April 21, 2020

Numerical Analysis

Last Time:

- Finished best approximation to a function in the 2-norm
- Constructing orthogonal polynomials under the inner product: $(f, g) = \int_a^b f(x)\, g(x)\, w(x)\, dx \;, \quad w > 0$

Numerical Integration

Almost no integral can be computed analytically, they must be evaluated numerically.

Ex:

$$\underbrace{\operatorname{erf}(x)}_{\text{error function}} = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt$$

Application ODEs, initial value problems

$$(*) \quad \begin{aligned} y'(t) &= f(t) \\ y(0) &= y_0 \end{aligned}$$

The analytic solution is

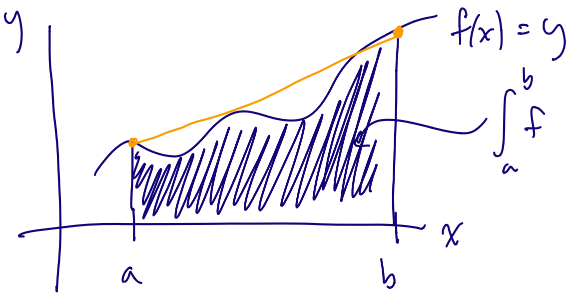
$$y(t) = y_0 + \int_0^t f(\tau)\, d\tau$$

All numerical methods for solving $(*)$ are based on numerically approximating the integral.

More to come later...

The Trapezoidal (Trapezium) Rule

The most basic numerical integration technique:



Option 1: Approximate f on $[a,b]$ by a line, integrate the line.

Area under this line is $\underbrace{(b-a)}_{\text{width}} \underbrace{\frac{(f(a)+f(b))}{2}}_{\text{average of edge heights.}} \approx \int_a^b f(x)\,dx.$

Area of a trapezoid.

① f was approximated by a line which interpolated f at $x=a$ and $x=b$.

② This interpolating line was integrated.

The trapezoidal rule is a special case of more general numerical integration formulas known as Newton-Cotes rules:

<u>Idea</u> Interpolate f on $[a,b]$, and then integrate the interpolating polynomial.

This can be done with arbitrarily high degree (high order interpolation) but remember: the interpolating polynomial may suffer from <u>Runge's Phenomena</u>.

In general: Interpolate f at the points $(x_0, f(x_0)), \ldots, (x_n, f(x_n))$

$$p_n(x) = \sum_{j=0}^{n} L_j(x) f(x_j)$$

Lagrange function $L_j(x) = \prod_{i \neq j} \frac{x - x_i}{x_j - x_i}$

Then the integral of f can be approximated as:

$$\int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx$$

$$= \int_a^b \sum_{j=0}^{n} L_j(x) f(x_j)\,dx$$

$$= \sum_{j=0}^{n} \underbrace{\left(\int_a^b L_j(x)\,dx \right)}_{w_j} f(x_j)$$

$$= \sum_{j=0}^{n} w_j f(x_j)$$

} Standard form of a (Numerical) <u>Quadrature Rule</u>

w_j = quadrature weights

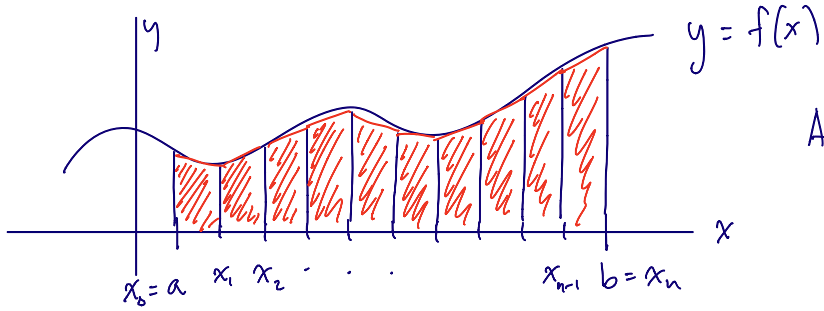
x_j = quadrature nodes (the locations where f is evaluated).

<u>Note</u>: $w_j = \int_a^b L_j(x)\,dx$ only depends on the location of the quadrature nodes, <u>not</u> the values of f.

<u>Note 2</u>: Warning: Large n may result in an inaccurate approximation by the interpolating polynomial due to Runge's Phenomena.

<u>Remedy</u>: Use many smaller lower-order interpolations, glue the results together.

The Composite Trapezoidal Rule



Apply the trapezoidal rule on each smaller interval (analogous to the Riemannian Integral).

$$x_j = a + jh$$
$$= a + j\left(\frac{b-a}{n}\right)$$

Then, the integral is approximated by:

$$\int_a^b f(x)\,dx \approx T_n f \quad \text{N-interval Trapezoidal Rule}$$

$$= \sum_{j=1}^{n} h\left(\frac{f(x_{j-1}) + f(x_j)}{2}\right)$$

$$= h\left(\sum_{j=0}^{n} f(x_j) - \frac{1}{2}\left(f(a) + f(b)\right)\right)$$

Question: What is the error $\left| \int_a^b f(x)\,dx - T_n f \right|$?

This error can be shown to be $\mathcal{O}(h^2)$.

Idea of the proof: on a single interval $[a,b]$, Taylor expand f about $x = \frac{a+b}{2}$ (the midpoint). Apply the Trapezoidal rule to this Taylor series.

In fact, a much more powerful formula exists that characterizes the error explicitly.

The Euler-MacLaurin Expansion

Theorem: Let $f \in C^{2k}[a,b]$, and $[a,b]$ be divided into n equal subintervals, $[x_{j-1}, x_j]$, with $x_j = a + jh$.

Then, $\int_a^b f(x)\,dx - T_n f$

I

$$= \sum_{r=1}^{k} c_r h^{2r} \left(f^{(2r-1)}(b) - f^{(2r-1)}(a) \right) - d_{2k} \left(\frac{h}{2}\right)^{2k}.$$

$$= \frac{h^2}{12}\left(f'(b) - f'(a) \right) - \frac{h^4}{720}\left(f^{(3)}(b) - f^{(3)}(a) \right) + \dots + (-1)^{k-1} \frac{B_{2n}}{(2k)!} h^{2k} f^{(2k)}(\xi)$$

$\xi \in [a,b]$

These coefficients are given by:

$$c_r = -\frac{B_{2r}}{(2r)!}, \quad B_{2r} \text{ is a Bernoulli number:}$$

$$\frac{x}{2}\coth\left(\frac{x}{2}\right) = \sum_{r=0}^{\infty} \frac{B_{2r}}{(2r)!} x^{2r}.$$

The calculation of B_{2r} was the output of arguably the first "computer program" written by Ada Lovelace and Charles Babbage.

Implications of Euler-MacLaurin

If $f \in C^\infty[a,b]$ and periodic with $f^{(j)}(a) = f^{(j)}(b)$ (think Fourier Series, or $\cos mx$, $\sin mx$, etc.) then this error $|I - T_n f|$ decays <u>superalgebraically</u> as $n \to \infty$.

Def: $\epsilon_n \to 0$ superalgebraically if

$$\lim_{n\to\infty} \frac{\epsilon_n}{h^{p\cdot n}} = 0 \quad \text{for any } p>0.$$

This means that $\epsilon_n \to 0$ faster than any power of h.

For this reason, the trapezoidal rule is very important important in various numerical methods.

Ex: $$J_0(x) = \frac{1}{\pi}\int_0^{\pi} e^{ix\cos\theta}\, d\theta.$$

$e^{ix\cos\theta}$ is not periodic on $[0,\pi]$, but it is on $[0,2\pi]$.

It can be shown that

$$J_0(x) = \frac{1}{\pi}\int_0^{\pi} e^{ix\cos\theta}\, d\theta = \underbrace{\frac{1}{2\pi}\int_0^{2\pi} e^{ix\cos\theta}\, d\theta}.$$

See mybessel.m for computing this via the trapezoidal rule.