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

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

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

- (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
$$Q(f) - I(f) = I(p) - I(f) = I(p - f)$$
apply Taylor's remainder theorem for $p - f$

Monte Carlo method

- interprete 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 ths interval
- approximation of $I(f)$ is then given by the sample mean

$$Q(f) = \frac{b-a}{n} \sum_{i=1}^{n} f(x_k)$$

- 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,\
             3.0, 4.0)
print("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,
     estimate of error of I: 1.63e-16
```

Composite rules

General construction

- use a base or component rule

$$q(f; \alpha, \beta) \approx \int_\alpha^\beta f(x)\, dx$$

- define a *grid*

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

- *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 $\overline{x}_k$ the chosen ξ for $\alpha = x_{k-1}$ and $\beta = x_k$
- **Riemannian sum**

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

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

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

- error

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

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

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

as $|\overline{x}_k - x| \le |x_k - x_{k-1}|$.

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 trapzoid under graph of p_1

composite trapezoidal rule for $x_k = a + kh$

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

- 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

$$e = q(f, \alpha, \beta) - \int_\alpha^\beta f(x)\,dx = \int_\alpha^\beta (p_1(x) - f(x))\,dx$$

- recall interpolation error formula

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

- insert in integral to get

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

- 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

- 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:

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

  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
$$\sum_{k=1}^{n} f''(\zeta_k) = \int_a^b f''(x)\,dx + O(h)$$
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):
$$\sum_{k=1}^{n} f''(\zeta_k) = f'(b) - f'(a) + O(h)$$
- insert this in (earlier) error formula to get
$$e = T(f,h) - I(f) = \frac{h^2}{12}(f'(b) - f'(a)) + O(h^3)$$

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

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

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

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