Notes about Thesis Project I

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1 Introduction

1.1 Numerical Quadrature

(Salgado and Wise, p. 397)

Let $f \in C([a,b])$. We seek calculate an approximation of

$$I^{(a,b)}[f] := \int_a^b f(x)\,\mathrm{d}x.$$

Suppose that $g \in C([a,b])$, whose antiderivative is simply obtained, and $\|f-g\|_\infty < \varepsilon$. Then,

$$\left| \int_a^b f(x)\,\mathrm{d}x - \int\limits_a^b g(x)\,\mathrm{d}x \right| \le \varepsilon(b-a).$$

Definition 1.1.1 (Nodal set)**.** Let $[a,b] \subset \mathbb{R}$. X is called a *nodal set* of size $n+1 \in \mathbb{N}$ iff $X = \{x_i\}_{i=0}^n \subset [a,b]$ is a set of distinct elements. The elements of X, x_i are called *nodes*.

Definition 1.1.2 (Interpolating polynomial)**.** Suppose that $X = \{x_i\}_{i=0}^n \subset [a,b]$ is a nodal set and $f\colon [a,b] \to \mathbb{R}$ is a function. The function $I\colon [a,b] \to \mathbb{R}$ is called an *interpolant of* f subordinate to X iff $\forall i = 0,\ldots,n : I(x_i) = f(x_i)$, we write $I(X) = f(X)$.

Theorem 1.1.3 (existence and uniqueness)**.** *Suppose that $X = \{x_i\}_{i=0}^n \subset [a,b]$ is a nodal set and $Y = \{y_i\}_{i=0}^n \subset \mathbb{R}$. There is a unique polynomial $p \in \mathbb{P}_n$ with the property that $p(X) = Y$.*

Definition 1.1.4 (Lagrange nodal basis)**.** Suppose that $X = \{x_i\}_{i=0}^n \subset [a,b]$ is a nodal set. The *Lagrange nodal basis* subordinate to X is the set of polynomials $\mathcal{L}_X = \{L_\ell\}_{\ell=0}^n \subset \mathbb{P}_n$ defined via

$$L_\ell(x) = \prod_{\substack{i=0\\ i\neq\ell}}^n \frac{x-x_i}{x_\ell - x_i}.$$

Definition 1.1.5 (Lagrange interpolating polynomial)**.** Suppose that $X = \{x_i\}_{i=0}^n \subset [a,b]$ is a nodal set, $\mathcal{L}_X = \{L_i\}_{i=0}^n \subset \mathbb{P}_n$ is the Lagrange nodal basis subordinate to X, and $f\colon [a,b] \to \mathbb{R}$. The *Lagrange interpolating polynomial* of the function f, subordinate to the nodal set X, is the polynomial

$$p(x) = \sum_{i=0}^n f(x_i)\,L_i(x) \in \mathbb{P}_n.$$

Suppose that $X = \{x_i\}_{i=0}^{n} \subset [a, b]$ is a nodal set and $p \in \mathbb{P}_n$ is the unique Lagrange interpolating polynomial of f subordinate to X. Then

$$\forall i = 0, \ldots, n : f(x_i) = p(x_i)$$

and

$$\forall x \in [a, b] : f(x) = p(x) + E(x),$$

where E is an expression of the interpolation error. Then

$$\int_a^b f(x)\ \mathrm{d}x = \int_a^b p(x)\ \mathrm{d}x + \int_a^b E(x)\ \mathrm{d}x.$$

But

$$\int_a^b p(x)\ \mathrm{d}x = \int_a^b \sum_{i=0}^{n} f(x_i) L_i(x) = \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x) = \sum_{i=0}^{n} f(x_i) \beta_i,$$

where $L_i \in \mathbb{P}_n$ is the ith Lagrange nodal basis element and β_i is its definite integral:

$$\beta_i = \int_a^b L_i(x)\ \mathrm{d}x.$$

The expression $\sum_{i=0}^{n} f(x_i) \beta_i$ is a typical numerical integration formula

$$\left| \int_a^b f(x)\ \mathrm{d}x - \sum_{i=0}^{n} f(x_i) \beta_i \right| = \left| \int_a^b E(x)\ \mathrm{d}x \right| \leq \int_a^b |E(x)|\ \mathrm{d}x.$$

The *quadrature weights*, β_i, depends only on the positions of the nodes within $[a, b]$, as well as the interval $[a, b]$ itself. We will consider the approximation of a weight integral

$$I_w^{(a,b)}[f] \coloneqq \int_a^b f(x) w(x)\ \mathrm{d}x.$$

Definition 1.1.6 (Quadrature rule)**.** Suppose that $n, r \in \mathbb{N}_0$, w is a weight function on $[a, b] \subset \mathbb{R}$, $h = b - a > 0$, and $f \in C^r([a, b])$. The expression

$$Q_{w,r}^{(a,b)}[f] = \sum_{i=0}^{r} \sum_{j=0}^{n} \beta_{i,j} f^{(i)}(x_j) = \sum_{j=0}^{n} \Big(\beta_{0,j} f(x_j) + \beta_{1,j} f'(x_j) + \cdots + \beta_{r,j} f^{(r)}(x_j) \Big),$$

where

$$\forall i \in \{0, \ldots, r\} : \forall j \in \{0, \ldots, n\} : \beta_{i,j} = h^{i+1} \widehat{\beta}_{i,j}$$

and

$$\forall j \in \{0, \ldots, n\} : x_j = a + h \cdot \widehat{x}_j,$$

is called a *quadrature rule of degree* r with *intrinsic nodes* $\widehat{X} = \{\widehat{x}_j\} \subset [0, 1]$ and *intrinsic weights* $\{\beta_{i,j}\} \subset \mathbb{R}$ are called the *effective nodes* and *effective weights*, respectively.

A quadrature rule of degree $r = 0$ is called a *simple quadrature rule*, and we simplify the notation by writing $\beta_j = \beta_{0,j}$ and

$$Q_{w,r}^{(a,b)}[f] = \sum_{j=0}^{n} \beta_j f^{(i)}(x_j).$$

The *quadrature rule error* is defined as

$$E_Q[f] = I_w^{(a,b)}[f] - Q_{w,r}^{(a,b)}[f].$$

Definition 1.1.7 (consistency)**.** The quadrature rule is *consistent of order at least* $m \in \mathbb{N}_0$ iff $E_Q[q] = 0$ for all $q \in \mathbb{P}_m$. The quadrature rule is *consistent of order exactly* m iff $E_Q[q] = 0$ for all $q \in \mathbb{P}_m$; however, for some $r \in \mathbb{P}_{m+1}$, $E_Q[r] \neq 0$.

Definition 1.1.8 (interpolatory quadrature rule)**.** Assume that $n \in \mathbb{N}_0$, w is a weight function on $[a,b] \subset \mathbb{R}$, and $f \in C([a,b])$. Suppose that $X = \{x_i\}_{i=0}^n \subset [a,b]$ is a nodal set and $p \in \mathbb{P}_n$ is the unique Lagrange Interpolating polynomial of f subordinate to X, with

$$p(x) = \sum_{j=0}^{n} f(x_j) L_j(x),$$

where $L_j \in \mathbb{P}_n$ is the jth Lagrange nodal basis element.

The expression

$$Q_w^{(a,b)}[f] = \sum_{j=0}^{n} f(x_j) \beta_j,$$

where

$$\beta_j = \int_a^b L_j(x) w(x) \, \mathrm{d}x,$$

is called an *interpolatory quadrature rule subordinate to* X *of Lagrange type* for approximating $I_w^{(a,b)}[f]$.

Theorem 1.1.9 (existence and uniqueness)**.** *Suppose that* $X = \{x_i\}_{i=0}^n \subset \mathbb{R}$ *is a nodal set. There exists uniqueness weights* $\{\beta_j\}_{j=0}^n$ *such that*

$$\forall q \in \mathbb{P}_n : \int_a^b q(x) w(x) \, \mathrm{d}x = \sum_{j=0}^{n} \beta_j q(x_j),$$

or, equivalently,

$$\forall q \in \mathbb{P}_n : E_Q[q] = 0.$$

Moreover, these weights are given by

$$\forall j \in \{0, \ldots, n\} : \beta_j = \int_a^b L_j(x) w(x) \, \mathrm{d}x,$$

where L_j *is the* j*th Lagrange nodal basis polynomial subject to* X*.*

Theorem 1.1.10 (consistency)**.** *The last result shows that the simple quadrature rule,*

$$Q_w^{(a,b)}[f] = \sum_{j=0}^{n} \beta_i f(x_i),$$

is consistent of order at least n iff it is a quadrature rule of Lagrange type.

Theorem 1.1.11 (Error estimate)**.** *Suppose that $n \in \mathbb{N}_0$, w is a weight function on $[a,b] \subset \mathbb{R}$. $f \in C^{n+1}([a,b])$, and $X = \{x_i\}_{i=0}^{n} \subset [a,b]$ is a nodal set. Suppose that $Q_w^{(a,b)}[f]$ is the interpolatory quadrature rule subordinate to X of Lagrange type. Then,*

$$|E_Q[f]| \leq \frac{M_{n+1}}{(n+1)!} \int_a^b |\omega_{n+1}(x)| \, w(x) \, \mathrm{d}x,$$

where

$$\omega_{n+1}(x) = \prod_{j=0}^{n} (x - x_j)$$

and

$$M_{n+1} = \left\| f^{(n+1)} \right\|_\infty .$$

Consequently, an interpolatory quadrature rule subordinate to X of Lagrange type is consistent of order at least n.

Definition 1.1.12 (characteristic function)**.** Suppose that $B \subset \mathbb{R}$. The *characteristic function* of B is the function

$$\chi_B(t) = \begin{cases} 1, & t \in B, \\ 0, & t \in \mathbb{R} \setminus B. \end{cases}$$

Theorem 1.1.13 (kernel)**.** *Suppose that $r \in \mathbb{N}_0$ and $m \in \mathbb{N}$, with $m > r$. Define the function $k_m \colon [a,b] \times [a,b] \to \mathbb{R}$ via*

$$k_m(x,y) = (x-y)^m \xi_{[a,x]}(y) = \begin{cases} (x-y)^m, & a \leq y \leq x \leq b, \\ 0, & a \leq x < y \leq b. \end{cases}$$

Then, for each $i \in \{0, \ldots, r\}$,

$$\frac{\partial^i k_m}{\partial x^i} \in C([a,b] \times [a,b])$$

and

$$\frac{\partial^i k_m(x,y)}{\partial x^i} = \begin{cases} \prod_{k=0}^{i-1} (m-k)(x-y)^{m-i}, & a \leq y \leq x \leq b, \\ 0, & a \leq x < y \leq b. \end{cases}$$

Theorem 1.1.14 (Peano Kernel Theorem)**.** *Suppose that $r \in \mathbb{N}_0$, $m \in \mathbb{N}$, with $m > n$, w is a weight function on $[a, b] \subset \mathbb{R}$, and $f \in C^{m+1}([a, b])$. Assume that $Q^{(a,b)}_{w,r}[f]$ is a quadrature rule of degree r, that is consistent of order at least m. Let the function $k_m \colon [a, b] \times [a, b] \to \mathbb{R}$. Set*

$$K_m(y) = E_Q[k_m(\cdot, y)] = \int_a^b k_m(x, y)\, w(x)\, \mathrm{d}x - \sum_{j=0}^{n} \sum_{i=0}^{r} \beta_{i,j} \frac{\partial^i k_m(x_j, y)}{\partial x^i}.$$

Then the quadrature error satisfies

$$E_Q[f] = \frac{1}{m!} \int_a^b f^{(m+1)}(y)\, K_m(y)\, \mathrm{d}y.$$

The function $K_m(y)$ is called the Peano Kernel*.*

Theorem 1.1.15 (quadrature error stability)**.** *We have*

$$|E_Q[f]| \le \frac{1}{m!} \left\| f^{(m+1)} \right\|_\infty \|K_m\|_1.$$

Since $\|K_m\|_1 < \infty$, there is a constant $C > 0$ that may depend on the size of the interval but is independent of f such that

$$|E_Q[f]| \le C \left\| f^{(m+1)} \right\|_\infty.$$

Theorem 1.1.16 (constant sign)**.** *If K_m does not change sign in $[a, b]$, then*

$$E_Q[f] = \frac{f^{(m+1)(\xi)}}{m!} \int_a^b K_m \,\mathrm{d}y$$

for some $\xi \in [a, b]$. Furthermore, we have the simple representation for the error

$$E_Q[f] = \frac{E_Q\left[x^{m+1}\right]}{(m+1)!} f^{(m+1)}(\xi)$$

for some $\xi \in [a, b]$, where $E_Q\left[x^{m+1}\right]$ is the quadrature error for the function $x \mapsto x^{m+1}$.

Definition 1.1.17 (Peano Kernel)**.** Let $M_1 = \chi_{[a,b]}$. For $k \in \mathbb{N}$ with $k \ge 2$, set

$$M_k(x) = \int_{\mathbb{R}} M_{k-1}(x - y)\, M_1(y)\, \mathrm{d}y.$$

For $k \in \mathbb{N}$ and $h > 0$, we define

$$M_k(x, h) = \frac{1}{h} M_k\left(\frac{x}{h}\right).$$

Definition 1.1.18 (Closed Newton-Cotes quadrature rule)**.** Suppose that w is a weight function on $[a,b] \subset \mathbb{R}$ and $n \in \mathbb{N}$. Set $h = b - a > 0$ and $\hbar = \frac{h}{n}$. Suppose that, for the simple quadrature rule, the nodal set $X = \{x_i\}_{i=0}^{n} \subset [a,b]$ is defined by

$$x_j = a + j\hbar, \quad j \in \{0, \dots, n\}.$$

The resulting method, denoting $Q_n[f]$, is called a *closed Newton-Cotes quadrature rule of order n.*

Example 1.1.19 (Newton-Cotes quadrature rules of order $n = 1, 2$ and weight function $w \equiv 1$ on $[a,b]$).

$$x_j = a + h\widehat{x}_j, \quad \beta_j = h\widehat{\beta}_j, \quad h = b - a.$$

n	rule	$\widehat{x}_j$	$\widehat{\beta}_j$	Error Formula
1	Trapezoidal	$0, 1$	$\frac{1}{2}, \frac{1}{2}$	$-\frac{1}{12}\hbar^3 f^{(2)}(\xi)$
2	Simpson's	$0, \frac{1}{2}, 1$	$\frac{1}{6}, \frac{4}{6}, \frac{1}{6}$	$-\frac{1}{90}\hbar^5 f^{(4)}(\xi)$

For $n = 2$, we observe the phenomenon of *super-convergence*, i.e., a higher than expected convergence.

For example, consider the case $n = 3$, Simpson's $\frac{3}{8}$ rule, on the reference interval $[0,1]$. The second Lagrange nodal basis element is

$$\widehat{L}_1(x) = \frac{x\left(x - \frac{2}{3}\right)(x-1)}{\frac{1}{3}\left(\frac{1}{3} - \frac{2}{3}\right)\left(\frac{1}{3} - 1\right)} = \frac{27}{2}\left(x^3 - \frac{5}{3}x^2 + \frac{2}{3}x\right).$$

Then,

$$\widehat{\beta}_1 = \int_0^1 \widehat{L}_1(x)\,\mathrm{d}x = \frac{27}{2}\left(\frac{1}{4}x^4 - \frac{5}{9}x^3 + \frac{1}{3}x^2\right)\Bigg|_{x=0}^{x=1} = \frac{3}{8}.$$

Theorem 1.1.20 (Error estimate)**.** *Let $[a,b] \subset \mathbb{R}$. Suppose that $Q_n^{(a,b)}[f]$ is a closed Newton-Cotes quadrature rule of order $n \in \mathbb{N}$. Then, the order of quadrature rule is consistent of order at least n. Moreover, if $f \in C^{n+1}([a,b])$, then*

$$|E_{Q_n}[f]| \le Ch^{n+2}\left\|f^{(n+1)}\right\|_\infty,$$

where $h = b - a$ and $C > 0$ is independent of h and f.

Theorem 1.1.21 (Integral Mean Value Theorem)**.** *Suppose that $-\infty < a < b < \infty$, $f \in C([a,b])$, and $g \in \mathcal{R}(a,b)$. Furthermore, suppose that $\forall x \in [a,b] : g(x) \ge 0$. Then there exists a point $\xi \in [a,b]$ such that*

$$\int_a^b f(x)\,g(x)\,\mathrm{d}x = f(\xi)\int_a^b g(x)\,\mathrm{d}x.$$

Thus, if $\forall x \in [a,b] : g(x) = 1$, there exists a point $\xi \in [a,b]$ such that

$$f(\xi) = \frac{1}{b-a}\int_a^b f(x)\,\mathrm{d}x.$$

1.2 Heuristic derivation of Advection Differential Equation

Definition 1.2.1 (Average concentration)**.** Let $h > 0$, $h \ll 1$. We define the *average concentration* $\overline{u}(x,t)$ in a space-time cell $\left[x - \frac{1}{2}h, +x\frac{1}{2}h\right] \times [0,T]$.

$$\overline{u}(x,t) = \frac{1}{h}\int_{x-\frac{1}{2}h}^{x+\frac{1}{2}h} u(s,t)\,\mathrm{d}s.$$

Definition 1.2.2 (Mass flux)**.** The mass flux is the product of

$$J_x = cv_x.$$

- J_x is the mass flux in x-direction.
- c is the concentration of the substance.
- v_x is the velocity of the substance in the x-direction.

Theorem 1.2.3 (Conservation law)**.** *If the species is carried along by a flowing medium with velocity $a(x,t)$, then the mass conservation law implies that the change of $\overline{u}(x,t)$ per unit of time is the net balance of inflow and outflow over the cell boundaries,*

$$\frac{\partial \overline{u}(x,t)}{\partial t} = \frac{1}{h}\left[a\left(x - \frac{1}{2}h, t\right)u\left(x - \frac{1}{2}h, t\right) - a\left(x + \frac{1}{2}h, t\right)u\left(x + \frac{1}{2}h, t\right)\right].$$

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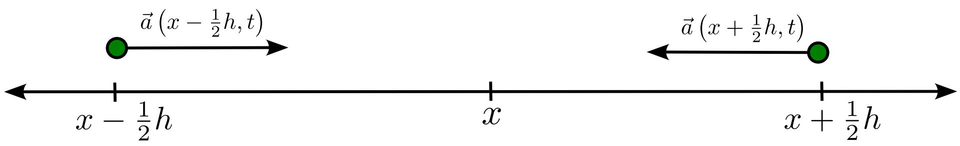
Definition 1.2.4 (Advection equation)**.**

$$\frac{\partial u(x,t)}{\partial t} + \frac{\partial a(x,t)\,u(x,t)}{\partial x} = 0.$$

Definition 1.2.5 (Diffusion equation)**.**

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(d(x,t)\,\frac{\partial u(x,t)}{\partial x}\right).$$



Theorem 1.2.6 (Mass conservation law)**.** *If $u(x,t)$ is a concentration and*

$$M(t) := \int_0^1 u(x,t)\,\mathrm{d}x$$

represents the mass in $[0,1]$ at time t, then M is a conserved quantity.

Proof.

$$\frac{\mathrm{d}M(t)}{\mathrm{d}t} = \int_0^1 u_t(x,t)\,\mathrm{d}x = \int_0^1 \left(-au_x(x,t) + du_{xx}(x,t)\right)\mathrm{d}x$$
$$= -a\left(u(1,t) - u(0,t)\right) + d\left(u_x(1,t) - u_x(0,t)\right) = 0.$$

□

1.3 The Advection Problem in One Dimension

Definition 1.3.1 (space-time grid)**.** Let $d \in \mathbb{N}$, $\Omega = (0,1)^d$, and $T > 0$. For $K, N \in \mathbb{N}$, we set $\tau = \frac{T}{K}$ and $h = \frac{1}{N+1}$. We define the *space-time grid domain*

$$\overline{\mathcal{C}}_h^\tau = \overline{\Omega}_h \times [0,T]_\tau = \left\{(\mathbf{x}, t_k) \mid \mathbf{x} \in \overline{\Omega}_h, t_k = k\tau, k \in \{0,\dots,K\}\right\},$$

where we recall that $\overline{\Omega}_h = \overline{\Omega} \cap \mathbb{Z}_h^d$. We define the *discrete interior* of $\overline{C}_h^\tau$ to be

$$\mathcal{C}_h^\tau = \Omega_h \times (0,T)_\tau\,.$$

Definition 1.3.2 (space-time grid functions)**.** Let $\mathcal{C}_h^\tau$ be a space-time grid domain. We denote by

$$\mathcal{V}\left(\overline{\mathcal{C}}_h^\tau\right) = \left\{v \mid \overline{C}_h^\tau \to \mathbb{R}\right\}$$

be the space of *space-time grid functions.* The spaces

$$\mathcal{V}\left(\mathcal{C}_h^\tau\right), \mathcal{V}\left(\partial_L \mathcal{C}_h^\tau\right)$$

Definition 1.3.3 (space-time discrete norms)**.** Let $d \in \{1,2\}$, $p \in [1,\infty]$, and $q \in [1,\infty)$. We define the *space-time* norm

$$\|v\|_{L_\tau^q(L_h^p)} = \left(\tau \sum_{k=1}^{K} \left\|v^k\right\|_{L_h^p}^q\right)^{\frac{1}{q}}$$

and

$$\|v\|_{L_\tau^\infty(L_h^p)} = \max_{k=0}^{K} \left\|v^k\right\|_{L_h^p}$$

Definition 1.3.4 (Péclet number)**.** Consider the simple constant-coefficient advection-diffusion equation

$$u_t + au_x = du_{xx}, \quad t > 0, \quad 0 < x < L,$$

with the given initial profile $u(x,0)$. If $d > 0$ we need boundary conditions at $x = 0$ and $x = L$, such as Dirichlet conditions. On the other hand, for the pure advection problem we need only to prescribe the solution at the *inflow* boundary, that is, at $x = 0$ if $a > 0$ and $x = L$ if $a < 0$. If $d > 0$ but $d \approx 0$, or more precisely if the *Péclet number*

$$|a|\,\frac{L}{d}$$

is large, the Dirichlet condition at the outflow boundary will give rise to a *boundary layer.*

If the Péclet number $\left|a\frac{L}{d}\right|$ is large, the problem is called *singularity perturbed.*

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