Simpson’s one third and three-eight rules

Simpson's 1/3 Rule

- If we use a 2nd order polynomial (need 3 points or 2 intervals):
  - Lagrange form.

$$\left(x_1 = \frac{x_0 + x_2}{2}\right)$$

$$I = \int_{x_0}^{x_2} \left[\frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \right] dx$$

Simpson's 1/3 Rule

- **Requiring** equally-spaced intervals:

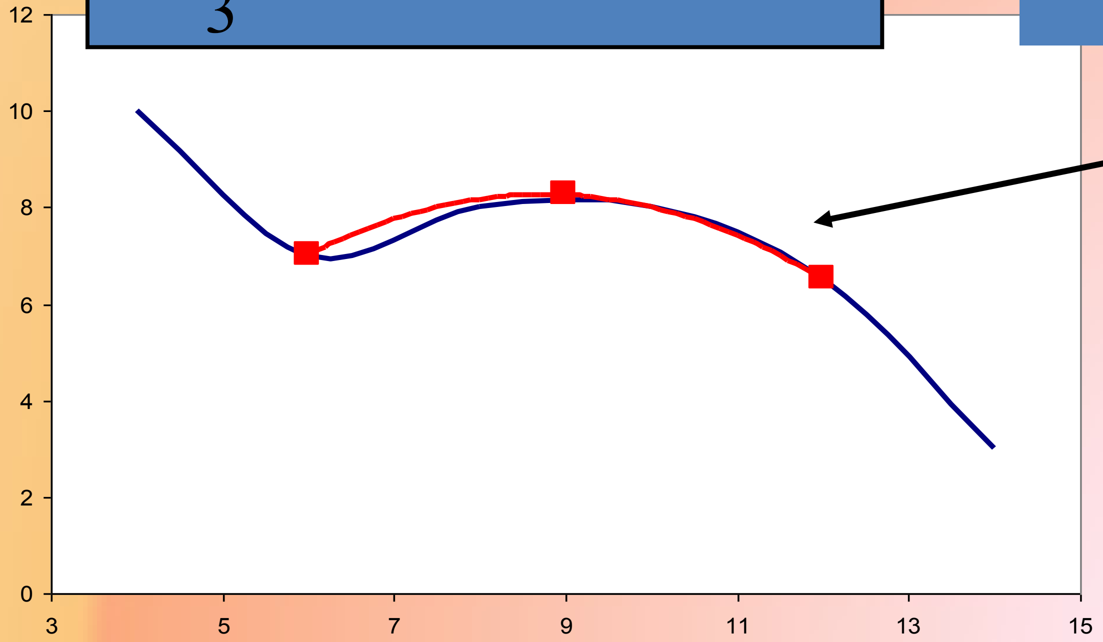
$$I = \int_{x_0}^{x_2} \left[\frac{(x - x_0 - h)(x - x_0 - 2h)}{-h(-2h)} f(x_0) + \frac{(x - x_0)(x - x_0 - 2h)}{(h)(-h)} f(x_1) \right.$$
$$\left. + \frac{(x - x_0)(x - x_0 - h)}{(2h)(h)} f(x_2) \right] dx$$

Simpson's 1/3 Rule

- Integrate and simplify:

$$I \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

$$h = \frac{b-a}{2}$$



Quadratic Polynomial

Simpson's 1/3 Rule

- If we use $a = x_0$ and $b = x_2$, and $x_1 = (b+a)/2$

$$I \approx \underbrace{(b-a)}_{\text{width}} \underbrace{\frac{f(x_0)+4f(x_1)+f(x_2)}{6}}_{\text{average height}}$$

Simpson's 1/3 Rule

- Error for Simpson's 1/3 rule

$$E_t = -\frac{h^5}{90} f^{(4)}(\xi) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

$$O(h^5)$$

$$h = \frac{b-a}{2}$$

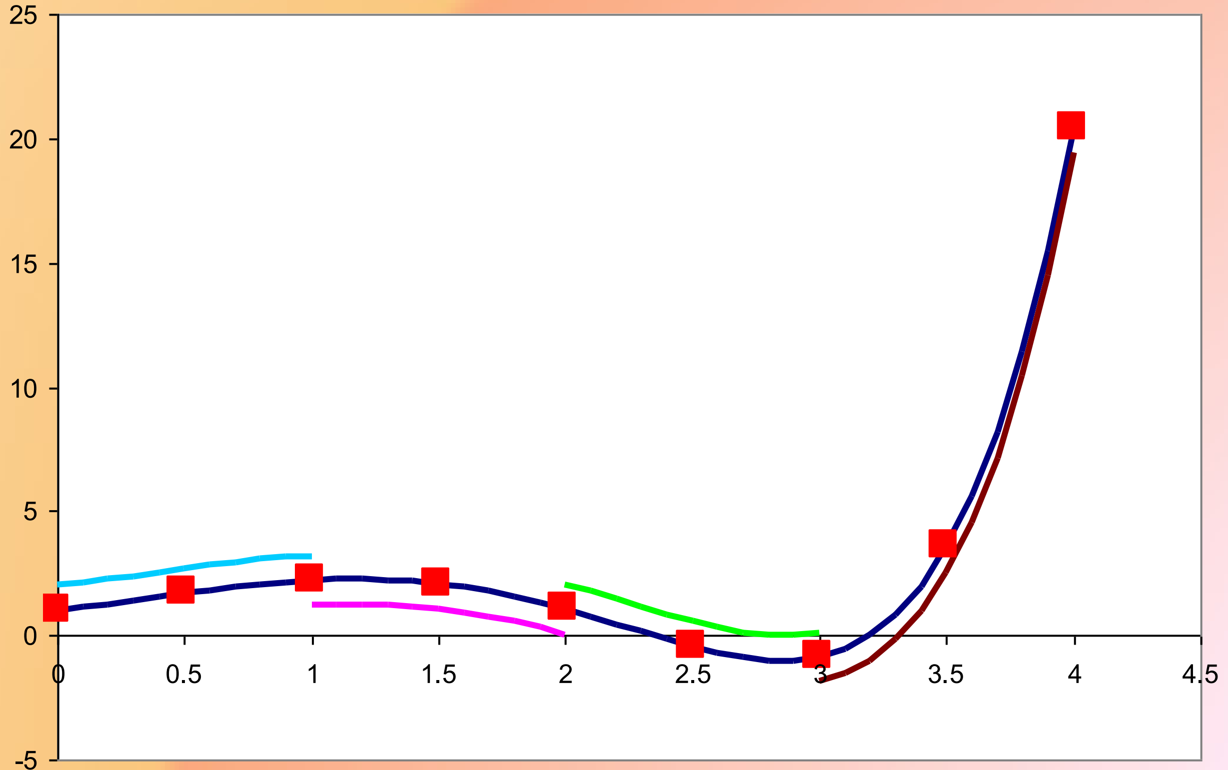
$\Rightarrow$Integrates a cubic exactly: $f^{(4)}(\xi) = 0$

Composite Simpson's 1/3 Rule

- As with Trapezoidal rule, can use multiple applications of Simpson's 1/3 rule.
- Need even number of intervals
  - An odd number of points are required.

Composite Simpson's 1/3 Rule

- Example: 9 points, 4 intervals



Composite Simpson's 1/3 Rule

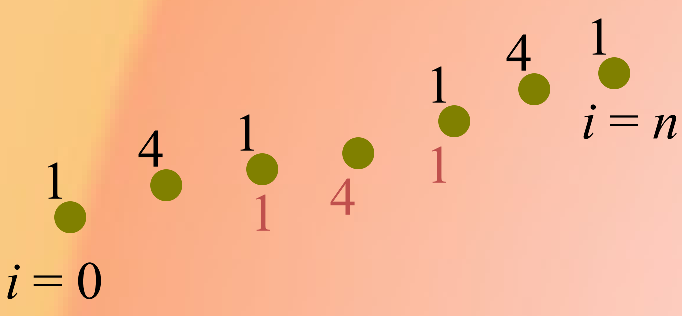
- As in composite trapezoid, break integral up into $n/2$ sub-integrals:
- Sub $$I=\int_{x_0}^{x_2} f(x)dx+\int_{x_2}^{x_4} f(x)dx+\ldots+\int_{x_{n-2}}^{x_n} f(x)dx$$ ch integral and collect terms.

$$I=(b-a)\frac{f(x_0)+4\sum_{i=1,3,5}^{n-1} f(x_i)+2\sum_{j=2,4,6}^{n-2} f(x_j)+f(x_n)}{3n}$$

$n+1$ data points, an odd number

Composite Simpson's 1/3 Rule

- Odd coefficients receive a weight of 4, even receive a weight of 2.
- Doesn't seem very fair, does it?



coefficients on numerator

Error Estimate

- The error can be estimated by:

$$E_a = \frac{nh^5}{180}\bar{f}^{(4)} = \frac{(b-a)h^4}{180}\bar{f}^{(4)} \qquad O(h^4)$$

- If n is doubled, $h \to h/2$ and $E_a \to E_a/16$

$\bar{f}^{(4)}$ is the average 4th derivative

Example

- Integrate from a = 0 to b = 2.
- Use Simpso $f(x) = e^{-x^2}$ e:

$$h = \frac{b-a}{2} = 1 \qquad x_0 = a = 0 \qquad x_1 = \frac{a+b}{2} = 1 \qquad x_2 = b = 2$$

$$I = \int_0^2 e^{-x^2}\,dx \approx \frac{1}{3} h\left[f\left(x_0\right) + 4f(x_1) + f\left(x_2\right)\right]$$

$$= \frac{1}{3}\left[f\left(0\right) + 4f(1) + f\left(2\right)\right]$$

$$= \frac{1}{3}(e^0 + 4e^{-1} + e^{-4}) = 0.82994$$

Example

- Error estimate:

$$E_t = -\frac{h^5}{90} f^{(4)}(\xi)$$

- Where $h = b - a$ and $a < \xi < b$
- Don't know ξ
  – use average value

$$E_t \approx E_a = -\frac{1^5}{90} \overline{f}^{(4)} = -\frac{1^5}{90} \frac{\left[f^{(4)}(x_0) + f^{(4)}(x_1) + f^{(4)}(x_2) \right]}{3}$$

Another Example

- Let's look at the polynomial again:

  – F

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

$$h = \frac{b-a}{2} = 0.4 \qquad x_0 = a = 0 \qquad x_1 = \frac{a+b}{2} = 0.4 \qquad x_2 = b = 0.8$$

$$I = \int_0^2 f(x)dx \approx \frac{1}{3}h\left[f\left(x_0\right) + 4f(x_1) + f\left(x_2\right)\right]$$

$$= \frac{(0.4)}{3}\left[f\left(0\right) + 4f(0.4) + f\left(0.8\right)\right]$$

$$= 1.36746667$$

Exact integral is 1.64053334

Error

- Actual Error: (using the known exact value)

$$E = 1.64053334 - 1.36746667 = 0.27306666 \quad 16\%$$

- Estimate error: (if the exact value is not available)

$$E_t = -\frac{h^5}{90} f^{(4)}(\xi)$$

- Where $a < \xi < b$.

Error

- Compute the fourth-derivative

$$f^{(4)}(x) = -21600 + 48000x$$

$$E_t \approx E_a = -\frac{0.4^5}{90} f^{(4)}(x_1) = -\frac{0.4^5}{90} f^{(4)}(\underset{\textit{middle point}}{0.4}) = 0.27306667$$

- Matches actual error pretty well.

Example Continued

- If we use 4 segments instead of 1:
  - **x** = [0.0 0.2 0.4 0.6 0.8]

$$h = \frac{b-a}{n} = 0.2$$

$$f(0) = 0.2 \qquad f(0.2) = 1.288 \qquad f(0.4) = 2.456$$
$$f(0.6) = 3.464 \qquad f(0.8) = 0.232$$

$$I = (b-a)\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}$$

$$= (0.8-0)\frac{f(0) + 4f(0.2) + 2f(0.4) + 4f(0.6) + f(0.8)}{(3)(4)}$$

$$= 0.8\frac{0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232}{12}$$

$$= 1.6234667$$

Exact integral is 1.64053334

Error

- Actual Error: (using the known exact value)

$$E = 1.64053334 - 1.62346667 = 0.01706667$$

1%

- Estimate error: (if the exact value is not available)

$$E_t \approx E_a = -\frac{0.2^5}{90} f^{(4)}(x_2) = -\frac{0.2^5}{90} f^{(4)}(0.4) = -0.0085$$

middle point

Error

- Actual is twice the estimated, why?
- Recall:

$$f^{(4)}(x) = -21600 + 48000x$$

$$\max_{x\in[0,0.8]}\left\{\left|f^{(4)}(x)\right|\right\} = \left|f^{(4)}(0)\right| = -21600$$
$$\left|f^{(4)}(0.4)\right| = 2400$$

Error

- Rather than estimate, we can bound the absolute value of the error:

$$|E_a| = \left| -\frac{0.2^5}{90} f^{(4)}(\xi) \right| \le \frac{0.2^5}{90} \left| f^{(4)}(0) \right| = 0.0768$$

- Five times the actual, but provides a safer error metric.

Simpon’s 1/3 Rule

- Simpson’s 1/3 rule uses a 2nd order polynomial
  - need 3 points or 2 intervals
  - This implies we need an even number of intervals.
- What if you don’t have an even number of intervals? Two choices:
  1. Use Simpson’s 1/3 on all the segments except the last (or first) one, and use trapezoidal rule on the one left.
     - Pitfall - larger error on the segment using trapezoid
  2. Use Simpson’s 3/8 rule.

Simpson's 3/8 Rule

- Simpson's 3/8 rule uses a third order polynomial
  - need 3 intervals (4 data points)

$$f(x) \approx p_3(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

$$I = \int_{x_0}^{x_3} f(x)dx \approx \int_{x_0}^{x_3} p_3(x)dx$$

Simpson’s 3/8 Rule

- Determine *a*’s with Lagrange polynomial
- For evenly spaced points

$$I = \frac{3}{8} h \left[f(x_0) + 3(x_1) + 3 f(x_2) + f(x_3) \right]$$

$$h = \frac{b-a}{3}$$

Error

- Same order as 1/3 Rule.
  - More function evaluations.
  - Interval width, *h*, is smaller.

$$E_t = -\frac{3}{80} h^5 f^{(4)}(\xi) \quad O(h^4)$$

- Integrates a cubic exactly:

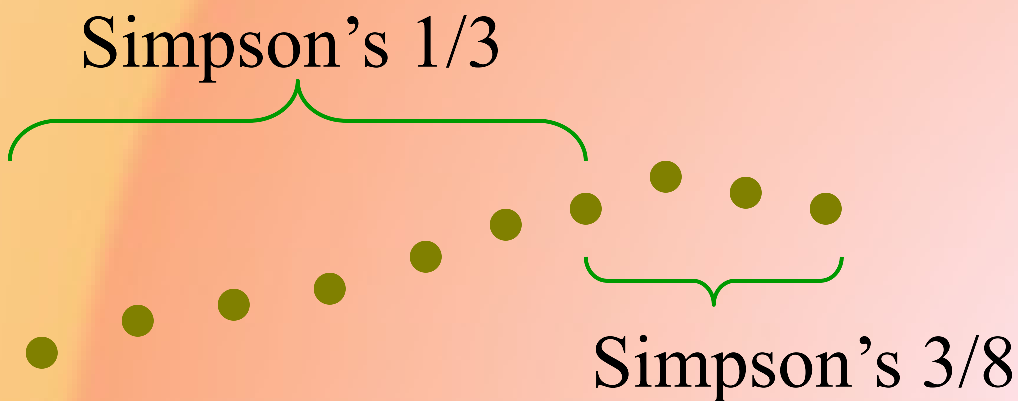
$$\Rightarrow \qquad f^{(4)}(\xi) = 0$$

Comparison

- Simpson's 1/3 rule and Simpson's 3/8 rule have the same order of error
  - $O(h^4)$
  - trapezoidal rule has an error of $O(h^2)$
- Simpson's 1/3 rule requires **even number** of segments.
- Simpson's 3/8 rule requires multiples of **three segments.**
- Both Simpson's methods require **evenly spaced** data points

Mixing Techniques

- n = 10 points $\Rightarrow$ 9 intervals
  - First 6 intervals - Simpson's 1/3
  - Last 3 intervals - Simpson's 3/8



Newton-Cotes Formulas

- We can examine even higher-order polynomials.
  - Simpson's 1/3 - 2nd order Lagrange (3 pts)
  - Simpson's 3/8 - 3rd order Lagrange (4 pts)
- Usually do not go higher.
- Use multiple segments.
  - But only where needed.

Adaptive Simpson's Scheme

- Recall Simpson's 1/3 Rule:

$$I \approx \frac{h}{3}\left[f\left(x_0\right)+4f\left(x_1\right)+f\left(x_2\right)\right]$$

- Where initially, we have $a=x_0$ and $b=x_2$.
- Subdividing the integral into two:

$$I \approx \frac{h}{6}\left[f\left(a\right)+4f\left(x_1\right)+2f\left(x_2\right)+4f\left(x_3\right)+f\left(b\right)\right]$$

Adaptive Simpson's Scheme

- We want to keep subdividing, until we reach a desired error tolerance, ε.
- Mathematically:

$$\left| \int_a^b f(x)\,dx - \left[\frac{h}{3}\left[f(a) + 4f(x_1) + f(b) \right] \right] \right| \le \varepsilon$$

$$\left| \int_a^b f(x)\,dx - \left[\frac{h}{6}\left[f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(b) \right] \right] \right| \le \varepsilon$$

Adaptive Simpson's Scheme

- This will be satisfied if:

$$\left|\int_a^c f(x)\,dx - \left[\frac{h}{6}\left[f(a)+4f(x_1)+f(x_2)\right]\right]\right| \le \frac{\varepsilon}{2}, \quad and$$

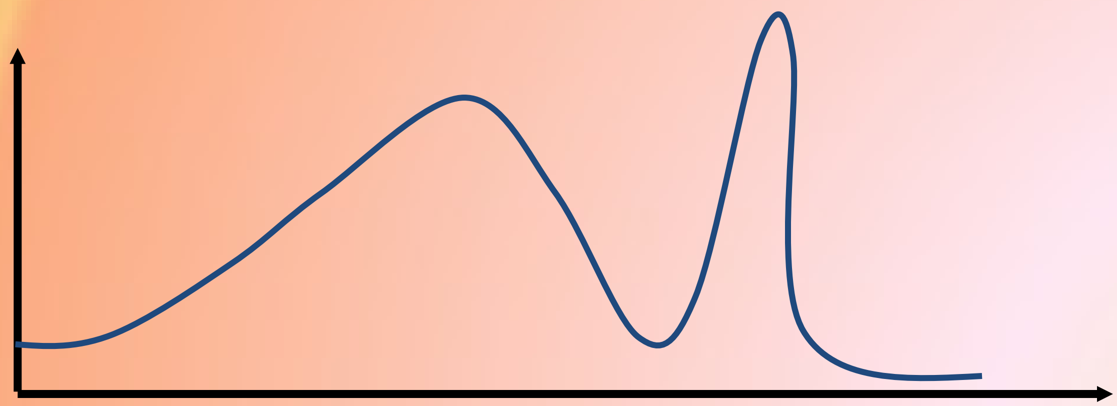
$$\left|\int_c^b f(x)\,dx - \left[\frac{h}{6}\left[f(x_2)+4f(x_3)+f(b)\right]\right]\right| \le \frac{\varepsilon}{2}, \quad where$$

$$c = x_2 = \frac{a+b}{2}$$

- Th ... or.

Adaptive Simpson's Scheme

- Okay, now we have two separate intervals to integrate.
- What if one can be solved accurately with an $h=10^{-3}$, but the other requires many, many more intervals, $h=10^{-6}$?



Adaptive Simpson's Scheme

- Adaptive Simpson's method provides a divide and conquer scheme until the appropriate error is satisfied everywhere.
- Very popular method in practice.
- Problem:
  - We do not know the exact value, and hence do not know the error.

Adaptive Simpson's Scheme

- How do we know whether to continue to subdivide or terminate?

$$I \equiv \int_a^b f(x)\,dx = S(a,b) + E(a,b), \;\; where$$

$$S(a,b) = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right], \;\; and$$

$$E(a,b) = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}$$

Adaptive Simpson's Scheme

- The first iteration can then be defined as:

$$I = S^{(1)} + E^{(1)}, \quad where$$

$$S^{(1)} = S\left(a,b\right),\ E^{(1)} = E\left(a,b\right)$$

- Subse … e defined as:

$$S^{(2)} = S\left(a,c\right) + S\left(c,b\right)$$

Adaptive Simpson's Scheme

- Now, since
- We $E^{(2)} = E(a,c) + E(c,b)$ erms of $E^{(1)}$.

$$E^{(2)} = -\frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)} - \frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)}$$

$$= \left(\frac{1}{2^4}\right) - \frac{1}{90}\left(\frac{h}{2}\right)^5 f^{(4)} = \frac{1}{16}E^{(1)}$$

Adaptive Simpson's Scheme

- Finally, using the identity:
- We $I = S^{(1)} + E^{(1)} = S^{(2)} + E^{(2)}$
- Plu $S^{(2)} - S^{(1)} = E^{(1)} - E^{(2)} = 15E^{(2)}$

$$I = S^{(2)} + E^{(2)} = S^{(2)} + \frac{1}{15}\left(S^{(2)} - S^{(1)}\right)$$

Adaptive Simpson's Scheme

- Our error criteria is thus:

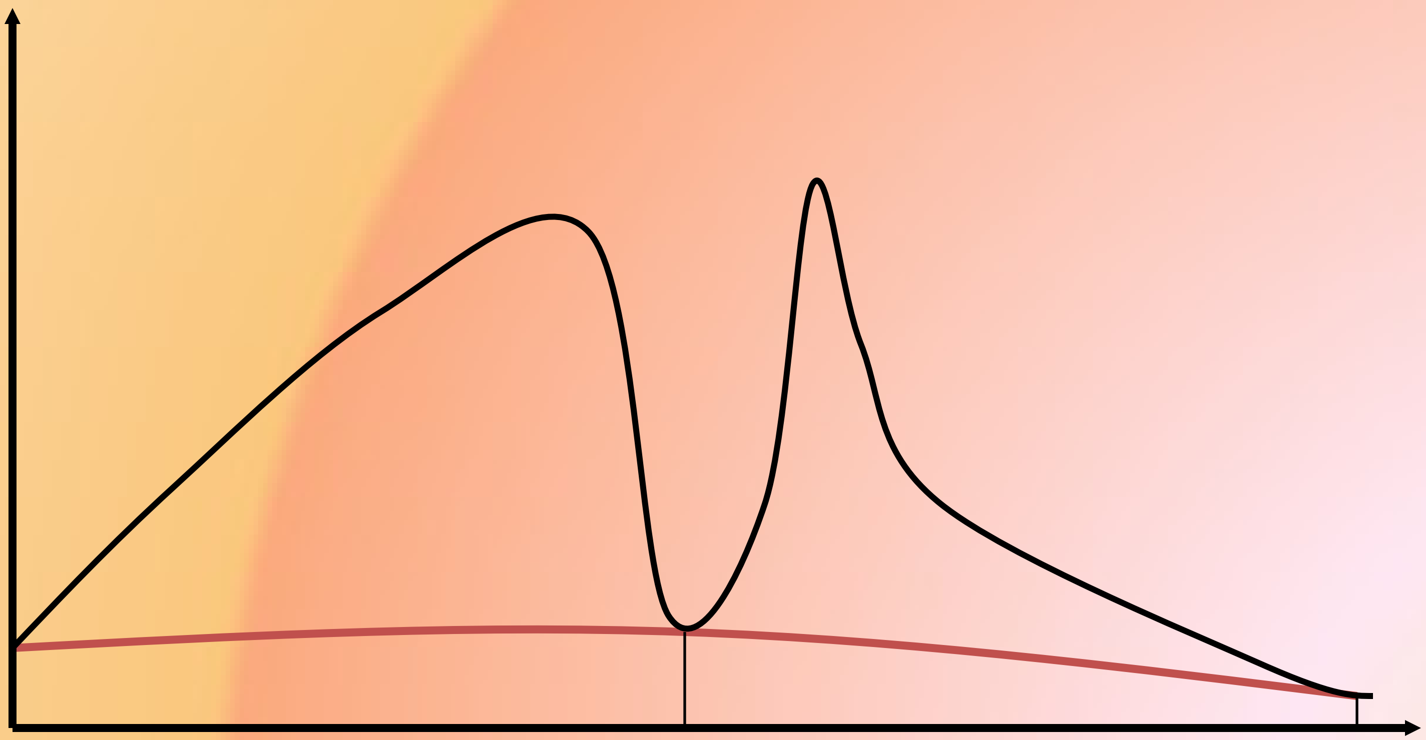
$$\left| I - S^{(2)} \right| = \left| \frac{1}{15}\left(S^{(2)} - S^{(1)} \right) \right| \leq \varepsilon$$

- Simplifying leads to the termination formula:

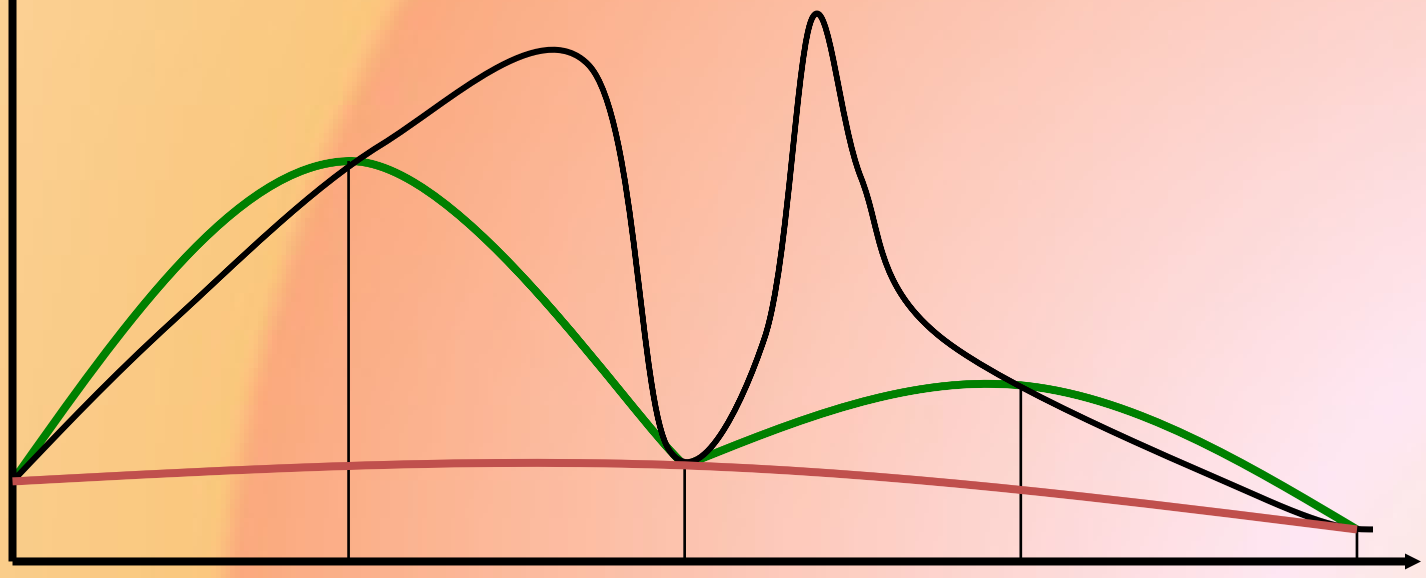
$$\boxed{\left| \left(S^{(2)} - S^{(1)} \right) \right| \leq 15\varepsilon}$$

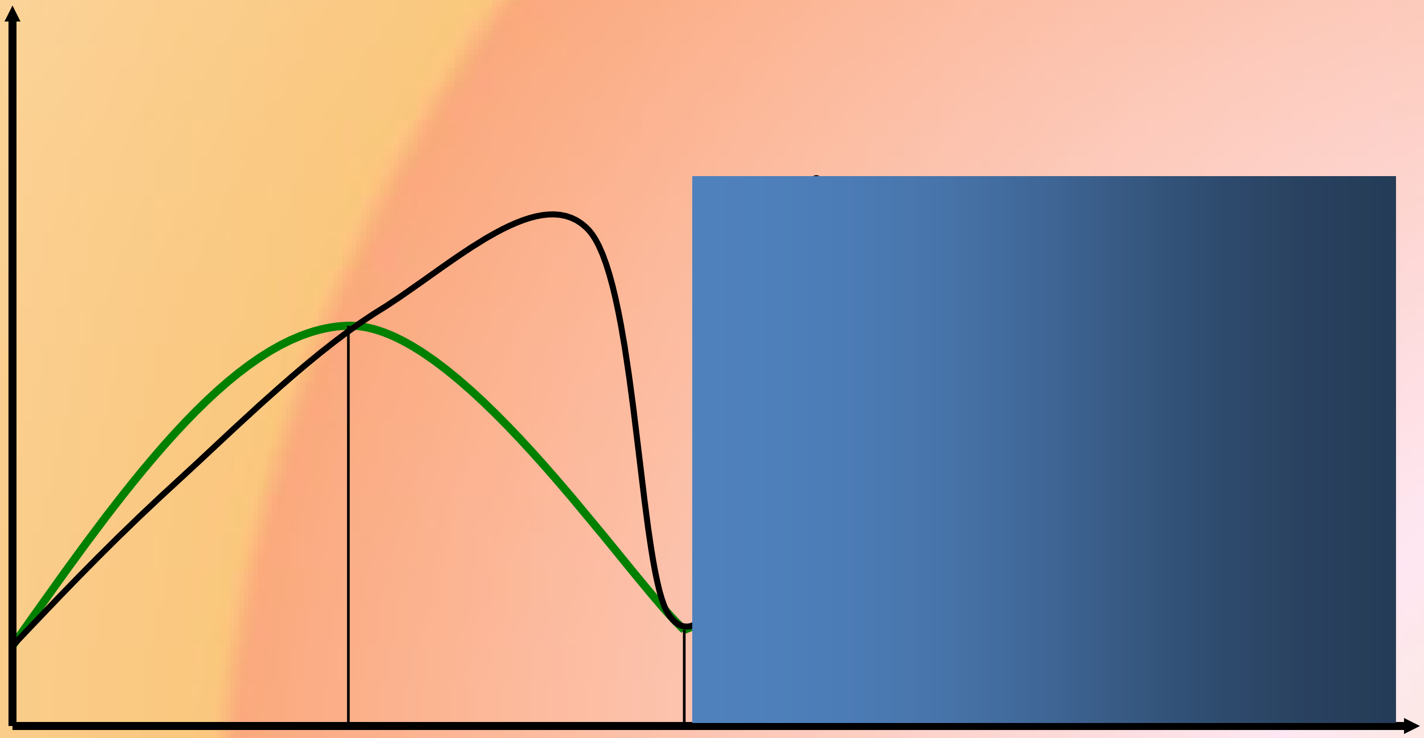
Adaptive Simpson's Scheme

- What happens graphically:

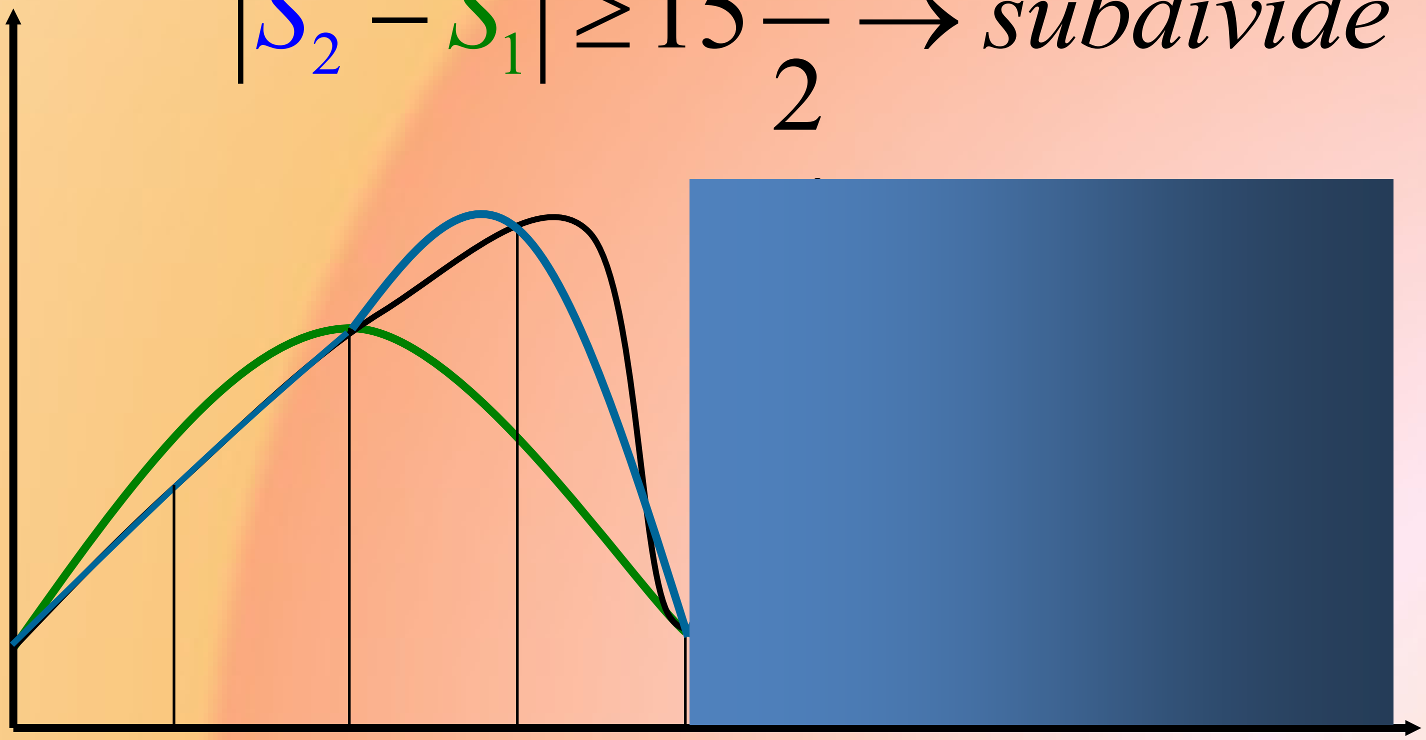


$$\left|S_2 - S_1\right| \geq 15\varepsilon \rightarrow subdivide$$



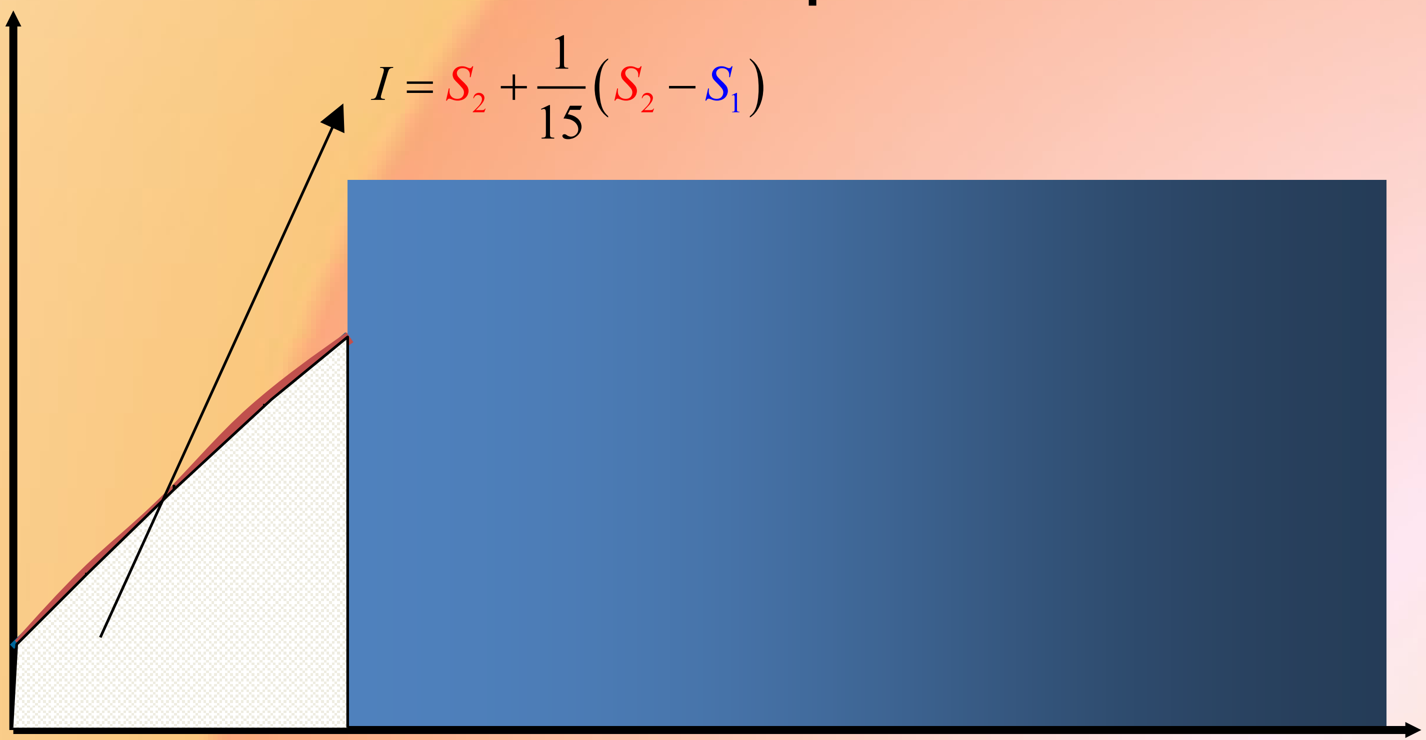


$$\left|S_2 - S_1\right| \geq 15\frac{\varepsilon}{2} \rightarrow subdivide$$

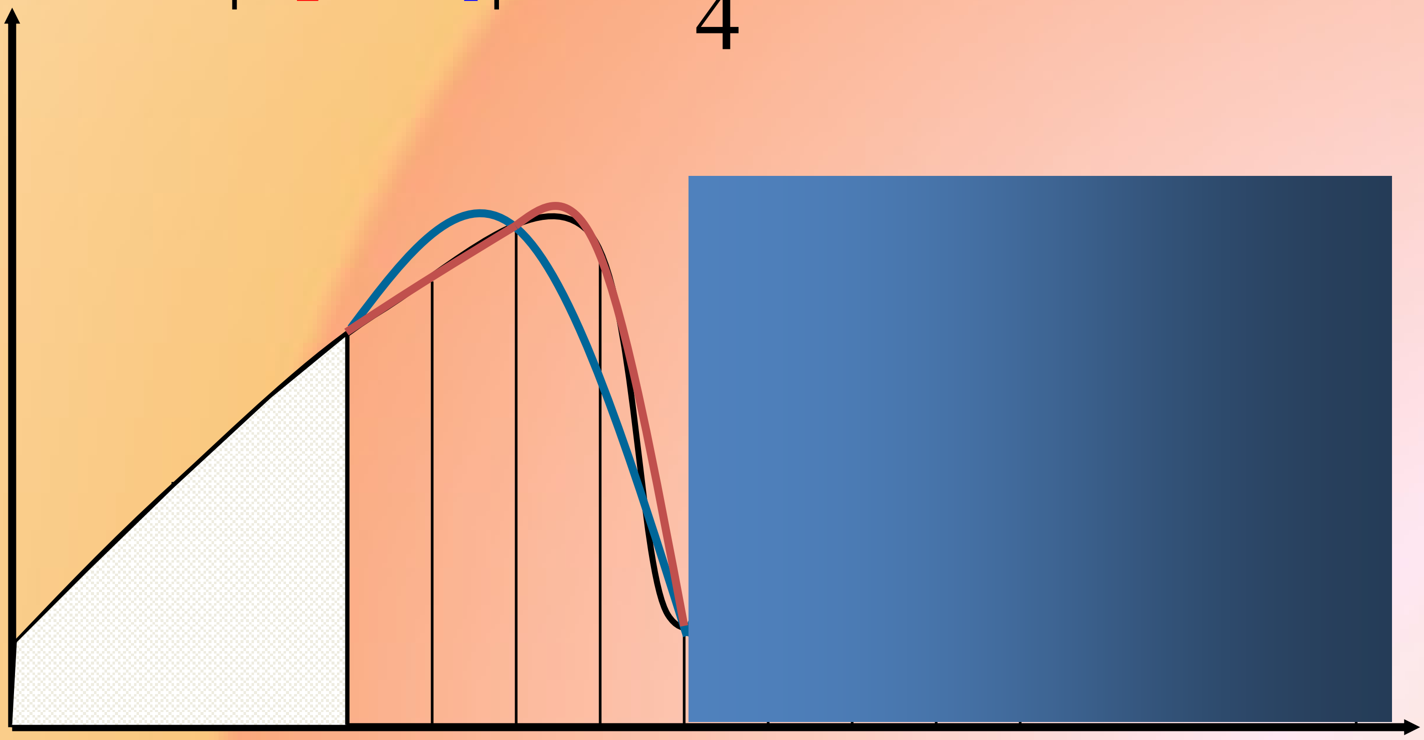


$$\left|S_2 - S_1\right| \le 15\frac{\varepsilon}{4} \rightarrow done$$

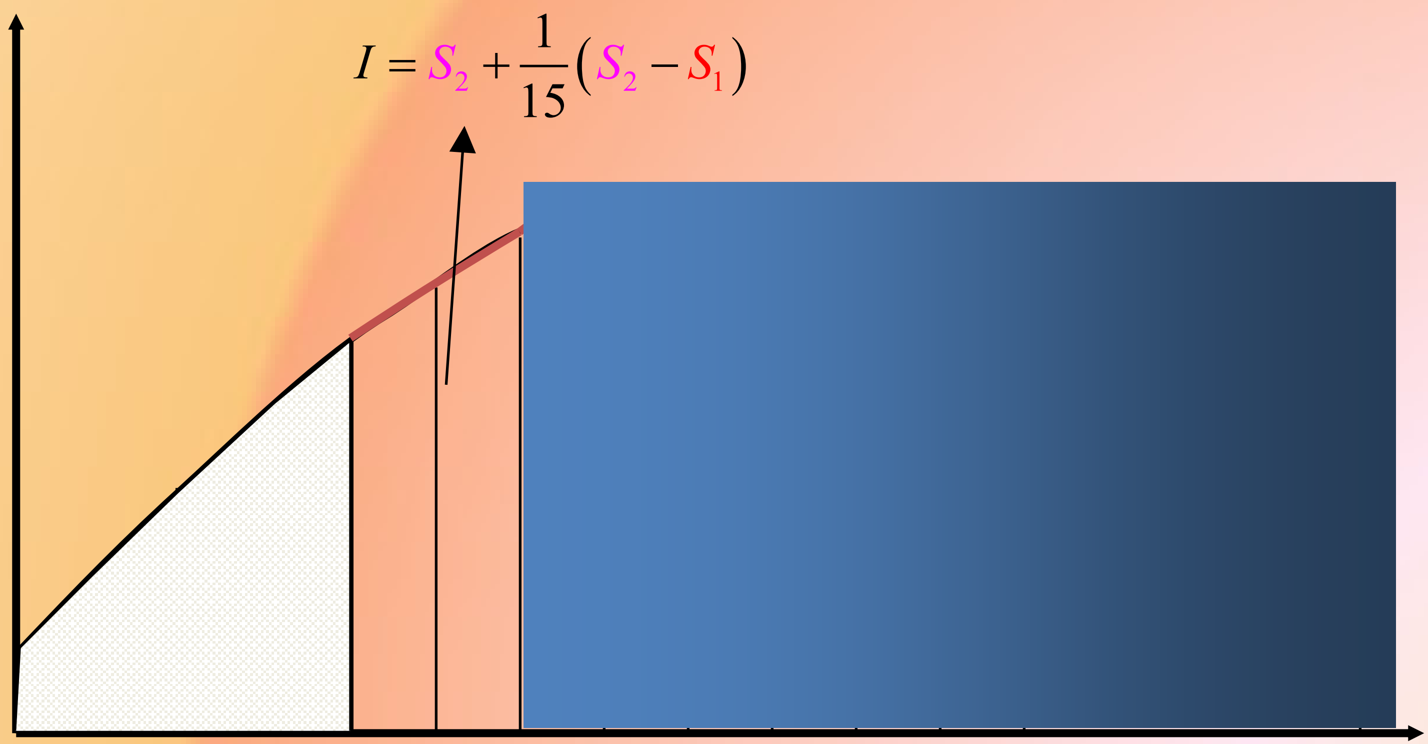
$$I = S_2 + \frac{1}{15}\left(S_2 - S_1\right)$$



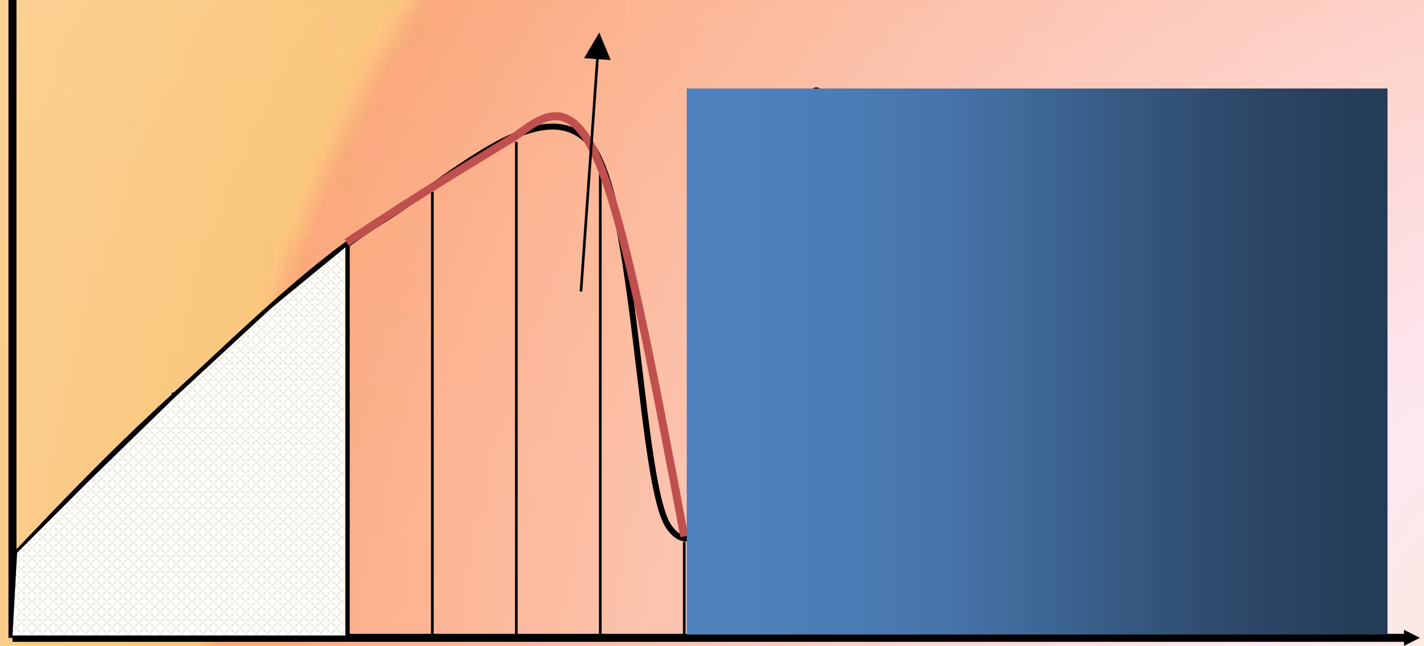
$$\left|S_2 - S_1\right| \geq 15\frac{\varepsilon}{4} \rightarrow subdivide$$

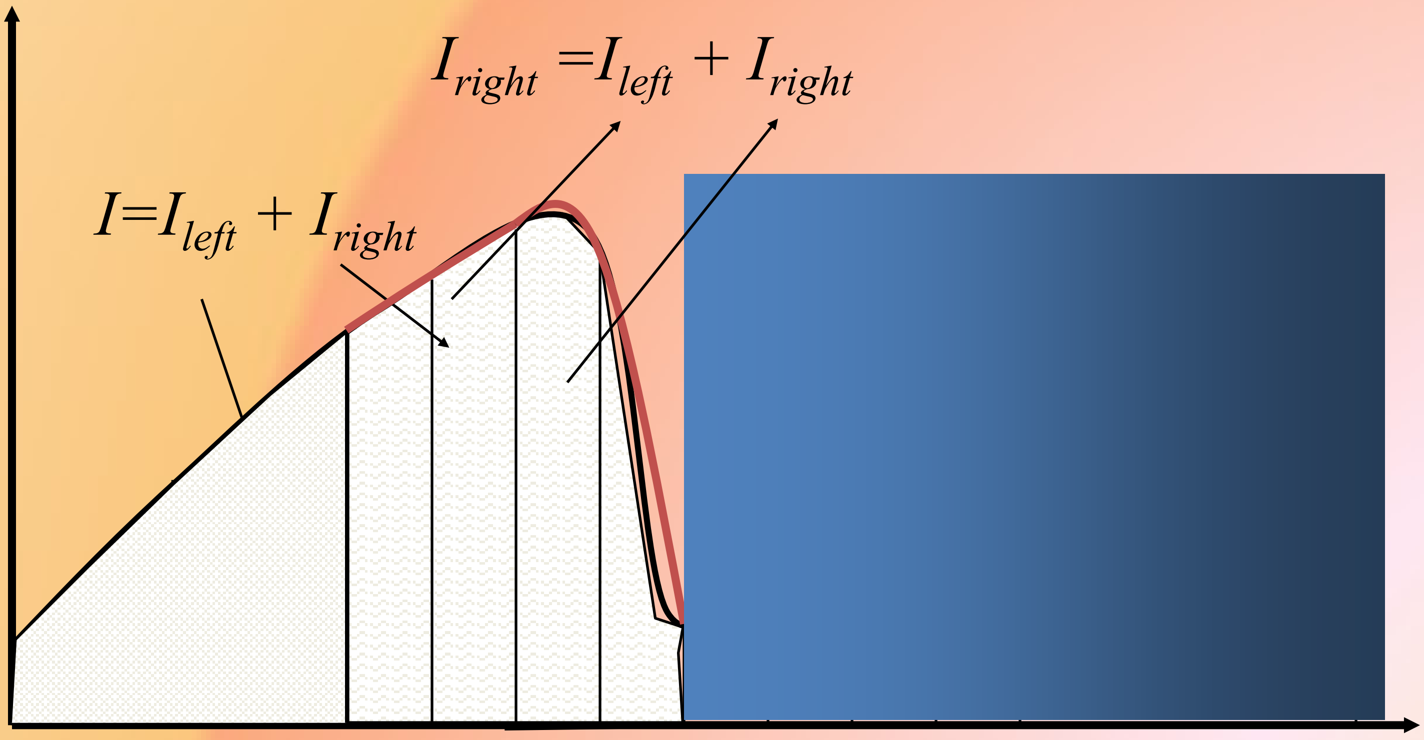


$$I = S_2 + \frac{1}{15}\left(S_2 - S_1\right)$$

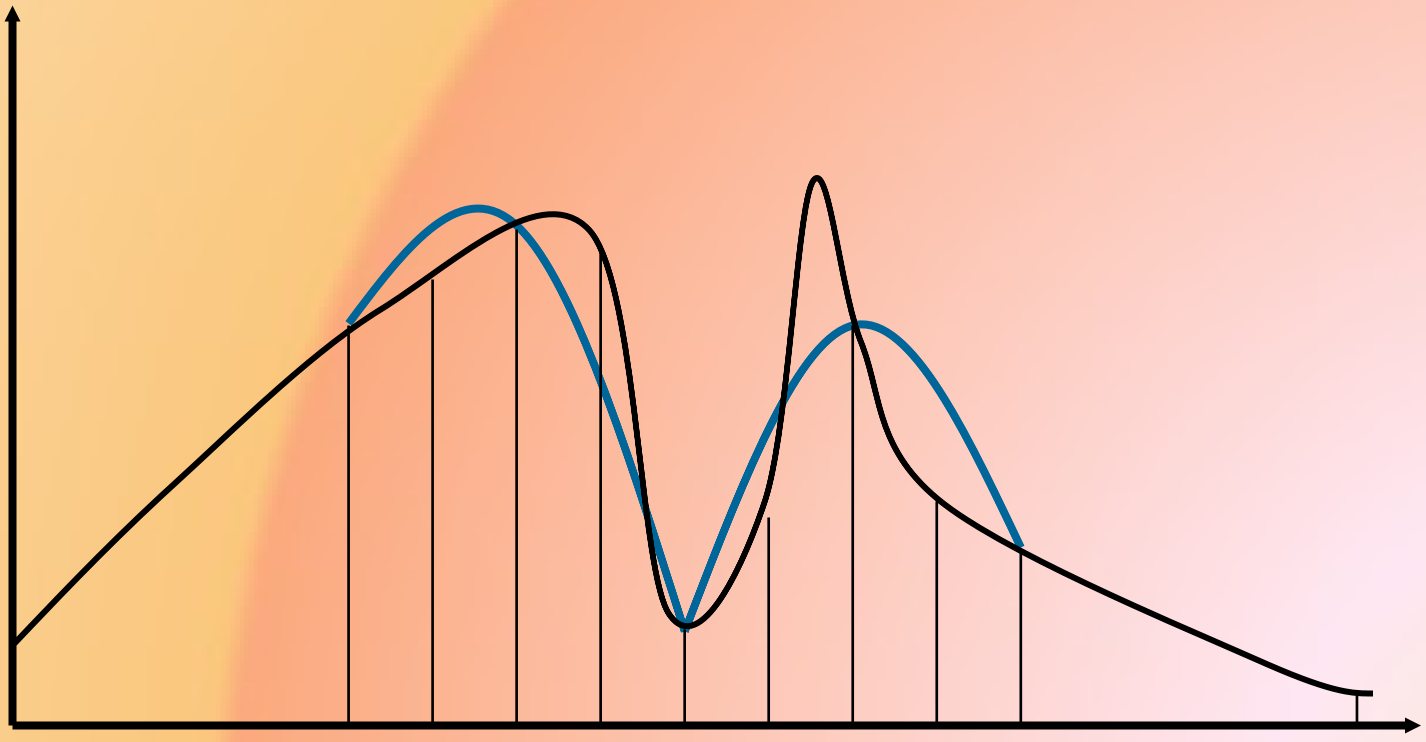


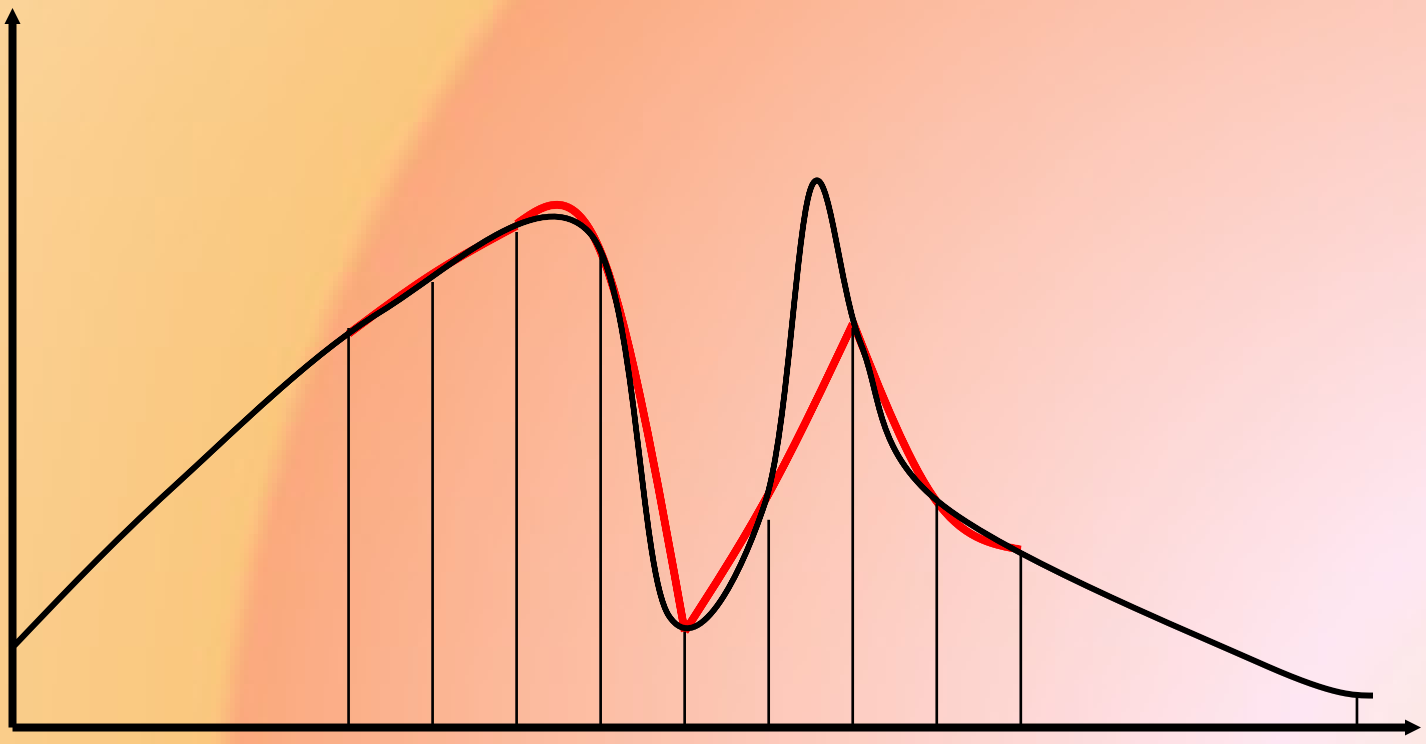
$$I = S_2 + \frac{1}{15}\left(S_2 - S_1\right)$$





$I_{right} = I_{left} + I_{right}$
$I = I_{left} + I_{right}$





Adaptive Simpson's Scheme

- We gradually capture the difficult spots.