Numerical introduction

It has been shown that some important integrals cannot be "solved" analytically (i.e. we cannot find $F(x)$). For example, the normal distribution (with mean and standard deviation both equal to 1) is described by this probability density function:

$$f(x) = \frac{1}{\sqrt{2\pi}}\ e^{-x^2/2}$$

To find the expected value or probability that the value lies between bounds a and b we should compute:

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

However, there is no function $F(x)$ such that $F'(x) = f(x)$, so we cannot solve the equation in the normal way by computing $F(b) - F(a)$.

To compute the integral, we fall back on Riemann sums. Divide the closed range $[a, b]$ into N rectangles whose individual height is the value $f(x)$ somewhere in the rectangle, and then compute the sum of $\Delta x \times f(x)$ over the whole interval. A simple approach uses rectangles of constant width (equal to $b - a/N$).

Using Python:

`https://gist.github.com/telliott99/5a1190217a130c7ee01dee17ea483f7b`

I hope the flow is clear. The function `get_xvalues` generates a list of x-values starting from the middle of the first step past a and continuing to the last step just before b. `integrate` simply computes $f(x)$ for each x-value, sums all of those values, and adjusts for the width of the steps (rectangles).

We integrate $f(x) = x^2$ over the ranges $[0, 1]$ and $[1, 2]$ and obtain the expected results (1/3 and 7/3).

We also integrate the normal probability density function over ranges $[-2, 2]$ to $[-10, 10]$. With standard deviation equal to 1, we obtain the expected result that 95% of the density lies within two standard deviations of the mean. Essentially all of the density lies within four standard deviations of the mean.

And finding that the total area equals 1 confirms that the normalization factor $1/\sqrt{2\pi}$ is correct. That is, the value of the unnormalized integral is equal to $\sqrt{2\pi}$. (This is not how the constant was actually determined. It turns out that in the special case of $(-\infty, \infty)$, the integral *can* be solved).

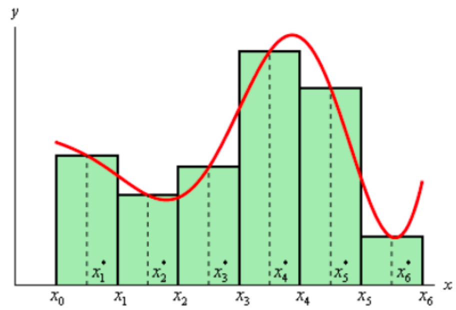
Refinements

Classically, the major improvement to be made to this algorithm is to make a more accurate estimation of the area for each small rectangle. This is not so important with fast computers. For example, with a million steps rather than 100, I obtain

```
> python numerical_int.py
0.333333333333
2.33333333333
>
```

for the first two integrations, in about two seconds.

The calculation above uses the midpoint rule, where $f(x)$ is evaluated at the midpoint of the range.



The step size is computed and used to generate a list of values where each rectangle starts, then half the step is added to give the midpoint.

If we think of a and b as the bounds for each small rectangle, then the average of a and b is the midpoint:

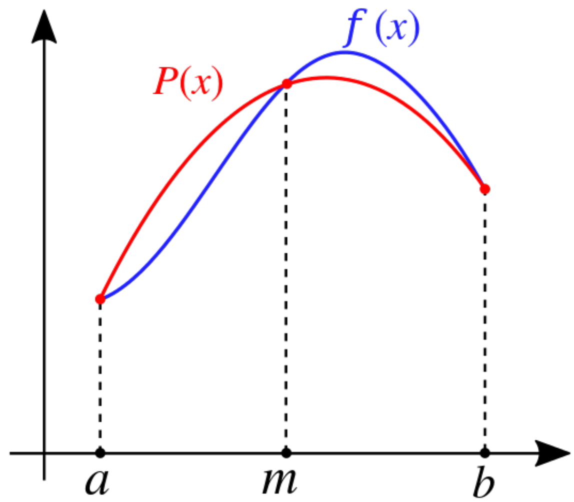
$$m = \frac{a+b}{2}$$

We evaluate $f(m)$, the function at the midpoint, and then multiply by the width:

$$M = f(m) \cdot (b - a)$$

Simpson's rule is a more sophisticated approach that uses:

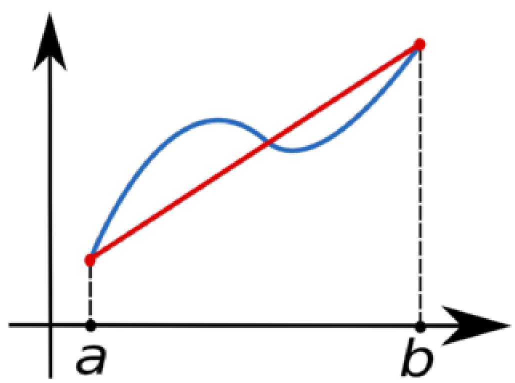
$$\frac{f(a) + 4f(m) + f(b)}{6} \cdot (b - a)$$



We sample once each from a and b, and four times from m, and average those samples.

The trapezoidal rule is

$$\frac{f(a) + f(b)}{2} \cdot (b - a)$$



Simpson's rule is really just a combination of the other two rules, namely, it is equal to $(2M + T)/3$. It weights the value at each endpoint as $1\times$ and then the midpoint as twice the combined values at the endpoints.

Essentially, this fits a parabola to the points a, m, b and then computes the area. It is really Archimedes' result (quadrature) in disguise.

Consider the parabola $y = -x^2 + 1$ between $x = -1 \to 1$ (the points where it crosses the x-axis on its way down). Our task is to find the correct y-value to use as the average height of the function in this region. Inverting the standard result for the area under $y = x^2$, the area under this parabola is 2/3 of the area above it. The result we seek is 2/3.

So a quadratic approximation to the area samples four times at the vertex plus once each at $x = \pm 1$. We sample because we understand that the curve is probably not exactly quadratic.