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Erratum from last lecture: Oct 25^{th} 2017

d_n instead of u_n. See uploaded notes for clarification.

Lecture 2: Numerical Integration

Consider the definite integral

$$I[f] := \int_a^b f(x)\,dx \qquad (*)$$

A quadrature scheme approximates $(*)$ as

$$I[f] \approx I_n[f] := \sum_{i=1}^{n} w_i f(x_i),$$

where $\{x_i\}_{i=1}^n$ are the <u>nodes</u> & $\{w_i\}_{i=1}^n$ the <u>weights</u>.

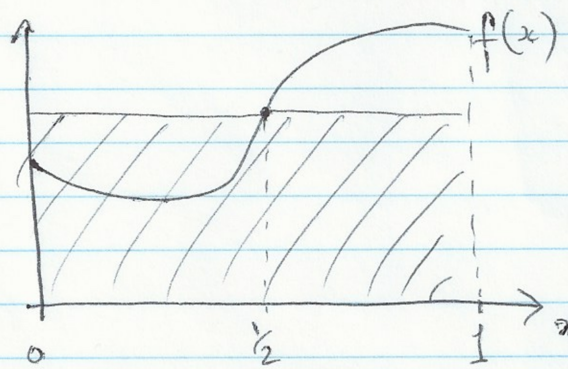
Define the error in the quad. scheme as

$$E_n[f] := \left| I[f] - I_n[f] \right| .$$

<u>Simplest method: Midpoint Rule.</u>

Consider $I[f] = \int_0^1 f(x)\,dx$, then the "midpoint rule" approximates I as

$$\int_0^1 f(x)\,dx \approx f\left(\frac{1}{2}\right).$$



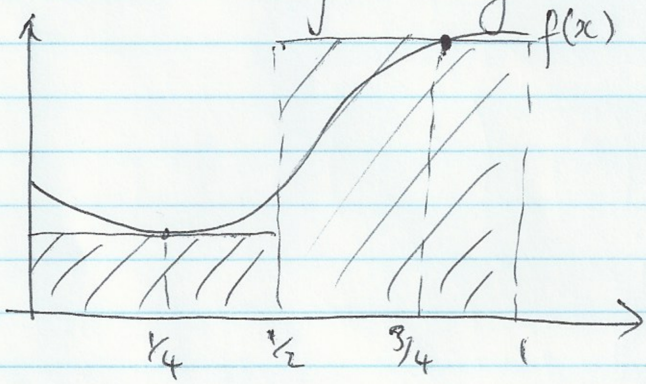
More generally, $\int_a^b f(x)\,dx \approx (b-a)\cdot f\left(\frac{b+a}{2}\right).$

Here $\frac{a+b}{2}$ is the node and $(b-a)$ is the weight.

In words: approximate area under $f(x)$ by the area of the rectangle of height $f\left(\frac{a+b}{2}\right)$.

Improving accuracy.

Increase the number of rectangles : "composite midpoint"



$$\int_0^1 f(x)\,dx \approx \frac{1}{2} f\left(\frac{1}{4}\right) + \frac{1}{2} f\left(\frac{3}{4}\right)$$

More generally,

$$\int_a^b f(x)\,dx \approx \left(\frac{b-a}{2}\right)\left[f\left(a+\frac{b-a}{4}\right) + f\left(a+\frac{3}{4}(b-a)\right)\right]$$

Now consider n subintervals :

$$\int_0^1 f(x) \approx \frac{1}{n}\sum_{i=1}^{n} f\left(\frac{2i-1}{2n}\right)$$

Generally,

$$\int_a^b f(x) \approx \underbrace{\frac{b-a}{n}}_{w_i} \sum_{i=1}^{n} f\underbrace{\left(a + \frac{b-a}{n}\left(i-\frac{1}{2}\right)\right)}_{x_i}$$

Error analysis

To derive the error of the midpoint rule, consider the interval $[0,h]$, $h>0$, and Taylor expand about $\frac{h}{2}$

$$f(x) = f\left(\frac{h}{2}\right) + \left(x-\frac{h}{2}\right)f'\left(\frac{h}{2}\right) + \underbrace{\frac{(x-h/2)^2}{2}f''(\xi)}_{\text{"Lagrange's form" of remainder}}$$

for some $\xi \in [0,h]$.

Then

$$\int_0^h f(x)\,dx = \int_0^h \left\{ f\left(\frac{h}{2}\right) + \left(x-\frac{h}{2}\right)f'\left(\frac{h}{2}\right) + \frac{(x-h/2)^2}{2}f''(\xi)\right\}dx$$

$$= \cancel{x}f\left(\frac{h}{2}\right)\Big|_0^h + \frac{(x-h/2)^2}{2}f'\left(\frac{h}{2}\right)\Big|_0^h + \left[\frac{(x-h/2)^3}{6}f''(\xi)\right]_0^h$$

$$= hf\left(\frac{h}{2}\right) + \frac{h^3}{24}f''(\xi)$$

Hence the error is

$$E_1[f] = I[f] - I_1[f]$$

$$= \cancel{hf\left(\frac{h}{2}\right)} + \frac{h^3}{24}f''(\xi) - \cancel{hf\left(\frac{h}{2}\right)}$$

So we see that the error depends on 2^{nd} derivative of f. Thus midpoint rule integrates 0^{th} & 1^{st} order polynomials exactly.

Composite midpoint $\quad E_n[f] = \frac{(b-a)^2}{24n^2}f''(\xi),\ \xi\in[a,b]$

Exercise: show this.

$$I_n[f] := \frac{h}{n}\sum_{i=1}^{n} f(x_i), \quad x_i = \frac{h}{n}(i-1/2).$$

$$I[f] = \int_0^h f(x)\,dx = \sum_{i=1}^{n} \int_{x_i - h/2}^{x_i + h/2} f(x)\,dx$$

$$\Rightarrow E_n[f] = \sum_{i=1}^{n} \int_{x_i - h/2}^{x_i + h/2} f(x)\,dx - \frac{h}{n} \sum_{i=1}^{n} f(x_i)$$

$$= \sum_{i=1}^{n} \left(\cancel{h f(x_i)} + \frac{h^3}{24} f''(\xi) - \cancel{h f(x_i)} \right)$$

$$= \frac{n h^3}{24} f''(\xi) \qquad , \; h = \frac{(b-a)}{n}$$

$$= \cancel{\left(b-a\right)^2}$$

$$= \frac{(b-a) h^2}{24} f''(\xi) = \frac{(b-a)^2}{24 n^2} f''(\xi)$$

So $O(h^2) / O\left(\frac{1}{n^2}\right)$ convergence.

MATLAB demo.

Can we derive a method for polys. of deg > 1?

Cubic example.

Want to determine w_1, w_2 & x_1, x_2 s.t.

$$I_2[f] = w_1 f(x_1) + w_2 f(x_2)$$

is ~~ex the~~ exactly equal to $I[f]$.

Cubic :

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

For exactness, require

$$\int_{-1}^{1}\left(a_0+a_1x+a_2x^2+a_3x^3\right)dx = w_1\left[a_0+a_1x_1+a_2x_1^2+a_3x_1^3\right]$$
$$+w_2\left[a_0+a_1x_2+a_2x_2^2+a_3x_2^3\right]$$

Gather like terms:

$$a_0: \quad w_1+w_2 = \int_{-1}^{1} dx = 2$$

$$a_1: \quad w_1x_1+w_2x_2 = \int_{-1}^{1} x\,dx = 0$$

$$a_2: \quad w_1x_1^2+w_2x_2^2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3}$$

$$a_3: \quad w_1x_1^3+w_2x_2^3 = \int_{-1}^{1} x^3\,dx = 0$$

Solve eqns. to give

$$w_1 = w_2 = 1, \quad x_1 = -\frac{1}{\sqrt{3}}, \quad x_2 = \frac{1}{\sqrt{3}}.$$

2 point rule integrates polys. of degree ≤ 3.

In general, an n pt. rule is exact for polys. of degree $\leq 2n-1$. Gives <u>spectral convergence</u> in n

To obtain nodes & weights for n point rule, could do as above and solve non-linear system using a Newton method. However this is difficult since the matrix becomes very ill-conditioned for large n. Instead use orthogonal polys. instead of above monomial to make rows linear independent. See other notes for more details.

<u>Transform Gauss to [a, b].</u>

Gauss rule always given on [−1, 1].

For [a, b], need to change variables:

$$\hat{x} = a + \left(\frac{x+1}{2}\right).(b-a)$$

So

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

<u>NB</u>: have modified weight by $\frac{b-a}{2}$ & mapped quad^{n} pts. to [a, b].

<u>Singular integrals</u>. (self-term)

If collocation pt. lies in element, have integral of form

$$I = \int_{-1}^{1} p(x)\log|x|\,dx \quad , \; p(x) \text{ poly. basis func}^{n}.$$

↖ singular at $x = 0$.

[Standard Gauss won't be accurate. MATLAB demo.].

Can construct <u>generalized</u> Gauss rule.

Say we want to exactly integrate

$$f(x) = a_0 \,,\; a_1\log x \,,\; a_2 x \,,\; a_3 x\log x$$

on [0, 1]. ← COMMENT.

~~For~~ As before ~~for~~ for polys.!
For exactness, require

$$a_0 : \int_0^1 dx = 1 = w_1 + w_2$$

$$a_1 : \int_0^1 \log x \, dx = -1 = w_1 \log(x_1) + w_2 \log(x_2)$$

$$a_2 : \int_0^1 x \, dx = \frac{1}{2} = w_1 x_1 + w_2 x_2$$

$$a_3 : \int_0^1 x \log x \, dx = -\frac{1}{4} = w_1 x_1 \log x_1 + w_2 x_2 \log x_2$$

[Ex: derive Gauss rule for a different set of func^{n}s].

Non-linear system more complicated but can still solve.

MATLAB Recovers spectral accuracy.

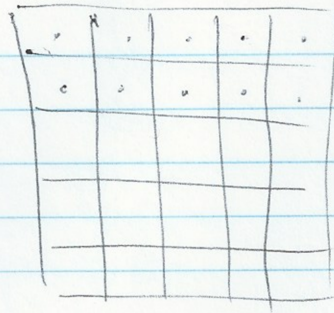
~~Two~~ 2D integrals

Galerkin method requires evaluation of 2D integrals:

$$I = \int_a^b \int_c^d G(x,y)\, p(x)\, q(y) \, dy \, dx$$

Just use product of 2 1D rules.

E.g., midpoint rule:



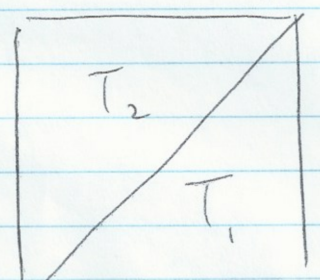
Gauss:
$$I \approx \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j f(x_i, x_j).$$

MATLAB: show nodes & weights in 2D.

Self term.

The self interaction term in Galerkin leads to a singularity along diag. of integration domain.

MATLAB



[How to integrate? Gen. Gauss would be OK if sing. along side]

E.g.
$$I = \int_0^1 \int_0^1 \log|x-y| \, dy \, dx.$$

Split int. dom. into 2 triangles T_1, T_2.

Consider T_1. T_2 for EX.

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$$I_{T_1} = \int_0^1 \int_0^x \log|x-y| \, dy \, dx \quad \leftarrow \text{sing. at } y = x.$$

Use <u>Duffy transform</u> to map $\triangle \to \square$.

Classical Duffy: $x = u$, $y = uv$, $\frac{dy}{dv} = u$

Gives

$$I_{T_1} = \int_0^1 \int_0^u \log|u-y| \, dy \, du$$

$$= \int_0^1 \int_0^1 \log|u - uv| \, u \, dv \, du$$

$$= \int_0^1 \int_0^1 \log|u(1-v)| \, u \, dv \, du$$

Integration now over square & singular at $u=0, v=1$.

To get sings. ~~at both~~ both at 0, let

$$s = 1-v$$

$$I_{T_1} = \int_0^1 \int_1^0 \log|u(1-(1-s))| \, u(-1) \, ds \, du$$

NB. Transforms out $\frac{1}{x}$ sing.

$$= \int_0^1 \int_0^1 \log|us| \, u \, ds \, du. \leftarrow \text{Sing. at } u=0 \text{ \& } s=0.$$

All-in-1 ~~Final~~ transform: $x = u$, $y = u(1-s)$.

MATLAB: Can use 2 1d generalized Gauss rules.

Note on Lagrange's remainder for Taylor series.

On page 3 we quoted the following form of Taylor's theorem:

Taylor's theorem.

Suppose that f is $(n+1)$ times differentiable on some interval containing the center of convergence c and x, and let

$$(1) \quad P_n(x) = f(c) + f'(c)(x-c) + \frac{f''(c)}{2}(x-c)^2 + \dots + \frac{f^{(n)}(c)}{n!}(x-c)^n$$

be the n^{th} order Taylor polynomial of f at $x=c$. Then

$$f(x) = P_n(x) + E_n(x)$$

where $E_n(x)$ is the error term. For ξ between c and x, the Lagrange Remainder form of the error E_n is given by

$$E_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1}.$$

In order to prove this form of the remainder, we shall use Cauchy's mean-value theorem which we quote without proof.

Cauchy's mean-value theorem.

Let F, G be continuous on $[a,b]$ and differentiable on (a,b), and $G'(x) \neq 0$ $\forall x \in (a,b)$. Then $\exists \xi \in (a,b)$ such that

$$\frac{F(b)-F(a)}{G(b)-G(a)} = \frac{F'(\xi)}{G'(\xi)}.$$

Proof of Lagrange's remainder in Taylor's thm.

Define

(2) $$F(\alpha) := f(\alpha) + f'(\alpha)(x-\alpha) + \frac{f''(\alpha)}{2}(x-\alpha)^2 + \ldots + \frac{f^{(n)}(\alpha)}{n!}(x-\alpha)^n$$

Notice that $F(x) = f(x)$ and $F(c) = P_n(x)$ from (1).

We want to find $f(x) - P_n(x)$, i.e., $E_n(x)$. From the above observation, we have that

(3) $$f(x) - P_n(x) = F(x) - F(c)$$

From Cauchy's mean-value theorem, we have

(4) $$F(x) - F(c) = \frac{F'(\xi)}{G'(\xi)}\left(G(x) - G(c)\right)$$

for ξ between x and c. Next observe, by differentiating (2), that

(5) $$F'(\alpha) = \frac{f^{(n+1)}(\alpha)}{n!}(x-\alpha)^n. \quad \text{(Exercise: show this)}$$

~~This gives~~ Substituting (5) into (4):

(6) $$F(x) - F(c) = \frac{f^{(n+1)}(\xi)(x-\xi)^n}{n!\, G'(\xi)}\left(G(x) - G(c)\right)$$

Judiciously choosing $G(\alpha) = (x-\alpha)^{n+1}$

$$\Rightarrow G'(\alpha) = -(n+1)(x-\alpha)^n$$

and substituting into (6):

$$F(x) - F(c) = \frac{f^{(n+1)}(\xi)\,\cancel{(x-\xi)^n}}{n!\left[-(n+1)\cancel{(x-\xi)^n}\right]} \cdot \left(-(x-c)^{n+1}\right)$$

$$\Rightarrow F(x) - F(c) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1}$$

Recall from (3) that $E_n(x) = F(x) - F(c)$, hence

$$E_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1}.$$