Numerical integration

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Problem and solution strategy

We want to find a numerical approximation to

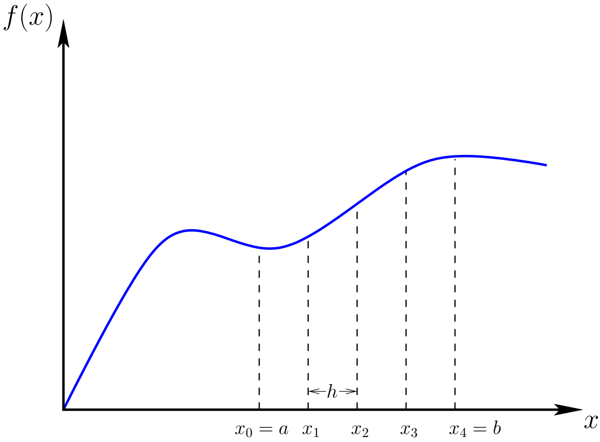
$$J = \int_a^b f(x)\,\mathrm{d}x.$$

We obtain this by approximating the integral as

$$J \approx \sum_{j=0}^{N} \int_{x_j}^{x_{j+1}} p_k(x)\,\mathrm{d}x = \sum_{j=0}^{N} J_j$$

where p_k is the interpolation polynomial of degree $k = 0, 1, 2$.

Geometric picture



We use $k = 0$.

In each subinterval we use a constant value for the function. This yields

$$J_j = \int_{x_j}^{x_{j+1}} f(t_j)\,\mathrm{d}x = hf(t_j)$$

$$J \approx h \sum_{j=0}^{N} f(t_j)$$

The best choice for the t_j is to choose them in the middle of each interval, that is

$$t_j = x_j + \frac{h}{2}$$

We use $k = 1$.

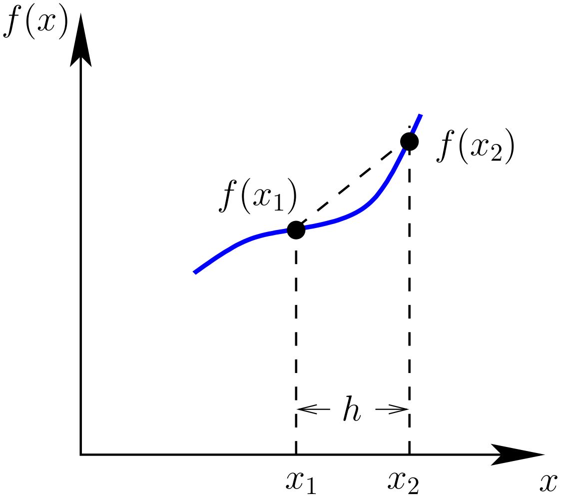


Figure: In each subinterval we approximate the function as a straight line.

We use $k = 1$.

We introduce the variable $s = (x - x_j)/h$. This means that in each subinterval we have

$$p_1(s) = f_j + (f_{j+1} - f_j)\, s$$

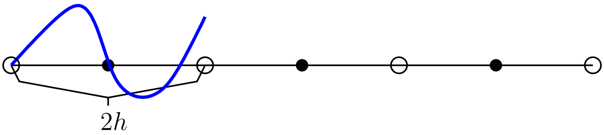
Taking the integral gives us

$$J_j = h \int_0^1 p_1(s)\,\mathrm{d}s = h \left(f_j s + \frac{1}{2}\,(f_{j+1} - f_j)\, s^2 \Big|_{s=0}^{1} \right) = \frac{h}{2}\,(f_j + f_{j+1})$$

Finally we take the sum. Every point except the end points will get two contributions:

$$J \approx \frac{h}{2} f_0 + h \sum_{j=1}^{N} f_j + \frac{h}{2} f_{N+1}$$

We use $k = 2$.



- Need an even number of subintervals.
- Divides in segments of three nodes.
- In each segment we approximate the function as a second order polynomial.

We use $k = 2$.

In one subinterval we find $p_2(x)$ using Lagrangian interpolation

$$p_2(x) = \frac{(x-x_{j+1})(x-x_{j+2})}{(x_j-x_{j+1})(x_j-x_{j+2})}f_j + \frac{(x-x_j)(x-x_{j+2})}{(x_{j+1}-x_j)(x_{j+1}-x_j)}f_{j+1} + \frac{(x-x_j)(x-x_{j+1})}{(x_{j+2}-x_j)(x_{j+2}-x_{j+1})}f_{j+2}$$

Introduce $s = (x - x_{j+1})/h$. This gives

$$p_2(s) = \frac{1}{2}s(s-1)f_j + (s+1)(s-1)f_{j+1} + \frac{1}{2}(s+1)sf_{j+2}$$

We use $k = 2$.

We then integrate of the segment $(s = -1 \cdots 1)$:

$$J_j \approx \frac{h}{3}\left(f_j + 4f_{j+1} + f_{j+2}\right)$$

- Every 'right' node get two contributions, apart from the end point.

We take the sum and obtain

$$J \approx \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_N + f_{N+1}\right)$$

Maximal polynomial order

- We now assume that $f(x)$ *IS* a polynomial.
- We allow weights in the integral points, i.e.

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \sum_{j=1}^{N} \omega_j f_j$$

  Note that we always work on a normalized interval.
- We can place the nodes whereever we want to within the subinterval. We are not restricted to having the nodes on the end points.
- This means that we have $2N$ degrees of freedom - N weights and N points.
- We know that with $2N$ parameters we can choose freely, we are able to interpolate a polynomial of degree $2N - 1$.

Maximal polynomial order

- This means that we can integrate a polynomial of degree 3 exactly using only 2 nodes.
- The nodes x_j are roots of Gaussian polynomials, we won't go into details here.
- With $n = 2$ we have:

$$\omega_1 = \omega_2 = 1$$
$$x_1 = -0.57, x_2 = 0.57$$

- Note that we need to be able to evaluate the function at any point within the subintervals to apply these methods.

Summary

Method	Order	Degree	Integrates exactly	Error estimate
Midpoint	1	0	1	
Trapezoidal	2	1	1	$\frac{1}{3}\left(J_{h/2} - J_h\right)$
Simpsons's	4	2	3	$\frac{1}{15}\left(J_{h/2} - J_h\right)$

All formulas have about the same amount of work $\Rightarrow$ use Simpsons if you can. Symmetry gives us the extra precision.

The Romberg method

- Idea: Use small h where the function has large variability ($f^{(n)}$ is large) and larger h where it is varies less.
- First we find an approximation using only one interval. We also decide a global error tolerance (which obviously should be less than the error we have using only one subinterval).
- We then half the interval and calculate the error using the error estimate.
- If this error is too large, divide again.
- This is called the Romberg method.
- Can be used with any numerical integration scheme as long as we have an error estimate.

Example: application of Romberg's method

$$J = \int_0^2 \frac{1}{4}\pi x^4 \cos\frac{\pi x}{4}\,\mathrm{d}x = 1.25953$$

- We use $h = 1$.
- We use $Tol = 0.0002$.
- We use Simpson's rule.
- First the entire segment:

$$J = 0.740480$$

Example: application of Romberg's method

$$J = \int_0^2 \frac{1}{4}\pi x^4 \cos\frac{\pi x}{4}\,\mathrm{d}x = 1.25953$$

Interval	Integral	Error	Tol	Decision
$[0, 2]$	0.740480		0.0002	
$[0, 1]$	0.1222794			
$[1, 2]$	1.10695			
	Sum=1.122974	0.032617	0.0002	Del
$[0.0, 0.5]$	0.004782			
$[0.5, 1.0]$	0.118934			
	Sum=0.123716*	0.000061	0.0001	Ok
$[1.0, 1.5]$	0.528176			
$[1.5, 2.0]$	0.605821			
	Sum=1.13300	0.001803	0.0001	Del

Example: application of Romberg's method

$$J = \int_0^2 \frac{1}{4}\pi x^4 \cos\frac{\pi x}{4}\,\mathrm{d}x = 1.25953$$

Interval	Integral	Error	Tol	Decision
$[1.00, 1.25]$	0.200544			
$[1.25, 1.50]$	0.328351			
	Sum=0.528895*	0.000048	0.00005	Ok
$[1.50, 1.75]$	0.388235			
$[1.75, 2.00]$	0.218457			
	Sum=0.606692	0.000058	0.00005	Del
$[1.500, 1.625]$	0.196244			
$[1.625, 1.750]$	0.192019			
	Sum=0.388263*	0.0000002	0.000025	Ok

Example: application of Romberg's method

$$J = \int_0^2 \frac{1}{4}\pi x^4 \cos\frac{\pi x}{4}\,\mathrm{d}x = 1.25953$$

Interval	Integral	Error	Tol	Decision
$[1.750, 1.875]$	0.153405			
$[1.875, 2.000]$	0.328351			
	Sum=0.218483*	0.000002	0.000025	Ok

We find our approximation as

$$J \approx 0.123716 + 0.528895 + 0.388263 + 0.218483 = 1.25936$$