UCLA Math151A
Fall 2021
Lecture 20
2021/11/10

1. Numerical Stability of Differentiation and Integration (continued)

2. Gaussian Quadrature

Last time: numerical differentiation under F.P.

$$|f'(x_0) - \frac{f(x_0+h) - f(x_0-h)}{2h}| = \frac{h^2}{6}|f'''(\xi)| \leq \frac{h^2}{6}M$$

$$f(x_0+h) = \tilde{f}(x_0+h) + \epsilon_1$$

$$f(x_0-h) = \tilde{f}(x_0-h) + \epsilon_2.$$

$$\frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} = \frac{f(x_0+h) - f(x_0-h)}{2h} + \frac{\epsilon_1 - \epsilon_2}{2h}$$

$$|f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h}| \leq \frac{M}{6}h^2 + |\frac{\epsilon_2 - \epsilon_1}{2h}|$$

$$\epsilon := |\frac{\epsilon_2 - \epsilon_1}{2}| \qquad \min_h \left(\frac{M}{6}h^2 + \frac{\epsilon}{h}\right) \quad \Rightarrow \quad h = \left(\frac{3\epsilon}{M}\right)^{1/3}$$

More generally, if an approximation is $O(h^p)$

(e.g., with Richardson Extrapolation, the centered difference formula becomes $O(h^4)$)

then the same analysis gives an optimal

$$h \sim \epsilon^{\frac{1}{p+1}}$$

The property of finite difference formulas for approximations of derivatives that *they do not produce a better approximation past a certain value* makes them numerically unstable.

Now: how about stability of integration?

Suppose $f : [a,b] \to \mathbb{R}$,

$[a,b]$ divided into n subintervals $[x_j, x_{j+1}]$

$j = 0, \ldots, n-1 \qquad x_0 = a, x_n = b.$

$h = (b-a)/n.$

Consider the C.S.R (assuming n is even).

Let $f(x_j) = \tilde{f}(x_j) + e_j$.

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right)$$

Under exact arithmetic:

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right)$$

$$\Big\downarrow \quad \text{Let } f(x_j) = \tilde{f}(x_j) + e_j.$$

Under floating points:

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(\tilde{f}(x_0) + 2\sum_{j=1}^{n/2-1} \tilde{f}(x_{2j}) + 4\sum_{j=1}^{n/2} \tilde{f}(x_{2j-1}) + \tilde{f}(x_n)\right)$$

$$+\boxed{\frac{h}{3}\left(e_0 + 2\sum_{j=1}^{n/2-1} e_{2j} + 4\sum_{j=1}^{n/2} e_{2j-1} + e_n\right)}$$

R.O. Error

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(\tilde{f}(x_0) + 2\sum_{j=1}^{n/2-1}\tilde{f}(x_{2j}) + 4\sum_{j=1}^{n/2}\tilde{f}(x_{2j-1}) + \tilde{f}(x_n)\right)$$

$$+\boxed{\frac{h}{3}\left(e_0 + 2\sum_{j=1}^{n/2-1} e_{2j} + 4\sum_{j=1}^{n/2} e_{2j-1} + e_n\right)}$$

R.O. Error

$$|E^{R.O.}(h)| \le \frac{h}{3}\left(|e_0| + 2\sum_{j=1}^{n/2-1}|e_{2j}| + 4\sum_{j=1}^{n/2}|e_{2j-1}| + |e_n|\right)$$

Let $\epsilon = \max|\epsilon_j|$, then

$$\le \frac{h}{3}(\epsilon + 2(n/2-1)\epsilon + 4(n/2)\epsilon + \epsilon) = nh\epsilon = \epsilon(b-a).$$

Independent of h or n. One can safely decrease h to improve numerical integration — Stable!

$\boxed{\textbf{Gaussian Quadrature}}$

The Q.R.s we so far are very naive.
They all use equispaced nodes.

That is likely not the best choice…

Recall the general definition of the quadrature formula

weights nodes

$$\sum_{i=1}^{n} w_i f(x_i). \qquad (*)$$

This gives $2n$ degrees of freedom.

The main idea for Gaussian Quadrature (G.Q.) is given n, maximize the degree of exactness (DOE).

Thinking about it…

$$\int_a^b f(x)dx = \sum_{i=1}^{n} w_i f(x_i)$$

We want this equality to be exact for f(x) being polynomials.

We want as high degree polynomial as possible.

We get to choose 2n numbers on the right.

We can at best hope it is good for polynomials that contain 2n coefficients.

That is: at most degree 2n-1 polynomials

$$\int_a^b f(x)dx = \sum_{i=1}^{n} w_i f(x_i) \qquad (*)$$

The main idea for Gaussian Quadrature (G.Q.):

choose $\{x_i\}$ adn $\{w_i\}$ so that $(*)$ is exact for all polynomials of degree d, with $0 \le d \le 2n-1$.

Assumption for the rest of the lecture:

the interval of integration $[a, b]$ is assumed to be $[-1, 1]$.

Note that quadrature formulas can be generalized to arbitrary [a, b] using u-substitution (change of variables).

$$x = \frac{b-a}{2}t + \frac{b+a}{2}$$

$$dx = \frac{b-a}{2}dt$$

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

So how to find $\{w_i\}$ and $\{x_i\}$?

Option 1 is brute force.

E.g., consider two nodes and weights: x_1, x_2, w_1, w_2

solving:

$$\int_{-1}^{1} x^k dx = w_1 x_1^k + w_2 x_2^k, \qquad k = 0, 1, 2, 3$$

When n is large we don't wanna do this –
very tedious to solve these nonlinear equation system.

So how to find $\{w_i\}$ and $\{x_i\}$?

Option 2 is to use orthogonal polynomials.

orthogonality…

vector space…

inner product…

linear algebra…

A **vector space** (over $\mathbb{R}$) consists of a set V along with two operations "$+$" and "$\cdot$" subject to these conditions.

1. For any $\vec{v}, \vec{w} \in V$: $\vec{v} + \vec{w} \in V$.
2. For any $\vec{v}, \vec{w} \in V$: $\vec{v} + \vec{w} = \vec{w} + \vec{v}$.
3. For any $\vec{u}, \vec{v}, \vec{w} \in V$: $(\vec{v} + \vec{w}) + \vec{u} = \vec{v} + (\vec{w} + \vec{u})$.
4. There is a **zero vector** $\vec{0} \in V$ such that $\vec{v} + \vec{0} = \vec{v}$ for all $\vec{v} \in V$.
5. Each $\vec{v} \in V$ has an **additive inverse** $\vec{w} \in V$ such that $\vec{w} + \vec{v} = \vec{0}$.
6. If r is a **scalar**, that is, a member of $\mathbb{R}$ and $\vec{v} \in V$ then the **scalar multiple** $r \cdot \vec{v}$ is in V .
7. If $r, s \in \mathbb{R}$ and $\vec{v} \in V$ then $(r + s) \cdot \vec{v} = r \cdot \vec{v} + s \cdot \vec{v}$.
8. If $r \in \mathbb{R}$ and $\vec{v}, \vec{w} \in V$, then $r \cdot (\vec{v} + \vec{w}) = r \cdot \vec{v} + r \cdot \vec{w}$.
9. If $r, s \in \mathbb{R}$ and $\vec{v} \in V$, then $(rs) \cdot \vec{v} = r \cdot (s \cdot \vec{v})$
10. For any $\vec{v} \in V$, $1 \cdot \vec{v} = \vec{v}$.

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The set $\mathbb{R}^2$ is a vector space if the operations "$+$" and "$\cdot$" have their usual meaning.

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \end{pmatrix} \qquad r \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} rx_1 \\ rx_2 \end{pmatrix}$$

The set $\mathcal{M}_{2\times2}$ of 2×2 matrices with real number entries is a vector space under the natural entry-by-entry operations.

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} + \begin{pmatrix} w & x \\ y & z \end{pmatrix} = \begin{pmatrix} a+w & b+x \\ c+y & d+z \end{pmatrix} \qquad r \cdot \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} ra & rb \\ rc & rd \end{pmatrix}$$

An **inner product** on a real spaces V is a function that associates a number, denoted $\langle \mathbf{u}, \mathbf{v} \rangle$, with each pair of vectors **u** and **v** of V. This function has to satisfy the following conditions for vectors **u**, **v**, and **w**, and scalar c.

1. $\langle \mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{v}, \mathbf{u} \rangle$ (symmetry axiom)
2. $\langle \mathbf{u} + \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{u}, \mathbf{w} \rangle + \langle \mathbf{v}, \mathbf{w} \rangle$ (additive axiom)
3. $\langle c\mathbf{u}, \mathbf{v} \rangle = c \langle \mathbf{u}, \mathbf{v} \rangle$ (homogeneity axiom)
4. $\langle \mathbf{u}, \mathbf{u} \rangle \geq 0$, and $\langle \mathbf{u}, \mathbf{u} \rangle = 0$ if and only if $\mathbf{u} = 0$ (position definite axiom)

A vector space V on which an inner product is defined is called an **inner product space**.

Orthogonal Polynomials

Definition 20.1. Recall **dot product** in $\mathbb{R}^3$.

Let $x = (2, -1, 2), y = (3, 1, -2)$, then

$$\langle x, y \rangle = 2 \cdot 3 - 1 \cdot 1 + 2 \cdot (-2) = 3$$

If $\mathbf{u}, \mathbf{v}$ non-zero, then

$\langle \mathbf{u}, \mathbf{v} \rangle = 0 \quad \Rightarrow \quad$ $\mathbf{u}$ and $\mathbf{v}$ are orthogonal: $\mathbf{u} \perp \mathbf{v}$.

$\square$

Definition 20.2.

(∞-dimensional vector space)

If f and g are functions on $[-1, 1]$ then an inner product can be defined:

$$\langle f, g \rangle := \int_{-1}^{1} f(x) d(x) dx$$

This is called an L^2 inner product.

As before, $\langle f, g \rangle = 0 \rightarrow f \perp g$. $\square$

Let's assume we got some cool polynomials.. (we'll worry about how to actually get them in a later lecture.) All we assume/require is that:

$\exists \ (n+1)$ polynomials $\{q_i\}_{i=0}^{n}$

each q_i is a polynomial of degree i

they are mutually orthonormal $\int_{-1}^{1} q_i(x) q_j(x) dx = \delta_{ij}$

$\exists \ (n+1)$ polynomials $\{q_i\}_{i=0}^n$ $\quad \int_{-1}^{1} q_i(x)q_j(x)dx = \delta_{ij}$
each q_i is a polynomial of degree i

Lemma 20.1 (Lemma 1).

$\mathbb{P}^n$

$\{q_i\}_{i=0}^n$ is a basis for space of polynmomails of degree n or less.

Proof. $\{q_i\}_{i=0}^n$ being orthonormal

$$\Rightarrow \quad \text{they are linearly independent}$$

contradition: $q_1 = q_2 + q_3, \quad < q_1, q_1 >=< q_2, q_1 > + < q_3, q_1 >, \quad 1 = 0$

$\mathbb{P}^n$ has dimension $n+1$
(counting the degrees of freedom, e.g., cubic polynomial has 4 dofs)

there are $n+1$ of the q_i's

thus q_i's are a basis. ■

$\exists$ $(n+1)$ polynomials $\{q_i\}_{i=0}^n$
each q_i is a polynomial of degree i $\int_{-1}^{1} q_i(x)q_j(x)dx = \delta_{ij}$

Lemma 20.1 (Lemma 1). $\mathbb{P}^n$

$\{q_i\}_{i=0}^n$ is a basis for space of polynmomails of degree n or less.

Lemma 20.2 (Lemma 2).
$\forall$ polynomail $p \in \mathbb{P}^{n-1}$, we have $\langle p, q_n \rangle = 0$,
where q_n is the last vector in the set $\{q_i\}_{i=0}^n$.

Proof. $\{q_i\}_{i=0}^{n-1}$ is a basis for $\mathbb{P}^{n-1}$ by lemma 1.

Thus $p(x) = \sum_{i=0}^{n-1} c_i q_i(x)$ for some c_i.

Therefore $\langle p, q_n \rangle = \cdots = 0$ (inner product is linear). ■

Theorem 20.1. [Gaussian Quadrature Theorem]

Let $\{x_i\}_{i=1}^{n}$ be the n roots of n degree polynomial $q_n(x)$, where q_n is the last in the set $\{q_i\}_{i=0}^{n}$.

We'll assume $\boxed{\text{they are real and distinct.}}$

(will give a theorem for this next time)

Let

$$w_i = \int_{-1}^{1} \Pi_{j=1,j\neq i}^{n} \frac{x - x_j}{x_i - x_j} dx, \qquad i = 1, 2, \ldots, n,$$

where the integrand equals to $L_i(x)$ from Lagnraigan interpolation polynomial. Then

$$\sum_{i=1}^{n} w_i f(x_i) \quad \text{is exact for any } f \in \mathbb{P}^{2n-1}. \qquad \square$$

In summary,

If I got n+1 orthonormal polynomials

$\{q_i\}_{i=0}^{n}$ each q_i is a polynomial of degree i

I just take the last one $q_n(x)$

I find its n roots: $\{x_i\}_{i=1}^{n}$

I construct Lagrangian polynomials on them $L_i(x)$

I compute some integrals $w_i = \int_{-1}^{1} L_i(x)dx$

Then $\sum_{i=1}^{n} w_i f(x_i)$ has DOE 2n-1

I can integrate a cubic exactly with just 2 points!

Recall T.R. which uses 2 points only has DOE=1.