Computational Techniques
Module 6: Differentiation and Integration

Dr. Niket Kaisare
Department of Chemical Engineering
Indian Institute of Technology - Madras

Differentiation: General Setup

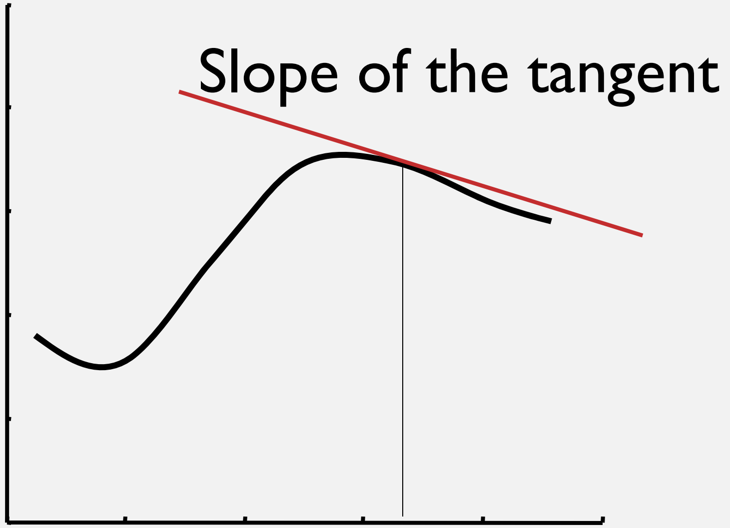
- Given a function $y = f(x)$ or data (x_i, y_i)
  Obtain: $\mathrm{d}y/\mathrm{d}x$

Differentiation:

Obtain slope of

tangent to the curve

at any point x

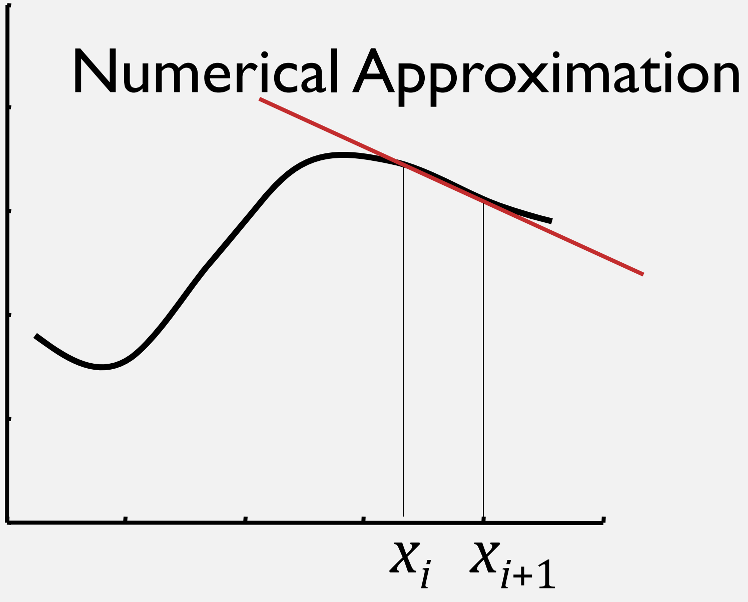


Differentiation: General Setup (2)

- Given a function $y = f(x)$ or data (x_i, y_i)
  Obtain: $\mathrm{d}y/\mathrm{d}x$

Differentiation:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} \approx \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$



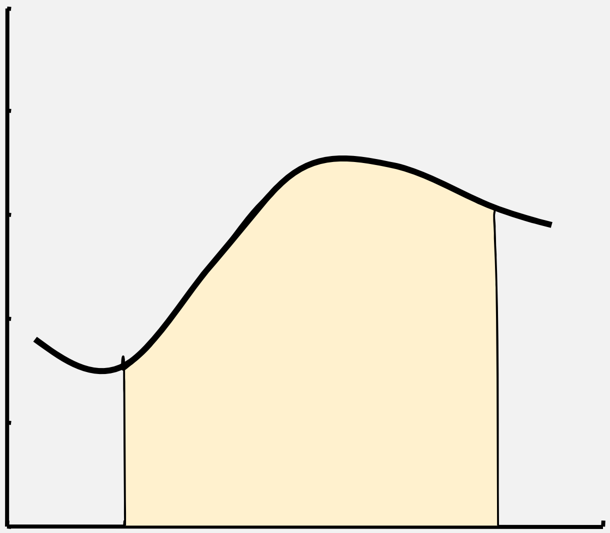
Integration: General Setup

- Given a function $y = f(x)$ or data (x_i, y_i)

  Obtain: $\int_a^b f(x)dx$

Integration:

Obtain area under the curve between two points *a* and *b*



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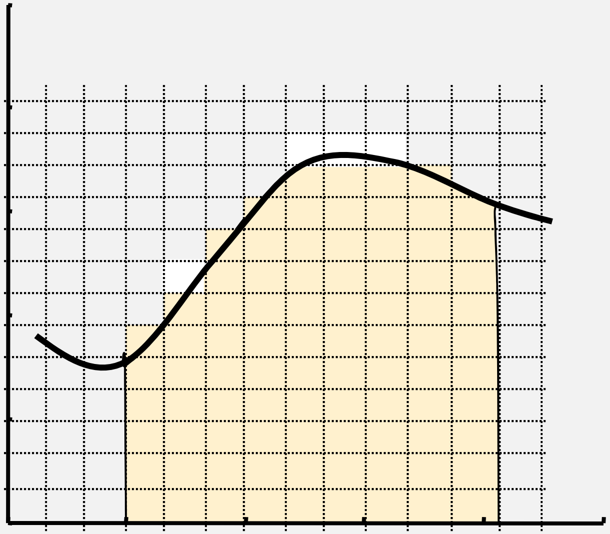

Applications of Differentiation

- Numerical Differentiation in Newton Raphson

$$x^{(i+1)} = x^{(i)} - \frac{f\left(x^{(i)}\right)}{f'\left(x^{(i)}\right)}$$

If derivative f'(x) is not available

$$x^{(i+1)} = x^{(i)} - \frac{\delta \cdot f\left(x^{(i)}\right)}{f\left(x^{(i)} + \delta\right) - f\left(x^{(i)}\right)}$$

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- Sensitivity Analysis (RDS in multiple reactions)

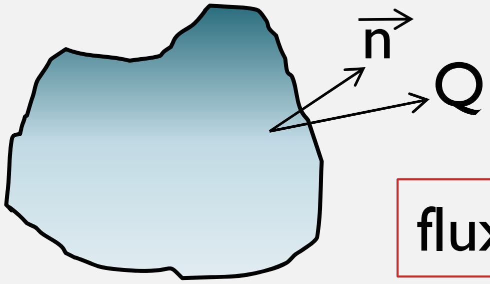
$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D \qquad s_i = \left(1/X\right)\frac{\partial X}{\partial k_i}$$

Applications of Integration

- To calculate mean $$\frac{1}{b-a}\int_a^b f(x)dx$$

- Mass flux calculation $$\iint_A (\rho u.w_k)dxdy$$

- Net heat flux or heat loss $$\oint_s \text{flux}\ ds$$

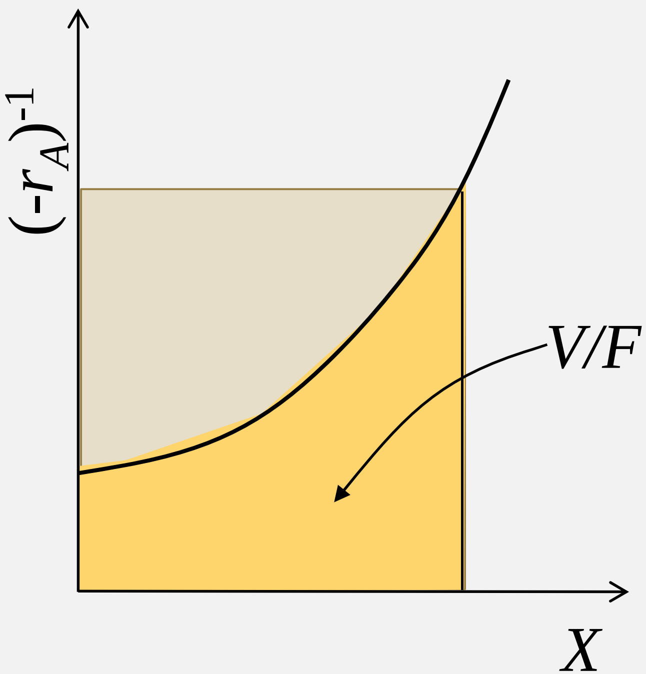


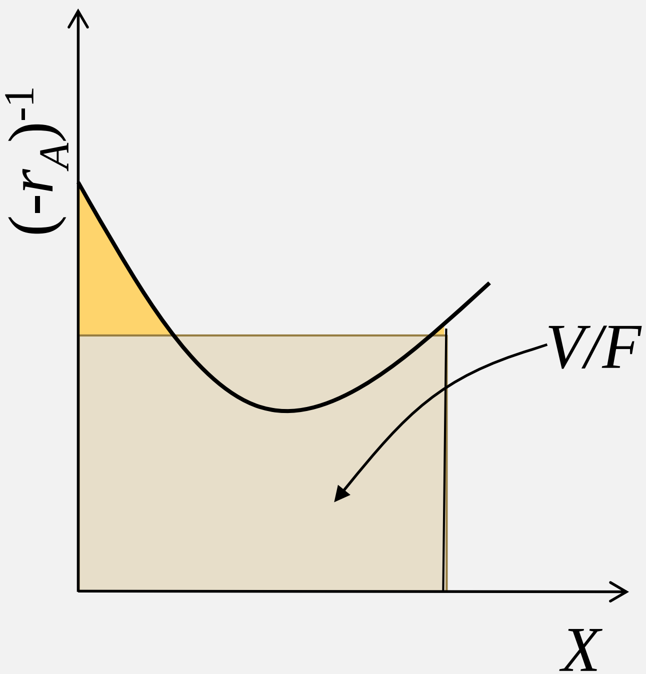
flux = Q.n

Applications of Integration (2)

- Design equation of a Plug Flow Reactor

$$V = F_{A0} \int_0^X \frac{dX}{-r_A}$$





Overview

- Numerical Differentiation
  - Forward and Backward Difference
  - Central Difference
  - Multi-Point methods
  - Error analysis
- Numerical Integration
  - Trapezoidal rule
  - Simpson's rules
  - Richardson's extrapolation
  - Gauss Quadrature

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Summary of Numerical Schemes

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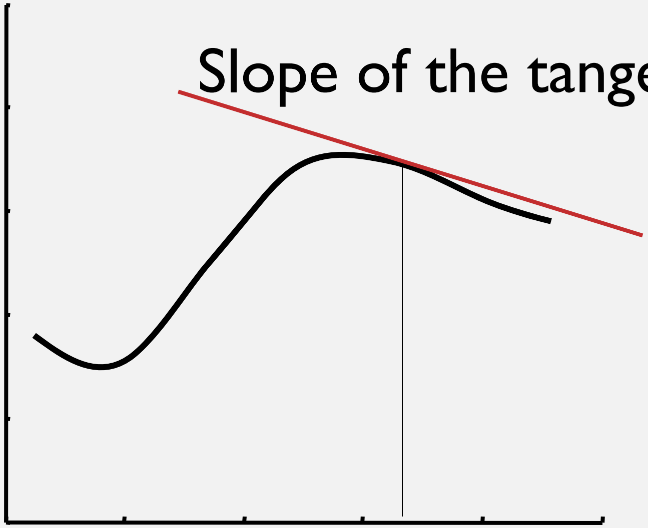
Differentiation:

Obtain slope of tangent to the curve at any point x



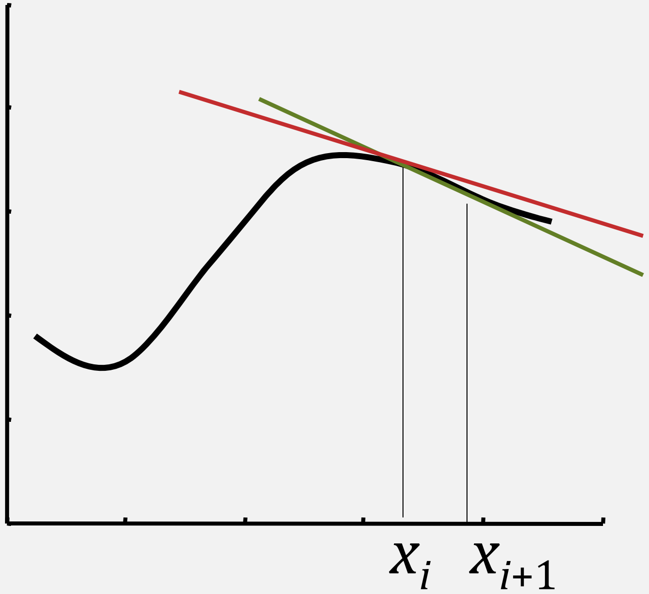
Differentiation: General Setup

- Given a function $y = f(x)$ or data (x_i, y_i)
  Obtain: $\mathrm{d}y/\mathrm{d}x$

Differentiation:

(Forward Difference)

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} \approx \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$



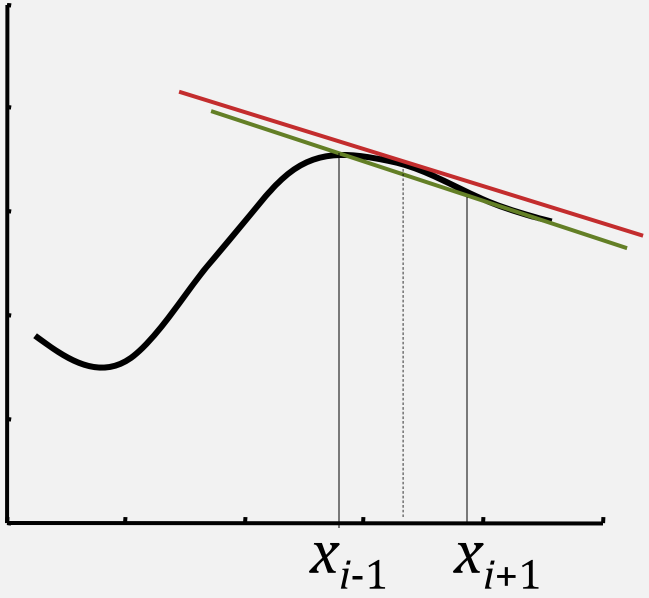
Differentiation: General Setup

- Given a function $y = f(x)$ or data (x_i, y_i)
  Obtain: $\mathrm{d}y/\mathrm{d}x$

Differentiation:

(Central Difference)

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} \approx \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}$$



Summary for Numerical *f'*(*x*)

- Method of characteristics: Using Taylor's Series

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

etc.

- The differential of interest is written as:

$$\frac{df}{dx}=a_1 f\left(x_{i-1}\right)+a_2 f\left(x_i\right)+a_3 f\left(x_{i+1}\right)$$

- Substitute and find values of a_1 a_2 and a_3.

Summary for Numerical $f'(x)$

Type	Differential	Error
Forward	$\dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Backward	$\dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
Central	$\dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
3-pt Forward	$\dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$

This is the truncation error

Higher Derivatives

- Second derivative (central difference)

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

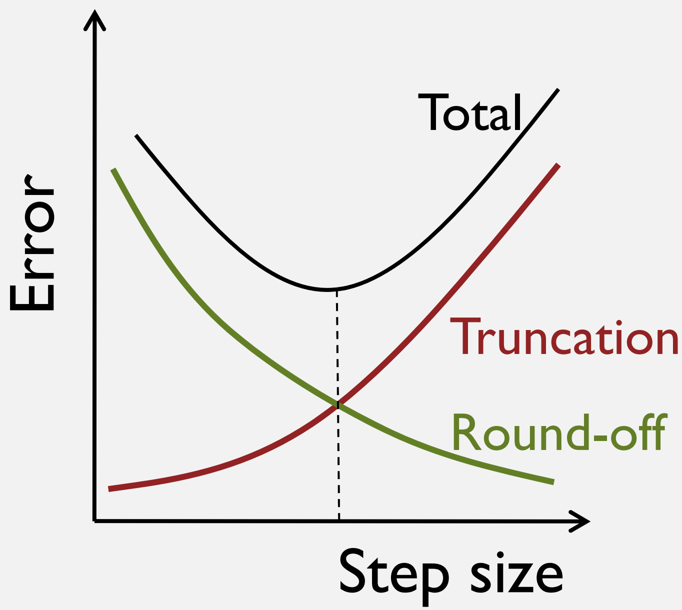
- Second derivative (forward difference)

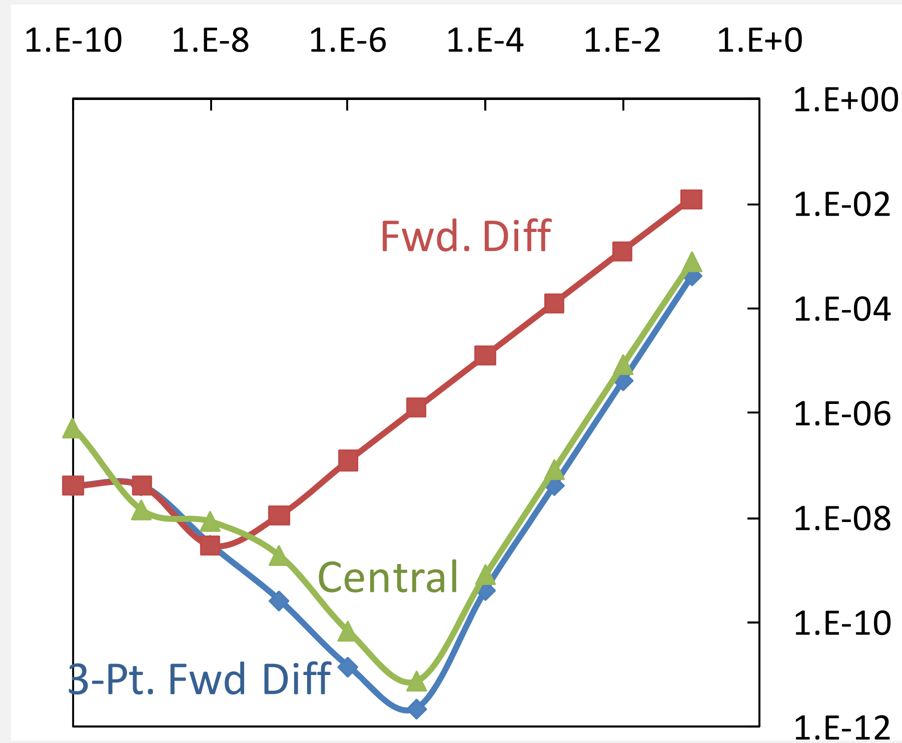
$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

- Third derivative (central difference)

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

Round-off and Truncation Errors





Step-size for minimum error

- Fwd Diff $h \propto \left[\varepsilon_{\text{machine}}\right]^{1/2}$
- Central $h \propto \left[\varepsilon_{\text{machine}}\right]^{1/3}$

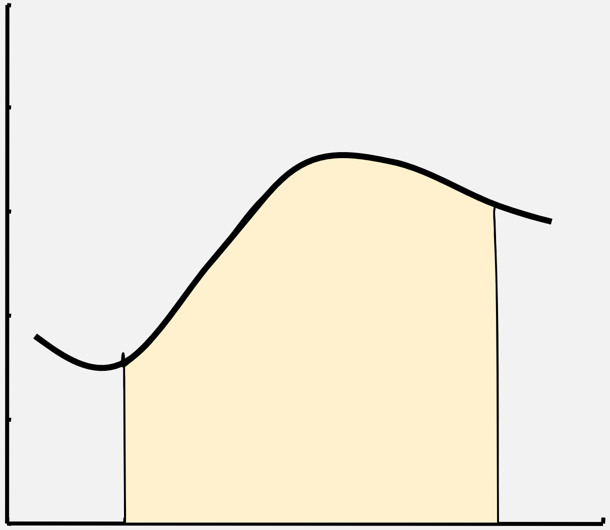
Integration: General Setup

- Given a function $y = f(x)$ or data (x_i, y_i)

  Obtain: $\int_a^b f(x)dx$

Integration:

Obtain area under the curve between two points *a* and *b*



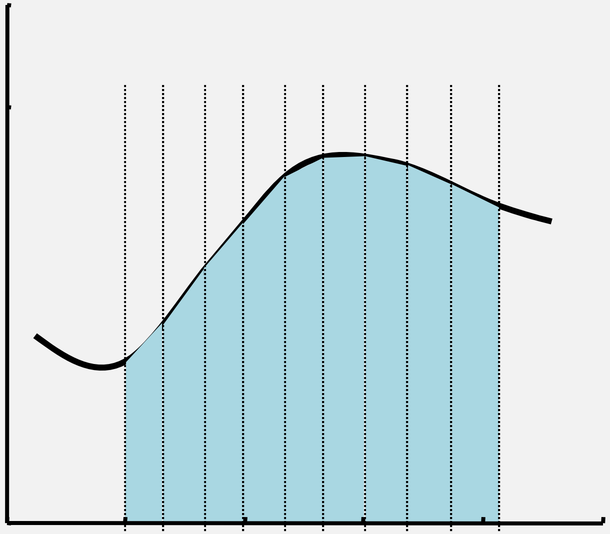
Numerical Integration

- Given a function $y = f(x)$ or data (x_i, y_i)

  Obtain: $\int_a^b f(x)dx$

Integration:

Split the region into various intervals and add the areas for each

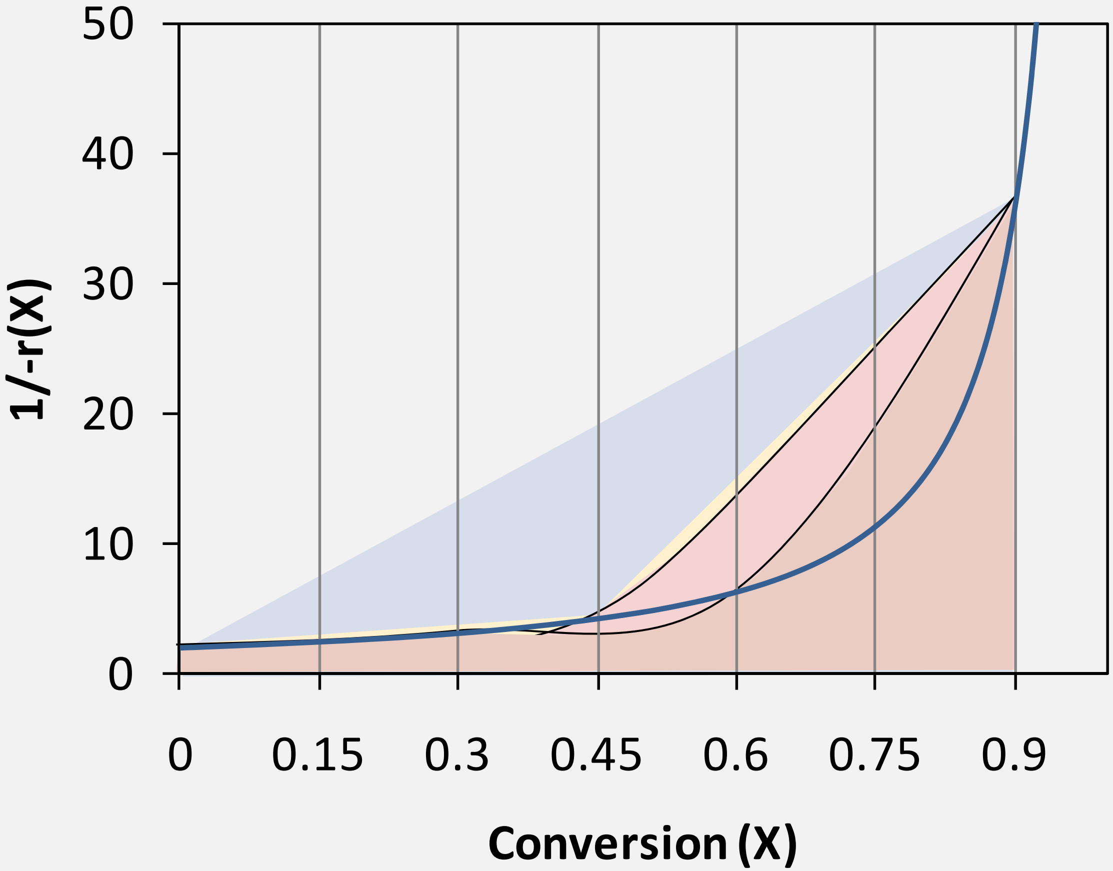


Integration Formulae

	Formula	Error
Trapezoidal	$\frac{h}{2}(y_1 + y_2)$	$O\left(h^3\right)$
Simpsons 1/3rd	$\frac{h}{3}(y_1 + 4y_2 + y_3)$	$O\left(h^5\right)$
Simpsons 3/8th	$\frac{3h}{8}(y_1 + 3y_2 + 3y_3 + y_4)$	$O\left(h^5\right)$
Richardson's	$\frac{2^n I(h_2) - I(h_1)}{2^n - 1}$	$O\left(h^{\overline{n}+1}\right)$
Quadrature	"Open-type" method	

Integration: PFR Example

- Design Equation $$V = F_{A0}\int_0^X \frac{dX}{-r(X)}$$



Trapezoidal Rule: Single Application

Trapezoidal Rule: Two Applications

1/3rd Rule: One Application

3/8th Rule: One Application

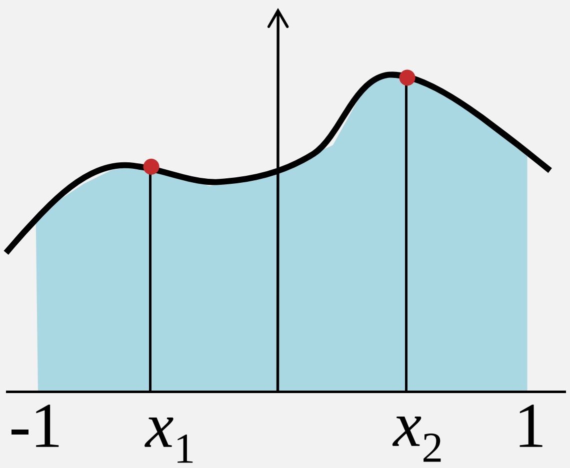
Results (comparison)

	Step Size (h)	0.15	0.075	0.015	0.0075
Trapezoidal	Volume	6.9271	6.4220	6.2345	6.2283
	# application	6	12	60	120
1/3rd Rule	Volume	6.4167	6.2536	6.2263	6.2262
	# application	3	6	30	60
3/8th Rule	Volume	6.4989	6.2711	6.2264	6.2262
	# application	2	4	20	40

Gauss Quadrature

- The integral is approximated as

$$\int_{-1}^{1} f(x)dx \approx \sum_{i\in[-1,1]} a_i f(x_i)$$



n	formula
2	$f\left(-1/\sqrt{3}\right) + f\left(1/\sqrt{3}\right)$
3	$\frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$
and so on …	

General Guidelines

- Numerical differentiation
  - Prefer central differences in general
  - Choose appropriate step size *h*
- Numerical integration
  - Prefer Simpson's 1/3rd rule due to accuracy
  - Multiple applications to improve accuracy
  - Richardson's extrapolation is effective, but requires more computation