Using interpolation to estimate integrals

In section 4.3 we are going to start developing estimates for integrals of the form

$$\int_a^b f(x)\,\mathrm{d}\,x$$

The strategy we will use is similar to the strategy we used in section 4.1 to develop derivative estimate formulas:

1. Sample the function $f(x)$ at two or more points and construct an interpolating polynomial that passes through those points.

2. Integrate the interpolating polynomial to derive an estimate for the integral of $f(x)$.

3. Integrate the error term to estimate the error we are making.

Here is the first simple application of this idea: we sample $f(x)$ at the points $x = a$ and $x = b$ and construct the interpolating polynomial that passes through $(a,f(a))$ and $(b,f(b))$.

In the calculations below I enlisted the aid of a computer algebra system. The DirectMath software that I use to write these lecture notes can do symbolic manipulation with the help of the Maxima computer algebra system. One special requirement of Maxima is that functions have to be written in a special way. Ordinary mathematical notation is ambiguous when it comes to functions. For example, in the expression

$$a(b+c)$$

it is not clear whether we should interpret the expression as "a times $(b+c)$" or as "apply the function a to the argument $b+c$". To disambiguate this expression Maxima forces us to use square braces in place of the usual parentheses for functions.

Here now is an interpolating polynomial that interpolates the points $(a,f(a))$ and $(b,f(b))$.

$$p[x] = f[a] + \frac{f[b]-f[a]}{b-a}\,(x-a)$$

Integrating this interpolating polynomial over the interval $[a,b]$ gives

$$\int_a^b p[t]\,\mathrm{d}\,t$$

$$= \frac{\left(b^2 - 2\,a\,b\right) f[b] + f[a]\,b^2}{2\,b - 2\,a} + \frac{a^2\,f[b] - 2\,a\,f[a]\,b + a^2\,f[a]}{2\,b - 2\,a}$$

$$= \frac{\left(b^2 - 2\,a\,b\right) f[b] + a^2 f[b] + f[a]\,b^2 - 2\,a\,f[a]\,b + a^2 f[a]}{2\,b - 2\,a}$$

$$= \frac{b^2 f[b] - 2\,a\,b\,f[b] + a^2 f[b] + f[a]\,b^2 - 2\,a\,f[a]\,b + a^2 f[a]}{2\,b - 2\,a}$$

$$= \frac{(b - a)^2\,(f[b] + f[a])}{2\,b - 2\,a}$$

$$= \frac{(b - a)^2\,(f[b] + f[a])}{2\,(b - a)}$$

$$= \frac{(b - a)\,(f[b] + f[a])}{2}$$

This is commonly referred to as the *trapezoid rule*, since the region under $p(x)$ over the interval $[a,b]$ has the shape of a trapezoid. The integral of $p(x)$ in this case just ends up being the area of that trapezoid.

Now, what about the error term? The error formula for polymial interpolation is

$$f(x) = P(x) + \frac{f^{(2)}(\xi(x))}{2!}\,(x - a)(x - b)$$

Integrating this error formula over the interval in question gives us

$$\int_a^b f(x)\,\mathrm{d}x = \int_a^b P(x)\,\mathrm{d}x + \int_a^b \frac{f^{(2)}(\xi(x))}{2!}\,(x - a)(x - b)\,\mathrm{d}x$$

To compute the integral of the error term we can enlist the help of the following

Theorem (Generalized Mean Value Theorem for Integrals) If the function $g(x)$ is non-negative on an interval $[a,b]$ and $f(x)$ is any integrable function then

$$\int_a^b f(x)\,g(x)\,\mathrm{d}x = f(c)\int_a^b g(x)\,\mathrm{d}x$$

where c is some point in the interval $[a,b]$.

We can apply this theorem in this case, since fortunately the expression $(x - a)(x - b)$ is non-negative on $[a,b]$:

$$\int_a^b \frac{f^{(2)}(\xi(x))}{2!}\,(x - a)(x - b)\,\mathrm{d}x = \frac{f^{(2)}(\xi(c))}{2!}\int_a^b (x - a)(x - b)\,\mathrm{d}x$$

$$= \frac{f^{(2)}(\xi(c))}{2!}\left(-\frac{b^3 - 3ab^2}{6} - \frac{3a^2 b - a^3}{6}\right) = \frac{f^{(2)}(\xi(c))}{2!}\left(-\frac{(b-a)^3}{6}\right)$$

Thus we see that the error term is proportional to $(b\text{-}a)^3$. This is only helpful if we can arrange to make b - a small. In this general case that won't happen, but in the section on composite integration below we can use this result to our advantage.

We now repeat these same arguments using a larger number of sample points. The next obvious step is to sample f(x) at the points $(a,f(a))$, $((b+a)/2, f((b+a)/2))$, and $(b,f(b))$.

$$p[x] = f[a] + \frac{f[(b+a)/2]\text{-}f[a]}{(b+a)/2\text{-}a}(x\text{-}a) + \frac{\frac{f[b]\text{-}f[(b+a)/2]}{b - (b+a)/2} - \frac{f[(b+a)/2] - f[a]}{(b+a)/2 - a}}{b - a}(x\text{-}a)(x\text{-}(b+a)/2)$$

$$\int_a^b p[t]\,\mathrm{d}t$$

$$= \frac{(4b^3 - 12ab^2)\,f[\frac{b+a}{2}] + (b^3 - 3ab^2 + 6a^2 b)\,f[b] + f[a]\,b^3 + 3a\,f[a]\,b^2}{6b^2 - 12ab + 6a^2} + \frac{(12a^2 b - 4a^3)\,f[\frac{b+a}{2}] + (-3a^2 b - a^3)\,f[b] - 6a\,f[a]\,b^2 + 3a^2 f[a]\,b - a^3 f[a]}{6b^2 - 12ab + 6a^2}$$

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

This result is known as Simpson's rule. An unfortunate problem with Simpson's rule is that we can't apply the generalized MVT for integrals to the error term in this case

$$\int_a^b \frac{f^{(3)}(\xi(x))}{3!}(x-a)\left(x - \frac{a+b}{2}\right)(x-b)\,\mathrm{d}x$$

since the expression $(x - a)(x - (a+b)/2)(x - b)$ is not non-negative on the interval $[a,b]$.

Here is an alternative argument that allows us to both derive Simpson's rule and get an error estimate. Instead of replacing $f(x)$ with the interpolating polynomial $p(x)$ we instead replace it with a Taylor expansion about the point $x_1 = (a+b)/2$:

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f^{(3)}(x_1)}{3!}(x - x_1)^3 + \frac{f^{(4)}(\xi(x))}{4!}(x - x_1)^4$$

Integrating this over the interval $[a,b]$ gives

$$\int_a^b f(x)\,\mathrm{d}x = (b-a)\,f(x_1) + \frac{1}{3}\left(\frac{b-a}{2}\right)^3 f''(x_1) + \int_a^b \frac{f^{(4)}(\xi(x))}{4!}\left(x-x_1\right)^4 \mathrm{d}x$$

This expression contains a second derivative term that we have to estimate somehow. To estimate that we can evaluate the second derivative of the $p(x)$ we constructed above and use it as an estimate for the $f''(x_1)$ term:

$$p''(x_1) = \frac{4\left(f(b) - 2\,f(x_1) + f(a)\right)}{\left(b-a\right)^2}$$

With this substitution we get

$$\int_a^b f(x)\,\mathrm{d}x = (b-a)\,f(x_1) + \frac{1}{3}\left(\frac{b-a}{2}\right)^3 \frac{4\left(f(b) - 2\,f(x_1) + f(a)\right)}{\left(b-a\right)^2} + \int_a^b \frac{f^{(4)}(\xi(x))}{4!}\left(x-x_1\right)^4 \mathrm{d}x + err$$

$$= \frac{\left(b-a\right)\left(f(a) + 4\,f(x_1) + f(b)\right)}{6} + \int_a^b \frac{f^{(4)}(\xi(x))}{4!}\left(x-x_1\right)^4 \mathrm{d}x + err$$

Where the *err* term is the error we introduced by replacing $f''(x_1)$ with $p''(x_1)$.

Finally, the remaining integral can be now be handled by the generalized MVT for integrals, since $\left(x-x_1\right)^4$ is non-negative on $[a,b]$.

$$\int_a^b f(x)\,\mathrm{d}x = \frac{\left(b-a\right)\left(f(a) + 4\,f(x_1) + f(b)\right)}{6} + \frac{f^{(4)}(c)}{4!}\int_a^b \left(x-x_1\right)^4 \mathrm{d}x + err$$

$$= \frac{\left(b-a\right)\left(f(a) + 4\,f(x_1) + f(b)\right)}{6} + \frac{f^{(4)}(c)}{4!}\,\frac{2}{5}\left(\frac{b-a}{2}\right)^5 + err$$

Finally, it is possible to show that the err term is proporational to

$$-\frac{1}{36}\left(\frac{b-a}{2}\right)^5$$

Thus, the entire error term in Simpson's rule is proporational to $\left(b-a\right)^5$.

Composite Integration

The results we derived in the last section were not immediately useful, since the error terms were simply too large. Fortunately, we can combine the results from the last section with another strategy, known as *composite integration*:

1. Divide the interval [a,b] into n equal sized subintervals of length $h = (b\text{-}a)/n$
2. Over each of the small subintervals we replace the original $f(x)$ with an interpolating polynomial $p(x)$ and integrate the polynomial.
3. Since the errors for each subinterval will now be proportional to powers of h, the errors are managable despite the fact that we now have n error terms instead of just one.

For example, in the composite version of Simpson's rule, the total error is proportional to

$$\frac{n}{2}\left(\frac{h^5}{90} f^{(4)}(\xi)\right) = \frac{b\text{-}a}{180}\, h^4 f^{(4)}(\xi)$$

For large enough n (and small enough h) this results in reasonable errors.