Online Lecture Notes

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1 Gauss Quadrature

The goal of this lecture is to derive numerical integration formulas with maximum order. Here, we use the notation

$$I(f) \;=\; \int_a^b f(x)\,\mathrm{d}x$$

to denote the exact integral. And we are using the notation

$$I_n(f) \;=\; \sum_{i=0}^{n} \alpha_i f(x_i)\;.$$

The numerical approximation error associated to this integration formulation is given by

$$|I(f) - I_n(f)|\;.$$

We want to find an bound on this error, which may have the form

$$|I(f) - I_n(f)| \leq \mathbf{O}(|b-a|^m)\;,$$

where m is the order of the approximation formula. Recall that Simpson formula uses $n = 2$ and we get a formula that has the approximation order $m = 5$. Now, Gauss asked the question whether we can get an even more accuract numerical integration formula by choosing the points

$$x_0, x_1, \ldots, x_n$$

in a better way. Recall that Simpson's formula is based on the closed Newton-Cotes points, which are equidistant—but this might not the possible choice. The goal of this is to show tha the maximum possible approximation order to given by

$$m = 2n + 2\;.$$

This is surprisingly accurate! In fact, this result predicts that there should exist integration formulas, which use $n = 2$, but get the order $m = 2 * 2 + 2 = 6$. This is more accurate than Simpson's formula!

This lecture is divided into two parts. In the first part we show that $m = 2n + 2$ is the maximum possible order of the numerical integration formula. And, in the second we show that it is possible to choose the points $x_0, x_1, \ldots, x_n$ in such a way that we obtain a formula, which has this order.

1.1 Proof of the fact that $m = 2n + 2$ is the maximum possible order

The main idea is to construct the auxiliary polynomial

$$p(x) = (x - x_0)^2 (x - x_1)^2 \ldots (x - x_n)^2 = N_{n+1}(x)^2 = \prod_{i=0}^{n} (x - x_i)^2 \ .$$

Since this is a product of squares, we can see that $p(x)$ is non-negative, since all factors are non-negative; that is $p(x) \geq 0$. We even have $p(x) > 0$ for all $x \neq x_i$ for all i. If we would have a numerical integration method that has order $m \geq 2n + 3$, then this method would need to be accurate for the polynomial $p(x)$, since the order of p is given by $2(n + 1) = 2n + 2$. This would mean that

$$0 \ < \ \int_a^b p(x) \, \mathrm{d}x \ = \ I_n(p) \ = \ \sum_{i=0}^{n} \alpha_i \underbrace{p(x_i)}_{=0} \ = \ 0 \ .$$

This is, of course, a contradiction! Consequently, our assumption that there exists a integration formula with order $m \geq 2n+3$ must be wrong. In summary, we know that $2n + 2$ is the maximum possible integration order.

1.2 Construction of Gauss' Quadrature Rule

The goal of this second part of this lecture is to actually construct a numerical formula that has order $m = 2n + 2$. For this aim, we first recall that we are using the divided difference notation

$$p(x) \ = \ \sum_{i=0}^{n} f[x_0, x_1 \ldots, x_i] N_i(x) \ = \ \sum_{i=0}^{n} f[x_0, x_1 \ldots, x_i] \prod_{j=0}^{i-1} (x - x_j) \qquad (1)$$

This is the same notation as in Lecture 2—we are essentially collecting the divided difference coefficients from the first row of the divided table and multiply them with the corresponding Newton basis. This construction is such that p is the interpolotation polynomial of f,

$$\forall i \in \{0, 1, \ldots, n\}, \qquad p(x_i) = f(x_i) \ .$$

So far our derivation steps are the same as for the derivation of the Newton-Cotes formulas via the Lagrange basis. The only difference here is that we now using the Newton basis. Our next step is to substitute this expression for p into the integral in order to work out the corresponding expression explicitly,

$$\begin{aligned} I_n(f) = \int_a^b p(x) \, \mathrm{d}x \quad &\overset{(1)}{=} \quad \int_a^b \sum_{i=0}^{n} f[x_0, x_1 \ldots, x_i] \prod_{j=0}^{i-1} (x - x_j) \, \mathrm{d}x \\ &= \quad \sum_{i=0}^{n} f[x_0, x_1 \ldots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j) \, \mathrm{d}x \qquad (2) \end{aligned}$$

Now, the main idea is to compare this formula with a corresponding formula that uses more interpolation points, namely, the additional points $x_{n+1}, x_{n+2}, \ldots, x_{2n+1}$, which eventually yields a more accurate integration formula of order $2n+2$ as we wish to find. This means that we analyze the auxiliary integration formula

$$\begin{aligned}
I_{2n+1} &= \sum_{i=0}^{2n+1} f[x_0, x_1 \ldots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j)\,\mathrm{d}x \\
&= \sum_{i=0}^{n} f[x_0, x_1 \ldots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j)\,\mathrm{d}x + \sum_{i=n+1}^{2n+1} f[x_0, x_1 \ldots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j)\,\mathrm{d}x \\
&= I_n(f) + \sum_{i=n+1}^{2n+1} f[x_0, x_1 \ldots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j)\,\mathrm{d}x \\
&= I_n(f) + \sum_{i=n+1}^{2n+1} f[x_0, x_1 \ldots, x_i] \int_a^b \prod_{j=0}^{n} (x - x_j) \prod_{j=n+1}^{i-1} (x - x_j)\,\mathrm{d}x
\end{aligned} \tag{3}$$

Now we see that we have two types of polynomials involved, we call them

$$q(x) = \prod_{j=0}^{n} (x - x_j) \qquad \text{and} \qquad r_i(x) = \prod_{j=n+1}^{i-1} (x - x_j)\ .$$

This means that we can write the above expression in the form

$$\begin{aligned}
I_{2n+1} &= I_n(f) + \sum_{i=n+1}^{2n+1} f[x_0, x_1 \ldots, x_i] \int_a^b q(x) r(x)\,\mathrm{d}x \\
&= I_n(f) + \sum_{i=n+1}^{2n+1} f[x_0, x_1 \ldots, x_i] \langle q, r_i \rangle_{L_2[a,b]}
\end{aligned} \tag{4}$$

Now, at this point the main idea is that we can choose the points $x_0, x_1, x_2, \ldots, x_n$, which essentially means that we can choose the polynomial $q(x)$. Since $q(x)$ is a polynomial of order $n+1$, our goal is to choose the points $x_0, x_1, x_2, \ldots, x_n$ in such a way that

$$q(x) = L_{n+1}(x)$$

is equal to the $(n+1)$-th Legendre polynomial. The reason for this choice is that $r_i(x)$ is a polynomial of degree $i-n-1$. Since i is in the above sum running to $2n+1$, we have that $\deg(r_i) \le n$. But this means that we have

$$\langle q, r_i \rangle_{L_2[a,b]} = 0$$

as long as q is equal to L_{n+1}. This means that if we are succeeding to choose the points $x_0, x_1, \ldots, x_n$ in such a way that $q = L_{n+1}$, then we would have

$$I_{2n+1}(f) = I_n(f)\ ,$$

which implies $I_n(f)$ is an integration formula of order $2n+2$. Thus, in order to complete our construction, it remains to discuss why we can always find points

$x_0, x_1, \ldots, x_n$ such that $q = L_{n+1}$. Since we have

$$q(x) = \prod_{j=0}^{n} (x - x_j),$$

we need to make sure that the x_js are the roots of the function L_{n+1}. However, this means that we need to show that L_{n+1} has indeed $n+1$ real-valued roots. In order to show this, we start by introducing the set

$$S = \{ \ \lambda \in [a, b] \ \mid \ \lambda \text{ is a real root of } L_{n+1} \text{ with odd multiplicity } \} \ .$$

Here, we use that the multiplicity of the root λ of a polynomial, $p(\lambda) = 0$, is defined to be the maximum order $m = m_\lambda$ for which

$$\frac{p(x)}{(x - \lambda)^m}$$

is a polynomial of reduced degree. For example for the polynomial

$$p(x) = x^3 (x-1)^4 (x-2)^7$$

we would have

$$S = \{0, 2\}.$$

Also recall that the sign of $p(x)$ changes in the neighborhood of a root with odd multiplicity. The next thing we can do is to construct the auxiliary polynomial

$$M(x) \ = \ \prod_{\lambda \in S} (x - \lambda)$$

This construction is such that the polynomial $M(x)L_{n+1}(x)$ has only roots with even multiplicity. This means that

$$0 \ < \ M(x)L_{n+1}(x) \qquad \Longrightarrow \qquad \langle M, L_{n+1} \rangle = \int_a^b M(x)L_{n+1}(x) \, \mathrm{d}x > 0 \ .$$

But this is a contradiction for $|S| < n+1$, since L_{n+1} would then be orthogonal on M. This implies that $|S| = n+1$. This means that L_{n+1} has exactly $n+1$ distinct real roots all with multiplicity 1. This means that we can indeed set $x_0, x_1, \ldots, x_n$ to these roots of L_{n+1}. This yields the Gauss Quadrature rule !!!

1.3 Example

If we set $n = 1$ and $a = -1$ and $b = 1$, we would need to work out the roots of the Legendre polynomial

$$L_2(x) = \frac{1}{2}(3x^2 - 1)$$

(see our previous lecture on orthogonal olynomials and Gauss approximation). This polynomial has roots at

$$x_0 = -\frac{1}{\sqrt{3}} \quad \text{and} \qquad x_1 = \frac{1}{\sqrt{3}}$$

By working out the corresponding coefficients, we find $\alpha_0 = \alpha_1 = 1$ and

$$I_2(f) = f(x_0) + f(x_1) = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \, .$$

This is the Gauss Quadrature rule for $n = 1$. The expected integration order is given by $m = 2n + 2 = 4$. This means that this integration formula should be accurate for polynomials of order 3. Let's check this: let us consider the example

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

The exact integral is given by

$$\int_{-1}^{1} (1 + x + x^3)\, \mathrm{d}x \;=\; x + \frac{1}{2}x^2 + \frac{1}{4}x^4 \bigg|_{-1}^{1} = 1 + \frac{1}{2} + \frac{1}{4} - \left[-1 + \frac{1}{2} + \frac{1}{4}\right] = 2 \, .$$

The corresponding Gauss-Quadrature based approximation is given by

$$I_2(f) = 1 - \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{3}}^3 + 1 + \sqrt{\frac{1}{3}} + \sqrt{\frac{1}{3}}^3 = 2 \, .$$

We see that for such third order polynomials we do indeed get exact results for the integral.