Lecture 25

Gauss Quadrature

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Today:

Objectives

- identify the most widely used quadrature method
- is it cheap?
- is it effective?
- how does it compare to Newton-Cotes (Trapezoid, Simpson, etc)?

Material

- Section 11.3

Quadrature

- up until now, our quadrature methods were of the form

$$\int_a^b f(x)\,dx \approx \sum_{j=1}^{n} w_j f(x_j)$$

  where x_j are equally spaced nodes
- Trapezoid:

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$

- Simpson:

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6} f(a) + \frac{2(b-a)}{3} f(\frac{a+b}{2}) + \frac{b-a}{6} f(b)$$

- Similar for higher order polynomial Newton-Cotes rules

Quadrature with Freedom

- These quadrature rules have one thing in common: they're restrictive
- Trapezoid, Simpson, etc (Newton-Cotes) are based on equally spaced nodes
- We know one thing already from interpolation: equally spaced nodes result in *wiggle*.
- Are they bad for interpolation?
- What are the other choices?

Gaussian Quadrature

- free ourselves from equally spaced nodes
- combine selection of the nodes and selection of the weights into one quadrature rule
- choose the nodes and coefficients optimally to maximize the order of accuracy of the quadrature rule:

$$\int_a^b f(x)\,dx \approx \sum_{j=1}^{n} c_j f(x_j)$$

- We want our formula to be *exact* for as fancy of a funcy as we can
- One thing we can do is seek c_j and x_j so that the quadrature rule is exact for really high polynomials

Gaussian Quadrature

$$\int_a^b f(x)\,dx \approx \sum_{j=1}^{n} c_j f(x_j)$$

- we have n points $x_j \in [a, b]$
- we have n real coefficients
- so there are $2n$ total unknowns to take care of
- this was 2 in the case of trapezoid
- this was 3 in the case of simpson

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$2n$ unknowns can be used to exactly interpolate and integrate polynomials of degree up to $2n - 1$

Better Nodes

The first thing we do is SIMPLIFY

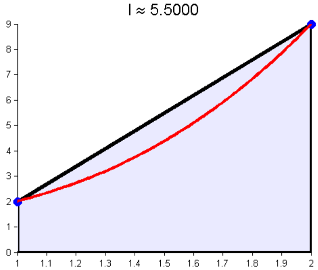
- consider the case of $n = 2$
- consider $[a, b] = [-1, 1]$ for simplicity
- we *know* how the trapezoid rule works
- Question: can we possibly do better using only 2 function evaluations?
- Goal: Find c_1, c_2, x_1, x_2 so that

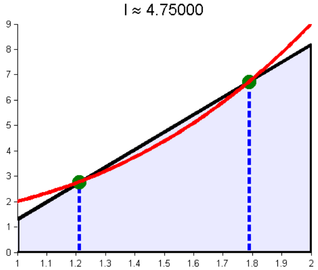
$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2)$$

Graphical View

Consider

$$\int_1^2 x^3 + 1\, dx = 4.75$$





Derive...

Again, we are considering $[a, b] = [-1, 1]$ for simplicity:

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

We would like this to be an exact representation for polynomials of degree as high as three. Assume the function is a cubic polynomial:

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

This implies that:

$$\begin{aligned} \int_{-1}^{1} f(x)\, dx &= \int_{-1}^{1} \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right)\, dx \\ &= c_1 \left(a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3\right) + \\ &\quad\; c_2 \left(a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3\right) \end{aligned}$$

Derive...

$$a_0\left(c_1 + c_2 - \int_{-1}^{1} dx\right) \quad + \quad a_1\left(c_1x_1 + c_2x_2 - \int_{-1}^{1} x\,dx\right) +$$
$$a_2\left(c_1x_1^2 + c_2x_2^2 - \int_{-1}^{1} x^2\,dx\right) \quad + \quad a_3\left(c_1x_1^3 + c_2x_2^3 - \int_{-1}^{1} x^3\,dx\right) = 0$$

Since a_0, a_1, a_2 and a_3 are arbitrary, then their coefficients must all be zero.

Derive...

This implies:

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

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

Some algebra leads to:

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

Therefore:

$$\int_{-1}^{1} f(x) \, dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

Over another interval?

$$\int_{-1}^{1} f(x)\,dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

- integrating over $[a, b]$ instead of $[-1, 1]$ needs a transformation: a change of variables
- let $t = \frac{2(x-a-b)}{b-a}$. Then $dx = \frac{b-a}{2}dt$. So

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

- so using two points, gave us exact integration for polynomails of degree less than 2*2-1 = 3.

Extending Gauss Quadrature

- we need more to make this work for more than two points
- hand calculation is tedius
- A sensible quadrature rule for the interval $[-1, 1]$ based on 1 node would use the node $x = 0$. This is a root of $\phi(x) = x$
- Notice: $\pm\frac{1}{\sqrt{3}}$ are the roots of $\phi(x) = x^2 - 3$

Orthogonal Polynomials

Orthogonality of Functions

Two functions $g(x)$ and $h(x)$ are *orthogonal* on $[a, b]$ if

$$\int_a^b g(x)h(x)\,dx = 0$$

- so the nodes we're using are roots of orthogonal polynomials
- these are the *Legendre* Polynomials

Legendre Polynomials

$$
\begin{aligned}
\phi_0 &= 1 \\
\phi_1 &= x \\
\phi_2 &= \frac{3x^2 - 1}{2} \\
\phi_3 &= \frac{5x^3 - 3x}{2} \\
&\vdots
\end{aligned}
$$

In general:

$$\phi_n(x) = \frac{2n-1}{n} x \phi_{n-1}(x) - \frac{n-1}{n} \phi_{n-2}(x)$$

Legendre Roots

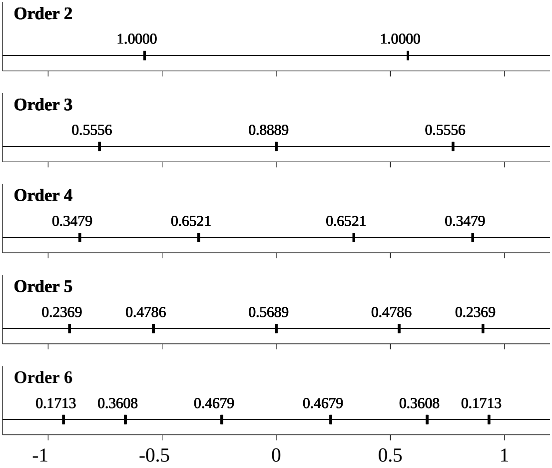
- The Legendre Polynomials are orthogonal (nice!)
- The Legendre Polynomials increase in polynomials order (like monomials)
- The Legendre Polynomials don't suffer from poor conditioning (unlike monomials)
- The Legendre Polynomials don't have a close form expression (recursion relation is needed)
- The roots of the Legendre Polynomials are the nodes for Gaussian Quadrature (GL nodes)

Quadrature Nodes

- Often listed in tables
- Weights determined by extension of above
- Roots are symmetric in $[-1, 1]$
- Example:

```
if(n==1)
  x = 0;    w = 2;
if(n==2)
  x(1) = -1/sqrt(3);      x(2) = -x(1);
  w(1) =  1;              w(2) =  w(1);
if(n==3)
  x(1) = -sqrt(3/5);     x(2) =  0;       x(3) = -x(1);
  w(1) =  5/9;           w(2) =  8/9;     w(3) =  w(1);
if(n==4)
  x(1) = -0.861136311594053;     x(4) = -x(1);
  x(2) = -0.339981043584856;     x(3) = -x(2);
  w(1) =  0.347854845137454;     w(4) =  w(1);
  w(2) =  0.652145154862546;     w(3) =  w(2);
if(n==5)
  x(1) = -0.906179845938664;     x(5) = -x(1);
  x(2) = -0.538469310105683;     x(4) = -x(2);
  x(3) =  0;
  w(1) =  0.236926885056189;     w(5) =  w(1);
  w(2) =  0.478628670499366;     w(4) =  w(2);
  w(3) =  0.568888888888889;
if(n==6)
  x(1) = -0.932469514203152;     x(6) = -x(1);
  x(2) = -0.661209386466265;     x(5) = -x(2);
  x(3) = -0.238619186083197;     x(4) = -x(3);
  w(1) =  0.171324492379170;     w(6) =  w(1);
  w(2) =  0.360761573048139;     w(5) =  w(2);
  w(3) =  0.467913934572691;     w(4) =  w(3);
```

View of Nodes



Theory

The connection between the roots of the Legendre polynomials and exact integration of polynomials is established by the following theorem.

Theorem

Suppose that $x_1, x_2, \ldots, x_n$ are 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

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

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

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

Do not!

!!!

When evaluating a quadrature rule

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

do not generate the nodes and weights each time. Use a lookup table...

Example

Approximate $\int_1^{1.5} x^2 \ln x \, dx$ using Gaussian quadrature with $n = 2$.

<u>Solution</u> As derived earlier we want to use $\int_{-1}^{1} f(x)\, dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$

From earlier we know that we are interested in

$$\int_1^{1.5} f(x)\, dx = \int_{-1}^{1} f\left(\frac{(1.5-1)t + (1.5+1)}{2}\right) \frac{1.5-1}{2}\, dt$$

Therefore, we are looking for the integral of

$$\frac{1}{4}\int_{-1}^{1} f\left(\frac{(x+5)}{4}\right) dx = \frac{1}{4}\int_{-1}^{1} \left(\frac{(x+5)}{4}\right)^2 \ln\left(\frac{(x+5)}{4}\right) dx$$

Using Gaussian quadrature, our numerical integration becomes:

$$\frac{1}{4}\left[\left(\frac{(-\frac{\sqrt{3}}{3}+5)}{4}\right)^2 \ln\left(\frac{(-\frac{\sqrt{3}}{3}+5)}{4}\right) + \left(\frac{(\frac{\sqrt{3}}{3}+5)}{4}\right)^2 \ln\left(\frac{(\frac{\sqrt{3}}{3}+5)}{4}\right)\right] = 0.19226$$

Example

Approximate $\int_0^1 x^2 e^{-x}\, dx$ using Gaussian quadrature with $n = 2$.

<u>Solution</u> We again want to convert our limits of integration to -1 to 1. Using the same process as the earlier example, we get:

$$\int_0^1 x^2 e^{-x} dx = \frac{1}{2}\int_{-1}^{1} \left(\frac{t+1}{2}\right)^2 e^{(t+1)/2} dt.$$

Using the Gaussian roots we get:

$$\int_0^1 x^2 e^{-x} dx \approx \frac{1}{2}\left[\left(\frac{-\frac{\sqrt{3}}{3}+1}{2}\right)^2 e^{(-\frac{\sqrt{3}}{3}+1)/2} + \left(\frac{\frac{\sqrt{3}}{3}+1}{2}\right)^2 e^{(\frac{\sqrt{3}}{3}+1)/2}\right] = 0.1594104$$

Examples

with matlab...

Example

gaussQuad.m: base routine for GL quadrature

Example

demoGauss.m: integrate $\int_0^5 xe^{-x}\,dx$ with

1. 1 interval (panel), increasing number of nodes
2. 3 nodes, increases number of intervals (panels)

Result: fewer total evaluations in GL quadrature with 1 panel and many nodes versus 3 nodes and many panels. Also more accurate.

Example

compIntRules.m: integrate $\int_0^5 xe^{-x}\,dx$ with

1. trapezoid
2. Simpson
3. Gauss

Keep the number of number of nodes and panels consistent. Result: fewer evals for GL

Questions

- With ____ nodes, basic Trapezoid integrates order ____ polynomials exactly.

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- The GL coeffiecient and weights with $n = 2$ are $c_{1,2} = 1.0$ and $x_{1,2} = \pm\frac{1}{\sqrt{3}}$. What are the coefficients and weights for $n = 3$?

Questions

- With ____ nodes, basic Trapezoid integrates order ____ polynomials exactly.
- With ____ nodes, basic Simpson integrates order ____ polynomials exactly.
- With ____ nodes, basic Gauss-Legendre Quadrature integrates order ____ polynomials exactly.
- The GL coeffiecient and weights with $n = 2$ are $c_{1,2} = 1.0$ and $x_{1,2} = \pm\frac{1}{\sqrt{3}}$. What are the coefficients and weights for $n = 3$?
- Use $n = 3$ GL quadrature to approximate $\int_0^1 e^{-x^2}, dx$. do not evaluate.

Read

- We are skipping the computation of the nodes and weights in general
- Read §11.3.4 for a good introduction on this