Numerical Analysis and Computing

Lecture Notes #08

— Numerical Differentiation and Integration — Composite Numerical Integration; Romberg Integration Adaptive Quadrature / Gaussian Quadrature

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Composite-Romberg-Adaptive-Gaussian

— (1/43)

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Divide and Conquer; Example — Simpson's Rule Collecting the Error.

Divide and Conquer with Simpson's Rule

1/111

The exact solution:

$$\int_0^4 e^x dx = e^4 - e^0 = 53.59815$$

Simpson's Rule with h = 2

$$\int_0^4 e^x dx \approx \frac{2}{3} (e^0 + 4e^2 + e^4) = 56.76958.$$

The error is -3.17143 (5.92%).

Divide-and-Conquer: Simpson's Rule with h = 1

$$\int_0^2 e^x dx + \int_2^4 e^x dx \approx \frac{1}{3} (e^0 + 4e^1 + e^2) + \frac{1}{3} (e^2 + 4e^3 + e^4) = 53.86385$$

The error is -0.26570. (0.50%) Improvement by a factor of 10!

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Outline

- Composite Quadrature
 - Divide and Conquer: Example Simpson's Rule
 - Generalization
 - Collecting the Error...
- Romberg Quadrature
 - Applying Richardson's Extrapolation
 - Romberg Quadrature Code Outline
- Adaptive Quadrature
 - Introduction
 - Building the Adaptive CSR Scheme
 - Example...
 - Putting it Together...
- Gaussian Quadrature
 - Ideas...
 - 2-point Gaussian Quadrature
 - Higher-Order Gaussian Quadrature Legendre Polynomials
 - Examples: Gaussian Quadrature in Action; HW#7

11/111

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Composite-Romberg-Adaptive-Gaussian

— (2/43)

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Divide and Conquer; Example — Simpson's Rule Collecting the Error.

Divide and Conquer with Simpson's Rule

The exact solution:

$$\int_0^4 e^x dx = e^4 - e^0 = 53.59815$$

Divide-and-Conquer: Simpson's Rule with h = 1/2

$$\int_{0}^{1} + \int_{1}^{2} + \int_{2}^{3} + \int_{3}^{4} e^{x} dx \approx \frac{1}{6} (e^{0} + 4e^{1/2} + e^{1}) + \frac{1}{6} (e^{1} + 4e^{3/2} + e^{2}) + \frac{1}{6} (e^{2} + 4e^{5/2} + e^{3}) + \frac{1}{6} (e^{3} + 4e^{7/2} + e^{4}) = 53.61622$$

The error has been reduced to -0.01807 (0.034%).

	h	abs-error	err/ <i>h</i>	err/ <i>h</i> ²	err/ <i>h</i> 3	err/ <i>h</i> ⁴
	2	3.17143	1.585715	0.792857	0.396429	0.198214
	1	0.26570	0.265700	0.265700	0.265700	0.265700
1/	/2	0.01807	0.036140	0.072280	0.144560	0.289120

Divide and Conquer with Simpson's Rule

111/111

Extending the table...

h	abs-error	err/h	err/h ²	err/h ³	err/h ⁴	err/ h^{5}
2	3.171433	1.585716	0.792858	0.396429	0.198215	0.099107
1	0.265696	0.265696	0.265696	0.265696	0.265696	0.265696
1/2	0.018071	0.036142	0.072283	0.144566	0.289132	0.578264
1/4	0.001155	0.004618	0.018473	0.073892	0.295566	1.182266
1/8	0.000073	0.000580	0.004644	0.037152	0.297215	2.377716

Clearly, the err/ h^4 column seems to converge (to a non-zero constant) as $h \setminus 0$. The columns to the left seem to converge to zero, and the err/ h^5 column seems to grow.

This is **numerical evidence** that the composite Simpson's rule has a convergence rate of $\mathcal{O}(h^4)$. But, isn't Simpson's rule 5th order???

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Composite-Romberg-Adaptive-Gaussian

— (5/43)

Romberg Quadrature

Divide and Conquer; Example — Simpson's Rule Collecting the Error.

Generalized Composite Simpson's Rule

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$\int_{a}^{b} f(x)dx = \frac{h}{3} \left[f(x_0) - f(x_n) + \sum_{i=1}^{n/2} \left[4f(x_{2i-1}) + 2f(x_{2i}) \right] \right]$ $-\frac{h^5}{90}\sum_{i=1}^{n/2}f^{(4)}(\xi_j).$

The error term is:

$$E(f) = -rac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j), \quad \xi_j \in [x_{2j-2}, x_{2j}]$$

Generalized Composite Simpson's Rule

For an even integer n: Subdivide the interval [a, b] into nsubintervals, and apply Simpson's rule on each consecutive pair of sub-intervals. With h=(b-a)/n and $x_i=a+jh$, $j=0,1,\ldots,n$, we have

$$\int_{a}^{b} f(x)dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx$$

$$= \sum_{j=1}^{n/2} \left\{ \frac{h}{3} \left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j}) \right] - \frac{h^{5}}{90} f^{(4)}(\xi_{j}) \right\},$$

for some $\xi_i \in [x_{2i-2}, x_{2i}]$, if $f \in C^4[a, b]$.

Since all the interior "even" x_{2i} points appear twice in the sum, we can simplify the expression a bit...

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Romberg Quadrature

Divide and Conquer; Example — Simpson's Rule Collecting the Error..

The Error for Composite Simpson's Rule

If $f \in C^4[a, b]$, the Extreme Value Theorem implies that $f^{(4)}$ assumes its max and min in [a, b]. Now, since

$$\min_{x \in [a,b]} f^{(4)}(x) \le f^{(4)}(\xi_j) \le \max_{x \in [a,b]} f^{(4)}(x),$$

$$\left[\frac{n}{2}\right] \min_{x \in [a,b]} f^{(4)}(x) \leq \sum_{i=1}^{n/2} f^{(4)}(\xi_i) \leq \left[\frac{n}{2}\right] \max_{x \in [a,b]} f^{(4)}(x),$$

$$\min_{x \in [a,b]} f^{(4)}(x) \le \left[\frac{2}{n}\right] \sum_{i=1}^{n/2} f^{(4)}(\xi_i) \le \max_{x \in [a,b]} f^{(4)}(x),$$

By the Intermediate Value Theorem $\exists \mu \in (a, b)$ so that

$$f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \quad \Leftrightarrow \quad \frac{n}{2} f^{(4)}(\mu) = \sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

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The Error for Composite Simpson's Rule

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We can now rewrite the error term:

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu),$$

or, since $h = (b - a)/n \Leftrightarrow n = (b - a)/h$, we can write

$$E(f) = -\frac{(b-a)}{180} \mathbf{h^4 f^{(4)}}(\mu).$$

Hence Composite Simpson's Rule has degree of accuracy 3 (since it is exact for polynomials up to order 3), and the error is proportional to h^4 — Convergence Rate $\mathcal{O}(h^4)$.

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— (9/43) Composite-Romberg-Adaptive-Gaussian

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Divide and Conquer; Example — Simpson's Rule Generalization Collecting the Error...

Homework #7 — Due Friday 11/13/2009, 12-noon

(Part-1)

Implement Composite Simpson's Rule, and use your code to solve BF-4.4.3-a,b,c,d.

Composite Simpson's Rule — Algorithm

Algorithm (Composite Simpson's Rule)

Given the end points a and b and an even positive integer n:

[1]
$$h = (b - a)/n$$

[2] ENDPTS =
$$f(a)+f(b)$$

ODDPTS = 0
EVENPTS = 0

[3] FOR
$$i = 1, ..., n-1$$
 — (interior points) $x = a + i * h$

if
$$i$$
 is even: EVENPTS += $f(x)$
if i is odd: ODDPTS += $f(x)$

END

INTAPPROX = h*(ENDPTS+2*EVENPTS+4*ODDPTS)/3

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(10/43)

Romberg Quadrature Adaptive Quadrature

Applying Richardson's Extrapolation omberg Quadrature — Code Outline

Romberg Integration

The Return of Richardson's Extrapolation

Romberg Integration is the combination of the Composite Trapezoidal Rule (CTR)

$$\int_{a}^{b} f(x)dx = \frac{h}{2} \left[f(a) + f(b) + 2 \sum_{j=1}^{n-1} f(x_{j}) \right] - \frac{(b-a)}{12} h^{2} f''(\mu)$$

and Richardson Extrapolation.

Here, we know that the error term for regular Trapezoidal Rule is $\mathcal{O}(h^3)$. By the same argument as for Composite Simpson's Rule, this gets reduced to $\mathcal{O}(h^2)$ for the composite version.

Romberg Integration

Step-1: CTR Refinement

Let $R_{k,1}$ denote the Composite Trapezoidal Rule with 2^{k-1} sub-intervals, and $h_k = (b-a)/2^{k-1}$. We get:

$$R_{1,1} = \frac{h_1}{2} [f(a) + f(b)]$$

$$R_{2,1} = \frac{h_2}{2} [f(a) + 2f(a + h_2) + f(b)]$$

$$= \frac{(b-a)}{4} [f(a) + f(b) + 2f(a + h_2)]$$

$$= \frac{1}{2} [R_{1,1} + h_1 f(a + h_2)]$$
.

 $R_{k,1} = \frac{1}{2} \left| R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k) \right|$

Update formula, using previous value + new points

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- (13/43)

Romberg Quadrature Adaptive Quadrature

Applying Richardson's Extrapolation Romberg Quadrature — Code Outline

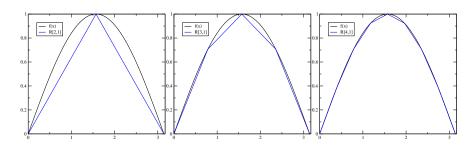
Extrapolate using Richardson

We know that the error term is $\mathcal{O}(h^2)$, so in order to eliminate this term we combine to consecutive entries $R_{k-1,1}$ and $R_{k,1}$ to form a higher order approximation $R_{k,2}$ of the integral.

$$R_{k,2} = R_{k,1} + \frac{R_{k,1} - R_{k-1,1}}{2^2 - 1}$$

$R_{k,2}$
0
2.09439510239
2.00455975498
2.00026916994
2.00001659104
2.00000103336
2.00000006453

Example: $R_{k,1}$ for $\int_0^{\pi} \sin(x) dx$



	k	$R_{k,1}$
ſ	1	0
	2	1.5707963267949
	3	1.8961188979370
	4	1.9742316019455
	5	1.9935703437723
	6	1.9983933609701
	7	1.9995983886400

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- (14/43)

Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Applying Richardson's Extrapolation Romberg Quadrature — Code Outline

Extrapolate, again...

It turns out (Taylor expand to check) that the complete error term for the Trapezoidal rule only has even powers of h:

$$\int_{a}^{b} f(x) = R_{k,1} - \sum_{i=1}^{\infty} E_{2i} h_{k}^{2i}.$$

Hence the $R_{k,2}$ approximations have error terms that are of size $\mathcal{O}(h^4)$.

To get $\mathcal{O}(h^6)$ approximations, we compute

$$R_{k,3} = R_{k,2} + \frac{R_{k,2} - R_{k-1,2}}{4^2 - 1}$$

Extrapolate, yet again...

In general, since we only have even powers of h in the error expansion:

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$

Revisiting $\int_0^{\pi} \sin(x) dx$:

	$R_{k,1}-\mathcal{O}\left(h^2\right)$	$R_{k,2}-\mathcal{O}\left(h^4\right)$	$R_{k,3}-\mathcal{O}\left(h^6\right)$	$R_{k,4} - \mathcal{O}\left(h^{8}\right)$
	0			
ll	1.570796326794897	2.094395102393195		
	1.896118897937040	2.004559754984421	1.998570731823836	
li	1.974231601945551	2.000269169948388	1.999983130945986	2.000005549979671
li	1.993570343772340	2.000016591047935	1.999999752454572	2.000000016288042
	1.998393360970145	2.000001033369413	1.999999996190845	2.000000000059674
	1.999598388640037	2.000000064530001	1.99999999940707	2.000000000000229



end disp(R)

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Composite-Romberg-Adaptive-Gaussian

— (17/43)

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Building the Adaptive CSR Scheme

More Advanced Numerical Integration Ideas

Adaptive and Gaussian Quadrature

Homework? No, enough already — Here's the code outline!

```
Code (Romberg Quadrature)
% Romberg Integration for sin(x) over [0,pi]
a = 0; b = pi; % The Endpoints
R = zeros(7,7);
R(1,1) = (b-a)/2 * (\sin(a) + \sin(b));
for k = 2:7
 h = (b-a)/2^{(k-1)};
 R(k,1)=1/2*(R(k-1,1)+2*h*\sum(\sin(a+(2*(1:(2^{(k-2)}))-1)*h)));
for j = 2:7
 for k = i : 7
  R(k,j) = R(k,j-1) + (R(k,j-1) - R(k-1,j-1))/(4^{(j-1)}-1);
```

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Composite-Romberg-Adaptive-Gaussian

- (18/43)

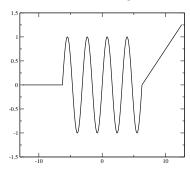
Adaptive Quadrature

Composite Quadrature Romberg Quadrature Adaptive Quadrature Introduction **Building the Adaptive CSR Scheme**

Introduction

The composite formulas require equally spaced nodes.

This is not good if the function we are trying to integrate has both regions with large fluctuations, and regions with small variations.



We need many points where the function fluctuates, but few points where it is close to constant or linear.

5050 (19/43)

Idea Cleverly predict (or measure) the amount of variation and automatically add more points where needed.

We are going to discuss this in the context of Composite Simpson's rule, but the approach can be adopted for other integration schemes.

First we are going to develop a way to measure the error a numerical estimate of the actual error in the numerical integration. Note: just knowing the structure of the error term is not enough! (We will however use the structure of the error term in our derivation of the numerical error estimate.)

Then we will use the error estimate to decide whether to accept the value from CSR, or if we need to refine further (recompute with smaller h).

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Composite-Romberg-Adaptive-Gaussian

- (21/43)

Romberg Quadrature Adaptive Quadrature

Building the Adaptive CSR Scheme Putting it Together..

Composite Simpson's Rule (CSR)

With this notation, we can write CSR with n = 4, and $h_2 = (b-a)/4 = h_1/2$:

$$\int_a^b f(x) dx = S(f; a, \frac{a+b}{2}) + S(f; \frac{a+b}{2}, b) - E(f; h_2, \mu_2).$$

We can squeeze out an estimate for the error by noticing that

$$E(f; h_2, \mu_2) = \frac{1}{16} \left(\frac{h_1^5}{90} f^{(4)}(\mu_2) \right) = \frac{1}{16} E(f; h_1, \mu_2).$$

Now, assuming $f^{(4)}(\mu_1) \approx f^{(4)}(\mu_2)$, we do a little bit of algebra magic with our two approximations to the integral...

Some Notation — One-step Simpson's Rule

S(f; a, b)

Notation — "One-step" Simpson's Rule:

$$\int_{a}^{b} f(x) dx = S(f; a, b) - \underbrace{\frac{h_{1}^{5}}{90} f^{(4)}(\mu_{1})}_{\mathbf{E}(f; \mathbf{h}_{1}, \mu_{1})}, \quad \mu_{1} \in (a, b),$$

where

$$S(f; a, b) = \frac{(b-a)}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right], \quad h_1 = \frac{(b-a)}{2}.$$

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Composite-Romberg-Adaptive-Gaussian

(22/43)

Adaptive Quadrature

Building the Adaptive CSR Scheme

Wait! Wait! — I pulled a fast one!

$$E(f; h_2, \mu_2) = \frac{1}{32} \left(\frac{h_1^5}{90} f^{(4)}(\mu_2^1) \right) + \frac{1}{32} \left(\frac{h_1^5}{90} f^{(4)}(\mu_2^2) \right)$$

where $\mu_2^1 \in [a, \frac{a+b}{2}], \, \mu_2^2 \in [\frac{a+b}{2}, b].$

If $f \in C^4[a, b]$, then we can use our old friend, the **intermediate** value theorem:

$$\exists \mu_2 \in [\mu_2^1, \mu_2^2] \subset [a, b] : f^{(4)}(\mu_2) = \frac{f^{(4)}(\mu_2^1) + f^{(4)}(\mu_2^2)}{2}.$$

So it follows that

$$E(f; h_2, \mu_2) = \frac{1}{16} \left(\frac{h_1^5}{90} f^{(4)}(\mu_2) \right).$$

Back to the Error Estimate...

Now we have

$$S(f; a, \frac{a+b}{2}) + S(f; \frac{a+b}{2}, b) - \frac{1}{16} \left(\frac{h_1^5}{90} f^{(4)}(\mu_2) \right)$$
$$= S(f; a, b) - \frac{h_1^5}{90} f^{(4)}(\mu_1).$$

Now use the assumption $f^{(4)}(\mu_1) \approx f^{(4)}(\mu_2)$ (and replace μ_1 and μ_2 by μ):

$$\frac{\mathbf{h_{1}^{5}}}{\mathbf{90}}\mathbf{f^{(4)}}(\mu) \approx \frac{16}{15} \left[S(f; a, b) - S(f; a, (a+b)/2) - S(f; (a+b)/2, b) \right],$$

notice that $\frac{h_1^5}{90}f^{(4)}(\mu) = E(f; h_1, \mu) = 16E(f; h_2, \mu)$. Hence

$$E(f; h_2, \mu) \approx \frac{1}{15} \bigg[S(f; a, b) - S(f; a, (a+b)/2) - S(f; (a+b)/2, b) \bigg],$$

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Composite-Romberg-Adaptive-Gaussian — (25/43)

Introduction
Building the Adaptive CSR Scheme

Adaptive Quadrature
Gaussian Quadrature

Example...
Putting it Together..

Example — Error Estimates

1/11

We will apply Simpson's rule to

$$\int_0^{\pi/2} \sin(x) dx = 1.$$

Here,

$$\mathbb{S}_1(\sin(x); 0, \pi/2) = S(\sin(x); 0, \pi/2)$$

$$= \frac{\pi}{12} \left[\sin(0) + 4\sin(\pi/4) + \sin(\pi/2) \right] = \frac{\pi}{12} \left[2\sqrt{2} + 1 \right]$$
$$= 1.00227987749221.$$

$$\mathbb{S}_2(\sin(x); 0, \pi/2) = S(\sin(x); 0, \pi/4) + S(\sin(x); \pi/4, \pi/2)$$

$$= \frac{\pi}{24} \left[\sin(0) + 4\sin(\pi/8) + 2\sin(\pi/4) + 4\sin(3\pi/8) + \sin(\pi/2) \right]$$

= 1.00013458497419.

Finally, we have the error estimate in hand...

Using the estimate of $\frac{h_1^5}{90}f^{(4)}(\mu)$, we have

Error Estimate for CSR

$$\begin{split} \left| \int_{a}^{b} f(x) dx - S(f; \ a, (a+b)/2) - S(f; \ (a+b)/2, b) \right| \\ \approx \frac{1}{15} \left| S(f; \ a, b) - S(f; \ a, (a+b)/2) - S(f; \ (a+b)/2, b) \right| \end{split}$$

Notice!!! S(f; a, (a + b)/2) + S(f; (a + b)/2, b) approximates $\int_a^b f(x) dx$ **15 times better** than it agrees with the known quantity S(f; a, b)!!!

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Composite-Romberg-Adaptive-Gaussian

(26/42)

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Introduction
Building the Adaptive CSR Scheme
Example...

Example — Error Estimates

The error estimate is given by

$$\frac{1}{15} \left[\mathbb{S}_1(\sin(x); 0, \pi/2) - \mathbb{S}_2(\sin(x); 0, \pi/2) \right] \\
= \frac{1}{15} \left[1.00227987749221 - 1.00013458497419 \right] \\
= 0.00014301950120.$$

This is a very good approximation of the actual error, which is 0.00013458497419.

OK, we know how to get an error estimate. How do we use this to create an adaptive integration scheme???

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Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Adaptive Quadrature

We want to approximate $\mathcal{I} = \int_a^b f(x) dx$ with an error less than ϵ (a specified tolerance).

- [1] Compute the two approximations $\mathbb{S}_1(f(x); a, b) = S(f(x); a, b)$, and $\mathbb{S}_2(f(x); a, b) = S(f(x); a, \frac{a+b}{2}) + S(f(x); \frac{a+b}{2}, b)$.
- [2] Estimate the error, if the estimate is less than ϵ , we are done. Otherwise...
- [3] Apply steps [1] and [2] recursively to the intervals $[a, \frac{a+b}{2}]$ and $[\frac{a+b}{2}, b]$ with tolerance $\epsilon/2$.

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Composite-Romberg-Adaptive-Gaussian

— (29/43)

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature Introduction
Building the Adaptive CSR Scheme
Example...
Putting it Together...

Adaptive Quadrature, Interval Refinement Example #2

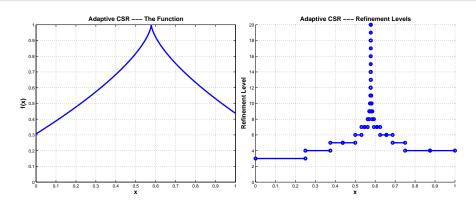
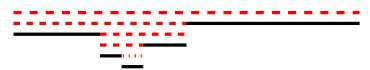


Figure: Application of adaptive CSR to the function $f(x)=1-\sqrt[3]{(x-\frac{\pi}{2e})^2}$. Here, we have required that the estimated error be less than 10^{-6} . The left panel shows the function, and the right panel shows the number of refinement levels needed to reach the desired accuracy. At completion we have the value of the integral being 0.61692712, with an estimated error of $3.93 \cdot 10^{-7}$.

Adaptive Quadrature, Interval Refinement Example #1



The funny figure above is supposed to illustrate a possible sub-interval refinement hierarchy. **Red** dashed lines illustrate failure to satisfy the tolerance, and **black** lines illustrate satisfied tolerance.

level	tol	interval	
1	ϵ	[a, b]	
2	$\epsilon/2$	$[a, a + \frac{b-a}{2}]$	$[\mathbf{a} + (\mathbf{b} - \mathbf{a})/2, \mathbf{b}]$
3	$\epsilon/4$	$[a, a + \frac{b-a}{4}]$ $[a + \frac{b-a}{4}, a + \frac{b-a}{2}]$	
:			

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Composite-Romberg-Adaptive-Gaussian

— (30/43)

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Ideas...
2-point Gaussian Quadrature

2-point Gaussian Quadrature

Higher-Order Gaussian Quadrature

Legendre Polynomials

Examples: Gaussian Quadrature in Action; HW#7

Gaussian Quadrature

Idea: Evaluate the function at a set of **optimally chosen** points in the interval.

We will choose $\{x_0, x_1, \dots, x_n\} \in [a, b]$ and coefficients c_i , so that the approximation

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

is exact for the largest class of polynomials possible.

We have already seen that the open Newton-Cotes formulas sometimes give us better "bang-for-buck" than the closed formulas (e.g. the mid-point formula uses only 1 point and is as accurate as the two-point trapezoidal rule). — Gaussian quadrature takes this one step further.

Examples: Gaussian Quadrature in Action; HW#7

Quadrature Types — A Comparison

	Newton-Cotes		Gaussian
	Open	Closed	
Quadrature Points	Degree of Accuracy	Degree of Accuracy	Degree of Accuracy
1	1*		1
2	1	1 [†]	3
3	3	3 #	5
4	3	3	7
5	5	5	9

* — The mid-point rule.

† — Trapezoidal rule.

— Simpson's rule.

The mid-point rule is the only optimal scheme we have see so far.



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Composite-Romberg-Adaptive-Gaussian

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Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

2-point Gaussian Quadrature Higher-Order Gaussian Quadrature — Legendre Polynomials

Higher Order Gaussian Quadrature Formulas

We could obtain higher order formulas by adding more points, computing the integrals, and solving the resulting non-linear system of equations... but it gets very painful, very fast.

The **Legendre Polynomials** come to our rescue!

The Legendre polynomials $P_n(x)$ are orthogonal on [-1,1] with respect to the weight function w(x) = 1, i.e.

$$\int_{-1}^{1} P_n(x) P_m(x) dx = \alpha_n \delta_{n,m} = \begin{cases} 0 & m \neq n \\ \alpha_n & m = n. \end{cases}$$

If P(x) is a polynomial of degree less than n, then

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

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Higher-Order Gaussian Quadrature — Legendre Polynomials Examples: Gaussian Quadrature in Action; HW#7

Gaussian Quadrature — Example

2-Point Formula

Suppose we want to find an optimal two-point formula:

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

Since we have 4 parameters to play with, we can generate a formula that is exact up to polynomials of degree 3. We get the following 4 equations:

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

$$c_1 = 1$$

$$c_2 = 1$$

$$x_1 = -\frac{\sqrt{3}}{3}$$

$$x_2 = \frac{\sqrt{3}}{3}$$

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Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

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2-point Gaussian Quadrature

Higher-Order Gaussian Quadrature — Legendre Polynomials

A Quick Note on Legendre Polynomials

We will see Legendre polynomials in more detail later. For now, all we need to know is that they satisfy the property

$$\int_{-1}^{1} P_n(x) P_m(x) dx = \alpha_n \delta_{n,m}.$$

and the first few Legendre polynomials are

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = x^2 - 1/3$$

$$P_3(x) = x^3 - 3x/5$$

$$P_4(x) = x^4 - 6x^2/7 + 3/35$$

$$P_5(x) = x^5 - 10x^3/9 + 5x/21$$

It turns out that the **roots** of the Legendre polynomials are the nodes in Gaussian quadrature.



Higher-Order Gaussian Quadrature — Legendre Polynomials Gaussian Quadrature in Action: HW#7

Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

Higher-Order Gaussian Quadrature — Legendre Polynomials es: Gaussian Quadrature in Action: HW#

Higher Order Gaussian Quadrature Formulas

Theorem

Suppose that $\{x_1, x_2, \dots, x_n\}$ are the roots of the n^{th} Legendre polynomial $P_n(x)$ and that for each i = 1, 2, ..., n, the coefficients c; are defined by

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

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

$$\int_{-1}^{1} P(x) dx = \sum_{i=1}^{n} c_{i} P(x_{i}).$$

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Romberg Quadrature

-noint Gaussian Quadrature Higher-Order Gaussian Quadrature — Legendre Polynomials

Proof of the Theorem

If the polynomial P(x) of degree [n, 2n) is divided by the n^{th} Legendre polynomial $P_n(x)$, we get:

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

where both Q(x) and R(x) are of degree less than n.

[1] Since deg(Q(x)) < n

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

[2] Further, since x_i is a root of $P_n(x)$:

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

Proof of the Theorem

Let us first consider a polynomial, P(x) with degree less than n. P(x) can be rewritten as an (n-1)-st Lagrange polynomial with nodes at the roots of the n^{th} Legendre polynomial $P_n(x)$. This representation is exact since the error term involves the n^{th} derivative of P(x), which is zero. Hence,

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

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

which verifies the result for polynomials of degree less than n.

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Romberg Quadrature

2-point Gaussian Quadrature Higher-Order Gaussian Quadrature — Legendre Polynomials

Proof of the Theorem

[3] Now, since deg(R(x)) < n, the first part of the proof implies

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

Putting [1], [2] and [3] together we arrive at

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

$$= \int_{-1}^{1} R(x) dx = \sum_{i=1}^{n} c_{i}R(x_{i})$$

$$= \sum_{i=1}^{n} c_{i}P(x_{i}),$$

which shows that the formula is exact for all polynomials P(x) of degree less than 2n. \square

Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature

deas... Project Gaussian Quadrature

Higher-Order Gaussian Quadrature — Legendre Polynomials Examples: Gaussian Quadrature in Action: HW#7

Gaussian Quadrature beyond the interval [-1, 1]

By a simple linear transformation,

$$t = \frac{2x - a - b}{b - a}$$
 \Leftrightarrow $x = \frac{(b - a)t + (b + a)}{2}$,

we can apply the Gaussian Quadrature formulas to any interval

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

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Composite Quadrature Romberg Quadrature Adaptive Quadrature Gaussian Quadrature Ideas...
2-point Gaussian Quadrature
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Examples

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$$\int_0^{\pi/4} (\cos(x))^2 dx = \frac{1}{4} + \frac{\pi}{8} = 0.642699081698724$$

	Degree	Quadrature points	Coefficients
ĺ	2	0.16597, 0.61942	1, 1
l	3	0.08851, 0.39270, 0.69688	0.55556, 0.88889, 0.55556
١	4	0.05453, 0.25919, 0.52621, 0.73087	0.34785, 0.65215, 0.65215, 0.34785

Table: Quadrature points translated to interval of interest; with weight coefficients.

	Degree	Integral approximation	Error
ſ	2	0.642317235049753	0.0003818466489
	3	0.642701112090729	0.0000020303920
İ	4	0.642699075999924	0.0000000056988

Table: Approximation and Error, for GQ.



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2-point Gaussian Quadrature
Higher-Order Gaussian Quadrature — Legendre Polynomials
Examples: Gaussian Quadrature in Action; HW#7

Examples

Degree	$P_n(x)$	Roots / Quadrature points
2	$x^2 - 1/3$	$\{-1/\sqrt{3}, \ 1/\sqrt{3}\}$
3	$x^3 - 3x/5$	$\{-\sqrt{3/5}, \ 0, \ \sqrt{3/5}\}$
4	$x^4 - 6x^2/7 + 3/35$	$\{-0.86114, -0.33998, 0.33998, 0.86114\}$

Table: Quadrature points on "standard interval.

$$\int_0^{\pi/4} (\cos(x))^2 dx = \frac{1}{4} + \frac{\pi}{8} = 0.642699081698724$$

Degree	Quadrature points	Coefficients
2	0.16597, 0.61942	1, 1
3	0.08851, 0.39270, 0.69688	0.55556, 0.88889, 0.55556
4	0.05453, 0.25919, 0.52621, 0.73087	0.34785, 0.65215, 0.65215, 0.34785

Table: Quadrature points translated to interval of interest; with weight coefficients.



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Composite-Romberg-Adaptive-Gaussian

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