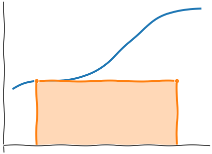
Numerical integration

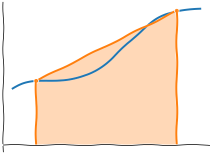
Quadratures

Elementary quadratures

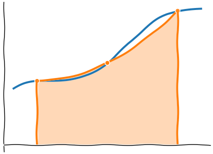
$$\int_a^b f(x)\,dx = \sum_{k=1}^{N} \int_{x_{k-1}}^{x_k} f(x)\,dx \approx \sum_{k=1}^{N} Q_k$$



Rectangles



Trapezoids



Simpson's rule

Elementary quadratures: Newton-Cotes formulas

On each elementary interval $[x_{k-1}, x_k]$, take $t_0, t_1, \cdots, t_m \in [0, 1]$,

approximate $f(x)$ on $[x_{k-1}, x_k]$ by an interpolating polynomial of degree m with nodes

$$z_j = x_{k-1} + ht_j, \qquad j = 0, \ldots, m$$

and values

$$y_j = f(z_j)$$

Elementary quadratures: Newton-Cotes formulas

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Equidistant nodes: *Newton-Cotes rules.*

Elementary quadratures: Newton-Cotes formulas

- An elementary Newton-Cotes rule of degree m integrates polynomials of degree m *exactly*.
- The error bound for a composite rule of degree m:

  $$\Delta \leqslant c_m M_{m+1}(b-a)h^{m+1}$$

  where

  $$M_{m+1} = \max_{x\in[a,b]} \left| f^{(m+1)}(x) \right|$$

- High m rules are poorly conditioned (Runge phenomenon)

Weighting functions

Newton-Cotes quadratures work well when $f(x)$ is locally well approximated by a polynomial.

However, consider, e.g.,

$$I = \int\limits_{-1}^{1} \frac{x^8}{\sqrt{1 - x^2}}\, dx$$

Split the integrand into a product

$$I = \int_a^b f(x)\omega(x)\, dx$$

Weighting functions

$$I = \int_a^b f(x)\omega(x)\,dx$$

Approximate $f(x)$ by a polynomial of degree m.

Need to be able to compute *moments* of $\omega(x)$,

$$\mu_k = \int_a^b x^k \omega(x)\,dx$$

for $k = 0, \cdots, m$.

Gaussian quadratures

Newton-Cotes quadratures

A *quadrature rule*

$$Q^{(N)} = \sum_{k=1}^{N} w_k f(x_k),$$

defined by its *nodes* and *weights*, approximates an integral

$$I = \int_a^b f(x)\omega(x)\,dx$$

Newton-Cotes rules

- fixed equidistant nodes
- m-point quadrature integrates polynomials of degree $m-1$

Can we do better?

Newton-Cotes quadratures

A *quadrature rule*

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Newton-Cotes rules

- fixed equidistant nodes
- m-point quadrature integrates polynomials of degree $m-1$

Idea: adjust both weights *and* nodes.

Gaussian quadratures

We want the quadrature rule

$$\int_a^b f(x)\omega(x)\,dx = \sum_{k=1}^{N} w_k f(x_k)$$

to be exact for polynomials of degree m, $\Longleftrightarrow$ exact for $f(x) = 1, x, \cdots, x^m$.

There are $2N$ unknowns: $w_1, \cdots, w_N$ and $x_1, \cdots, x_N$.

Expect the solution to exist for $m = 2N - 1$.

Example: A two-point Gaussian quadrature

Let $a = -1$, $b = 1$ and $\omega(x) = 1$:

$$I = \int_{-1}^{1} f(x)\,dx$$

Take $N = 2$:

$$I = w_1 f(x_1) + w_2 f(x_2)$$

Have four unknowns, expect the rule to integrate cubic polynomials.

Example: A two-point Gaussian quadrature

$$x^0: \qquad \int_{-1}^{1} 1\,dx = 2 = w_1 + w_2$$

$$x^1: \qquad \int_{-1}^{1} x\,dx = 0 = w_1 x_1 + w_2 x_2$$

$$x^2: \qquad \int_{-1}^{1} x^2\,dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2$$

$$x^3: \qquad \int_{-1}^{1} x^3\,dx = 0 = w_1 x_1^3 + w_2 x_2^3$$

Example: A two-point Gaussian quadrature

We find $w_1 = w_2 = 1$ and $x_1 = 1/\sqrt{3}$, $x_2 = -1/\sqrt{3}$, so that

$$I = \int_{-1}^{1} f(x)\,dx \approx f\left(\frac{1}{\sqrt{3}}\right) + f\left(-\frac{1}{\sqrt{3}}\right)$$

is exact for cubic polynomials.

Gaussian quadratures

Orthogonal polynomials

Orthogonal polynomials

Consider a space of polynomials of degree $\leqslant n$ on $x \in [a, b]$. A set of monomials,

$$1, x, x^2, \cdots, x^n$$

forms a basis of this space.

Can rotate to an alternative basis, $p_0(x), p_1(x), \cdots, p_n(x)$.

$$\begin{aligned} T(x) &= a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n \\ &= b_0 + b_1 p_1(x) + b_2 p_2(x) + \cdots + b_n p_n(x) \end{aligned}$$

Orthogonal polynomials

Integration with the weight functions defines a scalar product

$$\langle f \cdot g \rangle \equiv \int_a^b f(x)\, g(x)\, \omega(x)\, dx$$

A family of polynomials, $\{p_k(x)\}$, is called orthogonal on $x \in [a, b]$ with the weight function $\omega(x)$ if

$$\langle p_k \cdot p_m \rangle = \int_a^b p_k(x)\, p_m(x)\, \omega(x)\, dx = 0\ , \qquad m \neq k$$

Gaussian quadratures

The quadrature rule the with a weight function $\omega(x)$ on $x \in [a, b]$

$$\int_a^b f(x)\omega(x)\, dx = \sum_{k=1}^{n} w_k f(x_k)$$

is exact for $f(x)$ being polynomials of degree up to $2n - 1$ if

- the nodes, x_k, are the roots of $p_n(x)$, the n-th orthogonal polynomial, w.r.t. $\omega(x)$.
- the quadrature weights, w_k, are defined by the weighting function $\omega(x)$.

Classic orthogonal polynomials

	$p_n(x)$	$\omega(x)$	a, b
Legendre	$P_n(x)$	1	$-1, 1$
Hermite	$H_n(x)$	e^{-x^2}	$-\infty, \infty$
Chebyshev I kind	$T_n(x)$	$\frac{1}{\sqrt{1-x^2}}$	$-1, 1$
Chebyshev II kind	$U_n(x)$	$\sqrt{1-x^2}$	$-1, 1$
Laguerre	$L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$0, \infty$

See, e.g., DLMF 18.3