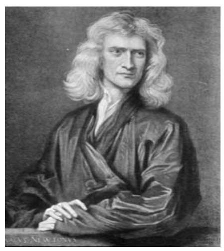
Chapter 12-b
Integral Calculus - Extra



Isaac Newton

Thomas Simpson

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BONUS
Introduction to Numerical Integration

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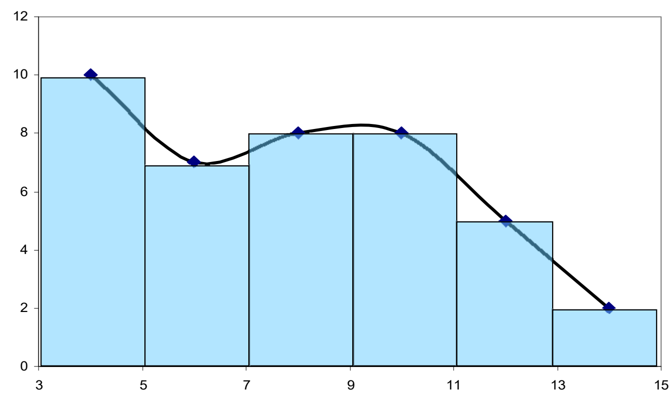
Numerical Integration

Idea: Do an integral in small parts, like the way we presented integration; i.e., *a summation.*

Numerical methods just try to make it faster and more accurate.



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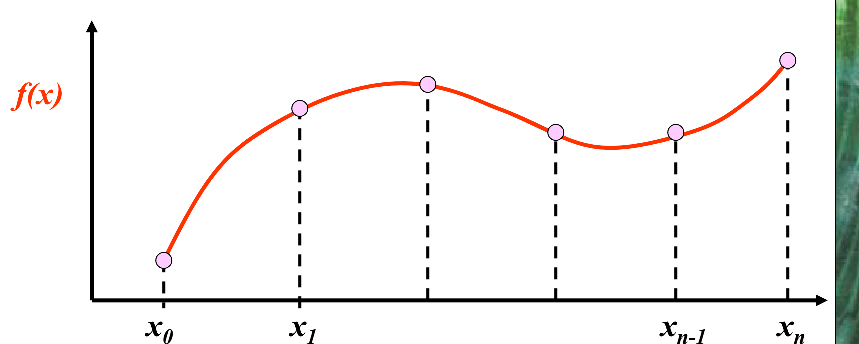
Basic Numerical Integration

- Idea: Weighted sum of function values to approximate integral

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} c_i f(x_i)$$
$$= c_0 f(x_0) + c_1 f(x_1) + \cdots\cdots + c_n f(x_n)$$



- Task: Find appropriate c_i's (weights) and the x_i's (nodes).

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Basic Numerical Integration

• We want to find integration of functions of various forms of the equation known as the *Newton-Cotes* integration formulas ("*rules*").

• Newton-Cotes formula

Assume the value of $f(x)$ defined on $[a, b]$ is known at equally spaced points x_i (i = 0, 1, ..., n), where $x_0 = a$, and $x_n = b$. Then,

$$\int_a^b f(x)\, dx = \sum_{i=1}^{n} c_i\, f(x_i),$$

where $x_i = h\, i + x_0$, with h ("*step size*") = $(x_n - x_0)/n = (b - a)/n$.

The c_i's are called *weights*. The x_i's are called *nodes*. The precision of the approximation depends on n.

Note: The N-C rules use nodes **equally spaced**. But, they do not have to be –unequally spaced nodes are OK too.

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Basic Numerical Integration

• Weights

In the N-C formulae, they are derived from an approximation required to be equal for a polynomial of order lower or equal to the degree of the polynomials used to approximate the function. In other methods, weights and nodes can be derived jointly.

• Error analysis

The error of the approximation is the difference between the value of the integral and the numerical result:

$$error = \varepsilon = \int_a^b f(x)\, dx - \sum_{i=1}^{n} c_i\, f(x_i)$$

The errors are frequently approximated using Taylor series for $f(x)$. The error analysis gives a strict upper bound on the error, if the derivatives of f are available.

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Newton-Cotes Formula

• The weights are derived from the Lagrange polynomials $L(x)$. The weight, $L_i(x)$, depend only on the x_i's (no two x_i's are the same); not on the function f.

$$L_i(x) = \prod_{0 \le j \le n, i \ne j} \frac{(x - x_j)}{(x_i - x_j)} = \frac{(x - x_0)...(x - x_{i-1})(x - x_{i+1})...(x - x_n)}{(x_i - x_0)...(x_i - x_{i-1})(x_i - x_{i+1})...(x_i - x_n)}$$

Recall that L(x) is used for polynomial interpolation of a function $f(x)$, given a set of points $(x_i, f(x_i))$.

Example: Interpolate $f(x) = 2\,x^3$ over [2, 4], with 3 points: (2, 3, 4). The interpolating Lagrange is:

$$L(x) = 16\frac{(x-3)}{2-3} * \frac{(x-4)}{2-4} + 54\frac{(x-2)}{3-2} * \frac{(x-4)}{3-4} + 128\frac{(x-2)}{4-2} * \frac{(x-3)}{4-3}$$
$$= 18\,x^2 - 52x + 48$$

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Newton-Cotes Formula

- Different methods use different polynomials to get the c_i's.
- Newton-Cotes Closed Formulae – Use both end points
  - Trapezoidal Rule : Linear
  - Simpson's 1/3-Rule : Quadratic
  - Simpson's 3/8-Rule : Cubic
  - Boole's Rule : Fourth-order
- Newton-Cotes Open Formulae – Use only interior points
  - midpoint rule

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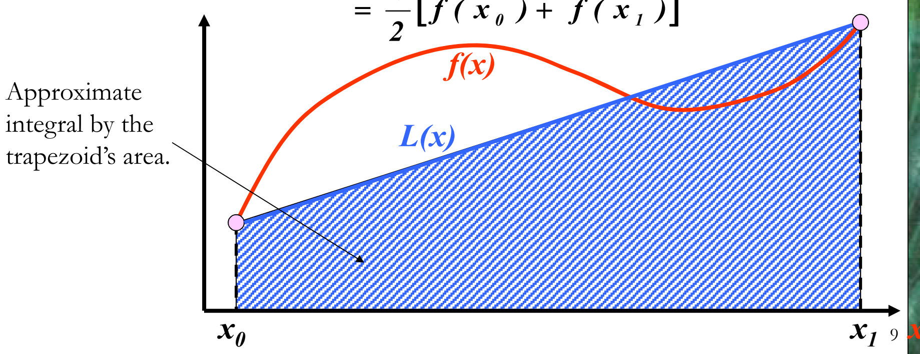
Trapezoid Rule

- Straight-line approximation

  The trapezoid rule approximates the region under the graph of the function $f(x)$ as a trapezoid and calculating its area.

$$\int_a^b f(x)dx \approx \sum_{i=0}^{1} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1)$$

$$= \frac{h}{2}[f(x_0) + f(x_1)]$$



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Trapezoid Rule – Derivation

• We use a Lagrange approximation (a polynomial) for $f(x)$ over the interval $(x_n - x_0)$ (*Lagrange interpolation*), given by

$$f(x) \approx f(x_0)L_0(x) + f(x_1)L_1(x) + \ldots + f(x_n)L_n(x)$$

• For the case, n = 2, with the interval $(x_1 - x_0)$:

$$L(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

$$let \quad \mathrm{a} = \mathrm{x}_0, \ \mathrm{b} = \mathrm{x}_1, \quad \xi = \frac{x-a}{b-a}, \quad \mathrm{d}\xi = \frac{\mathrm{dx}}{\mathrm{h}}; \quad h = b - a$$

$$\left\{\begin{array}{ll} x = a & \Rightarrow \xi = 0 \\ x = b & \Rightarrow \xi = 1 \end{array}\right\} \Rightarrow L(\xi) = (1-\xi)f(a) + (\xi)f(b)$$

• Then, we integrate the Lagrange polynomial to obtain the trapezoid rule

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Trapezoid Rule – Derivation

• Integrating: $\int_a^b f(x)dx \approx \int_a^b L(x)dx = h\int_0^1 L(\xi)d\xi$

$$= f(a)h\int_0^1 (1-\xi)d\xi + f(b)h\int_0^1 \xi d\xi$$

$$= f(a)h(\xi - \frac{\xi^2}{2})\Big|_0^1 + f(b)h\frac{\xi^2}{2}\Big|_0^1 = \frac{h}{2}\left[f(a)+f(b)\right]$$

⇒ The weights depend only on h!

• This approximation may be poor. The approximation error is:

$$\varepsilon = \int_a^b f(x)\,dx - \sum_{i=1}^n c_i\, f(x_i)$$

$$= -(b-a)^3/(12)\, f''(\eta), \qquad \eta \in [a, b].$$

• Thus, if the integrand is convex –i.e., positive second derivative–, the error is negative. That is, the trapezoidal rule overestimates the true value of the integral.

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Trapezoid Rule – Example

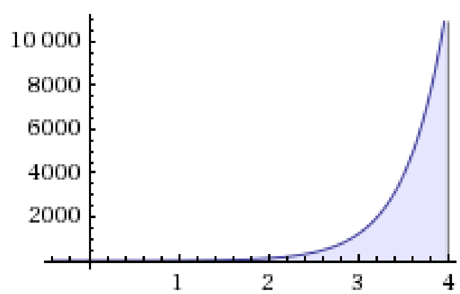
Evaluate the integral $\int_0^4 xe^{2x}dx$

• Exact solution

$$\int_0^4 xe^{2x}dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4$$

$$= \frac{1}{4}e^{2x}(2x-1)\Big|_0^1 = 5216.926477$$

• Graph



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Trapezoid Rule – Example

Evaluate the integral $\int_0^4 xe^{2x} dx$

- Trapezoidal Rule: Approximation Error

  ε = -(b – a)^3/(12) $f''(\eta)$, (η is a number between a and b).

  Let's take η =2. Then

  ε = -4^3/12 * [2*exp(2*2) + 2*exp(2*2) + 4*(2)*exp(2*2)]

  = -3494.282

- Trapezoidal Rule

$$I = \int_0^4 xe^{2x} dx \approx \frac{4-0}{2}\left[f(0) + f(4)\right] = 2(0 + 4e^8) = 23847.66$$

$$\varepsilon = \frac{5216.926 - 23847.66}{5216.926} = -357.12\%$$

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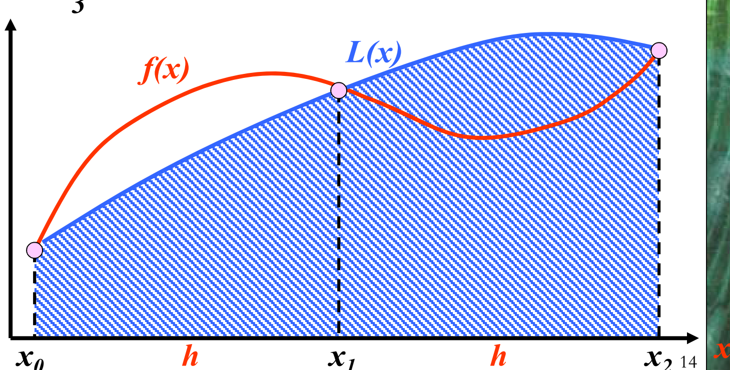
Simpson's 1/3-Rule (Kepler's Rule)

- Approximate the function by a parabola

$$\int_a^b f(x)dx \approx \sum_{i=0}^{2} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2)$$

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



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Simpson's 1/3-Rule – Derivation

- Use a quadratic Lagrange interpolation:

$$L(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

$$let \quad x_0 = a, x_2 = b, x_1 = \frac{a+b}{2}$$

$$h = \frac{b-a}{2}, \xi = \frac{x - x_1}{h}, \; d\xi = \frac{dx}{h}$$

$$\begin{cases} x = x_0 \Rightarrow \xi = -1 \\ x = x_1 \Rightarrow \xi = 0 \\ x = x_2 \Rightarrow \xi = 1 \end{cases}$$

$$\boxed{L(\xi) = \frac{\xi(\xi - 1)}{2} f(x_0) + (1 - \xi^2) f(x_1) + \frac{\xi(\xi + 1)}{2} f(x_2)}$$

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Simpson's 1/3-Rule – Derivation

- Integrate the Lagrange interpolation

$$\int_a^b f(x)dx \approx h\int_{-1}^{1} L(\xi)d\xi = f(x_0)\frac{h}{2}\int_{-1}^{1} \xi(\xi - 1)d\xi + f(x_1)h\int_0^1 (1 - \xi^2)d\xi + f(x_2)\frac{h}{2}\int_{-1}^{1} \xi(\xi + 1)d\xi$$

$$= f(x_0)\frac{h}{2}\left(\frac{\xi^3}{3} - \frac{\xi^2}{2}\right)\Bigg|_{-1}^{1} + f(x_1)h\left(\xi - \frac{\xi^3}{3}\right)\Bigg|_{-1}^{1} + f(x_2)\frac{h}{2}\left(\frac{\xi^3}{3} + \frac{\xi^2}{2}\right)\Bigg|_{-1}^{1}$$

$$\boxed{\int_a^b f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]}$$

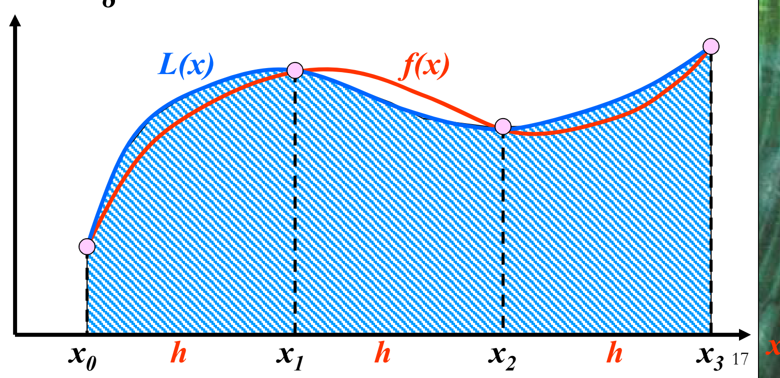
- Again, the weights depend only on h!

Thomas Simpson (1710 – 1761, England)

Simpson's 3/8-Rule

- Approximate by a cubic polynomial

$$\int_a^b f(x)dx \approx \sum_{i=0}^{3} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$
$$= \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]$$



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Simpson's 3/8-Rule

- Lagrange interpolation

$$L(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} f(x_0)$$
$$+ \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} f(x_1)$$
$$+ \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} f(x_2)$$
$$+ \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} f(x_3)$$

- Integrate to obtain the rule

$$\int_a^b f(x)dx \approx \int_a^b L(x)dx \quad ; \quad h = \frac{b-a}{3}$$
$$= \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]$$

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Simpson's Rule: Example

Evaluate the integral $\int_0^4 xe^{2x}dx$

- Simpson's 1/3-Rule: Approximation Error

  ε = -(b – a)^5/(2880) $f^{(4)}(\eta)$ ($\eta \in [a, b]$).

  Since $f^{(4)}(\eta) > 0$, the error is negative (overshooting).

  Let's take η=2.5. Then,

  ε = -4^5/(2880) [{exp(2*2.5)*[16*(2.5)+32]} =-3799.3769

- Simpson's 1/3-Rule

$$I = \int_0^4 xe^{2x}dx \approx \frac{h}{3}\left[f(0) + 4f(2) + f(4)\right]$$

$$= \frac{2}{3}\left[0 + 4(2e^4) + 4e^8\right] = 8240.411$$

$$\varepsilon = \frac{5216.926 - 8240.411}{5216.926} = -57.96\%$$

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Simpson's Rule: Example

Evaluate the integral $\int_0^4 xe^{2x}dx$

- Simpson's 3/8-Rule

$$I = \int_0^4 xe^{2x}dx \approx \frac{3h}{8}\left[f(0) + 3f(\frac{4}{3}) + 3f(\frac{8}{3}) + f(4)\right]$$

$$= \frac{3(4/3)}{8}\left[0 + 3(19.18922) + 3(552.33933) + 11923.832\right] = 6819.209$$

$$\varepsilon = \frac{5216.926 - 6819.209}{5216.926} = -30.71\%$$

- Simpson's 3/8-Rule: Approximation Error

  ε = -(b – a)^5 /(6480) $f^{(4)}(\eta)$ ($\eta \in [a, b]$).

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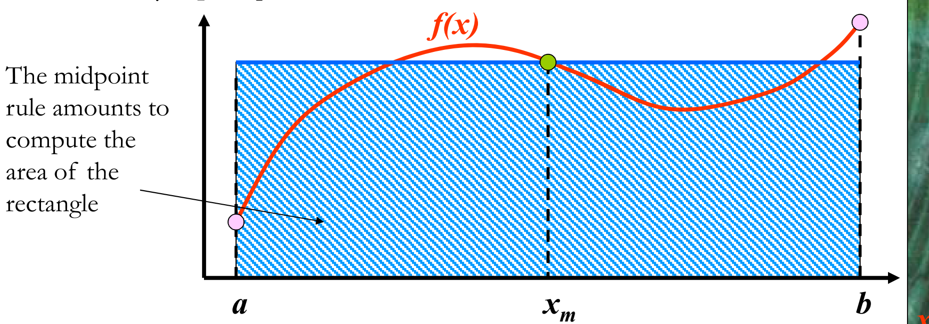
Midpoint Rule

- Newton-Cotes Open Formula

$$\int_a^b f(x)dx \approx (b-a)f(x_m)$$
$$= (b-a)f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24} f''(\eta)$$

where $\eta \in [a, b]$.



- Note: This rule does not make any use of the end points.

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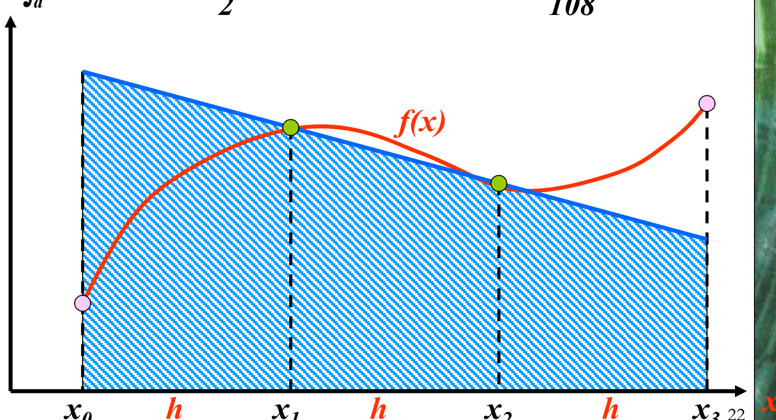
Two-point Newton-Cotes Open Formula

- Approximate by a straight line

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\left[f(x_1)+f(x_2)\right] + \frac{(b-a)^3}{108} f''(\eta)$$



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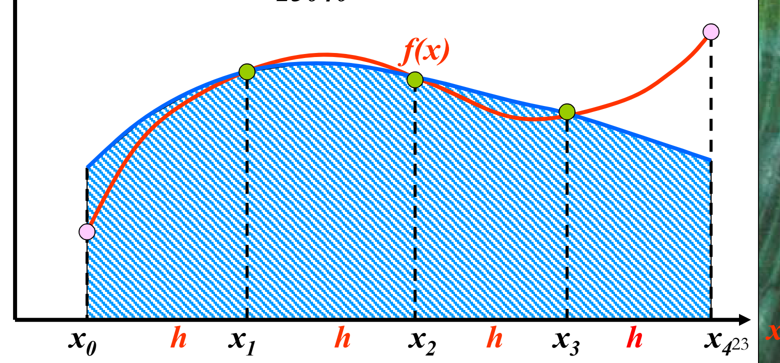
Three-point Newton-Cotes Open Formula

- Approximate by a parabola

$$\int_a^b f(x)dx \approx \frac{b-a}{3}\left[2f(x_1) - f(x_2) + 2f(x_3)\right] + \frac{7(b-a)^5}{23040} f''''(\eta)$$



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Better Numerical Integration

- Composite integration
  - Composite Trapezoidal Rule
  - Composite Simpson's Rule
- Richardson Extrapolation
- Romberg integration

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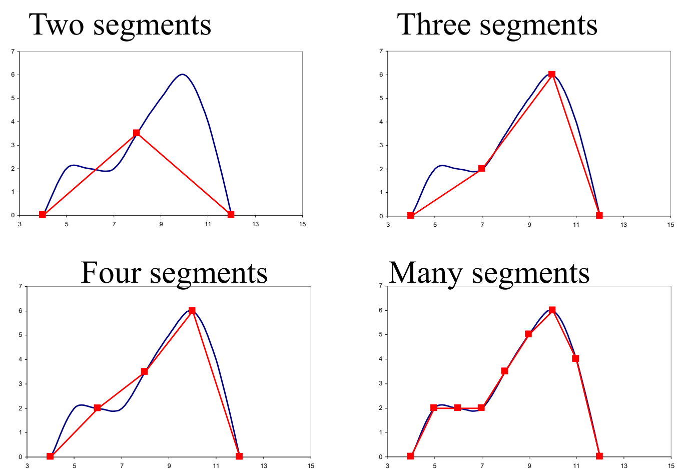
Composite Trapezoid Rule

To improve the Trapezoid Rule, first splits the interval of integration $[a, b]$ into N smaller, uniform subintervals, and then applies the trapezoidal rule on each of them.



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Composite Trapezoid Rule

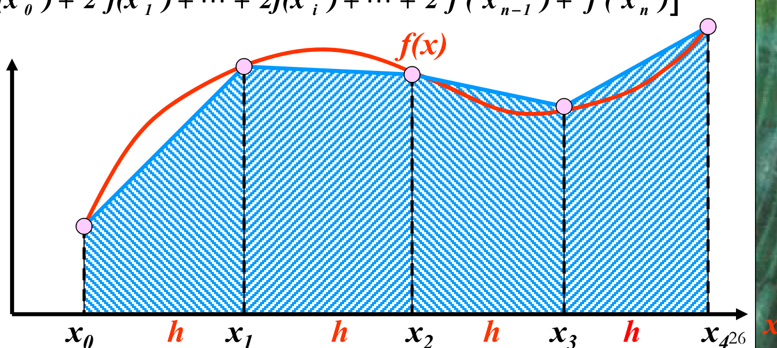
- Use the Trapezoid Rule in n intervals. Then, add them together.

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots\cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

$$= \frac{h}{2}[f(x_0) + f(x_1)] + \frac{h}{2}[f(x_1) + f(x_2)] + \cdots + \frac{h}{2}[f(x_{n-1}) + f(x_n)]$$

$$= \frac{h}{2}[f(x_0) + 2f(x_1) + \cdots + 2f(x_i) + \cdots + 2f(x_{n-1}) + f(x_n)]$$

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



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Composite Trapezoid Rule

- Evaluate the integral $I = \int_0^4 xe^{2x}dx$

$$n = 1, h = 4 \Rightarrow I = \frac{h}{2}\left[f(0) + f(4)\right] = 23847.66 \qquad \varepsilon = -357.12\%$$

$$n = 2, h = 2 \Rightarrow I = \frac{h}{2}\left[f(0) + 2f(2) + f(4)\right] = 12142.23 \qquad \varepsilon = -132.75\%$$

$$n = 4, h = 1 \Rightarrow I = \frac{h}{2}\left[f(0) + 2f(1) + 2f(2) + 2f(3) + f(4)\right] = 7288.79 \qquad \varepsilon = -39.71\%$$

$$n = 8, h = 0.5 \Rightarrow I = \frac{h}{2}\left[f(0) + 2f(0.5) + 2f(1) + 2f(1.5) + 2f(2) + 2f(2.5) + 2f(3) + 2f(3.5) + f(4)\right] = 5764.76 \qquad \varepsilon = -10.50\%$$

$$n = 16, h = 0.25 \Rightarrow I = \frac{h}{2}\left[f(0) + 2f(0.25) + 2f(0.5) + \cdots + 2f(3.5) + 2f(3.75) + f(4)\right] = 5355.95 \qquad \varepsilon = -2.66\%$$

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Composite Trapezoid Rule: Unequal Segments

- Evaluate the integral $I = \int_0^4 xe^{2x}dx$

  Use the following h_i's: $\{h_1=2,\ h_2=1,\ h_3=0.5,\ h_4=0.5\}$

$$I = \int_0^2 f(x)dx + \int_2^3 f(x)dx + \int_3^{3.5} f(x)dx + \int_{3.5}^4 f(x)dx$$

$$= \frac{h_1}{2}\left[f(0) + f(2)\right] + \frac{h_2}{2}\left[f(2) + f(3)\right] + \frac{h_3}{2}\left[f(3) + f(3.5)\right] + \frac{h_4}{2}\left[f(3.5) + f(4)\right]$$

$$= \frac{2}{2}\left[0 + 2e^4\right] + \frac{1}{2}\left[2e^4 + 3e^6\right] + \frac{0.5}{2}\left[3e^6 + 3.5e^7\right] + \frac{0.5}{2}\left[3.5e^7 + 4e^8\right] = 5971.58 \qquad \Rightarrow \varepsilon = -14.45\%$$

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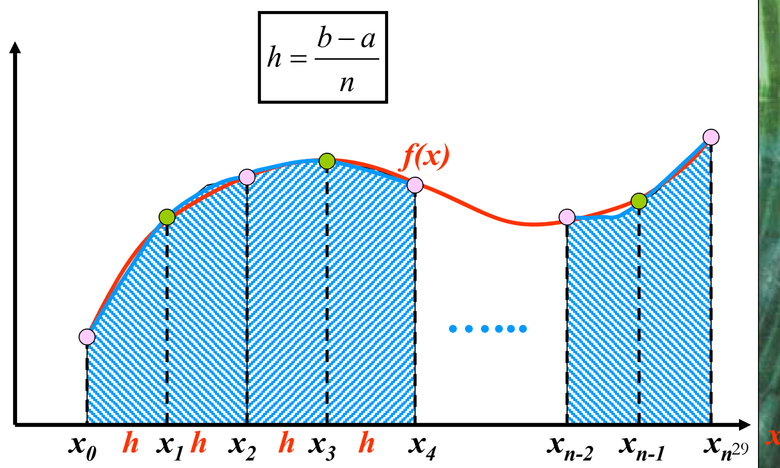
Composite Simpon's Rule

- Piecewise Quadratic approximations



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Composite Simpon's Rule

- Evaluate the integral $I = \int_0^4 xe^{2x}dx$
- Using $n = 2$, $h = 2$

$$I = \frac{h}{3}\left[f(0) + 4f(2) + f(4)\right]$$
$$= \frac{2}{3}\left[0 + 4(2e^4) + 4e^8\right] = 8240.411 \quad \Rightarrow \varepsilon = -57.96\%$$

- Using $n = 4$, $h = 1$

$$I = \frac{h}{3}\left[f(0) + 4f(1) + 2f(2) + 4f(3) + f(4)\right]$$
$$= \frac{1}{3}\left[0 + 4(e^2) + 2(2e^4) + 4(3e^6) + 4e^8\right]$$
$$= 5670.975 \quad \Rightarrow \varepsilon = -8.70\%$$

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Composite Simpson's Rule: Unequal Segments

- Evaluate the integral $I = \int_0^4 xe^{2x}dx$

  Using $h_1 = 1.5$, $h_2 = 0.5$

$$I = \int_0^3 f(x)dx + \int_3^4 f(x)dx$$
$$= \frac{h_1}{3}\left[f(0) + 4f(1.5) + f(3)\right]$$
$$+ \frac{h_2}{3}\left[f(3) + 4f(3.5) + f(4)\right]$$
$$= \frac{1.5}{3}\left[0 + 4(1.5e^3) + 3e^6\right] + \frac{0.5}{3}\left[3e^6 + 4(3.5e^7) + 4e^8\right]$$
$$= 5413.23 \quad \Rightarrow \varepsilon = -3.76\%$$

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Gaussian Quadratures

- Newton-Cotes Formulae
  - Nodes (x_i's): Use evenly-spaced functional values
  - Weights (c_i's): Derived from an approximation required to be equal for a polynomial of order lower or equal to the degree of the polynomials used to approximate the function. Given nodes, best!
  - Problem: Can explode for large *n* (Runge's phenomenon)

- Q: Can we use more efficient weights and nodes? Yes!

- Gaussian Quadratures
  - Gaussian quadrature rules set the nodes and the weights in such a way that the approximation is exact when *f*(.) is a low order polynomial. Best choice for both, nodes and weights!

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Gaussian Quadratures

• Gaussian quadrature computes an approximation to the integral:

$$\int_a^b f(x)dx = \sum_{i=1}^{n} c_i f(x_i),$$

c_i's are weights, x_i's are the *quadrature nodes*, also called *cusps*. These values are not predetermined, but unknowns to be determined in some "optimal" fashion.

Optimal Goal: Get an exact answer if *f* is a $(2n - 1)^{th}$-order polynomial. With n =2, we get an exact answer *f* is a 3^{th}-order polynomial. (With n = 5, we get an exact answer *f* is a 9^{th}-order polynomial).

Note: A Gauss quadrature rule with 3 points yields exact value of an integral for a polynomial of degree 2 × 3 – 1 = 5. Simpson's 1/3 rule also uses 3 points, but the order of accuracy is 3.

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Gaussian Quadratures – Features

- Gaussian Quadratures Features

- Select functional values at non-uniformly distributed points. The values are not predetermined, but unknowns determined by Legendre polynomials and integrating over a Lagrange interpolation.
- Several Gauss quadrature rules; we cover the Gauss-Legendre rules, which integrate from [-1, 1].
- A change of variables is needed:

$$t = \frac{b-a}{2}x + \frac{a+b}{h} \quad \Rightarrow \text{ the interval of integration is [-1,1].}$$

- Gauss-Legendre formulae for nodes and weights can be easily found online up to order n=100.
- With n nodes, delivers exact answer if *f* is $(2n - 1)^{th}$-order polynomial.
- Gauss-Legendre quadrature rule is not typically used for integrable functions with endpoint singularities.

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Gaussian Quadratures – Nodes and Weights

Example: For n = 2, we choose (c_1, c_2, x_1, x_2) such that the method yields "exact integral" for $f(x) = x^0, x^1, x^2, x^3$.

$$\begin{cases} f = 1 \Rightarrow \int_{-1}^{1} 1dx = 2 = c_1 + c_2 \\ f = x \Rightarrow \int_{-1}^{1} xdx = 0 = c_1 x_1 + c_2 x_2 \\ f = x^2 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \\ f = x^3 \Rightarrow \int_{-1}^{1} x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 \end{cases}$$

We solve this 4x4 system of equations to get (c_1, c_2, x_1, x_2).

• By construction we get right answer for

$f(x) = 1$ ($j = 0$), $f(x) = x$ ($j = 1$), ..., $f(x) = x^j$ ($j = 2n - 1$),

⇒ enough to get the right answer for any polynomial of order $2n$-1.

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Gaussian Quadratures – Nodes and Weights

Example (continuation): $n = 2$ ⇒ Solve the 4x4 system:

$$\begin{cases} f = 1 \Rightarrow \int_{-1}^{1} 1dx = 2 = c_1 + c_2 \\ f = x \Rightarrow \int_{-1}^{1} xdx = 0 = c_1 x_1 + c_2 x_2 \\ f = x^2 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \\ f = x^3 \Rightarrow \int_{-1}^{1} x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 \end{cases} \Rightarrow \begin{cases} c_1 = 1 \\ c_2 = 1 \\ x_1 = \frac{-1}{\sqrt{3}} \\ x_2 = \frac{1}{\sqrt{3}} \end{cases}$$

Note: This is not how it is done in practice:
- x_i's are chosen to be zeros of the degree-n Legendre polynomials $P_n(x)$ (not trivial to compute, but, they are tabulated).
- Then, find the Lagrange polynomial that interpolates the integral $f(x)$ at the selected x_i's and integrate to get c_i's.

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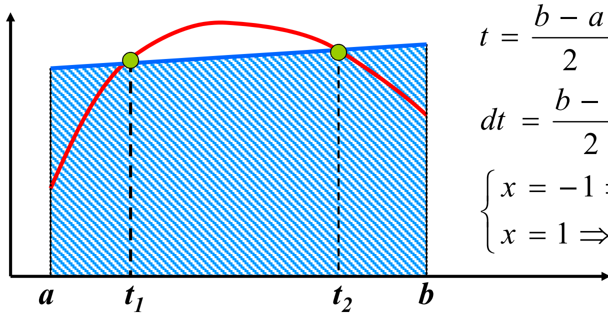
Gaussian Quadratures – Change of interval

• Coordinate transformation from $[a, b]$ to [-1, 1].

This can be done by an affine transformation on t and a change of variables.



$$t = \frac{b-a}{2}x + \frac{b+a}{2}$$

$$dt = \frac{b-a}{2}dx$$

$$\begin{cases} x = -1 \Rightarrow t = a \\ x = 1 \Rightarrow t = b \end{cases}$$

$$\int_a^b f(t)dt = \int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right)\left(\frac{b-a}{2}\right)dx \approx \frac{b-a}{2}\sum_{i=1}^{n} c_i f(x_i)$$

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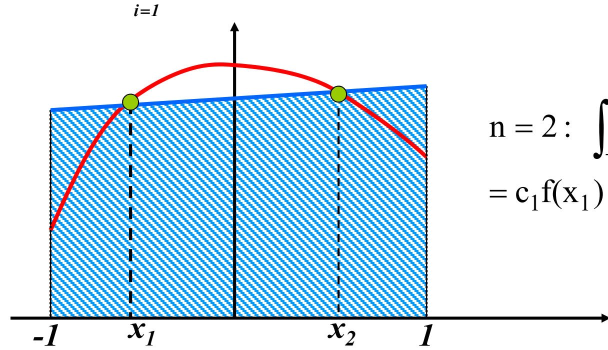
Gaussian Quadrature on [-1, 1]: $n = 2$

- Gauss Quadrature General formulation:

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i) = c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n)$$



$$n = 2: \int_{-1}^{1} f(x)dx = c_1 f(x_1) + c_2 f(x_2)$$

• For $n = 2$, we have four unknowns: (c_1, c_2, x_1, x_2)

• We have already solved this problem:

$c_1 = 1$; $c_2 = 1$; $x_1 = -1/\sqrt{3}$; & $x_2 = 1/\sqrt{3}$.

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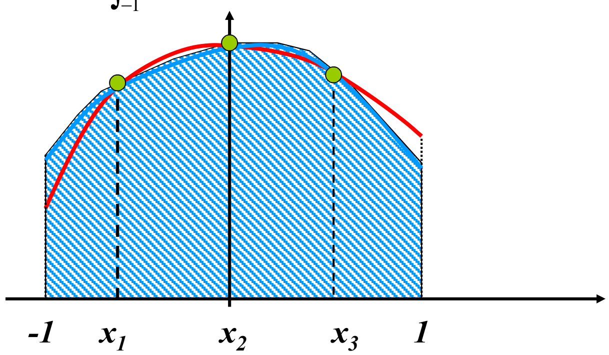
Gaussian Quadrature on [-1, 1]: $n = 3$

Case $n = 3$: $\int_{-1}^{1} f(x)dx = c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$



As for the $n = 2$ case, we choose $(c_1, c_2, c_3, x_1, x_2, x_3)$ such that the method yields "exact integral" for $f(x) = x^0, x^1, x^2, x^3, x^4, x^5$.

(Again, $(c_1, c_2, c_3, x_1, x_2, x_3)$ are calculated by assuming the formula gives exact expressions for integrating a 5th order polynomial).

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Gaussian Quadrature on [-1, 1]: $n = 3$

$$f = 1 \Rightarrow \int_{-1}^{1} 1 dx = 2 = c_1 + c_2 + c_3$$

$$f = x \Rightarrow \int_{-1}^{1} x dx = 0 = c_1 x_1 + c_2 x_2 + c_3 x_3$$

$$f = x^2 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 + c_3 x_3^2$$

$$f = x^3 \Rightarrow \int_{-1}^{1} x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 + c_3 x_3^3$$

$$f = x^4 \Rightarrow \int_{-1}^{1} x^4 dx = \frac{2}{5} = c_1 x_1^4 + c_2 x_2^4 + c_3 x_3^4$$

$$f = x^5 \Rightarrow \int_{-1}^{1} x^5 dx = 0 = c_1 x_1^5 + c_2 x_2^5 + c_3 x_3^5$$

$$\Rightarrow \begin{cases} c_1 = 5/9 \\ c_2 = 8/9 \\ c_3 = 5/9 \\ x_1 = -\sqrt{3/5} \\ x_2 = 0 \\ x_3 = \sqrt{3/5} \end{cases}$$

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Gaussian Quadrature on [-1, 1]: $n = 2$ & $n = 3$

- Approximation formula for $n = 2$:

$$I = \int_{-1}^{1} f(x)dx = f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}})$$

- Approximation formula for $n = 3$

$$I = \int_{-1}^{1} f(x)dx = \frac{5}{9} f(-\sqrt{\frac{3}{5}}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{\frac{3}{5}})$$

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Gaussian Quadratures: Example

Evaluate $$I = \int_0^4 te^{2t}dt = 5216.926477$$

First, a coordinate transformation

$$t = \frac{b-a}{2}x + \frac{b+a}{2} = 2x + 2; \quad \text{dt} = 2\text{dx}$$

$$I = \int_0^4 te^{2t}dt = \int_{-1}^{1} (4x+4)e^{4x+4}dx = \int_{-1}^{1} f(x)dx$$

- Two-point formula ($n = 2$)

$$I = \int_{-1}^{1} f(x)dx = f(\frac{-1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) = (4 - \frac{4}{\sqrt{3}})e^{4-\frac{4}{\sqrt{3}}} + (4 + \frac{4}{\sqrt{3}})e^{4+\frac{4}{\sqrt{3}}}$$

$$= 9.167657324 + 3468.376279 = 3477.543936 \qquad (\varepsilon = 33.34\%)$$

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Gaussian Quadratures: Example

- Three-point formula (n = 3)

$$I = \int_{-1}^{1} f(x)dx = \frac{5}{9} f(-\sqrt{0.6}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{0.6})$$
$$= \frac{5}{9}(4-4\sqrt{0.6})e^{4-\sqrt{0.6}} + \frac{8}{9}(4)e^{4} + \frac{5}{9}(4+4\sqrt{0.6})e^{4+\sqrt{0.6}}$$
$$= \frac{5}{9}(2.221191545) + \frac{8}{9}(218.3926001) + \frac{5}{9}(8589.142689)$$
$$= 4967.106689 \qquad (\varepsilon = 4.79\%)$$

- Four-point formula (n = 4)

$$I = \int_{-1}^{1} f(x)dx = 0.34785\left[f(-0.861136) + f(0.861136)\right]$$
$$+ 0.652145\left[f(-0.339981) + f(0.339981)\right]$$
$$= 5197.54375 \qquad (\varepsilon = 0.37\%)$$

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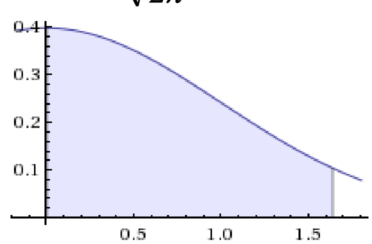
Gaussian Quadratures: Normal Curve

Evaluate $$I = \frac{1}{\sqrt{2\pi}} \int_{0}^{1.64} e^{-\frac{x^2}{2}} dx = .44949742$$



First, a coordinate transformation:

$$t = \frac{b-a}{2}x + \frac{b+a}{2} = .82x + .82 = .82(1+x); \quad dt = .82dx$$

$$I = \frac{1}{\sqrt{2\pi}} \int_{0}^{1.64} e^{-\frac{t^2}{2}} dt = \frac{.82}{\sqrt{2\pi}} \int_{-1}^{1} e^{-\frac{1}{2}[.82(1+x)]^2} dx = \frac{.82}{\sqrt{2\pi}} \int_{-1}^{1} f(x)dx$$

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Gaussian Quadratures: Normal Curve

- Two-point formula (n = 2)

$$I = \frac{.82}{\sqrt{2\pi}} \int_{-1}^{1} f(x)dx = \frac{.82}{\sqrt{2\pi}} \left(f(\frac{-1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) \right) = \frac{.82}{\sqrt{2\pi}} \left(e^{-\frac{1}{2}[.82(1-\frac{1}{\sqrt{3}})]^2} + e^{-\frac{1}{2}[.82(1+\frac{1}{\sqrt{3}})]^2} \right)$$

$$= 0.32713267 * (0.94171147 + 0.43323413) = .44978962 \qquad (\varepsilon = 0.065\%)$$

- Three-point formula (n = 3)

$$I = \frac{.82}{\sqrt{2\pi}} \int_{-1}^{1} f(x)dx = \frac{.82}{\sqrt{2\pi}} \left(\frac{5}{9} f(-\sqrt{0.6}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{0.6}) \right)$$

$$= \frac{.82}{\sqrt{2\pi}} \left(\frac{5}{9} e^{-\frac{1}{2}[.82(1-\sqrt{0.6})]^2} + \frac{8}{9} e^{-\frac{1}{2}[.82(1-0)]^2} + \frac{5}{9} e^{-\frac{1}{2}[.82(1+\sqrt{0.6})]^2} \right)$$

$$= .32713267 * (0.5461465\ 9 + 0.63509351 + 0.19271450)$$

$$= 0.44946544 \qquad (\varepsilon = 0.007\%)$$

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Gaussian Quadratures: Normal Curve

- Compare with Integration of Taylor series approximation (n = 6)

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \approx \frac{1}{\sqrt{2\pi}} \left(1 - \frac{x^2}{2} + \frac{x^4}{8} - \frac{x^6}{48}\right)$$

- Integrating Taylor approximation:

$$I = \int_0^{1.64} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}\, dx \approx \int_0^{1.64} \frac{1}{\sqrt{2\pi}} \left(1 - \frac{x^2}{2} + \frac{x^4}{8} - \frac{x^6}{48}\right) dx$$

$$I \approx \frac{1}{\sqrt{2\pi}} \left(x - \frac{x^3}{3*2} + \frac{x^5}{5*8} - \frac{x^7}{7*48}\right) + C\Big|_0^{1.64}$$

$$I \approx \frac{1}{\sqrt{2\pi}} \left(1.64 - \frac{1.64^3}{3*2} + \frac{1.64^5}{5*8} - \frac{1.64^7}{7*48}\right) = .4414171 \ (\varepsilon{=}0.0179\%)$$

Not as accurate as Gaussian quadrature with n = 2 (& more computations.

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Monte Carlo Integration

• In our motivation of integrals, we evaluated a one-dimensional integral by a sum of rectangles, using the end points of each interval to measure the height. Some of these rectangles overestimated the area, some underestimated the area.

• Let's focus on one of those rectangles, say with base [*a, b*]. We can also use as the height a *randomly* selected interior point, $x_1 \in [a, b]$ and estimate the integral, say $I(x_1)$. Of course, it may over- or under-estimate the area.

• But, we can *randomly* select N interiors points and get N estimations of the area. Some points will under-estimate, some points will over-estimate, but, statistical intuition suggests that the average may work.

• In fact, as N increases, the average of the integral converges to the integral.

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Monte Carlo Integration – Example 1

• **Example 1**: We want to do MC integration for (exact integral = 5,216.92):

$$\int_0^4 xe^{2x}dx$$

```
> M <- 200
> x <- runif(M,0,4)
> All_I <- matrix(0,M,1)
> a <- 0
> b <- 4
> m <- 1
> while (m <= M) {
+ Int <- (b-a)*(x[m] * exp(2*x[m]))
+ m <- m+ 1
+ All_I[m] <- Int
+ }
> IN <- sum(All_I)/M
> IN
[1] 5489.388
```

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Monte Carlo Integration – Example 2

- MC Integration can be applied to any area, like the area of a circle.

- **Example 2**: We want to estimate the area of a circle with radius, r=2 (exact area = π * r^2 = π * 4 =12.56637):

```
> M <- 100
> x <- runif(M,-2,2)
> y <- runif(M,-2,2)
> #box is area 16.
> distance.from.0 <- sqrt(x*x + y*y)
> inside.circle <- (distance.from.0 < 2)
> area <- 16*sum(inside.circle)/M
> area
[1] 12.48
```

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Monte Carlo Integration – Properties

- We formalize this idea with: $F_N = \frac{1}{N}\sum_{i=1}^{N} I(x_i)$

- This is our basic *Monte Carlo* (MC) estimator. Very simple.

- It can be shown it has good properties: unbiased, consistent (LLN applies), asymptotic normal (CLT applies).

- This results is very general and applies to many situations, for example, the trapezoid rule. Above, we selected two points to evaluate the integral (a and b). It produced a big over estimation.

We can also randomly select two points between [*a, b*], say x_1 and calculate the integral, say I($\mathbf{x_1}$). We repeat this evaluation of the integral at *N* randomly selected two points ∈ [*a, b*]: as *N* increases, the average of the integral converges to the integral.

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Monte Carlo Integration – Example 3

• **Example 3**: Back to the trapezoid example, where we wanted to integrate the following function:

$$\int_0^4 xe^{2x} dx$$

```
> M <- 1000
> All_I <- matrix(0,M,1)
> x <- runif(M,0,4)
> y <- runif(M,0,4)
>  a <- 0
>  b <- 4
>  m <- 1
>  while (m <= M) {
+  Int <- ((b-a)/2)* (x[m] * exp(2*x[m]) + y[m] * exp(2*y[m]))
+  m <- m+ 1
+  All_I[m] <- Int
+  }
>  IN <- sum(All_I)/M
>  IN
[1] 5134.759
```

Note: The exact integral is 5,216.93.

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Monte Carlo Integration & Multiple Integrals

• Q: Why use the MC estimator instead of the also very simple determinist quadrature rules?

• Quadrature rules do not extend very well to higher dimension. An approach is to rewrite the problem in terms of one-dimensional integrals. For two or three dimension it may work well, but for more than four dimensions it becomes imprecise.

• These rules suffer from the *curse of dimensionalitily.*

• Monte Carlo integration extends well to many dimensions. IT is based on repeated function evaluations, not repeated integrations using one-dimensional methods.

Popular MC algorithm: Markov chain Monte Carlo (MCMC), which include the Metropolis-Hastings algorithm and Gibbs sampling.

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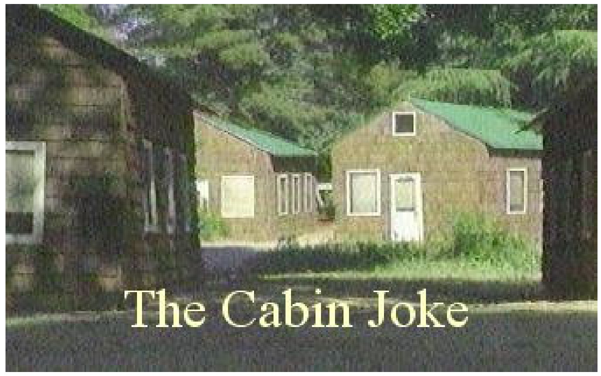

Q: What's the integral of (1/cabin)d(cabin)?

A: A natural log cabin!

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