Lecture 13 Numerical integration: basics

Weinan E[1,2] and Tiejun Li[2]

[1] Department of Mathematics,
Princeton University,
weinan@princeton.edu

[2] School of Mathematical Sciences,
Peking University,
tieli@pku.edu.cn
No.1 Science Building, 1575

Outline

Motivations and ideas

Basic techniques

Extrapolation algorithm

Motivations

- 在科学与工程问题中,经常需要计算各种积分,如

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

- 求解偏微分方程,如有限元求解

$$u''(x) = f(x), \quad u(0) = u(1) = 0.$$

转化为$a(u,v) = f(v)$, 对任意$v(x), v(0) = v(1) = 0$,

$$a(u,v) = \int_0^1 u(x)v(x)dx, \quad f(v) = \int_0^1 f(x)v(x)dx.$$

取$u(x), v(x)$均为分片线性函数,需要计算积分.

- 求解积分方程

$$\lambda \int_0^1 k(x,y)f(y)dy + g(x) = f(x)$$

取$f(x)$为分片线性函数,计算积分.

Ideas

- 每一种数值逼近就给出数值积分的一种技术

$$\int_a^b f(x)dx \approx \int_a^b P(x)dx$$

$P(x)$为多项式,为$f(x)$的某种逼近.

Outline

Lagrange interpolation integral

- To integrate
$$\int_a^b f(x)dx$$
where $f(x) \in C[a,b]$.
- Midpoint rule: Approximate $f(x)$ as $f\left(\frac{a+b}{2}\right)$ we have
$$\int_a^b f(x)\,dx \approx f\left(\frac{a+b}{2}\right)(b-a)$$
- Trapezoidal rule: Approximate $f(x)$ as
$$p_1(x) = \frac{x-b}{a-b}f(a) + \frac{x-a}{b-a}f(b)$$
we have
$$\int_a^b f(x)\,dx \approx \int_a^b p_1(x)\,dx = \frac{f(a)+f(b)}{2}(b-a)$$

Lagrange interpolation integral

- Simpson's rule: Approximate $f(x)$ as

$$p_2(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(a) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f\left(\frac{a+b}{2}\right) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(b)$$

we have

$$\int_a^b f(x)\,dx \approx \int_a^b p_2(x)\,dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

Lagrange interpolation integral

- Cubic interpolation quadrature:

$$\int_a^b f(x)\,dx \approx \int_a^b p_3(x)\,dx$$
$$= \frac{b-a}{8}\left[f(a) + 3f\left(a + \frac{b-a}{3}\right) + 3f\left(a + \frac{2(b-a)}{3}\right) + f(b)\right].$$

- Fourth order interpolation quadrature

$$\int_a^b f(x)\,dx \approx \int_a^b p_4(x)\,dx$$
$$= \frac{b-a}{90}\left[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)\right].$$

Lagrange interpolation integral

- Newton-Cotes quadrature: 对$[a,b]$作等距分割$x_0 = a < x_1 < \ldots < x_n = b,\ x_k = a + kh,\ (k = 0, 1, \ldots, n),$ $h = (b-a)/n$作Lagrange插值函数$P_n(x) \in \mathbb{P}_n$,并记$x = a + th \quad t \in [0, n]$,得到

$$
\begin{aligned}
P_n(x) &= \sum_{k=0}^{n} \Big(\prod_{\substack{j=0 \\ j\neq k}}^{n} \frac{x - x_j}{x_k - x_j}\Big) f(x_k) \\
&= \sum_{k=0}^{n} \Big(\prod_{\substack{j=0 \\ j\neq k}}^{n} \frac{t - j}{k - j}\Big) f(x_k) \\
&= \sum_{k=0}^{n} \frac{(-1)^{(n-k)}}{k!(n-k)!} \prod_{\substack{j=0 \\ j\neq k}}^{n} (t - j) f(x_k)
\end{aligned}
$$

Lagrange interpolation integral

- 作积分

$$\begin{aligned}\int_a^b f(x)dx &\approx \int_a^b P_n(x)dx \\ &= \frac{b-a}{n}\sum_{k=0}^{n}(\int_0^n \prod_{\substack{j=0\\ j\neq k}}^{n}\frac{t-j}{k-j}dt)f(x_k) \\ &= \sum_{k=0}^{n} A_k f(x_k)\end{aligned}$$

其中

$$A_k = (b-a)C_k^{(n)}, C_k^{(n)} = \frac{(-1)^{n-k}}{k!(n-k)!n}\int_0^n \prod_{\substack{j=0\\ j\neq k}}^{n}(t-j)dt \qquad (k=0,1,\ldots,n)$$

$C_k^{(n)}$称为Newton-Cotes求积系数。

- 当$n\geq 8$时，$C_k^{(n)}$有正有负，必然导致其中有的系数绝对值大于1，由于舍入误差的存在，误差会被更加放大导致计算的不准确。这种不稳定性使得在$n\geq 8$时的Newton-Cotes求积公式基本不被采用。

Piecewise interpolation integral

- 先把$[a,b]$区间剖分成一些小区间,例如,引进等距分点

$$x_i = a + ih, \quad h = \frac{b-a}{n}, i = 0, 1, \ldots n,$$

并记

$$x_{i+\frac{1}{2}} = a + (i + 1/2)h,$$

根据定积分的性质,有

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\,dx.$$

在每个小区间$[x_{i+1}, x_i]$上使用中点公式、梯形公式或Simpson公式, 便可得到复合求积公式.

Piecewise interpolation integral

- 复合中点公式:

$$\int_a^b f(x)\,dx \approx M(h) = h\sum_{i=0}^{n-1} f(x_{i+\frac{1}{2}})$$

- 复合梯形公式:

$$\int_a^b f(x)\,dx \approx T(h) = \frac{h}{2}\sum_{i=0}^{n-1}(f(x_i) + f(x_{i+1}))$$

- 复合Simpson公式:

$$\begin{aligned} &\int_a^b f(x)\,dx \\ \approx\quad & S(h) = \frac{h}{6}\sum_{i=0}^{n-1}(f(x_i) + 4f(x_{i+\frac{1}{2}}) + f(x_{i+1})). \end{aligned}$$

Error estimate

- Midpoint rule

$$\int_a^b f(x)\,dx - M_{ab} = \frac{(b-a)^3}{24} f''(\xi_1), \qquad \xi_1 \in (a,b)$$

- Trapezoidal rule

$$\int_a^b f(x)\,dx - T_{ab} = -\frac{(b-a)^3}{12} f''(\xi_2), \qquad \xi_2 \in (a,b)$$

- Simpson's rule

$$\int_a^b f(x)\,dx - S_{ab} = -\frac{(b-a)^5}{2880} f^{(4)}(\xi_3), \qquad \xi_3 \in (a,b)$$

- Note: high order convergence for midpoint rule and Simpson's rule.

Error estimate

- Composite midpoint rule

$$\left|\int_a^b f(x)\,dx - M(h)\right| \le \frac{h^2}{24} M_2(b-a)$$

- Composite trapezoidal rule

$$\left|\int_a^b f(x)\,dx - T(h)\right| \le \frac{h^2}{12} M_2(b-a)$$

- Composite Simpson's rule

$$\left|\int_a^b f(x)\,dx - S(h)\right| \le \frac{h^4}{2880} M_4(b-a)$$

where $M_2 = \max|f''|, M_4 = \max|f^{(4)}|$.

Numerical estimate for the convergence order

- Numerical estimate for the convergence order.

  Suppose
  $$|I(f) - I_h(f)| \leq Ch^p$$
  we take
  $$|I(f) - I_{\frac{h}{2}}(f)| \leq C(\frac{h}{2})^p$$
  then
  $$\frac{|I(f) - I_h(f)|}{|I(f) - I_{\frac{h}{2}}(f)|} \sim 2^p$$
  So
  $$p \approx \ln\Big(\frac{|I(f) - I_h(f)|}{|I(f) - I_{\frac{h}{2}}(f)|}\Big) / \ln 2$$

Basic observation

- We have the following relations

$$T(\frac{h}{2}) = \frac{1}{2}(T(h) + M(h))$$

$$S(h) = \frac{1}{3}T(h) + \frac{2}{3}M(h)$$

- We have

$$S(h) = \frac{4T(\frac{h}{2}) - T(h)}{4-1}$$

- Information:

  We combine $T(h)$ and $T(\frac{h}{2})$ to obtain higher accuracy!

Outline

Richardson's extrapolation

- 假设我们要用一个与步长h有关的量$Q_1(h)$（比如,一个复合求积公式），去近似一个与h无关的量Q（比如,一个定积分）,而且已知截断误差的渐进展开式为

$$Q - Q_1(h) = c_1h^{p_1} + c_2h^{p_2} + c_3h^{p_3} + \cdots + c_kh^{p_k} + \cdots , \tag{1}$$

其中c_k, p_k为常数且$0 < p_1 < p_2 < \cdots$.此时,Q_1逼近Q的截断误差精度就是$O(h^{p_1})$.

- 如果我们把步长缩小一倍,即取$h = h/2$,则有

$$\begin{aligned} Q - Q_1(h/2) &= c_1(h/2)^{p_1} + c_2(h/2)^{p_2} + c_3(h/2)^{p_3} + \cdots \\ &= 2^{-p_1}c_1h^{p_1} + 2^{-p_2}c_2h^{p_2} + 2^{-p_3}c_3h^{p_3} + \cdots \end{aligned} \tag{2}$$

把(1)乘上2^{-p_1}再减去(2),适当整理,得

$$Q - \frac{Q_1(h/2) - 2^{-p_1}Q_1(h)}{1 - 2^{-p_1}} = c_2^*h^{p_2} + c_3^*h^{p_3} + \cdots + c_k^*h^{p_k} + \cdots \tag{3}$$

其中常数c_k^*为

$$c_k^* = \frac{c_k(2^{-p_k} - 2^{-p_1})}{1 - 2^{-p_1}}, \quad k = 2, 3, \ldots .$$

Richardson's extrapolation

- 如果记

$$Q_2(h) = \frac{Q_1(h/2) - 2^{-p_1}Q_1(h)}{1-2^{-p_1}} \tag{4}$$

则Q_2与Q的截断误差精度就提高为$O(h^{p_2})$,即有

$$Q - Q_2(h) = c_2^* h^{p_2} + c_3^* h^{p_3} + \cdots + c_k^* h^{p_k} + \cdots. \tag{5}$$

- 我们完全可以从(5)出发,用与上面类似的方法再构造一个$Q_3(h)$,使得它与Q 的截断误差精度为$O(h^{p_3})$.而且这个过程可以不断地进行下去. 这种从低阶精度格式的截断误差的渐进展开式出发,做简单线性组合从而得到高阶逼近格式的方法称为Richardson外推加速收敛技术

Euler-Maclaurin formula

- **定理3.3.4** （Euler-Maclaurin公式）设$f \in C^m[a,b]$ $(m>2)$, $T_h(f) = \frac{h}{2}\sum_{k=0}^{n-1}[f(x_k)+f(x_{k+1})]$，则

$$\int_a^b f(x)dx = T_h(f) - \sum_{j=1}^{[\frac{m}{2}]} \frac{b_{2j}h^{2j}}{(2j)!}\left[f^{(2j-1)}(b) - f^{(2j-1)}(a)\right] + (-1)^m h^m \int_a^b \tilde{B}_m\left(\frac{x-a}{h}\right) f^{(m)}(x)dx.$$

这里$[\frac{m}{2}]$指小于或等于$\frac{m}{2}$的最大整数。

- 观察Euler-Maclaurin公式，不难发现如果$f(x)$是周期函数，将会出现h^{2j}中系数$f^{(2j-1)}(b) - f^{(2j-1)}(a) = 0$，最后仅剩下$h^m$！这表明梯形公式对周期函数积分具有极高的精度，换句话说，f 有多光滑，精度就有多高，这一现象称为具有谱精度。

Romberg quadrature

- 将Richardson外推加速收敛技术应用于复合梯形求积公式(12)就可以得到Romberg 求积方法.
- From Euler-Maclaurin formula

$$\int_a^b f(x)\,dx = T_1(h) + \sum_{k=1}^{\infty} c_{2k}^{(1)} h^{2k}. \tag{6}$$

- 利用外推加速技术我们容易推出

$$\int_a^b f(x)\,dx = T_2(h) + \sum_{k=2}^{\infty} c_{2k}^{(2)} h^{2k}, \tag{7}$$

其中

$$T_2(h) = \frac{T_1(h/2) - 4^{-1} T_1(h)}{1 - 4^{-1}}.$$

Romberg quadrature

- 再次使用外推加速技术,我们又可推出

$$\int_a^b f(x)\,dx = T_3(h) + \sum_{k=3}^{\infty} c_{2k}^{(3)} h^{2k}, \tag{8}$$

其中

$$T_3(h) = \frac{T_2(h/2) - 4^{-2} T_2(h)}{1 - 4^{-2}}.$$

- 一般地,我们可以得到递推定义的求积序列

$$T_{k+1}(h) = \frac{T_k(h/2) - 4^{-k} T_k(h)}{1 - 4^{-k}}, \quad k = 1, 2, 3, \ldots. \tag{9}$$

容易验证

$$\int_a^b f(x)\,dx - T_{k+1}(h) = O(h^{2(k+1)}). \tag{10}$$

这就是Romberg求积方法.它只需要编制一个复合梯形求积公式的程序,并不断折半初始步长h,以及做简单的线性组合,便能高精度地求出积分值.

Romberg quadrature

- Define

$$T_1^{(l)} = T\left(\frac{b-a}{2^l}\right), \quad l = 0, 1, 2, \ldots$$

and

$$T_{m+1}^{(k-1)} = \frac{4^m T_m^{(k)} - T_m^{(k-1)}}{4^m - 1}$$

- Romberg quadrature table

$$\begin{array}{ccc} T_1^{(0)} & T_2^{(0)} & T_3^{(0)} \\ T_1^{(1)} & T_1^{(1)} & \vdots \\ T_1^{(2)} & \vdots & \vdots \end{array}$$

Homework assignment

- 一个内接 n 边形的周长按照 $p_n = n\sin(\pi/n)$ 计算，外切的按照 $q_n = n\tan(\pi/n)$ 计算，这些值分别提供了 π 值的下界和上界。
  (a) 通过对 sin 和 tan 函数进行 Taylor 级数展开，证明 p_n 和 q_n 可以表示成如下形式

  $$p_n = a_0 + a_1h^2 + a_2h^4 + \cdots$$

  和

  $$q_n = b_0 + b_1h^2 + b_2h^4 + \cdots,$$

  其中 $h = 1/n$。a_0 和 b_0 的具体值是多少?
  (b) 试使用Richardson外推公式给出一个对 π 的数值计算格式.
- Compute the integral by Trapezoidal rule

$$\int_0^{2\pi} e^{\sin x}dx$$

and compute the numerical convergence order.