Set 14: Gaussian Quadrature

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Maximum Degree of Exactness

$$I(f) \approx I_n(f) = \sum_{i=0}^{n} \gamma_i f(x_i)$$

- $2n + 2$ parameters: $x_0, \ldots, x_n$ and $\gamma_0, \ldots, \gamma_n$
- $\therefore$ Intuition says we should be able get a degree of exactness of $2n + 1$.
- To do so we must choose the γ_i and the x_i, $0 \leq i \leq n$, specifically to maximize the degree of exactness.
- The methods that result are called Gauss Quadrature Methods of which there are several.

Review

We are interested in the degree of exactness so we can assume that $f \in \mathcal{C}^{n+1}[-1,1]$.

Recall

$$\int_{-1}^{1} f(x)dx \approx \int_{-1}^{1} p_n(x)dx$$

$$p_n(x) = \sum_{i=0}^{n} \ell_i(x) f(x_i)$$

$$f(x) = p_n(x) + R_n(x)$$

$$R_n(x) = \omega_{n+1}(x) f[x_0,\ x_1, \ldots, x_n,\ x] = \frac{\omega_{n+1}(x)}{(n+1)!} f^{(n+1)}(\xi(x))$$

$$E_n(x) = \int_{-1}^{1} R_n(x)dx$$

Review

- distinct $x_i \rightarrow p_n(x)$ is the unique interpolation polynomial
- $f \in \mathbb{P}_n \rightarrow f^{(n+1)}(x) \equiv 0$ and $\therefore E_n(x) \equiv 0$
- $\therefore$ the degree of exactness is at least n for an interpolatory quadrature formula.
- Note that we have not set the x_i to any particular values.

Maximum Degree of Exactness

Suppose f is a polynomial of degree $2n+1$ or less, i.e., $f \in \mathbb{P}_{2n+1}$

$$R_n(x) = \omega_{n+1}(x) f[x_0,\ x_1, \ldots, x_n,\ x]$$

$$E_n(x) = \int_{-1}^{1} R_n(x) dx = (\omega_{n+1}(x), f[x_0,\ x_1, \ldots, x_n,\ x])$$

where (x, y) is the inner product defined for $\mathcal{L}^2[-1, 1]$ with a weight function identically 1.

Divided Differences of Polynomials

Theorem 14.1. *If* $f \in \mathbb{P}_r$ *then*

$$\forall x \neq x_0, \quad f[x_0,\ x] = \frac{f(x) - f(x_0)}{x - x_0} \in \mathbb{P}_{r-1}$$

Proof. Since $f \in \mathbb{P}_r$, there exists $q_{r-1}(x) \in \mathbb{P}_{r-1}$ such that

$$f(x) = (x - x_0)q_{r-1}(x) + f(x_0)$$

It follows trivially that

$$\forall x \neq x_0, \quad f[x_0,\ x] = \frac{f(x) - f(x_0)}{x - x_0} = q_{r-1}(x)$$

□

Divided Differences of Polynomials

Corollary 14.2. *If* $f \in \mathbb{P}_{2n+1}$ *and* x_i*,* $0 \le i \le n$*, are distinct points then*

$$\forall x \neq x_i, \quad f[x_0,\ x_1, \ldots,\ x_n,\ x] \in \mathbb{P}_n$$

Proof. Apply Theorem 14.1 repeatedly. $\square$

So we can treat $f[x_0,\ x_1, \ldots,\ x_n,\ x]$ as a polynomial of degree n when discussing the integral that defines the error.

Maximum Degree of Exactness

To get the maximum degree of exactness we must have

$$\forall f \in \mathbb{P}_{2n+1}, \quad E_n(x) = 0$$

$$\text{or equivalently,} \quad \forall q_n(x) \in \mathbb{P}_n, \quad (\omega_{n+1}(x), q_n(x)) = 0$$

- maximum degree of exactness $\Leftrightarrow$ orthogonality in $\mathcal{L}^2[-1,1]$
- Newton-Cotes and similar interpolatory quadrature methods achieved d.o.e. of n by forcing $q_n(x) \equiv 0$ for any choice of x_i.
- $q_n(x) \equiv 0$ **is not required for maximum degree of exactness**!
- x_i, $0 \leq i \leq n$, are not yet specified. They define $\omega_{n+1}(x)$ and the method.

Gauss Legendre Quadrature

Let $P_i(x)$, $i = 0, 1, \ldots$ be the Legendre polynomials.

$$\forall q_n(x) \in \mathbb{P}_n, \quad \exists \alpha_0, \ldots, \alpha_n$$

$$q_n(x) = \sum_{i=0}^{n} \alpha_i P_i(x)$$

We have

$$(\omega_{n+1}(x), q_n(x)) = \sum_{i=0}^{n} \alpha_i (\omega_{n+1}(x), P_i(x))$$

$$(\omega_{n+1}(x), q_n(x)) = 0 \leftrightarrow (\omega_{n+1}(x), P_i(x)) = 0, \;\; 0 \leq i \leq n$$

Gauss Legendre Quadrature

Lemma. *Let $P_i(x)$, $i = 0, 1, \ldots$ be the Legendre polynomials. Let $P_{n+1}(x_i) = 0, \quad 0 \leq i \leq n$, i.e., the x_i are the $n+1$ roots of $P_{n+1}(x)$. We then have*

$$\forall q_n(x) \in \mathbb{P}_n, \quad (\omega_{n+1}(x), q_n(x)) = 0$$

$$\textit{where} \quad \omega_{n+1}(x) = \prod_{i=0}^{n}(x - x_i)$$

$$\textit{and} \quad \forall f \in \mathbb{P}_{2n+1}, \quad E_n(x) = 0$$

Proof. $\omega_{n+1}(x) \sim P_{n+1}(x)$ and by definition $(P_{n+1}(x), P_i(x)) = 0$ for any $0 \leq i \leq n$. Therefore, $\forall q_n(x) \in \mathbb{P}_n, \quad (\omega_{n+1}(x), q_n(x)) = 0$ and $E_n(x) = 0$ follows $\forall f \in \mathbb{P}_{2n+1}$ as desired. $\square$

Gauss Legendre Quadrature

- x_i are the roots of the $n+1-$st Legendre polynomial.
- the weights are

$$\gamma_i = \int_{-1}^{1} \ell_i(x)$$

- The approximation

$$\int_{-1}^{1} f(x)dx \approx \int_{-1}^{1} p_n(x)dx = \sum_{i=0}^{n} \gamma_i f(x_i)$$

has degree of exactness $2n+1$

- The formula are open since the roots of the orthogonal polynomials are interior to the interval of definition

Example

Two-point formula Gauss-Legendre uses linear interpolant with

$$x_\pm = \pm\frac{1}{\sqrt{3}}, \quad \gamma_\pm = 1$$

$$f(x) = x^3 + x^2 + x + 1 \rightarrow \int_{-1}^{1} f(x)dx = \frac{8}{3}$$

$$f(x_-) = \frac{4}{3}(1 - \frac{1}{\sqrt{3}}), \quad f(x_+) = \frac{4}{3}(1 + \frac{1}{\sqrt{3}})$$

$$\therefore I_2(f) = f(x_-) + f(x_+) = \frac{8}{3} \quad exact$$

Example

Consider midpoint rule, trapezoidal rule, and Simpson's rule.

$$f(x) = x^3 + x^2 + x + 1$$

$$I_{mp} = (b-a)f(0) = 2$$

$$I_{trap} = \frac{(b-a)}{2}\big[f(-1) + f(1)\big] = 0 + 4 = 4$$

$$I_{simp} = \frac{(b-a)}{2}\Big[\frac{f(-1)}{3} + \frac{4f(0)}{3} + \frac{f(1)}{3}\Big] = \Big[\frac{0}{3} + \frac{4}{3} + \frac{4}{3}\Big] = \frac{8}{3}, \quad \text{exact}$$

Gauss Quadrature Parameters

- x_i and γ_i must be computed and tabulated in general.
- roots of orthogonal polynomials
- eigenvalues of the Jacobi matrix associated with the recurrence that defines each family of polynomials
- text gives further details on points
- text has code for points and weights
- web is a good source of tabulation of parameters

Other Intervals

We can integrate over $[a, b]$ by a change of variables to $[-1, 1]$

$$a \leq x \leq b \text{ and } -1 \leq z \leq 1$$

$$x = \frac{z(b-a)+b+a}{2} \rightarrow dx = \frac{b-a}{2} dz$$

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

$$I_n(f) = \frac{b-a}{2} \sum_{i=0}^{n} \gamma_i f(u_i)$$

$$u_i = \frac{z_i(b-a)+b+a}{2} \text{ and } P_{n+1}(z_i) = 0$$

Example

$$\int_1^2 \frac{1}{x} dx = [\ln x]_1^2 \approx 0.69314718$$

$$f(x) = \frac{1}{x} \text{ and } F(z) = \frac{2}{z+3}$$

$$\int_1^2 \frac{1}{x} dx = \frac{1}{2} \int_{-1}^1 F(z) = \int_{-1}^1 \frac{1}{z+3} dz$$

$$I_1(f) = 9/13 \approx 0.69230769$$

$$I_4(f) \approx 0.69314712$$

Example Details

Carnahan, Luther, Wilkes – Wiley, 1969

i	z_i	γ_i	$\frac{F(z_i)}{2}$	$\gamma_i \frac{F(z_i)}{2}$
0	0.00000000	0.56888889	0.33333333	0.18962962
1	+0.53846931	0.47862867	0.28260808	0.13526433
2	−0.53846931	0.47862867	0.40625128	0.19444351
3	+0.90617985	0.23692689	0.25600460	0.06065437
4	−0.90617985	0.23692689	0.47759593	0.11315529

$I_4(f) = 0.69314712$

Other Formulas

- The Gauss Legendre quadrature formula have $a < x_0 < \cdots < x_n < b$
- If $x_0 = a$ and $x_n = b$ are added as a constraint then Gauss Lobatto quadrature formulas result.
- degree of exactness becomes $2n - 1$
- The $n - 1$ free x_i are the roots of the derivative of $P_n(x)$
- Gauss Radau formulas are those that only require $x_0 = a$ or $x_n = b$.
- Adaptive strategies are more difficult due to lack of sharing of x_i as n changes

Gauss Legendre Error

Theorem 14.3. *If a Gauss Legendre quadrature formula is used to approximate a definite integral on $[-1, 1]$ we have*

$$E_n(x) = \frac{2^{2n+3}\{(n+1)!\}^4}{(2n+3)\{(2n+2)!\}^3} f^{(2n+2)}(\xi)$$

with $-1 < \xi < 1$.

Other Weight Functions

Same idea but the family of orthogonal polynomials is determined by the interval and the weight function

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x)dx \rightarrow \text{ Gauss Chebyshev}$$

$$\int_{0}^{\infty} e^{-x} f(x)dx \rightarrow \text{ Gauss Laguerre}$$

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)dx \rightarrow \text{ Gauss Hermite}$$

Other Weight Functions

The weighting can be used to evaluate more general integrals

$$\int_a^b f(x)dx = \int_a^b w(x)\frac{f(x)}{w(x)}dx = \int_a^b w(x)g(x)dx$$

Singularity in $f(x)$ can be handled by isolating a weight function, e.g.,

$$f(x) = \frac{g(x)}{\sqrt{1-x^2}} \rightarrow \text{ Gauss Chebyshev}$$