AMSC/CMSC 460 Computational Methods, Fall 2007
UNIT 3: Numerical Integration
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A new unit: Numerical Integration

Also known as quadrature.

Read: Chapter 4. Skip: Section 4.5.

Problem:

Compute an approximation $Q(f)$ to

$$I(f) \equiv \int_a^b f(t)dt$$

given either

1. a definition of the function f
2. or the values of f at some points $t_i \in [a, b]$.

Our approximation will be of the form

$$Q(f) = \sum_{i=1}^{m} \alpha_i f(t_i)\,,$$

for some fixed (scalar) weights α_i.

Our plan

- Present Newton-Cotes formulas (trapezoidal formula, Simpson's formula, etc.)
- Study Gaussian integration.
- Investigate the anatomy of a practical algorithm: adaptive integration.
- Discuss singular integrals.
- Discuss multidimensional integration.

Newton-Cotes Formulas for integration

The basic idea:

- Let
$$h = \frac{b-a}{n}$$
for some integer n.
- Suppose we are given a set of function values for f at equally spaced points
  - Closed formulas:
  $$t_i = a + (i-1)h, \;\; i = 1, \ldots, n+1,$$
  - or, alternatively, for Open formulas:
  $$t_i = a + ih, \;\; i = 1, \ldots, n-1.$$

- We approximate f by a polynomial $p(t)$ that interpolates f at the given points.
- Then we integrate the polynomial
$$Q(f) \equiv \int_a^b p(t)dt$$
- We immediately have an error estimate:
$$I(f) - Q(f) = \int_a^b f[t_1, t_2, \ldots, t_m, t](t-t_1)\ldots(t-t_m)dt$$
($m = n+1$ for closed; $m = n-1$ for open).

Note: Newton-Cotes formulas have the properties that

- $\sum_{i=1}^{m} \alpha_i = b - a$, since if $f(t) = 1$, the error must be zero.
- $\alpha_i > 0$ for the low-order formulas, but not for all.

An example

Take $n = 1$ and derive the closed formula.

– $h = b - a$, so $t_1 = a$ and $t_2 = b$.
– We approximate f by a polynomial $p(t)$ that interpolates f at the given points:
$$p(t) = f(a) + (t-a)\frac{f(b)-f(a)}{b-a}.$$
– Then we integrate the polynomial

$$\begin{aligned}
Q(f) &\equiv \int_a^b p(t)dt \\
&= f(a)(b-a) + \left[\frac{b^2-a^2}{2} - a(b-a)\right]\frac{f(b)-f(a)}{b-a} \\
&= f(a)(b-a) + \left[\frac{b+a}{2} - a\right](f(b)-f(a)) \\
&= \frac{b-a}{2}(f(b)+f(a)).
\end{aligned}$$

- We immediately have an error estimate:
$$I(f) - Q(f) = \int_a^b f[a,b,t](t-a)(t-b)dt$$

This is the Trapezoidal Rule formula for integration.

Make sure you understand how the formula is derived vs. how the algorithm is programmed.

A second example

For $n = 2$, the closed formula is
$$Q(f) = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

This is Simpson's Rule.

A third example

For $n = 1$, the open formula is

$$Q(f) = f\left(\frac{a+b}{2}\right)(b-a)\,.$$

This is the Midpoint Formula.

Other integration formulas

We can derive integration formulas other than Newton-Cotes by

- using different polynomial approximations, such as Taylor series.
- using spline interpolants,
- or using composite formulas , where we break the interval $[a, b]$ into pieces and use one of our basic formulas on each piece.

What these formulas have in common

- The formulas all have the form

$$Q(f) = \sum_{i=1}^{m} \alpha_i f(t_i)$$

- The error function

$$R(f) = I(f) - Q(f)$$

  is a linear operator; i.e., for every two functions f and g, and for every two scalars β and γ,

$$R(\beta f + \gamma g) = \beta R(f) + \gamma R(g)\,.$$

  (We restrict f and g to lie in some function space; for example, we need a certain number of continuous derivatives in order for the polynomial error formula to apply.)

Error Formula for the Newton-Cotes Rules

Your book finds the formula for Simpson's rule. We'll do trapezoidal rule here.

Theorem: If $f(t)$ and its first 3 derivatives are continuous on $[a, b]$, then

$$\int_a^b f(t)dt - T = -\frac{(b-a)^3}{12} f''(\eta)$$

where $\eta \in [a, b]$.

Proof: The trapezoidal rule is computed by integrating the linear interpolant to $f(t)$ at a and b.

From our work on polynomial interpolation, we know that, for the linear interpolant,

$$f(t) - p(t) = f[a, b, t](t-a)(t-b)\,,$$

so

$$\int_a^b f(t)dt - T \quad = \quad \int_a^b f[a, b, t](t-a)(t-b)dt$$

Recall the Integral Mean Value Theorem: If $w(t)$ doesn't change sign on $[a, b]$ then

$$\int_a^b w(t)f(t)dt = f(\xi)\int_a^b w(t)dt$$

for some point $\xi \in [a, b]$.

Therefore,

$$\begin{aligned}
\int_a^b f(t)dt - T \quad &= \quad f[a, b, \xi]\int_a^b (t-a)(t-b)dt \\
&= \quad f[a, b, \xi](-\frac{1}{6}(b-a)^3)
\end{aligned}$$

The result follows from the fact that

$$f[a, b, \xi] = \frac{1}{2} f''(\eta)\,.[]$$

Practical Use of These Rules: Composite Rules

Idea: If $b - a$ is big, then our error bound is also big.

In order to reduce it, we can apply our favorite rule to subintervals of $[a, b]$.

Divide our interval into n pieces by choosing points z_i with $a = z_1 < z_2 < \ldots < z_{n+1} = b$.

Note that

$$\int_a^b f(t)dt = \sum_{i=1}^n \int_{z_i}^{z_{i+1}} f(t)dt.$$

If we apply our integration rule to each of the n integrals in this expression, the interval lengths will be smaller, so our polynomials will be better approximations, and we may get smaller error bounds.

Picture.

Note the importance of reusing function values.

Example: Composite Trapezoidal Rule. Let's divide $[a, b]$ into n pieces of equal length $h = (b - a)/n$.

$$\int_a^b f(t)dt$$

$$\approx \frac{h}{2}(f(a)+f(a+h))+\frac{h}{2}(f(a+h)+f(a+2h)+\ldots+\frac{h}{2}(f(a+(n-1)h)+f(a+nh))$$

$$= h[\frac{1}{2}f(a) + f(a+h) + f(a+2h) + \ldots + f(a+(n-1)h) + \frac{1}{2}f(b)]$$

$$\equiv T_n\,.$$

The Error formula for the Composite Trapezoidal Rule is

$$\int_a^b f(t)dt - T_n = -\sum_{i=1}^n \frac{h^3}{12} f''(\eta_i)$$

where $\eta_i \in [a + (i-1)h, a + ih]$. Since $nh = b - a$, and

$$\frac{1}{n}\sum_{i=1}^n f''(\eta_i)$$

is an average value of f'' on $[a, b]$, we obtain

$$\int_a^b f(t)dt - T_n = -\frac{(b-a)h^2}{12} f''(\eta)$$

for some $\eta \in [a, b]$. []

Recall our plan:

- Study Newton-Cotes formulas (trapezoidal formula, Simpson's formula, etc.)
- YOU ARE HERE! Study Gaussian integration.
- Investigate the anatomy of a practical algorithm: adaptive integration.
- Discuss singular integrals.
- Discuss multidimensional integration.

Gaussian integration

Gaussian integration

Problem: Compute an approximation to

$$I(f) = \int_a^b w(t) f(t) dt$$

under these assumptions:

- a and/or b may be infinite.
- $w(t) \geq 0$ for $t \in [a, b]$.
- The moments
$$\mu_k = \int_a^b w(t) t^k dt$$
exist and are finite for $k = 0, 1, \ldots$.
- If $s(t)$ is a polynomial, and $s(t) \geq 0$ on $[a, b]$ and
$$\int_a^b w(t) s(t) dt = 0\,,$$
then $s(t) = 0$. (This assumption is satisfied if w is positive and continuous.)

As before, our approximation will be of the form

$$Q(f) = \sum_{i=1}^{n} \omega_i f(t_i)\,,$$

but now we will try to choose not only ω_i but also t_i in the best possible way.

By counting the number of parameters, we see that we have enough to make the formula exact for polynomials of degree $2n - 1$ and less.

How do we compute the parameters in the formula?

There are some very elegant ways to do it, using the theory of orthogonal polynomials, but we will use brute force!

Example: Suppose we want a rule of the form

$$Q(f) = \omega_1 f(t_1) + \omega_2 f(t_2) + \omega_3 f(t_3)$$

for the interval $[a, b] = [-1, 1]$.

We have 6 parameters to choose, so let's write down the conditions to make it exact for polynomials of degree 5 or less:

$$\begin{aligned}
I(1) &= 2 = \omega_1 + \omega_2 + \omega_3 \\
I(t) &= 0 = \omega_1 t_1 + \omega_2 t_2 + \omega_3 t_3 \\
I(t^2) &= 2/3 = \omega_1 t_1^2 + \omega_2 t_2^2 + \omega_3 t_3^2 \\
I(t^3) &= 0 = \omega_1 t_1^3 + \omega_2 t_2^3 + \omega_3 t_3^3 \\
I(t^4) &= 2/5 = \omega_1 t_1^4 + \omega_2 t_2^4 + \omega_3 t_3^4 \\
I(t^5) &= 0 = \omega_1 t_1^5 + \omega_2 t_2^5 + \omega_3 t_3^5
\end{aligned}$$

This is a system of 6 nonlinear equations in 6 unknowns. We study methods for solving such systems later, but for this one, the work has already been done and the solution tabulated in programs such as `GLWeights`.

Convergence result

Theorem: Suppose we have a function $f \in \mathcal{C}^{2n}[a, b]$. If n is the number of function values used, then

$$I(f) - Q(f) = \frac{f^{(2n)}(\xi)}{(2n)!}(p_n, p_n)$$

where

$$p_n(t) = (t - t_1) \dots (t - t_n)$$

for some point $\xi \in [a, b]$.

How does this compare with other integration formulas?

Consider Gauss-Legendre integration. The interval is $[-1, 1]$ and $w(t) = 1$.

Composite trapezoidal formula:

$$I(f) - Q(f) = \frac{f^{(2)}(\xi_1)}{2!} \frac{\text{constant}}{n^2}$$

Composite Simpson formula:

$$I(f) - Q(f) = \frac{f^{(4)}(\xi_2)}{4!} \frac{\text{constant}}{n^4}$$

Gauss-Legendre:

$$I(f) - Q(f) \quad \approx \quad \frac{f^{(2n)}(\xi_3)}{(2n)!} \frac{\pi}{4^n}$$

for large n.

Recall our plan:

- Study Newton-Cotes formulas (trapezoidal formula, Simpson's formula, etc.)
- Study Gaussian integration.
- YOU ARE HERE! Investigate the anatomy of a practical algorithm: adaptive integration. The Matlab function is `quad`.
- Discuss singular integrals.
- Discuss multidimensional integration.

We'll pick up the remaining ideas in a set of powerpoint notes.