Unit 27: Numerical integration

LECTURE

27.1. We look here at some numerical techniques for computing integrals. There are variations of basic Riemann sums but allow speed up or adjust the computation to more complex situations.

### Riemann sum with nonuniform spacing

Definition: A more general Riemann sum is obtained by choosing n points $\{x_j\}$ in $[a, b]$ and then to look at

$$S_n = \sum f(x_j)(x_{j+1} - x_j) = \sum_{y_j} f(x_j)\Delta x_j \ ,$$

where $\Delta x_j = x_{j+1} - x_j$.

27.2. This generalization of Riemann and allows to use a small mesh size where the function fluctuates a lot. The function $f(x) = \sin(1/(x^2 + 0.1))$ for example fluctuates near the origin more. We need more division points there.

Definition: The sum $L = \sum f(x_j)\Delta x_j$ is called the **left Riemann sum**, the sum $R = \sum f(x_{j+1})\Delta x_j$ the **right Riemann sum**.
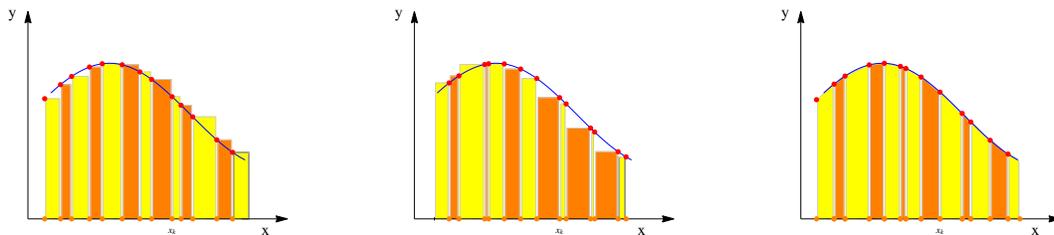
If $x_0 = a$, $x_n = b$ and $\max_j \Delta x_j \to 0$ for $n \to \infty$ then S_n converges to $\int_a^b f(x) \, dx$.

Example: If $x_j - x_k = 1/n$ and $z_j = x_j$, then we have the Archimedes sum defined initially.

Example: You numerically integrate $\sin(x)$ on $[0, \pi/2]$ with a Riemann sum. What is better, the left Riemann sum or the right Riemann sum? Look also at the interval $[\pi/2, \pi]$? **Solution:** you see that in the first case, the left Riemann sum is smaller than the actual integral. In the second case, the left Riemann sum is larger than the actual integral.

Trapezoid rule

Definition: The average $(L + R)/2$ between the left and right hand Riemann sum is called the **Trapezoid rule**. Geometrically, it sums up areas of trapezoids instead of rectangles.

27.3. The trapezoid rule does not change things in the Archimedescase. For the interval $[0, 1]$ for example, with $x_k = k/n$ we have

$$S_n = \frac{1}{2n}[f(0) + f(1)] + \frac{1}{n}\sum_{k=1}^{n-1} f(x_k) \ .$$

Simpson rule

Definition: The **Simpson rule** computes the sum

$$S_n = \frac{1}{6n}\sum_{k=1}^{n}[f(x_k) + 4f(y_k) + f(x_{k+1})] \ ,$$

where $y_k = (x_k + x_{k+1})/2$ is the midpoint between x_k and x_{k+1}.

27.4. The Simpson rule is exact for quadratic functions: for $f(x) = ax^2 + bx + c$, the formula

$$\frac{1}{v - u}\int_u^v f(x) \ dx = [f(u) + 4f((u + v)/2) + f(v)]/6$$

holds exactly. To prove it just run the following two lines in Mathematica: (== means "is equal")

```
f [ x_ ]  := a x^2 + b x + c ;
( f [ u]+f [ v]+4 f [ ( u+v)/2])/6==Integrate [ f [ x] ,{ x ,u , v }]/( v−u )]
Simplify [%]
```

27.5. With a bit more calculus one can show that if f is 4 times differentiable then the Simpson rule is n^{-4} close to the actual integral. For 100 division points, this can give accuracy to 10^{-8} already.

There are other variants which are a bit better but need more function values. If x_k, y_k, z_k, x_{k+1} are equally spaced, then

Definition: The **Simpson 3/8 rule** computes

$$\frac{1}{8n} \sum_{k=1}^{n} [f(x_k) + 3f(y_k) + 3f(z_k) + f(x_{k+1})] \ .$$

This formula is again exact for quadratic functions: for $f(x) = ax^2 + bx + c$, the formula

$$\frac{1}{v-u} \int_{u}^{v} f(x)\, dx = [f(u) + 3f((2u+v)/3) + 3f((u+2v)/3) + f(v)]/6$$

holds. Just run the two Mathematica lines to check this:

```
f[x_] := a x^2 + b x + c;  L=Integrate[f[x],{x,u,v}]/(v−u);
Simplify[(f[u]+f[v]+3f[(2u+v)/3]+3f[(u+2v)/3])/8==L]
```

This **Simpson 3/8 method** can be slightly better than the first Simpson rule.

Monte Carlo Method

27.6. A powerful integration method is to chose n random points x_k in $[a, b]$ and look at the sum divided by n. Because it uses randomness, it is called **Monte Carlo method**.

**Definition:** The **Monte Carlo** integral is the limit S_n to infinity

$$S_n = \frac{(b-a)}{n} \sum_{k=1}^{n} f(x_k) \ ,$$

where x_k are n random values in $[a, b]$.

27.7. The law of large numbers in probability shows that the **Monte Carlo integral** is equivalent to the **Lebesgue integral** which is more powerful than the Riemann integral. Monte Carlo integration is interesting especially if the function is complicated.

Example: The following two lines evaluate the **area of the Mandelbrot fractal** using Monte Carlo integration. The function F is equal to 1, if the parameter value c of the quadratic map $z \to z^2 + c$ is in the Mandelbrot set and 0 else. It shoots 100'000 random points and counts what fraction of the square of area 9 is covered by the set. Numerical experiments give values close to the actual value around 1.51.... One could use more points to get more accurate estimates.
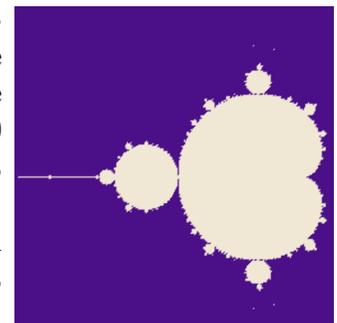

```
F[c_]:=Block[{z=c,u=1},Do[z=N[z^2+c]; If[Abs[z]>3,u=0;z=3],{99}];u];
M=10^5;  Sum[F[−2.5+3 Random[]+I(−1.5+3 Random[])],{M}]*(9.0/M)
```

Homework

Problem 27.1: Use the generalized left Riemann sum with $x_0 = 0$, $x_1 = \pi/6$, $x_2 = \pi/2$, $x_3 = 2\pi/3$ and $x_4 = \pi$ to compute the integral

$$\int_0^\pi \sin(x)\ dx$$

without a computer.

Problem 27.2: Use a computer to generate 10 random numbers x_k in $[0, 1]$. If you do not have a computer to do that for you, make up some random numbers on your own. Try to be as random as possible. Sum up the cubes x_k^3 of these numbers and divide by 10. Compare your result with $\int_0^1 x^3\ dx$.

Remark. If using a program, increase the value of n as large as you can. Here is a Mathematica code:

```
n=10; Sum[ Random[]^3 ,{ n }]/n
```

Problem 27.3: Use the Simpson rule to compute $\int_0^\pi \sin(x)\ dx$ using $n = 2$ intervals $[a, b] = [0, \pi/2]$ or $[a, b] = [\pi/2, \pi]$. On each of these two intervals $[a, b]$, compute the Simpson value

$$\frac{[f(a) + 4f((a + b)/2) + f(b)]}{6}(b - a)$$

with $f(x) = \sin(x)$ then add up. Compare with the actual integral.

Problem 27.4: Now use the 3/8 Simpson rule to estimate $\int_0^\pi \sin(x)\ dx$ using $n = 1$ intervals $[0, \pi]$. Again compare with the actual integral.

Problem 27.5: a) Use a computer to numerically integrate

$$\int_0^1 \sin(\frac{1}{x^2})\frac{1}{x^2}\ dx\ .$$

b) Do the same with

$$\int_0^1 \sin(\frac{1}{x^2})\frac{1}{x^4}\ dx\ .$$