Introduction to Scientific Computing
Lecture 7

Professor Hanno Rein

Last updated: October 29, 2018

Integrals over infinite ranges

We often encounter integrals over infinite ranges like

$$\int_0^\infty f(x)dx$$

How can we possible integrate those using one of the algorithms we discussed? One way is to use a coordinate transformation such as

$$z = \frac{x}{1+x}$$

or equivalently

$$x = \frac{z}{1-z}$$

Then

$$dx = \frac{dz}{(1-z)^2}$$

and therefore

$$\int_0^\infty f(x)dx = \int_0^1 \frac{1}{(1-z)^2} f\left(\frac{z}{1-z}\right) dz$$

Let's do an example with the Bell Curve

$$I = \int_0^\infty e^{-t^2} dt$$

Using the above coordinate transformation we get

$$I = \int_0^1 \frac{1}{(1-z)^2} e^{-z^2/(1-z)^2} dz$$

Let's use Simpson's rule to calculate this value.

```python
from math import exp
def f(x):
    return 1./(1.-x)**2*exp(-x**2/(1.-x)**2)
N = 100
a = 0
b = 0.9999999999999999
h = (b-a)/N
s = f(a)
s += f(b)
for k in range(1,N,2):
    s += 4.*f(a+k*h)
for k in range(2,N,2):
    s += 2.*f(a+k*h)
s *= h/3.
print(s)
```

Code 1: Python code of Simpson's rule

Note that $\pi = (2I)^2$.

Multiple integrals

We won't go into details, but consider you want to solve the integral

$$I = \int_0^1 \int_0^1 f(x, y) dx dy.$$

We can rewrite this as

$$I = \int_0^1 F(y) dy$$

where

$$F(y) = \int_0^1 f(x, y) dx$$

So we can solve the two dimensional integral by solving a series of one dimensional integrals. Note that this now scales as $O(N^2)$ if N is the number of grid points in each dimension. Thus for very large dimensions, this becomes prohibitively large. We will discuss one alternative method to solve integrals in high dimensions.

1 Differential equations

Differential equations are equations where we are solving for a function rather than a variable. For example, instead of solving for x in a normal algebraic equation such as

$$a \cdot x = b$$

we now solve for a function $y(t)$ in a differential equation such as

$$y(t) = a \cdot \frac{\partial y(t)}{\partial t}.$$

Differential equations are closely related to integral equations. The differential and the integral operators are the inverse of each other. So for every differential equation there is one corresponding integral equation. For the above example, this would be

$$\int y(t)\, dt = a \cdot y(t).$$

We'll usually work with differential equations rather than integral equations because they are more intuitive most of the time.

Let's discuss a few examples of differential equations. For these differential equations we can write down exact solutions.

Example 1: The following differential equation pops up in a variety of places in biology and physics:

$$N(t) = a \cdot N'(t).$$

It says that the growth of the function, $N'(t)$, is proportional to the value of the function $N(t)$. The solution is an exponential:

$$N(t) = N_0 \cdot e^{a \cdot t}$$

Here, N_0 is an initial value that is determined by the boundary conditions.

Example 2: The first example leads to a exponentially growing or decreasing function. Another class of differential equations leads to periodic solutions. For example

$$m \cdot x''(t) = -k \cdot x(t)$$

has a solution

$$x(t) = A \cdot \cos(\omega t + \phi) \qquad \text{with} \qquad \omega^2 = \frac{k}{m}.$$

This is the solution for a harmonic oscillator, a very common problem in physics.

So, let's go back to the initial conditions. What are these values N_0, A and ϕ? They are given to you as part of the problem description. For example, in the first example, if you think of N as the number of creatures in a biology model, then N_0 is the number od creatures at the beginning of the experiment. Similarly, in the second example, the initial position and velocity of your pendulum determine the constants A and ϕ.

The unknown function is not entirely specified by the differential equation itself. We also need to define certain boundary conditions. The nature of the boundary conditions varies depending on the problem. They can be as simple as requiring that the function has a certain value at $t = 0$. But they can also be complex algebraic equations. Different boundary conditions lead to qualitatively different problems and solutions. There are two main kinds of differential equations.

- The first kind has the boundary conditions specified at one point.
- The second kins has boundary conditions for two points

In this course we will focus on the first kind.