Numerical Differentiation & Integration

Gaussian Quadrature

Numerical Analysis (9th Edition)

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Beamer Presentation Slides
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Outline

1 Gaussian Quadrature & Optimal Nodes

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1. Gaussian Quadrature & Optimal Nodes
2. Using Legendre Polynomials to Derive Gaussian Quadrature Formula

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2. Using Legendre Polynomials to Derive Gaussian Quadrature Formulae
3. Gaussian Quadrature on Arbitrary Intervals

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Gaussian Quadrature: Contrast with Newton-Cotes

Features of a Newton-Cotes Formula

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Gaussian Quadrature: Contrast with Newton-Cotes

Features of a Newton-Cotes Formula

- The Newton-Cotes formulas were derived by integrating interpolating polynomials.
- The error term in the interpolating polynomial of degree n involves the $(n+1)$st derivative of the function being approximated, ...
- so a Newton-Cotes formula is exact when approximating the integral of any polynomial of degree less than or equal to n.

Gaussian Quadrature: Contrast with Newton-Cotes

Features of a Newton-Cotes Formula (Cont'd)

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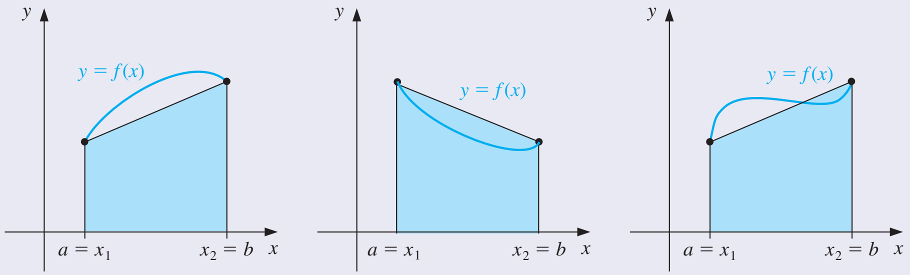
Gaussian Quadrature: Contrast with Newton-Cotes

Features of a Newton-Cotes Formula (Cont'd)

- All the Newton-Cotes formulas use values of the function at equally-spaced points.
- This restriction is convenient when the formulas are combined to form the composite rules which we considered earlier, . . .
- but it can significantly decrease the accuracy of the approximation.

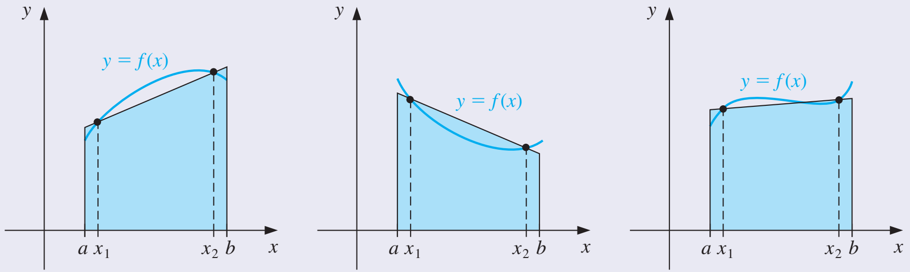
Consider, for example, the Trapezoidal rule applied to determine the integrals of the functions whose graphs are as shown.



It approximates the integral of the function by integrating the linear function that joins the endpoints of the graph of the function.

Gaussian Integration: Optimal integration points

But this is not likely the best line for approximating the integral. Lines such as those shown below would likely give much better approximations in most cases.



Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally-spaced, way.

Gaussian Quadrature: Introduction

Choice of Integration Nodes

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Choice of Integration Nodes

- The nodes $x_1, x_2, \ldots, x_n$ in the interval $[a, b]$ and coefficients $c_1, c_2, \ldots, c_n$, are chosen to minimize the expected error obtained in the approximation

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

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- that is, the choice that gives the greatest degree of precision.

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- The coefficients $c_1, c_2, \ldots, c_n$ in the approximation formula are arbitrary, and the nodes $x_1, x_2, \ldots, x_n$ are restricted only by the fact that they must lie in $[a, b]$, the interval of integration.

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- This gives us $2n$ parameters to choose.

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- This, then, is the largest class of polynomials for which it is reasonable to expect a formula to be exact.
- With the proper choice of the values and constants, exactness on this set can be obtained.

Gaussian Quadrature: Illustration ($n = 2$)

Example: Formula when $n = 2$ on $[-1, 1]$

Suppose we want to determine c_1, c_2, x_1, and x_2 so that the integration formula

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2)$$

gives the exact result whenever $f(x)$ is a polynomial of degree $2(2) - 1 = 3$ or less, that is, when

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3,$$

for some collection of constants, a_0, a_1, a_2, and a_3.

Gaussian Quadrature: Illustration ($n = 2$)

Finding the Formula Coefficients (1/3)

Because

$$\int (a_0 + a_1 x + a_2 x^2 + a_3 x^3)\, dx$$
$$= a_0 \int 1\, dx + a_1 \int x\, dx + a_2 \int x^2\, dx + a_3 \int x^3\, dx$$

this is equivalent to showing that the formula gives exact results when $f(x)$ is 1, x, x^2, and x^3.

Gaussian Quadrature: Illustration ($n = 2$)

Finding the Formula Coefficients (2/3)

Hence, we need c_1, c_2, x_1, and x_2, so that

$$c_1 \cdot 1 + c_2 \cdot 1 = \int_{-1}^{1} 1\, dx = 2$$

Gaussian Quadrature: Illustration ($n = 2$)

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c_1 \cdot 1 + c_2 \cdot 1 &= \int_{-1}^{1} 1\, dx = 2 \\
c_1 \cdot x_1 + c_2 \cdot x_2 &= \int_{-1}^{1} x\, dx = 0 \\
c_1 \cdot x_1^2 + c_2 \cdot x_2^2 &= \int_{-1}^{1} x^2\, dx = \frac{2}{3} \\
c_1 \cdot x_1^3 + c_2 \cdot x_2^3 &= \int_{-1}^{1} x^3\, dx = 0
\end{aligned}$$

Gaussian Quadrature: Illustration ($n = 2$)

Finding the Formula Coefficients (3/3)

A little algebra shows that this system of equations has the unique solution

$$c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3} \quad \text{and} \quad x_2 = \frac{\sqrt{3}}{3},$$

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This formula has degree of precision 3, that is, it produces the exact result for every polynomial of degree 3 or less.

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Gaussian Quadrature: Legendre Polynomials

An Alternative Method of Derivation

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Gaussian Quadrature: Legendre Polynomials

An Alternative Method of Derivation

- We will consider an approach which generates more easily the nodes and coefficients for formulas that give exact results for higher-degree polynomials.
- This will be achieved using a particular set of orthogonal polynomials (functions with the property that a particular definite integral of the product of any two of them is 0).
- This set is the is the Legendre polynomials, a collection $\{P_0(x), P_1(x), \ldots, P_n(x), \ldots, \}$ with properties:
  - **(1)** For each n, $P_n(x)$ is a monic polynomial of degree n.
  - **(2)** $\displaystyle\int_{-1}^{1} P(x)P_n(x)\,dx = 0$ whenever $P(x)$ is a polynomial of degree less than n.

Gaussian Quadrature: Legendre Polynomials

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The first few Legendre Polynomials

$$P_0(x) = 1, \qquad P_1(x) = x, \qquad P_2(x) = x^2 - \frac{1}{3}$$

$$P_3(x) = x^3 - \frac{3}{5}x \qquad \text{and} \qquad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}$$

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The nodes $x_1, x_2, \ldots, x_n$ needed to produce an integral approximation formula that gives exact results for any polynomial of degree less than $2n$ are the roots of the nth-degree Legendre polynomial.

Gaussian Quadrature: Legendre Polynomials

Theorem

Suppose that $x_1, x_2, \ldots, x_n$ are the roots of the nth Legendre polynomial $P_n(x)$ and that for each $i = 1, 2, \ldots, n$, the numbers c_i are defined by

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \, dx$$

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If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^{1} P(x) \, dx = \sum_{i=1}^{n} c_i P(x_i)$$

Gaussian Quadrature: Legendre Polynomials

Proof (1/5)

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- The error term for this representation involves the nth derivative of $P(x)$.
- Since $P(x)$ is of degree less than n, the nth derivative of $P(x)$ is 0, and this representation of is exact. So

Gaussian Quadrature: Legendre Polynomials

Proof (2/5)

Gaussian Quadrature: Legendre Polynomials

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Therefore

$$P(x) = \sum_{i=1}^{n} P(x_i)L_i(x) = \sum_{i=1}^{n} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} P(x_i)$$

Gaussian Quadrature: Legendre Polynomials

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and

$$\int_{-1}^{1} P(x)\, dx = \int_{-1}^{1} \left[\sum_{i=1}^{n} \prod_{\substack{j=1 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} P(x_i) \right] dx$$

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and

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$$= \sum_{i=1}^{n} \left[\int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx \right] P(x_i) = \sum_{i=1}^{n} c_i P(x_i)$$

Hence the result is true for polynomials of degree less than n.

Gaussian Quadrature: Legendre Polynomials

Proof (3/5)

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Gaussian Quadrature: Legendre Polynomials

Proof (3/5)

- Now consider a polynomial $P(x)$ of degree at least n but less than $2n$.
- Divide $P(x)$ by the nth Legendre polynomial $P_n(x)$.
- This gives two polynomials $Q(x)$ and $R(x)$, each of degree less than n, with

$$P(x) = Q(x)P_n(x) + R(x)$$

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$$P(x) = Q(x)P_n(x) + R(x)$$

- Note that x_i is a root of $P_n(x)$ for each $i = 1, 2, \ldots, n$, so we have

$$P(x_i) = Q(x_i)P_n(x_i) + R(x_i) = R(x_i)$$

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- Note that x_i is a root of $P_n(x)$ for each $i = 1, 2, \ldots, n$, so we have
$$P(x_i) = Q(x_i)P_n(x_i) + R(x_i) = R(x_i)$$
- We now invoke the unique power of the Legendre polynomials.

Gaussian Quadrature: Legendre Polynomials

Proof (4/5)

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First, the degree of the polynomial $Q(x)$ is less than n, so (by the Legendre orthogonality property),

$$\int_{-1}^{1} Q(x)P_n(x)\,dx = 0$$

Gaussian Quadrature: Legendre Polynomials

Proof (4/5)

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$$\int_{-1}^{1} Q(x)P_n(x)\,dx = 0$$

Then, since $R(x)$ is a polynomial of degree less than n, the opening argument implies that

$$\int_{-1}^{1} R(x)\,dx = \sum_{i=1}^{n} c_i R(x_i)$$

Gaussian Quadrature: Legendre Polynomials

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Putting these facts together verifies that the formula is exact for the polynomial $P(x)$:

$$\int_{-1}^{1} P(x)\,dx = \int_{-1}^{1} [Q(x)P_n(x) + R(x)]\,dx$$

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Putting these facts together verifies that the formula is exact for the polynomial $P(x)$:

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Gaussian Quadrature: Roots & Coefficients

The constants c_i needed for the quadrature rule can be generated from the equation given in the theorem:

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \, dx$$

but both these constants and the roots of the Legendre polynomials are extensively tabulated.

The following table lists these values for $n = 2, 3, 4$, and 5.

Gaussian Quadrature Rules: Roots & Coefficients

n	Roots $r_{n,i}$	Coefficients $c_{n,i}$
2	0.5773502692	1.0000000000
	−0.5773502692	1.0000000000
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	−0.7745966692	0.5555555556
4	0.8611363116	0.3478548451
	0.3399810436	0.6521451549
	−0.3399810436	0.6521451549
	−0.8611363116	0.3478548451
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286705
	0.0000000000	0.5688888889
	−0.5384693101	0.4786286705
	−0.9061798459	0.2369268850

Gaussian Quadrature: Legendre Polynomials

Example ($n = 2$)

Approximate $\int_{-1}^{1} e^x \cos x \, dx$ using Gaussian quadrature with $n = 3$.

Solution

The entries in the table of roots and coefficients ▸ See Table

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The entries in the table of roots and coefficients ▸ See Table give us

$$\begin{aligned}\int_{-1}^{1} e^x \cos x \, dx &\approx 0.\overline{5}e^{0.774596692} \cos 0.774596692 + 0.\overline{8} \cos 0 \\ &+ 0.\overline{5}e^{-0.774596692} \cos(-0.774596692) \\ &= 1.9333904.\end{aligned}$$

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Integration by parts can be used to show that the true value of the integral is 1.9334214, so the absolute error is less than 3.2×10^{-5}.

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Gaussian Quadrature on Arbitrary Intervals

Transform the Interval of Integration to $[-1, 1]$

An integral $\int_a^b f(x)\,dx$ over an arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using the change of variables See Diagram:

$$t = \frac{2x - a - b}{b - a} \iff x = \frac{1}{2}[(b - a)t + a + b]$$

Gaussian Quadrature on Arbitrary Intervals

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This permits Gaussian quadrature to be applied to any interval $[a, b]$, because

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b - a)t + (b + a)}{2}\right)\frac{(b - a)}{2}\,dt$$

Gaussian Quadrature on Arbitrary Intervals

Example: Comparing Formulae

Consider the integral

$$\int_1^3 x^6 - x^2 \sin(2x)\, dx = 317.3442466.$$

Gaussian Quadrature on Arbitrary Intervals

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Gaussian Quadrature on Arbitrary Intervals

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(a) Compare the results for the closed Newton-Cotes formula with $n = 1$, the open Newton-Cotes formula with $n = 1$, and Gaussian Quadrature when $n = 2$.

(b) Compare the results for the closed Newton-Cotes formula with $n = 2$, the open Newton-Cotes formula with $n = 2$, and Gaussian Quadrature when $n = 3$.

Solution: Part (a): Newton-Cotes Formulae ($n = 1$)

Each of the formulas in this part requires 2 evaluations of the function $f(x) = x^6 - x^2 \sin(2x)$. The Newton-Cotes approximations ▸ See Formulae are:

$$\textbf{Closed n} = \mathbf{1}: \quad \frac{2)}{2}[f(1) + f(3)] = 731.6054420$$

$$\textbf{Open n} = \mathbf{1}: \quad \frac{3(2/3)}{2}[f(5/3) + f(7/3)] = 188.7856682$$

Gaussian Quadrature on Arbitrary Intervals

Solution: Part (a): Gaussian Quadrature ($n = 2$)

Gaussian quadrature applied to this problem requires that the integral first be transformed into a problem whose interval of integration is $[-1, 1]$. Using the ▸ transformation gives

$$\int_1^3 x^6 - x^2 \sin(2x)\, dx = \int_{-1}^1 (t+2)^6 - (t+2)^2 \sin(2(t+2))\, dt.$$

Gaussian Quadrature on Arbitrary Intervals

Solution: Part (a): Gaussian Quadrature ($n = 2$)

Gaussian quadrature applied to this problem requires that the integral first be transformed into a problem whose interval of integration is $[-1, 1]$. Using the transformation gives

$$\int_1^3 x^6 - x^2 \sin(2x)\, dx = \int_{-1}^1 (t+2)^6 - (t+2)^2 \sin(2(t+2))\, dt.$$

Gaussian quadrature with $n = 2$ then gives

$$\begin{aligned} & \int_1^3 x^6 - x^2 \sin(2x)\, dx \\ \approx\ & f(-0.5773502692 + 2) + f(0.5773502692 + 2) \\ =\ & 306.8199344 \end{aligned}$$

Gaussian Quadrature on Arbitrary Intervals

Solution: Part (b): Newton-Cotes Formulae ($n = 2$)

Each of the formulas in this part requires 3 function evaluations. The Newton-Cotes approximations ▸ See Formulae are:

$$\textbf{Closed n} = \textbf{2}: \quad \frac{1)}{3}[f(1) + 4f(2) + f(3)] = 333.2380940$$

$$\textbf{Open n} = \textbf{2}: \quad \frac{4(1/2)}{3}[2f(1.5) - f(2) + 2f(2.5)] = 303.5912023$$

Gaussian Quadrature on Arbitrary Intervals

Solution: Part (b): Gaussian Quadrature ($n = 3$)

Gaussian quadrature with $n = 3$, once the ▸ transformation has been done, gives

$$\begin{aligned}
&\int_1^3 x^6 - x^2 \sin(2x)\, dx \\
\approx\;& 0.\overline{5} f(-0.7745966692 + 2) + 0.\overline{8} f(2) + 0.\overline{5} f(-0.7745966692 + 2) \\
=\;& 317.2641516
\end{aligned}$$

Gaussian Quadrature on Arbitrary Intervals

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Gaussian Quadrature on Arbitrary Intervals

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Comparison of Results

	Newton-Cotes		
	Closed	Open	Gaussian Quadrature
2-Point Rule	731.6054420	188.7856682	306.8199344
3-Point Rule	333.2380940	303.5912023	317.2641516

The Gaussian quadrature results are clearly superior in each instance.

Questions?

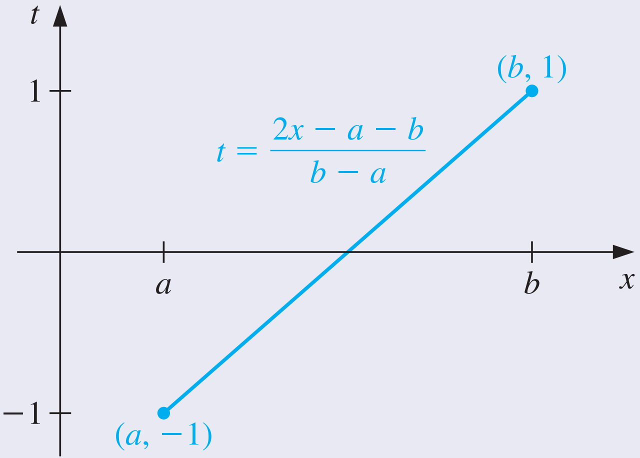
Reference Material

Gaussian Quadrature Rules: Roots & Coefficients

n	Roots $r_{n,i}$	Coefficients $c_{n,i}$
2	0.5773502692	1.0000000000
	−0.5773502692	1.0000000000
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	−0.7745966692	0.5555555556
4	0.8611363116	0.3478548451
	0.3399810436	0.6521451549
	−0.3399810436	0.6521451549
	−0.8611363116	0.3478548451
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286705
	0.0000000000	0.5688888889
	−0.5384693101	0.4786286705
	−0.9061798459	0.2369268850

Return to $\int_{-1}^{1} e^x \cos(x)\,dx$ Example

Mapping Interval $[a, b]$ onto $[-1, 1]$



◂ Return to Gaussian Quadrature on Arbitrary Intervals (Introduction)

◂ Return to Gaussian Quadrature on Arbitrary Intervals (Example Part (a))

◂ Return to Gaussian Quadrature on Arbitrary Intervals (Example Part (b))

Open & Closed Newton-Cotes Formulae ($n = 1$)

- **Closed $n = 1$**: Trapezoidal Rule:

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi)$$

  where $x_0 < \xi < x_1$.

- **Open $n = 1$**:

$$\int_{x_{-1}}^{x_2} f(x)\,dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4} f''(\xi)$$

  where $x_{-1} < \xi < x_2$.

Return to arbitrary intervals Example (where $n = 1$)

Open & Closed Newton-Cotes Formulae ($n = 2$)

- $n = 0$: Midpoint Rule:

$$\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi)$$

  where $x_{-1} < \xi < x_1$.

- **Open** $n = 2$

$$\int_{x_{-1}}^{x_3} f(x)\,dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45} f^{(4)}(\xi)$$

  where $x_{-1} < \xi < x_3$.

◂ Return to arbitrary intervals Example (where $n = 1$)