LECTURE 7: QUADRATURE

Introduction

- Given an integrand f and an interval $[a, b]$, approximate

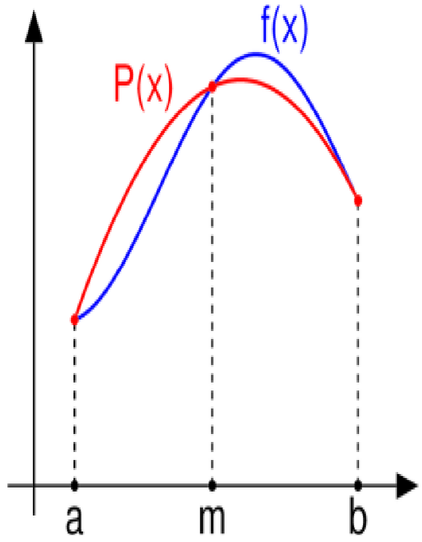
$$I(f) = \int_a^b \mu(x) f(x) dx \approx I_n(f) = \sum_{j=0}^{n} w_k f(x_k)$$

  - $\mu(x)$ is a non-negative, integrable weight function (take $\mu(x) = 1$ for now).
  - n is the degree of the quadrature (i.e., number of evaluations).
  - x_j are the nodes and w_j are the weights.
- Most integrals do not have closed form solutions. For example

$$\int_{-1}^{1} \exp(-x^2) dx = \cdots ?$$

  (Liouville's theorem of differential algebra)
- Idea: Approximate the complicated integrand by a proxy.

Examples



Examples:

- Trapezium rule:
  - Integrate a piecewise linear interpolant.
  - $I_2(f) = (b - a)\frac{f(a)+f(b)}{2}$.
- Simpson's rule:
  - Integrate a quadratic interpolant.
  - $I_2(f) = \frac{b-a}{6} \frac{f(a)+4f(\frac{a+b}{2})+f(b)}{2}$.
- Newton-Cotes:
  - Interpolate f at $x_j = a + jh, j = 0, \ldots, n$, where h
  - Integrate this interpolant exactly. (It's just a polynomial, after all).
  - $I_n(f) = I(g_n) = \sum_{j=0}^{n} f(x_j) \int_a^b l_j(x) dx$
  - This is almost always a bad idea if n is large!

Integration error

- Recall the interpolation error formula:

$$e(x) = g_n(x) - f(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{k=0}^{n} (x - x_k) : \xi \in (a, b)$$

- Integrating gives a error formula for this type of quadrature:

$$\left| \int_a^b g_n(x)dx - \int_a^b f(x)dx \right| \leq \frac{\max_{\xi \in (a,b)} |f^{(n+1)}(\xi)|}{(n+1)!} \left| \int_a^b \prod_{k=0}^{n} (x - x_k)dx \right|$$

- Points are good/bad for interpolation ⇒ good/bad for quadrature.

Two approaches

Newton-Cotes is unstable for large degrees.

- Use smaller degrees on sub-intervals ⇒ composite rules.
- Use better interpolants / nodes ⇒ Gauss quadrature / Clenshaw-Curtis.

In both cases, can use adaptive methods to further increase efficiency.

COMPOSITE RULES

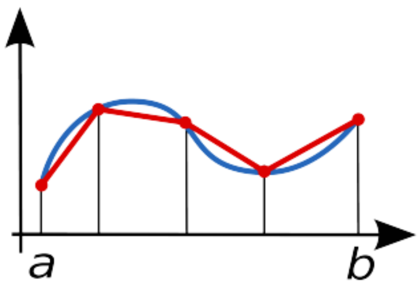
Composite trapezium rule:

- Local linear interpolants ($x_k = a + kh$)

$$I_n(f) = \frac{h}{2} \sum_{k=0}^{n} (f(x_{k+1}) + f(x_k)).$$

- Approximation error: (quadratic in h)

$$\left| I_n(f) - I(f) \right| \leq \max_{\xi \in (a,b)} \frac{h^2(b-a)}{12} \left| f''(\xi) \right|.$$

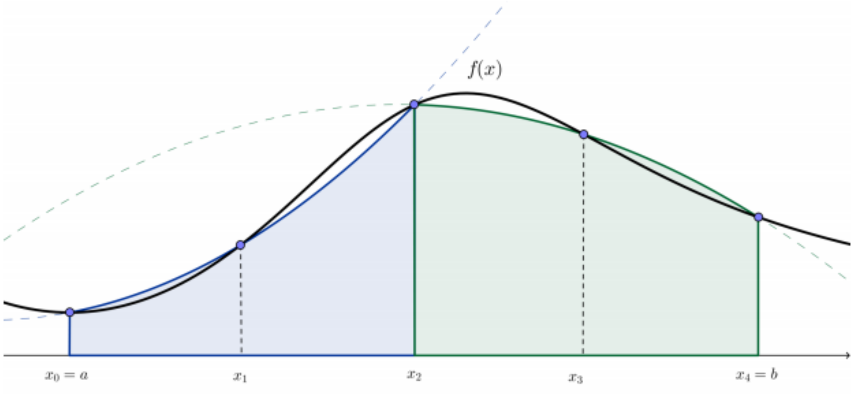


- Convergence for periodic analytic functions is geometric
- Can be applied on a non-equispaced grid (without geometric convergence)

Composite Simpson's rule:

- Local quadratic interpolants

$$I_n(f) = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right].$$



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- Approximation error becomes (for sufficiently smooth f)

$$\left|I_n(f) - I(f)\right| \leq \max_{\xi\in(a,b)} \frac{h^4}{180}(b-a)\left|f^{(4)}(\xi)\right|.$$

CLENSHAW CURTIS QUADRATURE

- Chebyshev points and Chebyshev polynomials were great interpolants.
- Why don't we use them for quadrature? (We do!)
- Clenshaw-Curtis quadrature integrates Chebyshev interpolants.
- Inherits accuracy of interpolant, so that $|I(f) - I_n(f)| \sim O(\rho^{-n})$ as $n \to \infty$.
- Can do this is either of the convenient representations of the interpolants:
  - Coefficient space
  - Value space

Clenshaw-Curtis: Coefficient space

- Interpolate f by g_n at Chebyshev points.
- Compute the Chebyshev coefficients $\{f(x_j)\} \leftrightarrow \sum_{j=0}^{n} \alpha_j T_j(x)$.
- Observe that
$$I(f) \approx I(g_n) = \sum_{j=0}^{n} \alpha_j \int_{-1}^{1} T_j(x)dx.$$
- Now
$$\int_{-1}^{1} T_j(x)dx = \int_{-1}^{1} \cos(j\cos^{-1}(x))dx = \int_{0}^{\pi} \cos(j\theta)\sin(\theta)d\theta = \begin{cases} 0 & : j \text{ odd} \\ \frac{2}{1-j^2} & : j \text{ even.} \end{cases}$$
- Therefore
$$I(g_n) = \sum_{\substack{j=0 \\ j \text{ even}}}^{n} \frac{2\alpha_j}{1-j^2}.$$

Clenshaw-Curtis: Value-space

- Task: Find $\{w_k\}_{k=0}^{n}$ such that $I(g_n) = \sum_{k=0}^{n} w_k f(x_k)$.
- We can do this by ensuring we integrate each T_k exactly:

$$\begin{aligned} T_0(x_0)w_0 + T_0(x_1)w_1 + \ldots + T_0(x_n)w_n &= \int_{-1}^{1} T_0(x)dx = 2 \\ T_1(x_0)w_0 + T_1(x_1)w_1 + \ldots + T_1(x_n)w_n &= \int_{-1}^{1} T_1(x)dx = 0 \\ &\vdots \\ T_n(x_0)w_0 + T_n(x_1)w_1 + \ldots + T_n(x_n)w_n &= \int_{-1}^{1} T_n(x)dx = \frac{2}{1-n^2} \end{aligned}$$

- I.e., $V^T\underline{w} = \underline{b}$, where $b_k = \int_{-1}^{1} T_k(x)dx$. ($V$ is the Vandermonde matrix!)
- (V^{-T} can actually be applied in $O(n\log n)$ operations via an FFT/DCT.)

Aside: Scaling to different domains

- When deriving quadrature routines, it's convenient to work on $[-1,1]$.
- We can easily map this to a different domain by a linear change of variables:

$$l : [-1,1] \to [a,b] \quad : \quad l(y) = \frac{b(y+1) + a(1-y)}{2}.$$

- If we do this, then

$$\begin{aligned} \int_a^b f(x)dx &= \int_{-1}^1 f(l(y))l'(y)dy \\ &= \int_{-1}^1 f\left(\frac{b(y+1)+a(1-y)}{2}\right)\frac{b-a}{2}dy \\ &= \int_{-1}^1 F(y)dy \end{aligned}$$