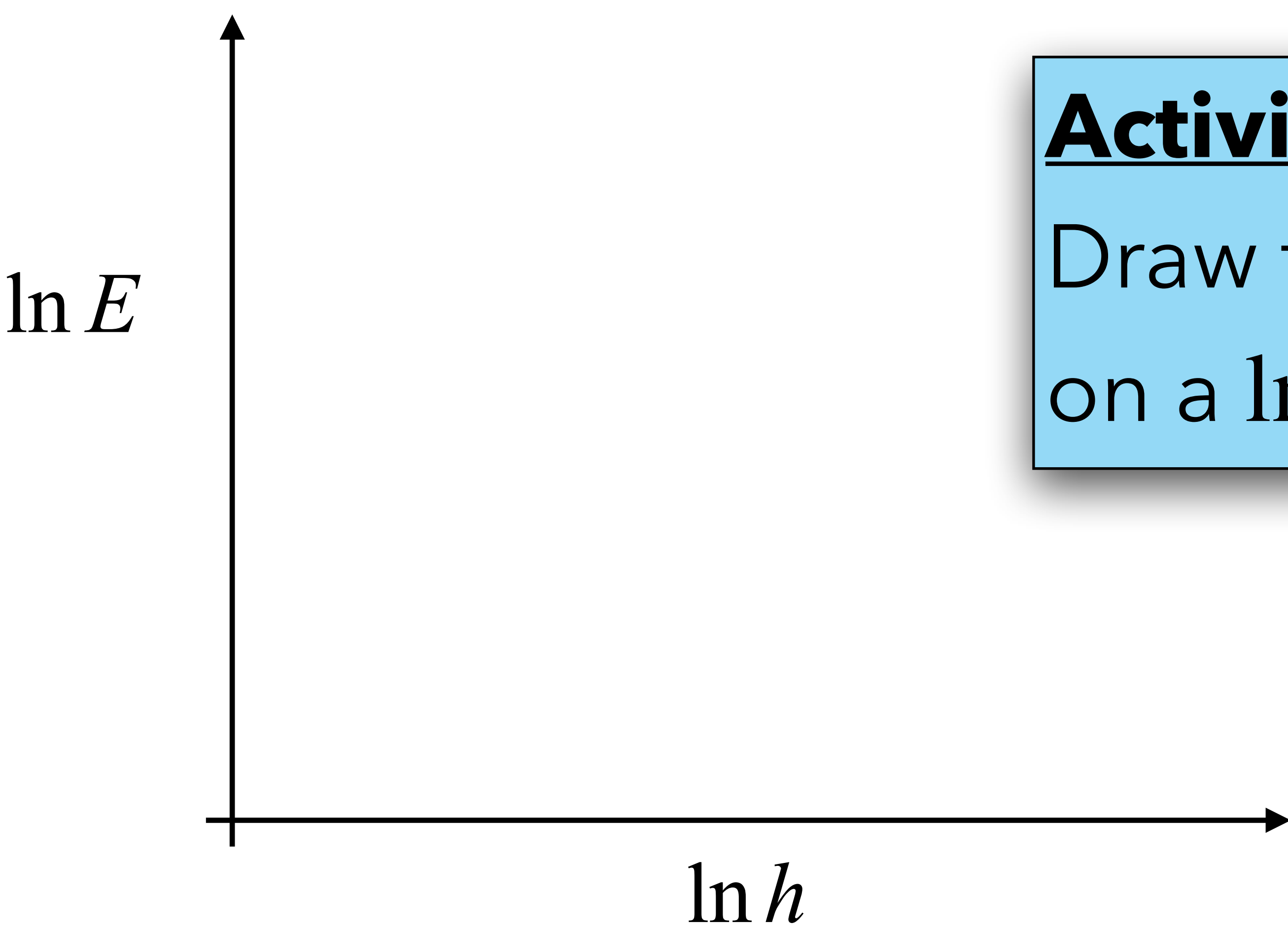
Show that if a method is $\mathcal{O}(h^2)$, then, if $h$ is cut in half the error will be cut by a factor of 4.

$$E_h = Ch^2$$

$$E_{h/2} = C\left(\frac{h}{2}\right)^2 = C\frac{h^2}{4} = \frac{E_h}{4}$$

**In general**, an approximation is said to be of order $p$ if the truncation error is $\mathcal{O}(h^p)$ or $E = Ch^p$

$$\ln E = \ln C + p \ln h$$

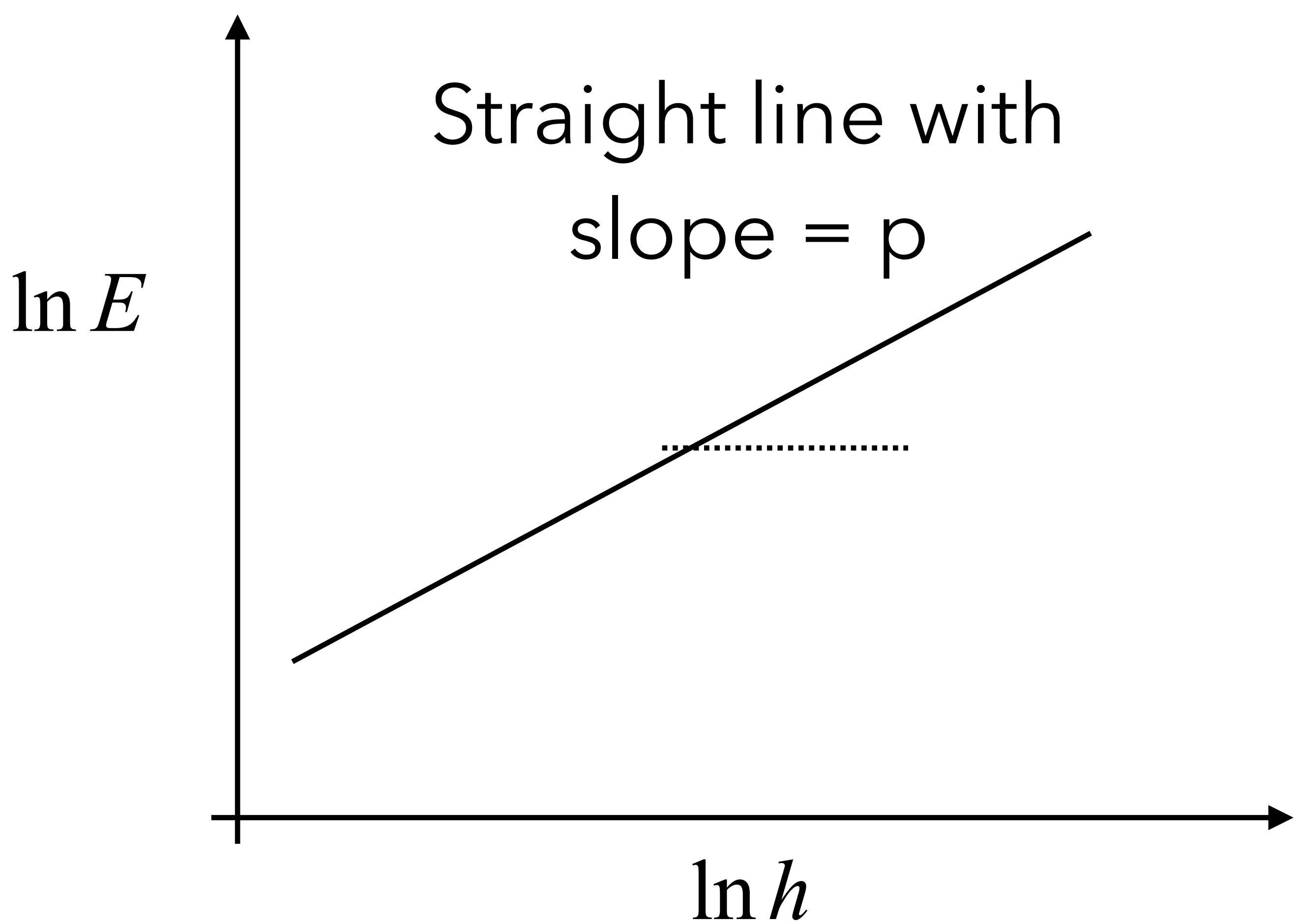



**<u>Activity (2 min, Group):</u>**

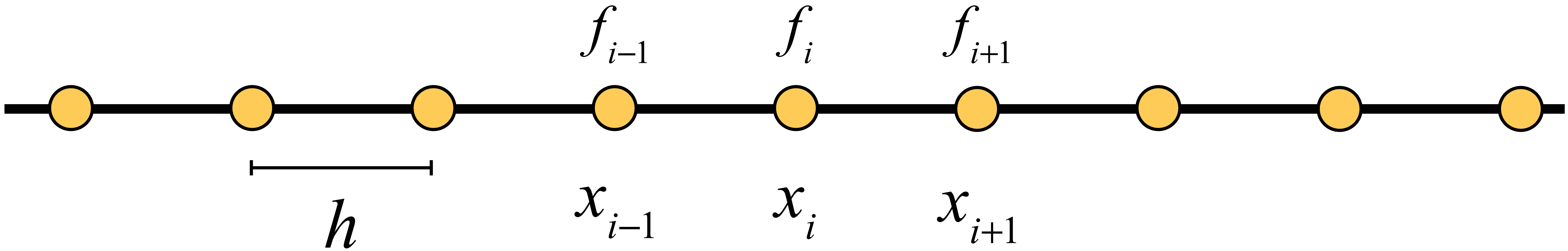
Draw the curve $\ln E = \ln C + p \ln h$ on a $\ln E$ vs $\ln h$ plot.

**In general**, an approximation is said to be of order $p$ if the truncation error is $\mathcal{O}(h^p)$ or $E = Ch^p$

$$\ln E = \ln C + p \ln h$$



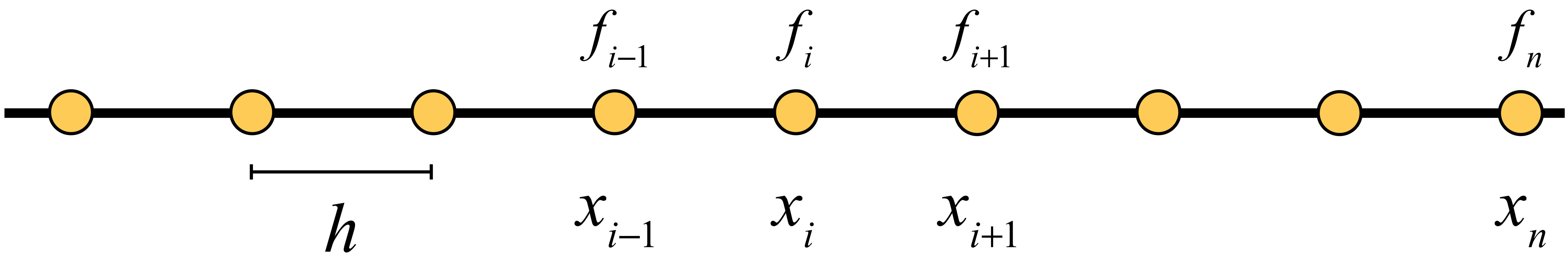

This type of plot is referred to as the convergence rate of an approximation




$$f_i' \approx \frac{f_{i+1} - f_i}{h}$$

**Coding Activity 1 (2 min, Group):**

For $f(x) = \exp(x)$, plot the absolute true error for $f'(2)$ using the forward difference formula versus values of $h$ ranging from 1e-5 to 1. Use a loglog plot. (download notebook with gaps from canvas)



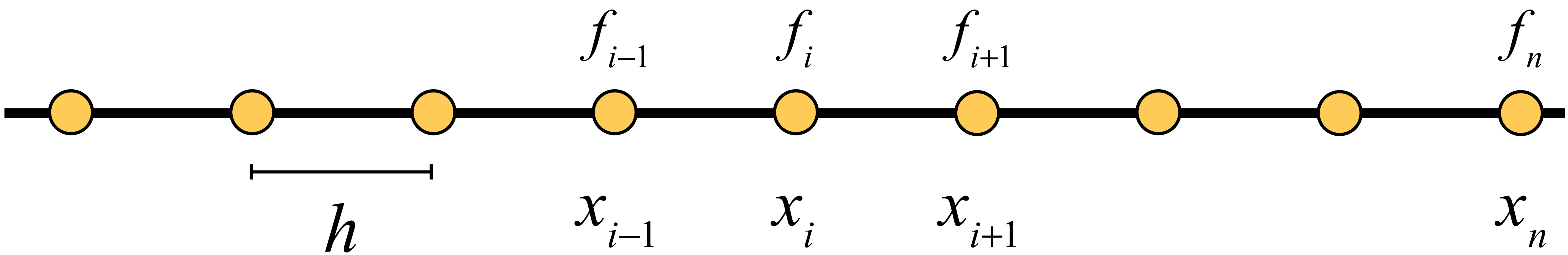

$$f_i' \approx \frac{f_{i+1} - f_i}{h}$$

We can apply this formula to any point in a set of discrete data.

**Activity (1 min, individual):**
What about the last point in the sequence?

$$f'(x_n) = \frac{f(x_{n+1}) - f(x_n)}{h}$$

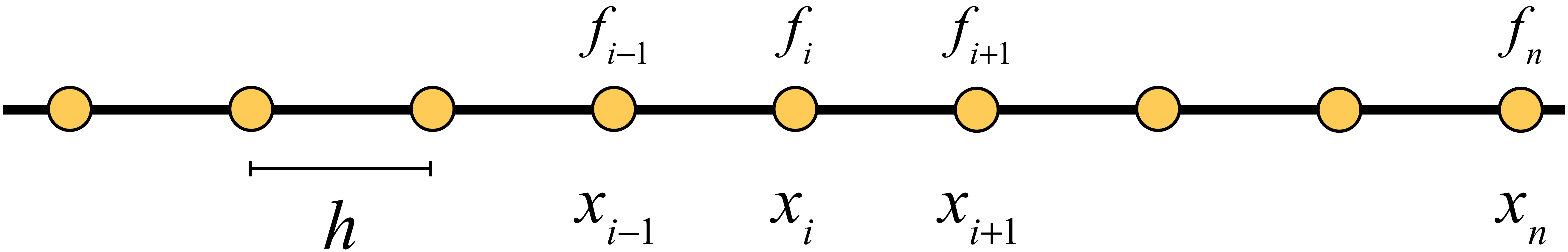
But we don't have $f(x_{n+1})$




In this case, we need to derive another formula that uses interior points only.

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

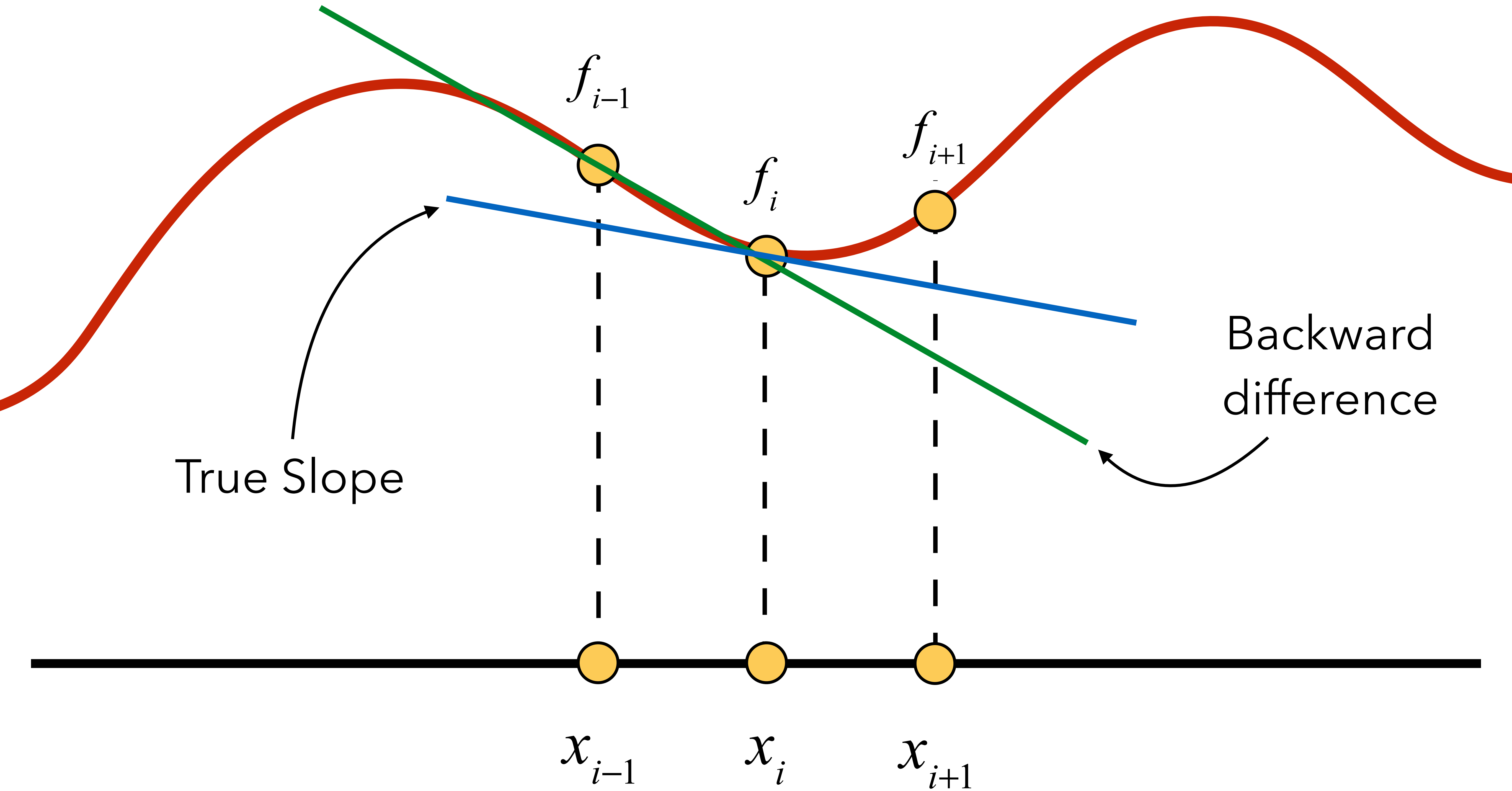
$$f_{i-1} = f_i - h f_i' + \frac{1}{2} h^2 f_i'' + \ldots$$

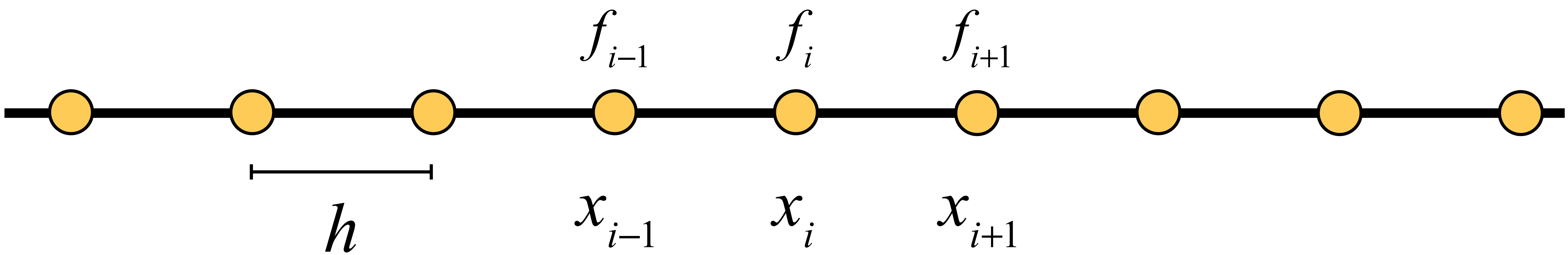



$$f_{i-1} = f_i - h f_i' + \frac{1}{2} h^2 f_i'' + \ldots$$

$$\boxed{f_i' = \frac{f_i - f_{i-1}}{h} + \mathcal{O}(h)}$$

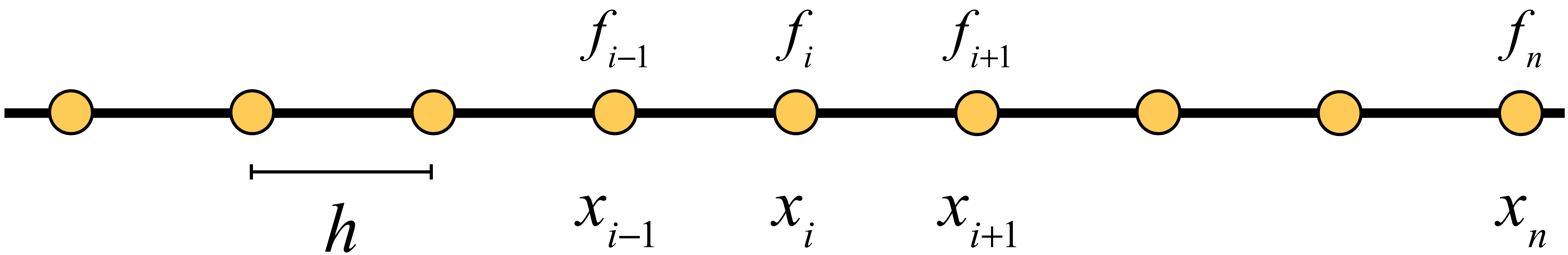
Backward difference formula


$f_{i-1}$
$f_i$
$f_{i+1}$
True Slope
Backward difference
$x_{i-1}$
$x_i$
$x_{i+1}$




What about formulas with smaller errors, such as O(h2)?

One can develop high-order approximations to derivatives by combining Taylor series expansions around different points

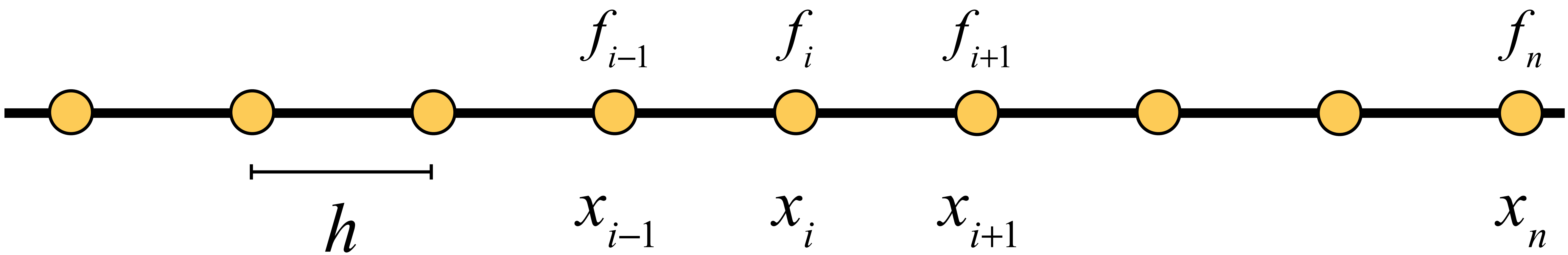



$$f_{i+1} = f_i + hf_i' + \frac{1}{2}h^2 f_i'' + \frac{1}{3!}h^3 f_i''' \ldots$$

$$f_{i-1} = f_i - hf_i' + \frac{1}{2}h^2 f_i'' - \frac{1}{3!}h^3 f_i''' \ldots$$

**Activity (3 min, group):**

Combine these two formulas to develop a second order approximation for the first derivative. HINT: Your goal is to eliminate the $h^2 f_i''$ term.



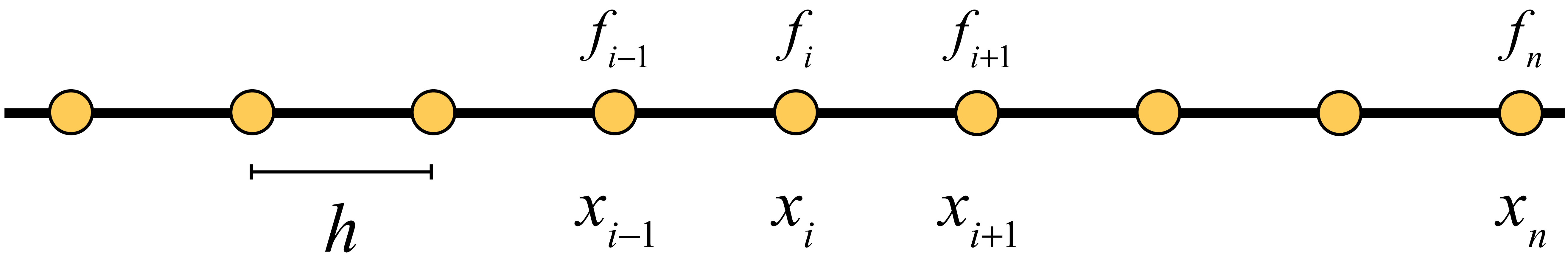

$$f_{i+1} = f_i + hf_i' + \frac{1}{2}h^2 f_i'' + \frac{1}{3!}h^3 f_i''' \ldots$$

$$-$$

$$f_{i-1} = f_i - hf_i' + \frac{1}{2}h^2 f_i'' - \frac{1}{3!}h^3 f_i''' \ldots$$

---

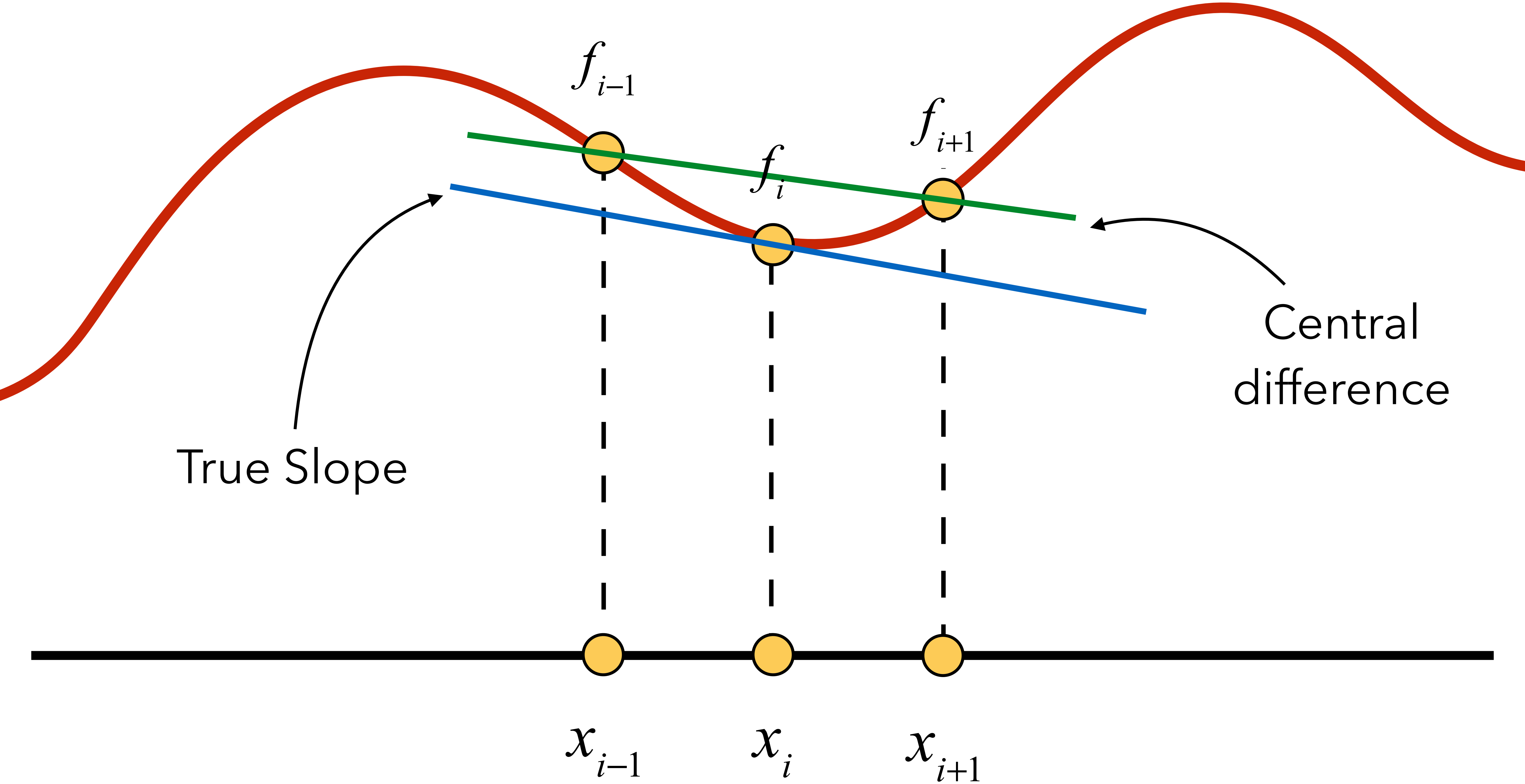
$$f_{i+1} - f_{i-1} = \quad 0 + 2h f'(x_i) + 0 + \frac{2}{3!}h^3 f'''(x_i) + \ldots$$




$$f_{i+1} - f_{i-1} = 0 + 2h\, f_i' + 0 + \frac{2}{3!} h^3 f_i''' + \ldots$$

$$\boxed{f_i' = \frac{f_{i+1} - f_{i-1}}{2h} + \mathcal{O}(h^2)}$$

Central difference formula

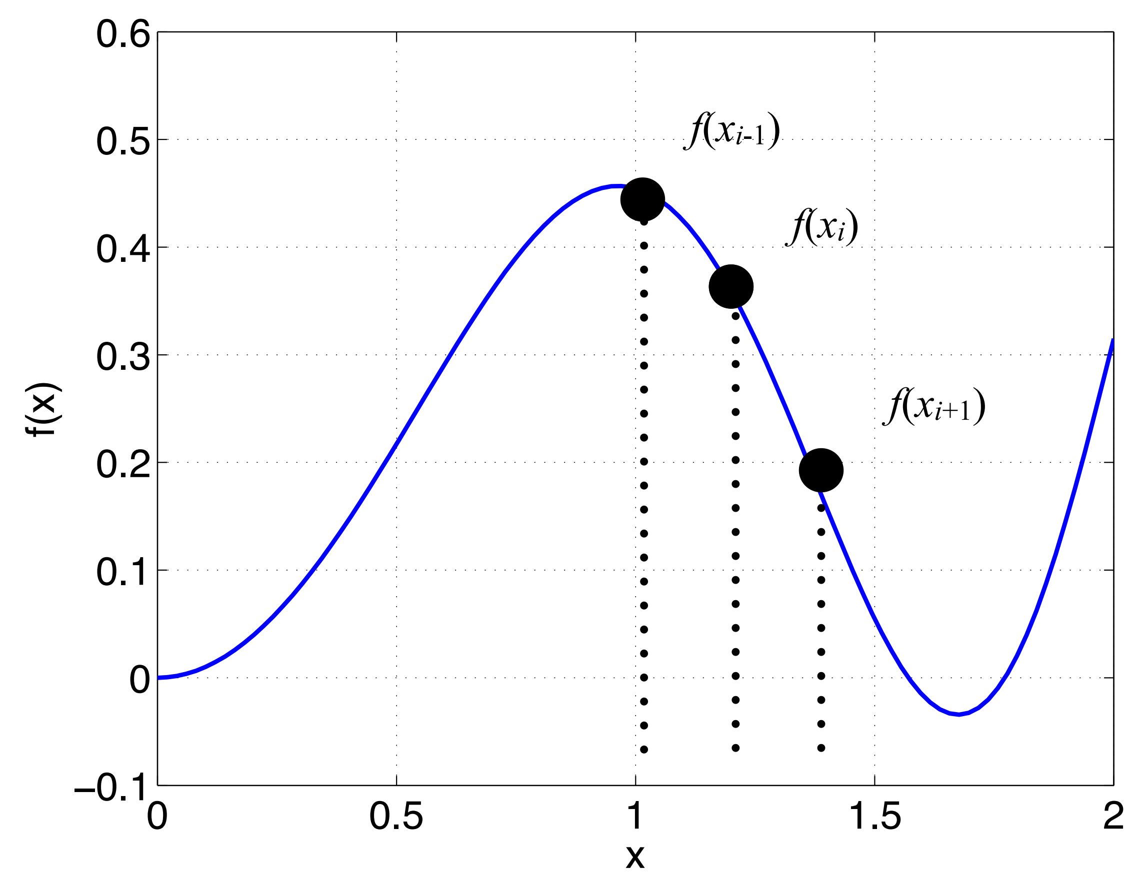

$f_{i-1}$
$f_i$
$f_{i+1}$
Central difference
True Slope
$x_{i-1}$
$x_i$
$x_{i+1}$

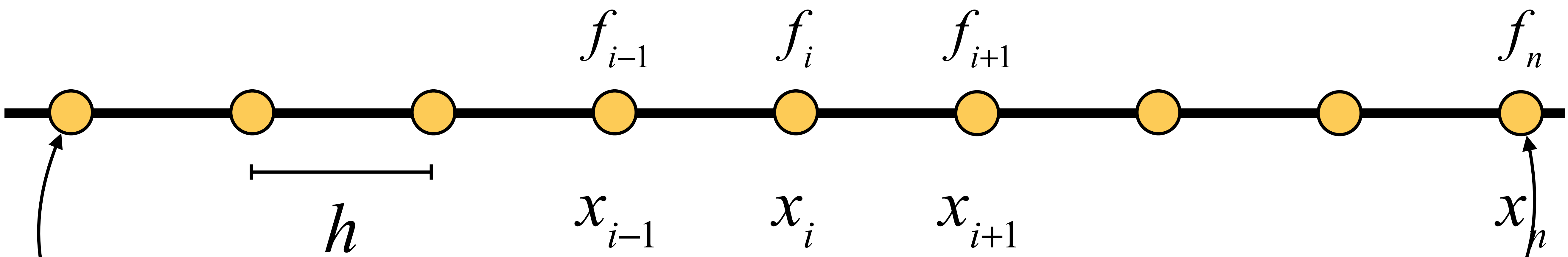
# Summary

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

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

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






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

Forward difference

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

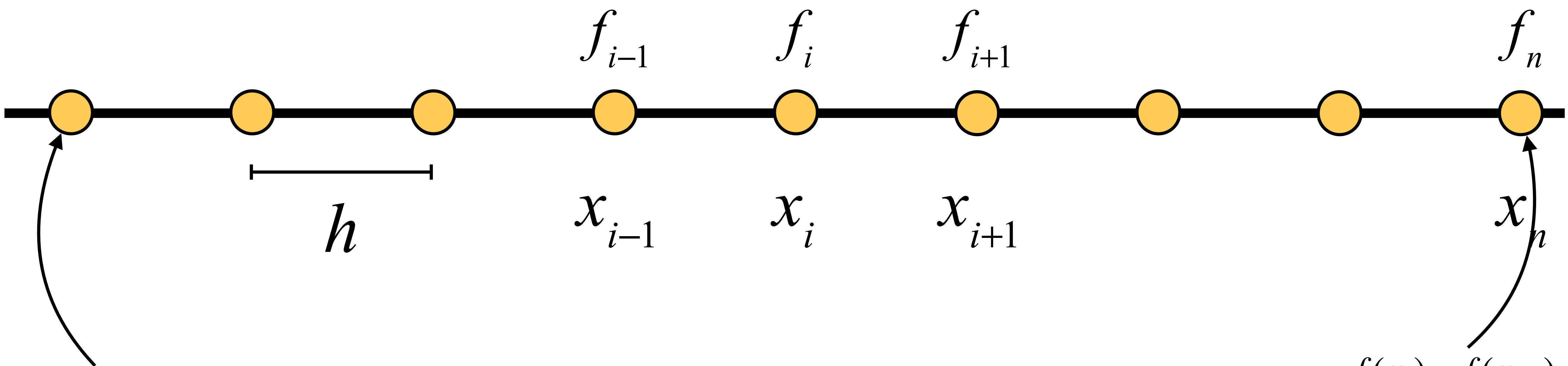
$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{h}$$

Backward difference

We now have enough ammo to tackle discrete data

**Coding Activity 2 (5 min, Group):**

Develop a Python code that to find the first derivative of discrete data and apply the code to analyze the CoVid19 cases. Your code should use central differencing for interior points, forward and backward for the first and last points.




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

Forward difference

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

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

Backward difference

We now have enough ammo to tackle discrete data

**Activity (2 min, group):**

List one problem with this approach.

# First Derivatives

| formula | order | | Constant $\Delta x$ ? |
|---|---|---|---|
| $\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\rvert_i \approx \frac{f_{i+1}-f_i}{\Delta x}$ | $\Delta x$ | Forward difference | no |
| $\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\rvert_i \approx \frac{f_i-f_{i-1}}{\Delta x}$ | $\Delta x$ | backward difference | no |
| $\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\rvert_i \approx \frac{f_{i+1}-f_{i-1}}{2\Delta x}$ | $\Delta x^2$ | central difference | yes |
| $\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\rvert_i \approx \frac{-3f_i+4f_{i+1}-f_{i+2}}{2\Delta x}$ | $\Delta x^2$ | Forward difference | yes |
| $\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\rvert_i \approx \frac{3f_i-4f_{i-1}+f_{i-2}}{2\Delta x}$ | $\Delta x^2$ | backward difference | yes |

# Some Approximations for Second Derivatives

All assume constant $\Delta x$.

| $\frac{\partial^2 f}{\partial x^2}$ | Order | Comments |
|---|---|---|
| $\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{f_i - 2f_{i+1} + f_{i+2}}{\Delta x^2}$ | $\Delta x$ | Forward difference |
| $\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{f_i - 2f_{i-1} + f_{i-2}}{\Delta x^2}$ | $\Delta x$ | Backward difference |
| $\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$ | $\Delta x^2$ | Central difference |
| $\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{2f_i - 5f_{i+1} + 4f_{i+2} - f_{i+3}}{\Delta x^2}$ | $\Delta x^2$ | Forward difference |
| $\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{-f_{i-3} + 4f_{i-2} - 5f_{i-1} + 2f_i}{\Delta x^2}$ | $\Delta x^2$ | Backward difference |