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Set 10

Issued: 03.05.2019; Due: 12.05.2019

In this exercise, you will learn about improving the numerical integration scheme by changing the integration points. Instead of using a uniformly distributed grid, you will experience two other methods: (1) Adaptive Quadrature, and (2) Gauss Quadrature.

Question 1: Integrating Batman with Adaptive Quadrature

Gotham city needs your help. Police Commissioner James Gordon accidentally broke the Bat-Signal, and a new one needs to be built. You have been provided with an explicit mathematical function that defines the upper and lower curves of the Batman symbol on the range $x \in [-7, 7]$:

$$\begin{aligned}\mathrm{batman\_upper}(x) =& (\mathrm{h}(x) - \mathrm{l}(x)) \cdot \mathrm{H}(x+1) + (\mathrm{r}(x) - \mathrm{h}(x)) \cdot \mathrm{H}(x-1) + \\ & (\mathrm{l}(x) - \mathrm{w}(x)) \cdot \mathrm{H}(x+3) + (\mathrm{w}(x) - \mathrm{r}(x)) \cdot \mathrm{H}(x-3) + \mathrm{w}(x)\end{aligned}$$

$$\begin{aligned}\mathrm{batman\_lower}(x) = \frac{1}{2}\left[\left|\frac{1}{2}x\right| + \sqrt{1-(||x|-2|-1)^2} - \frac{1}{112}\left(3\sqrt{33}-7\right)x^2 + 3\sqrt{1-\left(\frac{x}{7}\right)^2} - 3\right] \times \\ [\mathrm{sgn}(x+4) - \mathrm{sgn}(x-4)] - 3\sqrt{1-\left(\frac{x}{7}\right)^2}\end{aligned}$$

where $\mathrm{H}(x)$ is the Heaviside step function, $\mathrm{sgn}(x)$ is the sign function, and:

$$\begin{aligned}
\mathrm{w}(x) &= 3\sqrt{1-\left(\frac{x}{7}\right)^2} \\
\mathrm{l}(x) &= \frac{1}{2}(x+3) - \frac{3}{7}\sqrt{10}\sqrt{4-(x+1)^2} + \frac{6}{7}\sqrt{10} \\
\mathrm{h}(x) &= \frac{1}{2}\left[3\left(\left|x+\frac{1}{2}\right| + \left|x-\frac{1}{2}\right| + 6\right) - 11\left(x+\frac{3}{4}\right) + \left|x-\frac{3}{4}\right|\right] \\
\mathrm{r}(x) &= \frac{1}{2}(3-x) - \frac{3}{7}\sqrt{10}\sqrt{4-(x-1)^2} + \frac{6}{7}\sqrt{10}
\end{aligned}$$

These functions have been provided to you in *helpers.py*. You **do not** need to implement them yourself. A visualization of the upper and lower curves (with areas shaded in) is provided in Figure 1.

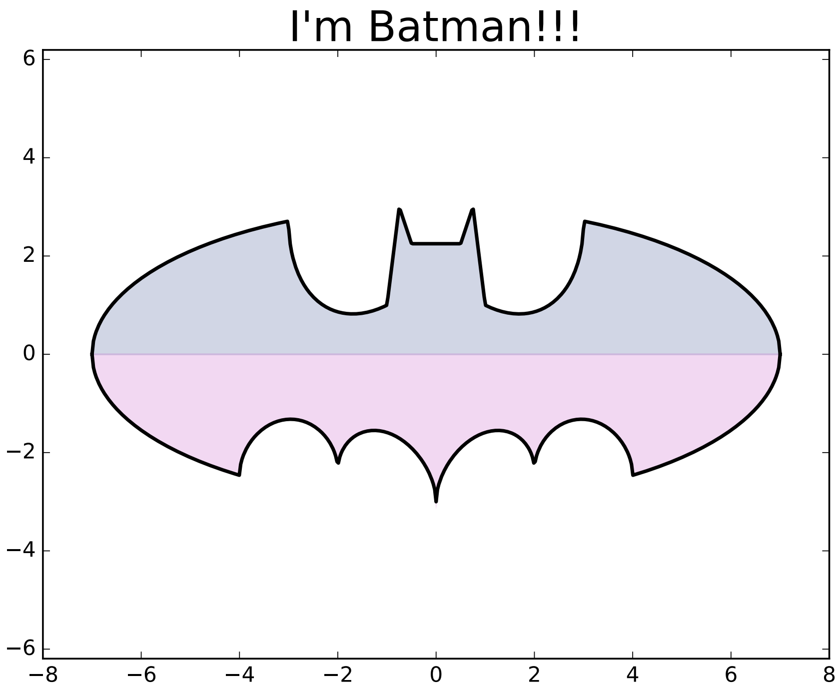

Figure 1: Upper and Lower Batman Curves

Your task will be to estimate the area of the Batman figure using Simpsons based Adaptive Quadrature. Taking advantage of the Romberg integration to estimate the error, one can refine the numerical integration points at regions that have a large error. This adaptive scheme can efficiently use computational power in important regions (where the function is not very smooth and hence is difficult to be estimated accurately). In this exercise, you will verify the benefits of an adaptive quadrature rule compared to the rules based on uniformly distributed quadrature points. And you'll help save Gotham City.

a) Intuitively, where (in Figure 1) do you expect the largest amount of 'clustering' of small intervals to occur? Where do you expect the intervals to be larger?

b) Write a Python program for numerical integration using an adaptive Simpson's scheme. To do so, you will need to perform numerical integration starting with a single interval (in this case $[-7, 7]$). Then you will need to recursively split the interval into two equal intervals and apply Simpson's rule within each of them. Afterwards, use Richardson's extrapolation to estimate the quadrature error in the given interval. If the error is smaller than the tolerance $\epsilon = 10^{-6}$, then we keep the approximated value (in this interval), otherwise we split the interval into two equal subintervals and repeat the error-estimation procedure in each of them. You need to continue such recursive splitting procedure until the error is smaller than tolerance in **all** intervals. There are many ways to implement such adaptive quadrature. One of them is using recursion. The algorithm is listed below:

Algorithm 1 Adaptive integration using recursion

```
function ADAPTIVESIMPSON(a, b)
    apply Simpson's rule in interval [a, b]
    subdivide the interval into [a, m] and [m, b] with m = (a + b)/2
    apply Simpson's rule in intervals [a, m] and [m, b]
    estimate error in [a, b] using Richardson's extrapolation
    if accuracy is worse than desired then
        return ADAPTIVESIMPSON(a, m) + ADAPTIVESIMPSON(m, b)
    else
        return value of Simpson's rule (the accurate one)
    end if
end function
```

c) Visualize the results of the numerical integration scheme by plotting vertical lines corresponding to where the optimal intervals were computed. Do this for both the upper and lower Batman curves. Where does the most clustering of small intervals occur?

d) Compare the efficiency of the adaptive Simpson's scheme and a uniform composite Simpson's scheme. For the upper curve, what was the total number of subintervals generated (N) and what was the smallest interval generated (h_{min})? If we were to use this subinterval width, h_{min}, to perform a uniform composite Simpson's method, how many intervals would we need to compute over the domain of the Batman curve?

e) Believe it or not, there is a closed form expression for the total area under the Batman curves. It is given by:

$$A_{batman} = \tfrac{955}{48} - \tfrac{2}{7}\left(2\sqrt{33} + 7\pi + 3\sqrt{10}(\pi - 1)\right) + 21\left(\arccos(\tfrac{3}{7}) + \arccos(\tfrac{4}{7})\right)$$

Compare the true value of the integral to your estimate from Adaptive Simpson's Quadrature. What is the final percentage error of the estimate?

Question 2: Gauss Quadrature

Gauss Quadrature is a set of carefully designed integration points that can achieve high accuracy for numerical integration of sufficiently smooth functions. In this exercise, you will first experience the advantages of the Gauss Quadrature and its limitations. You need to evaluate by hand two integrals with different types of integrands: a smooth and a non-smooth integrand. You need to perform three types of numerical integration methods: Trapezoidal rule, Newton-Cotes formula and Gauss Quadrature. The integration points and corresponding weights of different orders of the Gauss Quadrature are typically recorded in a table. In this exercise, you will be using the order 3 Gauss Quadrature (see Table 1). Typically, the integration points are given based on the interval [-1,1]. One should first convert the definite integral to be between -1 and 1 before using the tabulated values.

Procedure of using the Gauss Quadrature to evaluate $I = \int_a^b f(x)\,\mathrm{d}x$:

1. Change the boundary of the integral using change of variables, i.e., let $z = \frac{2x}{b-a} + 1 - \frac{2b}{b-a}$, then, $I = \int_{-1}^{1} \frac{b-a}{2} f\left(\frac{b-a}{2}(z-1) + b\right)\,\mathrm{d}z$.
2. Read out the integration points z_i for z and the corresponding weights w_i from the table (see Table 1).

3. Evaluate $I \approx \frac{b-a}{2} \sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}(z_i - 1) + b\right)$, where n is the order of Gauss Quadrature chosen.

z_i	w_i
0.7745966692	$0.555\ldots$
0.0	$0.888\ldots$
-0.7745966692	$0.555\ldots$

Table 1: Order three ($n = 3$) Gauss Quadrature integration points and weights.

a) Perform numerical quadrature with:

   (i) the composite Trapezoidal rule with uniform grid spacing and $n = 3$ points,

   (ii) the Newton-Cotes (closed) formula for $n = 2$,

   (iii) the Gauss Quadrature for $n = 3$,

   for the following two integrals:

   (a) $I = \int_1^3 x^6 - x^2 \sin(2x)\,\mathrm{d}x = 317.3442467$,

   (b) $I = \int_0^2 1 - |x - 1|\,\mathrm{d}x = 1$.

   Which method is better for which integrand? Do you suspect why?

b) What can you do to improve the accuracy of the poorly behaved quadrature schemes?