UCLA Math151A
Fall 2021
Lecture 18
2021/11/05

Simpson's Rule,
Newton-Cotes,
Composite Quadrature

$$\int_a^b f(x)dx = \int_a^b P(x)dx + \int_a^b E(x)dx$$

$$P(x) = \sum_{i=0}^{n} f(x_i)L_i(x)$$

If we use Lagrangian polynomial

$$E(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)\dots(x-x_n)$$

$$\int_a^b P(x)dx = \sum_{i=0}^{n} f(x_i)\int_a^b L_i(x)dx$$

Compare with $\sum_{i=0}^{n} w_i f(x_i)$

$$\boxed{\Rightarrow w_i := \int_a^b L_i(x)dx.}$$

We can also compute the error (integral of E(x)).

Big Picture

The traperzoidal Rule, Simpsons' rule, Newton-Cotes, etc. are quadrature rules to approximate

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

where f(x) is replaced by a polynomial approximation (e.g., Lagrange polynomial,

Taylor polynomial – see homework 6 deriving Simpson's rule using Taylor polynomial.).

We can estimate error and easily see degree of exactness.

D.O.E. of a quadrature formula is the largest non-zero integer N s.t. the quadrature formula is exact for

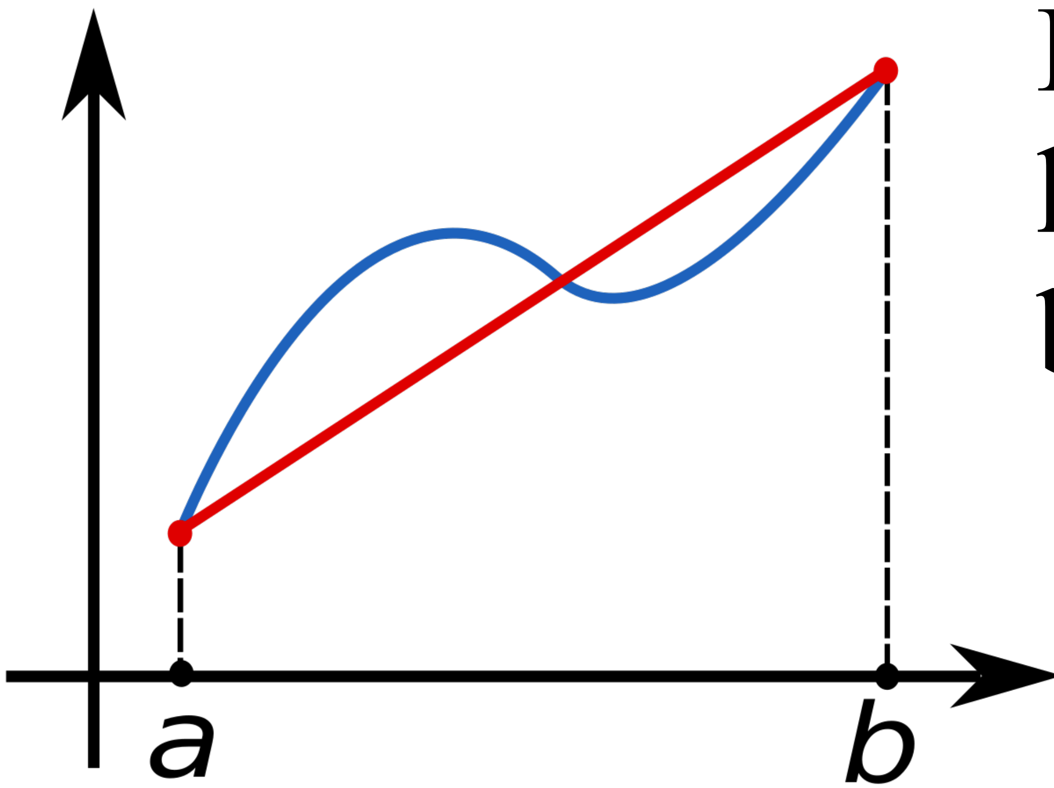
$$f(x) = x^k, k = 0, 1, \ldots, N.$$

I.e., reproducing up to degree N polynomials. $\square$

For example, $$\int_a^b f(x)dx = \frac{h}{2}(f(a) + f(b)) - \frac{f''(c)}{12}h^3$$

for Trasperzopdal rule ($h = b - a$), DOE: $N = 1$.

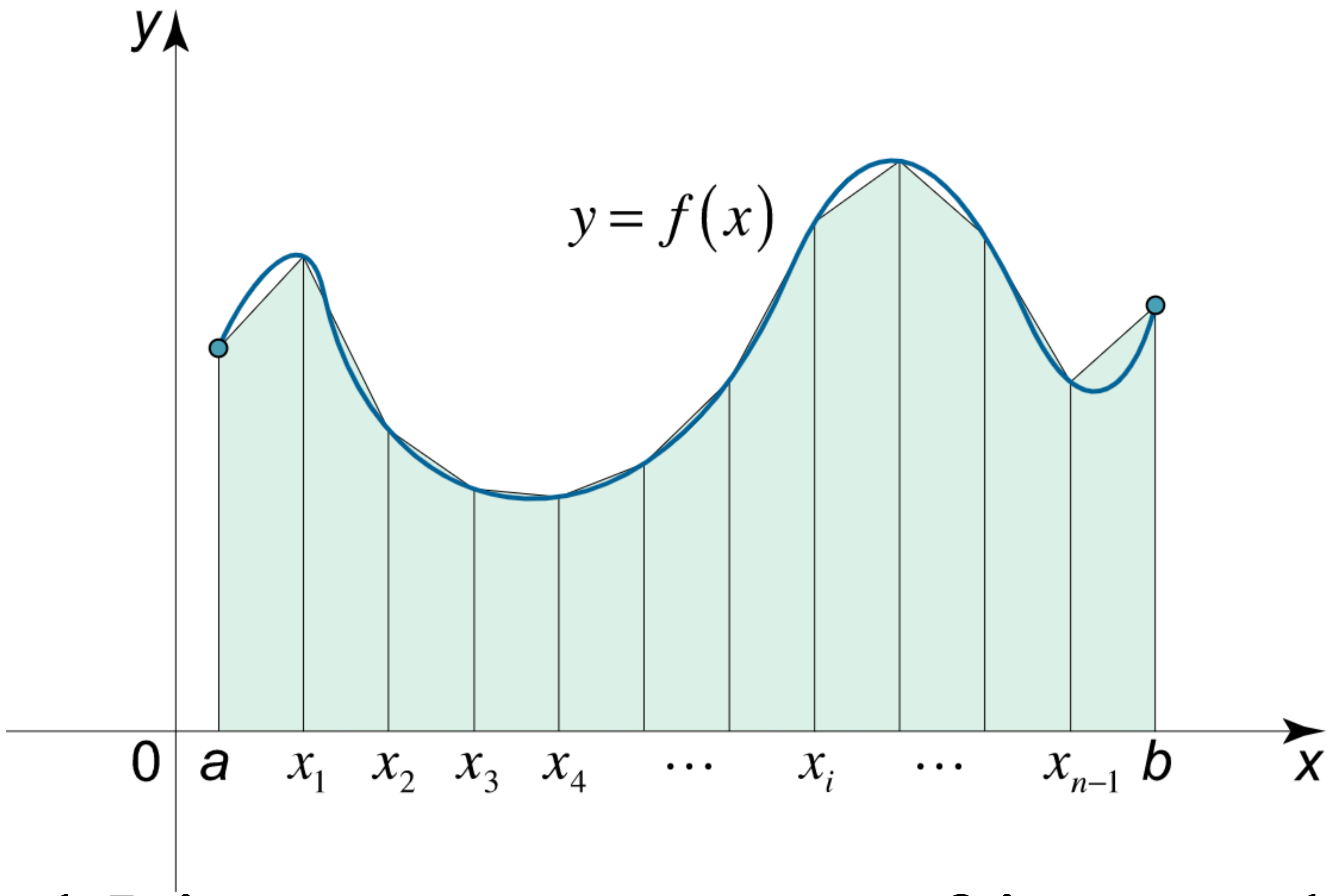
However in practice, replacing f(x) with a **single** low order polynomial across x = a to x = b, e.g., with linear, or quadratic, is not sufficient.



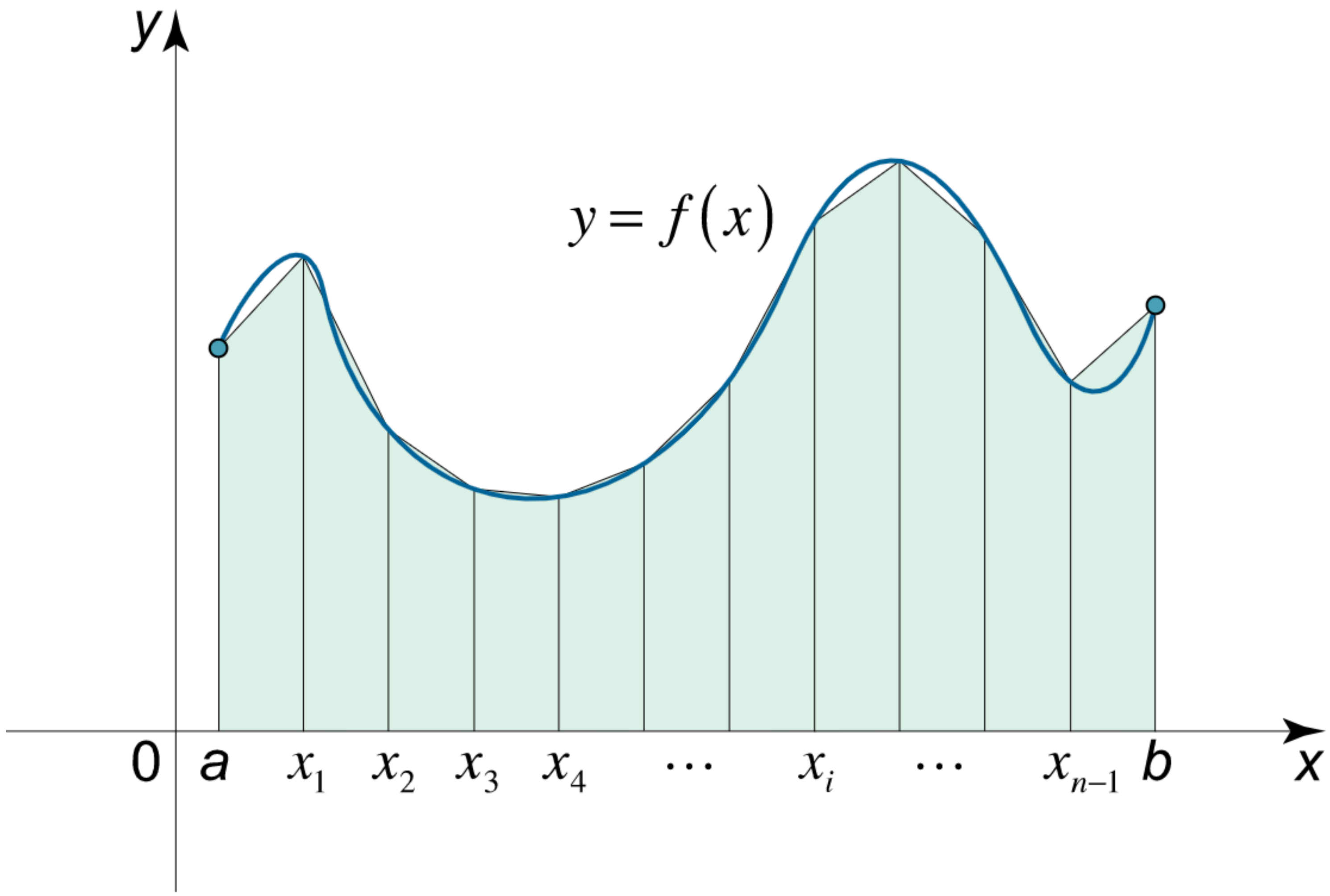
But also, if replacing with a high order polynomial, can be a bad choice too. Why?

Runge's Phenomenon!

In practice, we should replace f(x) with pieceiweise polymonials. That is more accurate.



Break up [a,b] into a sequence of intervals and approximate f(x) with a polynomial on each one – use splines.



The piecewise polynomial approach is called ***Composite Quadrature Formulas.***

To analyze the properties of the composite formulas, we still need to understand the properties of the "original" (not piecewise) approach.

We derived the error for Trapezoidal Rule using weighted mean value theorem:

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{f''(c)}{2}\frac{h^3}{6}$$

Now let's deal with Simpson's Rule.

Simpson's Rule: a "Bad" Derivation

"Bad" means the result is correct but not optimal.

The "good" derivation is in homework, it doesn't use Lagrangian polynomial!

The bad derivation uses Lagrange Polynomial

$$f(x) \ = \ P(x) + E(x)$$

using 3 points: $x_0 = a, x_1 = a + h, x_2 = b, h = \frac{b-a}{2}$

$$f(x) = P(x) + E(x)$$

using 3 points: $x_0 = a, x_1 = a + h, x_2 = b, h = \frac{b-a}{2}$

$$\int_{x_0}^{x_2} f(x)dx = \int_{x_0}^{x_2} P(x)dx + \int_{x_0}^{x_2} E(x)dx$$

$$f(x_0)\int_{x_0}^{x_2} L_0(x)dx + f(x_1)\int_{x_0}^{x_2} L_1(x)dx + f(x_2)\int_{x_0}^{x_2} L_2(x)dx$$

$$\int_{x_0}^{x_2} \frac{f'''(\xi(x))}{3!}(x - x_0)(x - x_1)(x - x_2)dx$$

Since when $f(x) = x^2$, $f''(x) = 0$, we know DOE $N = 2$.

$$\int_{x_0}^{x_2} \frac{f'''(\xi(x))}{3!}(x-x_0)(x-x_1)(x-x_2)dx$$

The error is bounded by

$$M = \max_{a \le x \le b} |f'''(x)|$$

$$|\text{error}| \le \left(\max_{a \le x \le b} |f'''(x)| \right) \frac{1}{6} \int_{x_0}^{x_2} \underline{|x-x_0|}\,\underline{|x-x_1|}\,\underline{|x-x_2|}dx$$

$$\le M \frac{1}{6} 8h^4 = O(h^4)$$

bounded by 2h
bounded by h
bounded by 2h

In summary, using Lagrange polynomial for Simpson's rule gives

DOE N=2 and Error $O(h^4)$

"Bad derivation" tells us that Simpson's Rule has

$$\text{DOE N=2 and Error } O(h^4)$$

In HW6 you will use Taylor Polynomial to re-derive Simpson's Rule.

$$\text{"Good derivation"}$$
$$\text{DOE } N = 3, \text{ Error } O(h^5)$$

To be clear, however, both results in quadrature formula

$$\int_{x_0}^{x_2} f(x)dx \approx \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$$

The good derivation just gives us a better theoretical knowledge of the error.

$\boxed{\textbf{Newton-Cotes}}$

Trapezoidal Rule uses 2 points.
Simpson's rule uses 3 points.

uses $\{x_0, x_1, \ldots, x_{n-1}, x_n\}$ uses $n+1$ points.

It's defined to be the quadrature formula $\sum_{i=0}^{n} w_i f(x_i)$ where $a = x_0 \leq x_1 \leq \cdots \leq x_n = b$ are equispaced and

$$w_i = \int_a^b L_i(x)dx = \int_a^b \Pi_{j=0,j\neq i}^{n} \left(\frac{x - x_j}{x_i - x_j}\right) dx.$$

Note $f(x) = P(x) + E(x)$, $P(x) = \sum_{i=0}^{n} f(x_i)L_i(x)$.

It's good to know what Newton-Cotes is. But in practice it's not useful. Why? *Runge's Phenomenon!*

Composite Quaduature Formulas

Similar to splines. In each subinterval we approximate the function with a linear/quadratic function.

Then we integrate.

dividing $[a, b]$ into n subintervals of equal width, $h = \frac{b-a}{n}$
$a = x_0, x_1 = x_0 + h, x_2 = x_1 + h = x_0 + 2h, \ldots, x_n = x_0 + nh = b.$

Let's derive the **composite traperzoidal rule** (C.T.R.)

Let $f \in C^2([a,b])$,

$$\int_a^b f(x)dx = \sum_{j=0}^{n-1} \int_{x_j}^{x_{j+1}} f(x)dx$$

$$= \sum_{j=0}^{n-1} \left(\frac{h}{2} \left(f(x_j) + f(x_{j+1}) \right) - \frac{h^3}{12} f''(\xi_j) \right), \qquad \xi_j \in (x_j, x_{j+1})$$

Thus,

$$C.T.R. = \sum_{j=0}^{n-1} \frac{h}{2} \left(f(x_j) + f(x_{j+1}) \right) = \frac{h}{2} \left(f(x_0) + 2\sum_{j=1}^{n-1} f(x_j) + f(x_n) \right)$$

$$Error = -\frac{h^3}{12}\sum_{j=0}^{n-1} f''(\xi_j) = -\frac{h^3}{12} n \frac{\sum_{j=0}^{n-1} f''(\xi_j)}{n}$$

$f \in C^2([a,b])$, so $\exists$ a min and max of f'' on $[a,b]$.

Extreme Value Theorem

$$MIN = \min_{a \le x \le b} f''(x) \le f''(\xi_j) \le \max_{a \le x \le b} f''(x) = MAX, \quad \forall j$$

summing it up we get $\boxed{MIN} \le \boxed{\frac{\sum_{j=0}^{n-1} f''(\xi_j)}{n}} \le \boxed{MAX}$

f''(A) a number in-between f''(B)

By the I.V.T., $\exists \mu \in (a,b)$ s.t. $f''(\mu) = \frac{\sum_{j=0}^{n-1} f''(\xi_j)}{n}$

$$Error = -\frac{h^3}{12} n f''(\mu) = -\frac{h^2}{12}\frac{b-a}{n} n f''(\mu) = -\frac{h^2}{12}(b-a) f''(\mu)$$

Continue next time on C.S.R.