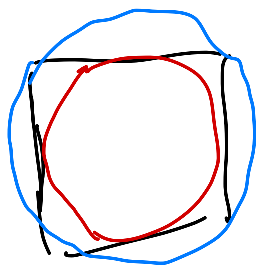
Numerical Analysis, Lecture 8

Numerical Integration

Integration scheme = Quadrature
(Quadrature rules)

Classically:

"squaring the circle"



also sometimes
"cubature"
in higher
dim.

There are no simple integration schemes in higher dim. Already in 2D ~ cases are complicated.

IDEA:

Randomized quadrature rules

→ Monte Carlo integration

- Central limit theorem → Convergence rate
- Law of large numbers → Convergence

Let X_i be i.i.d. (independent and identically distributed) random variables, mean μ variance σ^2.

Law of large numbers

$$A_N = \frac{1}{N} \sum_{i=1}^{N} X_i$$ Césaro-sum

$$\frac{1}{N} \sum_{i=1}^{N} X_i \longrightarrow \mu$$

also

$$\mathrm{var}(A_N) = \frac{1}{N^2} \sum_{i=1}^{N} \mathrm{var}(X_i) = \frac{\sigma^2}{N}$$

Central limit theorem "right" unit is the standard deviation $\sigma(A_N) = \frac{\sigma}{\sqrt{N}} \sim \varepsilon$

Consequence

If the integration problem can be cast into averaging problems (Césaro sum), the convergence rate will be $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$

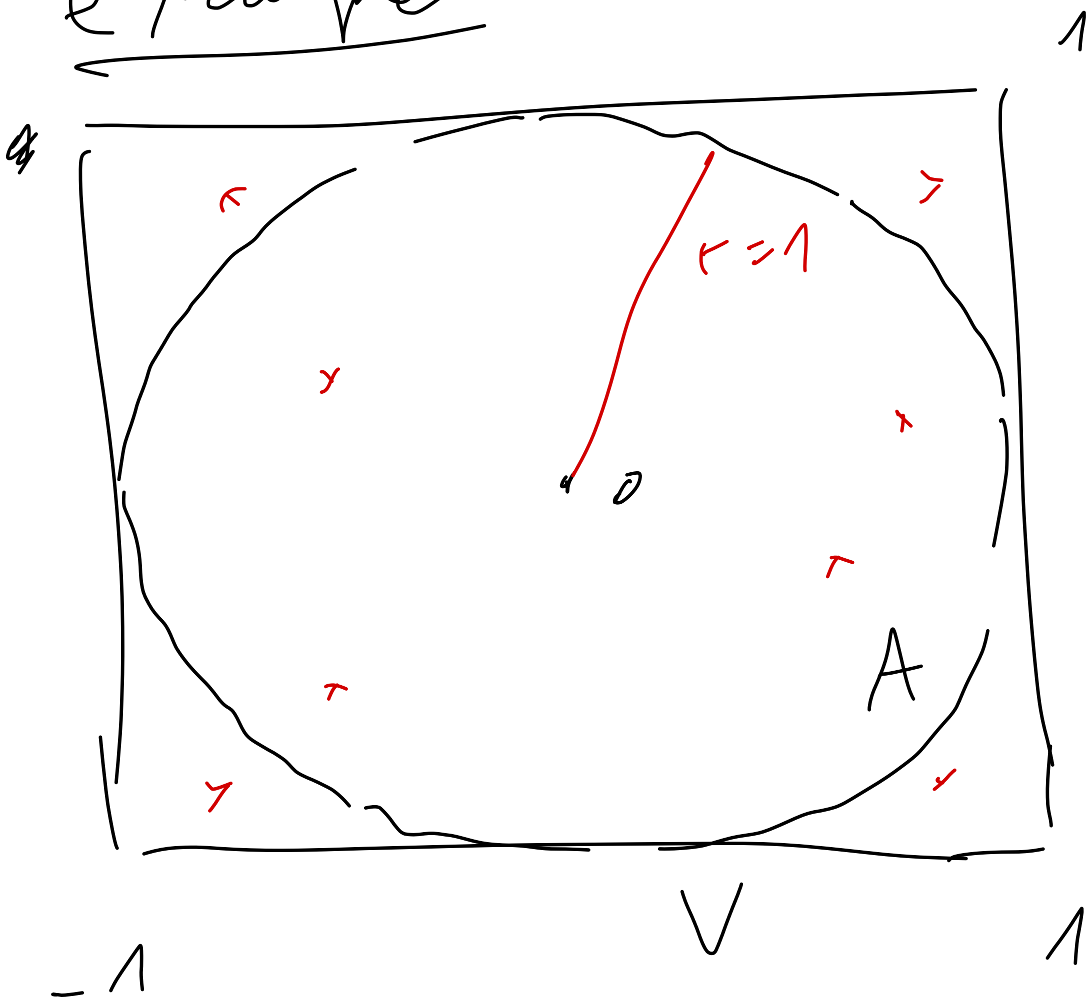
Drawback:

"Error is halving for quadrupling the number of samples"

Advantage:

The rate is independent of the spatial dim.

Example



Estimating the value of π

Area of circle is $A = \pi r^2$, $r = 1$

$$V = [-1,1] \times [-1,1]$$

$$|V| = 2^2 = 4$$

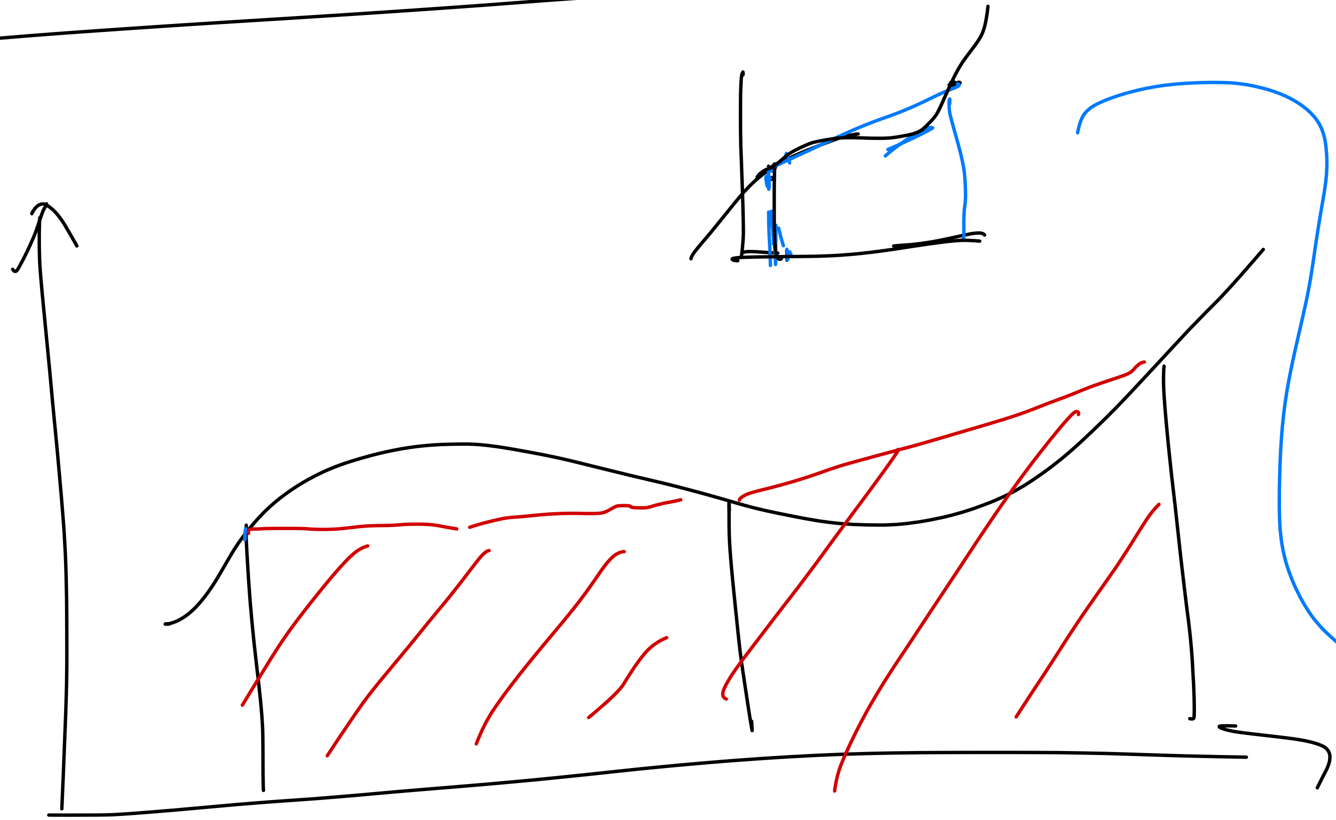
Ratio $\frac{\pi}{4}$

Let $g_i = \begin{cases} 1, & \text{if } p_i \text{ is inside } A \\ 0, & \text{otherwise} \end{cases}$

Idea: Let us sample random points p_i uniformly in V.

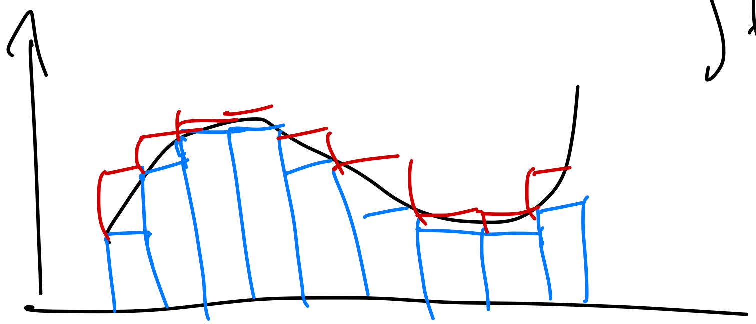
In the limit the number of "hits" over all samples tends to the ratio $= \frac{\pi}{4}$.

Newton-Cotes quadrature rules (1 dim)



always ok

so-called piecewise "Trapezoid rule"



usually integral

$\int f$ = limit of (upper sum) − (lower sum)

Riemann sum

"numerical algorithm" -7-

Idea:

Approximate $\int_a^b f(x)\,dx = I$

$$I \approx \int_a^b p_K(x)\,dx = Q(p)$$

p_K is an interpolation polynomial of f.

We know how to integrate polynomials!

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Lagrange

$a = x_0 \ , \ b = x_n$

$$\int_a^b f(x)\,dx \simeq \sum_{i=0}^{n} \underbrace{f(x_i)}_{\text{data}} \underbrace{\int_a^b \Bigg(\prod_{\substack{j=0 \\ i \neq j}}^{n} \frac{x - x_j}{x_i - x_j} \Bigg) dx}_{\text{just depends on the nodes}}$$

Let $n = 1$

$$p_1(x) = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a}$$

linear interpolation

$$\int_a^b f(x)\,dx \approx \int_a^b p_1(x)\,dx = \frac{b-a}{2}\left[f(a)+f(b)\right]$$

"Trapezoid rule"

Let's assume $f'' \in C^2$. (piecewise always ok for integrals)

Error formulations:

$$\underbrace{\int_a^b f(x)\,dx - \int_a^b p_1(x)\,dx}$$

Interpolation error

$$= \frac{1}{2} \int_a^b f''(\xi)\,(x-a)(x-b)\,dx \qquad \xi = \xi(x)$$

Now, $(x-a)(x-b) < 0$ for $x \in (a,b)$

therefore by mean value thm. for integrals

$$= \frac{1}{2} f''(\eta) \underbrace{\int_a^b (x-a)(x-b)\,dx}_{= \frac{1}{6}(a-b)^3} = -\frac{1}{12} f''(\eta)(b-a)^3$$

~10~

Mean value theorem for integrals $f \in C[a,b]$

$\exists\, \eta \in [a,b]$ and $\exists\, \tilde{\eta} \in [a,b]$,

such that

$$\int_a^b f(x)\,dx = (a-b)\, f(\eta)$$

(used for fundamental theorem of calculus)

and

$$\int_a^b f(x)\, g(x)\, dx = f(\tilde{\eta}) \int_a^b g(x)\, dx \,.$$

Break until 15:05

piecewise always ok!

$\longrightarrow$ Composite rule

Interdivision $\quad h = \frac{b-a}{n} \qquad x_i = a + ih$

$i = 0, \dots, n$

$x_0 = a, \; x_n = b$

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\Big[f(x_0) + 2f(x_1) + \dots + 2f(x_{n-1}) + f(x_n)\Big]$$

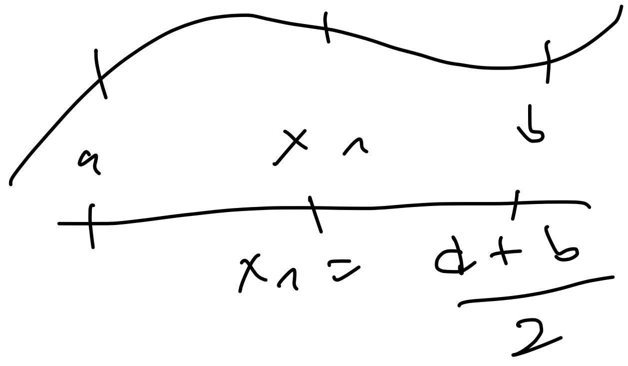
piecewise trapezoid rule!

Total error $\quad O(h^2) \sim O\left(\frac{1}{n^2}\right)$

We say that the method is quadratic

Let $n = 2$

Exact for degree 2 (or lower).



$$\int_a^b f(x)\,dx = A_1 f(a) + A_2 f\left(\frac{a+b}{2}\right) + A_3 f(b)$$

$$\int_a^b 1 = b-a \Rightarrow A_1 + A_2 + A_3 = b-a$$

$$\int_a^b x\,dx = \frac{b^2-a^2}{2} \Rightarrow A_1 a + A_2 \left(\frac{a+b}{2}\right) + A_3 b = \frac{b^2-a^2}{2}$$

$$\int_a^b x^2\,dx = \frac{1}{3}(b^3 - a^3)$$

$$\Rightarrow \quad A_1 a^2 + A_2 \left(\frac{a+b}{2}\right)^2 + A_3 b^2$$

$$= \frac{1}{3}(b^3 - a^3)$$

Solution: $\quad A_1 = A_3 = \dfrac{b-a}{6}$

$$A_2 = \frac{4(b-a)}{6}$$

Simpson's rule

(In contrast to Trapezoid rule. $A_1 = A_3 = 1$, $A_2 = 2$)

— u —

Simpson's rule (exact for degree 2 and less)

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$$

Composite rule

$$\int_a^b f(x)\,dx \approx \frac{h}{6}\Big[f(x_0)+4f(x_1)+\dots$$
$$\dots+2f(x_2)+4f(x_3)+\dots$$
$$\dots 4f(x_{n-1})+f(x_n)\Big]$$

$\boxed{\text{Greenbaum \& Chartier}}$

Error: $n=2$ $\quad \frac{1}{4!5!}(b-a)^5 f^{(4)}(\eta)$ $\quad f\in C^4$

Composite: $O(h^4)$ $\quad 4!5! = 2880$

Exact for cubic

Gauss quadrature

Idea: choose the nodes and the weights simultaneously.

One interval:

$$\int_a^b f(x) = A_0 f(x_0) + A_1 f(x_1)$$

weights: A_0, A_1

nodes: x_0, x_1 , $n=1$, $(n+1)$-rule

Coefficients are determined by usual process

$$\int_a^b 1\, dx = b-a = A_0 + A_1$$

$$\int_a^b x\, dx = \frac{1}{2}(b^2-a^2) = A_0 x_0 + A_1 x_1$$

$$\int_a^b x^2\, dx = \frac{1}{3}(b^3-a^3) = A_0 x_0^2 + A_1 x_1^2$$

$$\vdots$$

Need 4 equations (up to order 3)

$\rightarrow$ Problem: Resulting system is nonlinear!

Orthogonal polynomials

Define inner product of two polynomials

$$\langle p, q \rangle := \int_a^b p(x)\, q(x)\, dx$$

(There is a certain relation to Fourier series.)

Norm: $$\| p \| = \left(\int_a^b p(x)^2 \, dx \right)^{1/2}$$

Norm:

$$\|x+y\| \leq \|x\| + \|y\|$$

$$\|\alpha x\| = |\alpha| \, \|x\| \quad \forall \alpha \in \mathbb{R}$$

$$\|x\| = 0 \iff x = 0 .$$

(Real)

Inner product:

Cauchy-Schwarz:

$$|\langle p, q\rangle| \leq \|p\| \, \|q\|$$

$$\langle p_1 + p_2, q \rangle = \langle p_1, q\rangle + \langle p_2, q\rangle$$

$$\langle p, q_1 + q_2\rangle = \langle p, q_1\rangle + \langle p, q_2\rangle$$

$$\langle \alpha p, q\rangle = \alpha \langle p, q\rangle , \quad \langle p, \beta q\rangle = \beta \langle p, q\rangle$$

$$\langle p, q\rangle = \langle q, p\rangle \qquad \alpha, \beta \in \mathbb{R}$$

Def. (orthogonality)

Two polynomials are said to be <u>orthogonal</u> on $[a, b]$ if their inner product is zero.

$\langle p, q \rangle = 0$ orthogonal $p \perp q$

orthonormal: $\langle p, p \rangle = 1 = \langle q, q \rangle$

$(\|p\| = 1, \|q\| = 1)$

polynomials form a vector space.

Gram-Schmidt procedure (orthogonalization)

Idea: transform a basis to an orthogonal basis:

$$\{1, x, x^2, x^3, \dots, x^k, \dots\}$$

$$\xrightarrow[G.-S.]{} \{q_0, q_1, \dots, q^k, \dots\}$$

orthonormal

$$q_0 = \frac{1}{\|1\|} = \frac{1}{\left[\int_a^b 1^2\,dx\right]^{\frac{1}{2}}} = \frac{1}{\sqrt{b-a}}$$

Recursion

for $j = 1, 2, \ldots$

$$\tilde{q}_j = x\, q_{j-1}(x) - \sum_{i=0}^{j-1} \langle x\, q_{j-1}(x), q_i(x) \rangle q_i(x)$$

orthogonal

$$q_j(x) = \frac{\tilde{q}_j(x)}{\|\tilde{q}_j(x)\|}$$

orthonormal

Observation

$q_{j-1}(x)$ is orthogonal to all polynomials of degree $j-2$ or less.

but it's an integral!

thus

$$\langle x\, q_{j-1}(x), q_i(x)\rangle$$

$$= \langle q_{j-1}(x), x\, q_i(x)\rangle = 0$$

$$i+1 \leq j-2$$

$$\boxed{\deg(x\, q_i) = i+1} \qquad \Rightarrow i \leq j-3$$

$$\tilde{q}_j = x\, q_{j-1}(x) - \sum_{i=0}^{j-1} \langle x\, q_{j-1}(x), q_i(x)\rangle q_i(x)$$

$$= x\, q_{j-1}(x) - \sum_{i=j-2}^{j-1} \langle x\, q_{j-1}(x), q_i(x)\rangle q_i(x)$$

$$= x\, q_{j-1}(x) - \langle x\, q_{j-1}(x), q_{j-1}(x)\rangle q_{j-1}(x)$$

$$- \langle x\, q_{j-1}(x), q_{j-2}(x)\rangle q_{j-2}(x)$$

Two step recursion ~~recurrence~~ tree term rule.

Orthogonality?

Gram Schmidt works!

$$\langle \tilde{q}_j(x), q_{j-1}(x) \rangle$$

$$= \langle x\, q_{j-1}(x), q_{j-1}(x) \rangle$$

$$- \langle x\, q_{j-1}(x), q_{j-1}(x) \rangle \overbrace{\langle q_{j-1}(x), q_{j-1}(x) \rangle}^{1 \,=\, \|q_{j-1}\|^2 \,=}$$

$$- \langle x\, q_{j-1}(x), q_{j-2}(x) \rangle \underbrace{\langle q_{j-2}(x), q_{j-1}(x) \rangle}_{=0}$$

If q_{j-1} is normalized, $\|q_{j-1}\|^2 = 1$

$\Rightarrow \; = 0 \quad \Rightarrow \quad \tilde{q}_j \perp q_{j-1}$