

Quadrature

integrals

- ▶ aim: to compute

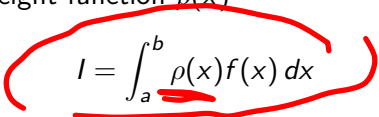
$$I(f) = \int_a^b f(x) dx$$

for given $a, b \in \mathbb{R}$ and function $f(x)$

- ▶ data:

- ▶ a, b and procedure defining $f(x)$
- ▶ data points $a \leq x_0 < \dots x_n \leq b$ and $y_k = f(x_k)$
- ▶ from computations and from observations

- ▶ integral with weight function $\rho(x)$


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

- ▶ we call the process of computing the integral **quadrature**

[https://en.wikipedia.org/wiki/Numerical_integration]



applications

- ▶ geometric properties like volume, areas or length
- ▶ physics: mass energy, total force on an object
- ▶ probability: expectation, averages, covariance, cumulative distribution
- ▶ decision making: risk
- ▶ finance: costs, values, utility
- ▶ weather prediction: average rainfall, expected rainfall

quadrature in scientific computing

$$\int_0^x k(x,y)f(y)dy = g(x)$$

- ▶ solution of integral and partial differential equations
- ▶ solving ordinary differential equations by recasting as integral equations

history

- ▶ Archimedes: area of a circle – he provides a numerical technique!

quadrature and calculus

- ▶ given continuous $f : [a, b] \rightarrow \mathbb{R}$
- ▶ determine any *anti-derivative* $F(x)$ such that

$$\frac{dF(x)}{dx} = \underline{f(x)}$$

- ▶ (second) fundamental theorem of calculus:

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

- ▶ use this theorem to compute integrals of polynomials, exponential functions, sin and cos and many others
- ▶ but for most functions f we don't know F

two simple methods (or rules)

► rectangle rule

- approximate $f(x)$ by a constant (interpolation) function

$$f(x) \approx p(x) = f(x_0)$$

- integrate approximation exactly to get

$$Q(f) = (b - a)f(x_0) \approx I(f) = \int_a^b f(x) dx$$

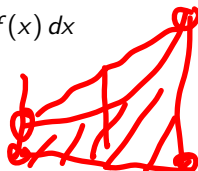
► trapezoidal rule

- approximate $f(x)$ by linear interpolant

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

- integrate approximation exactly to get

$$Q(f) = \frac{b-a}{2} (f(a) + f(b)) \approx I(f) = \int_a^b f(x) dx$$



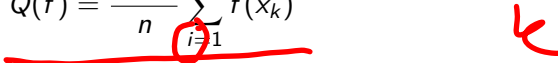
- ▶ these methods by themselves are not too exciting but they form the basis for quite effective methods
- ▶ error

$$\underline{Q(f) - I(f)} = I(p) - I(f) = I(p - f)$$

apply Taylor's remainder theorem for $p - f$

Monte Carlo method

- ▶ interpret the integral $I(f)$ as an expectation for a uniform distribution with density $\rho(x) = 1/(b - a)$ over the interval $[a, b]$
- ▶ draw samples x_k from this interval
- ▶ approximation of $I(f)$ is then given by the sample mean

$$Q(f) = \frac{b - a}{n} \sum_{i=1}^n f(x_k)$$
A red handwritten underline is drawn under the entire equation. A red arrow points from the right side of the slide towards the summation index $i=1$.

- ▶ expected squared error can be shown to be bounded by $1/n$ so that the error decreases with n proportional to $1/\sqrt{n}$

Quadrature and Python

- ▶ input: a function $f(x)$ and integration boundaries a and b
- ▶ output: integral $I(f)$ and indication of accuracy
- ▶ handy function in module `scipy.integrate`: `quad`
- ▶ example:

$$I(f) = \int_3^4 \frac{\exp(x)}{(1+x^2)^{-3}} dx$$

- ▶ python code:

```
I = sci.quad(lambda x : m.exp(x)/(1.0+x*x)**3,\n              3.0, 4.0)\nprint("approximation of integral I: {0[0]:3.3g},\\n \\  
      estimate of error of I: {0[1]:3.3g}".format(I))
```

```
approximation of integral I: 0.0147,\n      estimate of error of I: 1.63e-16
```

Composite rules

General construction

- ▶ use a base or component rule

$$- \quad \curvearrowright \quad q(f; \alpha, \beta) \approx \int_{\alpha}^{\beta} f(x) dx$$

- ▶ define a *grid*

$$x_0 = a < x_1 < \dots < x_n = b$$

- ▶ *composite rule* using q and the x_k :

$$Q(f) = \sum_{k=1}^n q(f; x_{k-1}, x_k)$$



Riemannian sums

- ▶ base rule is the rectangle rule

$$q(f; \alpha, \beta) = (\beta - \alpha)f(\xi)$$

where ξ is chosen as a function of α, β , 3 typical choices are

- ▶ $\xi = \alpha$
 - ▶ $\xi = \beta$
 - ▶ $\xi = (\alpha + \beta)/2$ (midpoint rule)
- ▶ we denote by \bar{x}_k the chosen ξ for $\alpha = x_{k-1}$ and $\beta = x_k$
- ▶ **Riemannian sum**

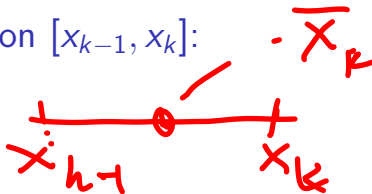
$$Q(f) = \sum_{k=1}^n (x_k - x_{k-1}) f(\bar{x}_k)$$

application of Riemannian sums

- ▶ in calculus to define the Riemann integral which is the limit of the Riemannian sum for continuous f
 - ▶ **this is an example where the numerical technique is driving the theory**
- ▶ the Riemannian sums are generally not very accurate and not very widely used
- ▶ they are related to the Euler method for solving PDEs and ODEs
- ▶ an exception is if the base rule is the midpoint rule – this method has the same accuracy as the widely used trapezoidal rule

error of rectangular rule on $[x_{k-1}, x_k]$:

- ▶ component rule



$$q_k(f) = (x_k - x_{k-1})f(\bar{x}_k)$$

- ▶ error

$$e_k(x) = q_k(f) - \int_{x_{k-1}}^{x_k} f(x) dx = \int_{x_{k-1}}^{x_k} (f(\bar{x}_k) - f(x)) dx$$

- ▶ assumption: f Lipschitz continuous with Lipschitz constant M .
Then

$$|e_k(x)| \leq M(x_k - x_{k-1})^2$$

as $|\bar{x}_k - x| \leq |x_k - x_{k-1}|$.

error for Riemannian sum

- ▶ error = sum of component errors

$$e(x) = \sum_{k=1}^n e_k(x)$$

- ▶ include the error bound for the components

$$|e(x)| \leq M \sum_{k=1}^n |x_k - x_{k-1}|^2$$


- ▶ use bound $0 \leq x_k - x_{k-1} \leq h$ (define h as maximum)

$$|e(x)| \leq Mh \sum_{k=1}^n (x_k - x_{k-1}) = M(b-a)h$$

- ▶ one achieves a lower error using the midpoint rule and C^2 functions

(composite) trapezoidal rule

- ▶ the (base) trapezoidal rule


$$q(f, \alpha, \beta) = (\beta - \alpha) \frac{f(\alpha) + f(\beta)}{2} .$$

- ▶ equals integral $\int_{\alpha}^{\beta} p_1(x) dx$ where p_1 is the linear interpolant
- ▶ area of trapezoid under graph of p_1

composite trapezoidal rule for $x_k = a + kh$

$$T(f) = \sum_{k=1}^n q(f, x_{k-1}, x_k) = h \left(\frac{f(x_0)}{2} + \sum_{k=1}^{n-1} f(x_k) + \frac{f(x_n)}{2} \right)$$

- ▶ equals the integral $\int_a^b s(x) dx$ of the piecewise linear interpolant

error of base rule

- ▶ error equals the integral of the interpolation error


$$e = q(f, \alpha, \beta) - \int_{\alpha}^{\beta} f(x) dx = \int_{\alpha}^{\beta} \underbrace{(p_1(x) - f(x))}_{\text{interpolation error}} dx$$

- ▶ recall interpolation error formula

$$\underbrace{p_1(x) - f(x) = -\frac{f''(\xi_x)}{2}(x - \alpha)(x - \beta)}$$

- ▶ insert in integral to get

$$e = \int_{\alpha}^{\beta} \underbrace{\frac{(x - \alpha)(\beta - x)}{2} f''(\xi_x)}_{\text{interpolation error}} dx$$



- ▶ this looks like an expectation ...

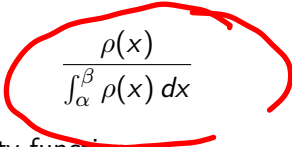
mean value theorem for integration

Theorem

If $\rho(x)$ and $f(x)$ continuous and $\rho(x) \geq 0$ then there exists some $\zeta \in [\alpha, \beta]$ such that

$$\int_{\alpha}^{\beta} \rho(x) f(x) dx = f(\zeta) \int_{\alpha}^{\beta} \rho(x) dx$$

- ▶ prove using Riemann sums
- ▶ note that the function


$$\frac{\rho(x)}{\int_{\alpha}^{\beta} \rho(x) dx}$$

is a probability density function

- ▶ there is also a version for Lebesgue integrals

error formula

- ▶ as $f(\xi_x)$ in the error formula is continuous function of x and $(x - \alpha)(\beta - x)/2 \geq 0$ one has

$$e = \int_{\alpha}^{\beta} \frac{(x - \alpha)(\beta - x)}{2} f''(\xi_x) dx = \frac{f''(\zeta)}{2} \int_{\alpha}^{\beta} (x - \alpha)(\beta - x) dx$$

- ▶ compute the integral by transformation $x = \alpha + (\beta - \alpha)t$
 - ▶ $x - \alpha = (\beta - \alpha)t$
 - ▶ $\beta - x = \beta - \alpha - (x - \alpha) = (\beta - \alpha)(1 - t)$
 - ▶ $dx = (\beta - \alpha)dt$

$$\int_{\alpha}^{\beta} (x - \alpha)(\beta - x) dx = (\beta - \alpha)^3 \int_0^1 t(1 - t) dt = \frac{(\beta - \alpha)^3}{6}$$

- ▶ final error formula for base rule for some $\zeta \in [\alpha, \beta]$:

$$e = \frac{(\beta - \alpha)^3}{12} f''(\zeta)$$

error formula for the composite rule – case of equidistant grid

$$h = x_k - x_{k-1}$$

- ▶ sum the errors of all intervals $[x_{k-1}, x_k]$:

$$T(f, h) - I(f) = \sum_{k=1}^n e_k = \frac{h^3}{12} \sum_{k=1}^n f''(\zeta_k)$$

- ▶ use the mean value theorem for sums of values of continuous functions g :

$$\sum_{k=1}^n g(x_k) = ng(\xi)$$

for some ξ in the range of x_k

- ▶ final error result: there exists some $\xi \in [a, b]$ such that

$$e = T(f, h) - I(f) = \frac{h^2(b-a)}{12} f''(\xi)$$

using Riemann sum to get an approximate error formula

- ▶ The following sum occurring in the error formula is a Riemann sum

$$h \sum_{k=1}^n f''(\zeta_k) = \int_a^b f''(x) dx + \underline{O(h)}$$

where $O(h)$ stands for the error of the Riemann sum which we know is bounded by h times some constants depending on f

- ▶ integrate (fundamental theorem of calculus):

$$e \sum_{k=1}^n f''(\zeta_k) = f'(b) - f'(a) + O(h)$$

- ▶ insert this in (earlier) error formula to get

$$e = T(f, h) - I(f) = \frac{h^2}{12}(f'(b) - f'(a)) + \underline{O(h^3)}$$

case of non-equidistant grids

- ▶ sum the errors of all intervals $[x_{k-1}, x_k]$:

$$T(f, h) - I(f) = \sum_{k=1}^n e_k = \frac{1}{12} \sum_{k=1}^n (x_k - x_{k-1})^3 f''(\zeta_k)$$

- ▶ let $h = \max_k (x_k - x_{k-1})$ to get with triangle inequality

$$|T(f, h) - I(f)| = \sum_{k=1}^n |e_k| \leq \frac{h^2}{12} \sum_{k=1}^n |f''(\zeta_k)|$$

- ▶ if $|f''|$ is continuous, we can use the mean value theorem for sums and get
- ▶ the final error bound

$$|e| = |T(f, h) - I(f)| \leq \frac{h^2(b-a)}{12} |f''(\xi)|$$
