Lecture 14 Numerical integration: advanced topics

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Outline

Gaussian quadrature

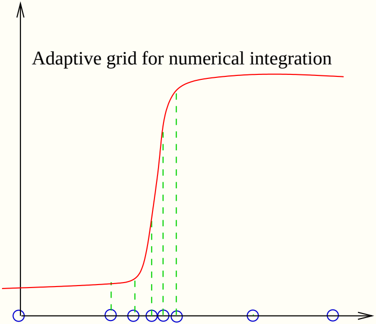
- 定积分的n点求积公式一般可写为

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

- How to obtain the maximal accuracy with fixed number of node points n and suitable choice of coefficients A_k?

Adaptive integration

- Adaptive integration



- The information of the function itself must be taken into account.

Outline

Interpolated integration

- 一般的数值积分可表示为

$$I = \int_a^b f(x)dx \approx \sum_{k=0}^{n} A_k f(x_k) = I_N$$

其中x_k称求积节点，A_k称求积系数，可定义误差

$$E_n(f) = I(f) - I_N(f).$$

- **定义** 如果$\forall f \in \mathbb{P}_n$, $E_n(f) = 0$, 则称数值积分为插值型的。
- **定理** 下面两个命题是等价的:

(1) $I_N(f)$为插值型积分;

(2) $I_N(f)$可由对$x_0, x_1, \dots, x_n$的n次插值积分得到。

代数精度

- **定义:** 设m是一个正整数,如果数值积分公式的截断误差对

$$f(x) = 1, x, x^2, \ldots, x^m$$

都为零,但对$f(x) = x^{m+1}$不为零,则称数值积分公式的代数精度为m.

- 例子: 考察中点公式

$$\int_a^b f(x)dx \approx f(\frac{a+b}{2})(b-a).$$

取$f(x) = 1, x$, 等式均精确成立, 取$f(x) = x^2$等式不成立, 故中点公式代数精度为1。

代数精度

- 下面定理精确刻划了n次代数精度与$n+k$次代数精度的差异。
  定理: 对$\forall 0 \le k \le n+1$, $I_N(f)$为$d = n+k$次代数精度等价于
  (1) $I_N(f)$为插值型的;
  (2) $\omega_n(x) = \prod_{k=0}^{n}(x - x_k)$满足$\int_a^b \omega_n(x)p(x)dx = 0, \quad \forall p \in \mathbb{P}_{k-1}$.

- **定理:** Newton-Cotes求积公式至少具有n次代数精度，如n为偶数，则具有$n+1$次代数精度。

Gauss积分

- 关于定积分的n点求积公式一般可写为

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{n} A_k f(x_k), \tag{1}$$

- 更一般的如果考虑带有权函数的定积分的计算

$$\int_a^b \rho(x) f(x)\,dx \approx \sum_{k=1}^{n} A_k f(x_k), \tag{2}$$

  其中$\rho(x) > 0$为已知的权函数.

- 我们的目标是把节点个数n固定,而让节点的位置x_k与系数A_k都待定,而让求积公式的代数精度达到最高.这种在取定节点数目的条件下,代数精度达到最高的求积公式，我们称之为Gauss求积公式. 由于此时共有$2n$个自由度，设想最大可能的代数精度为$2n-1$.

Gauss积分

- 不失一般性，我们可以设积分区间$[a,b]=[-1,1]$,这是因为有积分变量替换公式
$$\int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{a+b}{2}+\frac{b-a}{2}t\right)dt. \tag{3}$$
- 待定的参数有$2n$个(n个节点,n个系数),取$f(x)$分别为$1,x,x^2,\ldots,x^{2n-1}$,并令求积公式对这些函数准确成立. 首先考虑$\rho(x)\equiv 1$,得到一个$2n$个方程
$$\sum_{k=1}^{n} A_k f(x_k) = \frac{1}{j+1}(b^{j+1}-a^{j+1}),\quad j=0,1,2,\ldots,2n-1.$$
非线性方程组,难以求解!

Gauss积分

- $n=1$情形

  方程$\int_{-1}^{1} f(x)\,dx = A_1 f(x_1)$中,令$f(x)=1$和$f(x)=x$得

$$A_1 = 2, \quad x_1 = 0.$$

于是得到一个节点的Gauss求积公式为

$$\int_a^b f(x)dx \approx f(\frac{a+b}{2})(b-a).$$

这就是中点公式.

Gauss积分

- $n=2$情形
  等式$\int_{-1}^{1} f(x)\,dx = A_1 f(x_1) + A_2 f(x_2)$中,令$f(x)=1, f(x)=x,$
  $f(x)=x^2, f(x)=x^3$得方程组

$$\begin{cases} A_1 + A_2 = 2, \\ A_1 x_1 + A_2 x_2 = 0, \\ A_1 x_1^2 + A_2 x_2^2 = \frac{2}{3}, \\ A_1 x_1^3 + A_2 x_2^3 = 0. \end{cases}$$

- 此方程组有唯一解$A_1 = A_2 = 1,\ x_1 = -\frac{1}{\sqrt{3}}, x_2 = \frac{1}{\sqrt{3}}$. 于是得到两个节点的Gauss求积公式为

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}\Big(f\Big(\frac{a+b}{2} - \frac{b-a}{2\sqrt{3}}\Big) + f\Big(\frac{a+b}{2} + \frac{b-a}{2\sqrt{3}}\Big)\Big).$$

易证此求积公式的代数精度为3.

正交多项式

- Gauss积分一般情形难以求解!
- **定义:**设$\rho(x)$为(a,b)区间上的一个给定的非负函数，任取两个函数f,$g \in C[a,b]$，我们称数值

$$(f,g) = \int_a^b \rho(x)f(x)g(x)dx$$

为函数f与g的带权内积,并称

$$\|f\|_2 = \sqrt{(f,f)} = \sqrt{\int_a^b \rho(x)f(x)f(x)dx}$$

为函数f的带权2范数,其中的$\rho(x)$称为权函数.

- **定义:** 函数f,$g \in C[a,b]$称为是正交的,如果它们的内积

$$(f,g) = \int_a^b \rho(x)f(x)g(x)dx = 0$$

正交多项式

- **定义** 设(a,b)区间上实系数多项式函数

$$\{\varphi_0(x), \varphi_1(x), \varphi_2(x), \cdots, \},$$

满足

$$\int_a^b \rho(x)\varphi_j(x)\varphi_l(x)dx = 0, \quad \text{当} j \neq l \text{ 时}, \tag{4}$$

则称之为区间$[a,b]$上关于权函数$\rho(x)$的正交多项式系.

- 按照给定的内积,可用Gram-Schmidt正交化方法把基函数$\{1, x, x^2, \ldots, x^k, \ldots\}$化成正交多项式系

$$\begin{cases} \varphi_0(x) = 1 \\ \varphi_{j+1}(x) = x^{j+1} - \sum_{i=0}^{j} \frac{(x^{j+1}, \varphi_i(x))}{(\varphi_i(x), \varphi_i(x))}\varphi_i(x), \quad \text{对} j = 0, 1, \ldots \end{cases}$$

正交多项式

- (1)Legendre多项式: $[a,b]=[-1,1]$, $\rho(x)\equiv 1$,

$$\begin{cases}\varphi_0(x)=1, \quad \varphi_1(x)=x,\\ \varphi_{k+1}(x)=\dfrac{2k+1}{k+1}x\varphi_k(x)-\dfrac{k}{k+1}\varphi_{k-1}(x),\\ \qquad\qquad \text{对}k=1,2,\dots\end{cases}$$

- (2)Chebyshev多项式: $[a,b]=[-1,1]$, $\rho(x)=1/\sqrt{1-x^2}$

$$\begin{cases}T_0(x)=1, \quad T_1(x)=x,\\ T_{k+1}(x)=2xT_k(x)-T_{k-1}(x),\\ \qquad\qquad \text{对}k=1,2,\dots\end{cases}$$

- (3)Laguerre多项式: $[a,b)=[0,+\infty)$, $\rho(x)=\exp(-x)$

$$\begin{cases}Q_0(x)=1, \quad Q_1(x)=1-x,\\ Q_{k+1}(x)=(1+2k-x)Q_k(x)-k^2Q_{k-1}(x),\\ \qquad\qquad \text{对}k=1,2,\dots\end{cases}$$

Hermite多项式等等.

Gauss积分

- **定理:** 区间$[a,b]$上的n阶带权正交多项式必有n个实单根. 取这些实单根做节点x_j 即可得到Gauss积分.
- Gauss-Legendre公式: 此时$[a,b]=[-1,1]$,$\rho(x)\equiv 1$, 求积节点x_j为n阶Legendre多项式的零点.几个低阶具体情形为:
  $n=1$时$\int_{-1}^{1} f(x)\,dx \approx 2f(0)$
  $n=2$时$\int_{-1}^{1} f(x)\,dx \approx f\Big(-\frac{1}{\sqrt{3}}\Big)+f\Big(\frac{1}{\sqrt{3}}\Big)$
  $n=3$时$\int_{-1}^{1} f(x)\,dx \approx \frac{5}{9}f\Big(-\sqrt{\frac{3}{5}}\Big)+\frac{8}{9}f(0)+\frac{5}{9}f\Big(\sqrt{\frac{3}{5}}\Big)$
  其它的可以从数学手册中查到.
- Gauss-Chebyshev公式

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\,dx \approx \frac{\pi}{n}\sum_{j=1}^{n} f(x_j)$$

其中x_j是$[-1,1]$区间上的n阶Chebyshev多项式$T_n(x)$的零点

$$x_j=\cos\left(\frac{2j-1}{2n}\pi\right)$$

Gauss积分

- Gauss-Laguerre公式

$$\int_0^{\infty} e^{-x} f(x)\, dx \approx \sum_{j=1}^{n} A_j f(x_j)$$

节点x_j为$(-\infty, 0]$区间上的n阶Laguerre多项式$Q_n(x)$的零点.
当$n=2$时,Gauss-Laguerre公式为

$$\int_0^{\infty} e^{-x} f(x)\, dx \approx \frac{2+\sqrt{2}}{4} f(2-\sqrt{2}) + \frac{2-\sqrt{2}}{4} f(2+\sqrt{2})$$

其它的可以从数学手册中查到.

- **定理:** 设权函数$\rho(x)=1$相应$[a,b]$上首1的$n+1$次正交多项式记为$q_{n+1}(x)$则当$f \in C^{2n+2}[a,b]$时，Gauss-Legendre积分误差:

$$E(f) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \int_a^b (\omega_n(x))^2 dx.$$

Outline

Composite trapezoid rule

- Consider, for example, the general composite trapezoid rule

$$I_N(f) = \sum_{i=1}^{N} \frac{x_i - x_{i-1}}{2} [f(x_{i-1} + f(x_i)]$$

and the error estimate

$$I(f) - I_N(f) = -\sum_{i=1}^{N} \frac{f''(\eta_i)(x_i - x_{i-1})^3}{12}$$

where the nodes x_i are not necessarily equally spaced.

- The contribution

$$-\frac{f''(\eta_i)(x_i - x_{i-1})^3}{12}, \quad \eta_i \in (x_{i-1}, x_i)$$

depends on both the size of $f''(x)$ on the interval (x_{i-1}, x_i) and the size of $|x_i - x_{i-1}|$.

Adaptive idea

- In those parts of the interval of integration (a, b) where $|f''(x)|$ is "small", we can take subintervals of "large" size, while in regions where $|f''(x)|$ is "large", we can take subintervals of "small" size.
- This equi-partition policy of errors is best if the goal is to minimize the number of subintervals and hence the number of function evaluations, necessary to calculate $I(f)$ to a given accuracy.

Adaptive quadrature

- Suppose the object is to compute an approximation P to the integral $I(f) = \int_a^b f(x)dx$ such that

$$|P - I(f)| \leq \epsilon$$

and to do this using as small a number of function evaluations as possible.

- Define $I_i(f) = \int_{x_i}^{x_{i+1}} f(x)dx$, and

$$S_i = \frac{h}{6}\Big(f(x_i) + 4f(x_i + \frac{h}{2}) + f(x_{i+1})\Big)$$

$$\bar{S}_i = \frac{h}{12}\Big(f(x_i) + 4f(x_i + \frac{h}{4}) + 2f(x_i + \frac{h}{2}) + 4f(x_i + \frac{3h}{4}) + f(x_{i+1})\Big)$$

Adaptive quadrature

- From error estimates

$$I_i(f) - S_i = -\frac{f^{(4)}(\eta_1)}{90}(\frac{h}{2})^5$$

$$I_i(f) - \bar{S}_i = -\frac{2f^{(4)}(\eta_2)}{90}(\frac{h}{4})^5$$

- Assume $\eta_1 = \eta_2$, then

$$\bar{S}_i - S_i = \frac{f^{(4)} \cdot h^5}{2^5 \cdot 90}\left(\frac{1-2^4}{2^4}\right)$$

thus

$$\frac{f^{(4)} \cdot h^5}{2^5 \cdot 90} = \frac{2^4(\bar{S}_i - S_i)}{1-2^4}$$

- Substitute it back we have

$$I_i(f) - \bar{S}_i = \frac{\bar{S}_i - S_i}{1-2^4} = \frac{1}{15}(\bar{S}_i - S_i)$$

Adaptive quadrature

- So the principle of equipartition of errors gives

$$E_i = \frac{1}{15}(\bar{S}_i - S_i) \leq \frac{h}{b-a}\epsilon$$

and the approximate integration is taken as

$$P = \sum_{i=1}^{N} \bar{S}_i$$

- Adaptive quadrature essentially consists of applying the Simpson's rule to each of the subintervals covering $[a, b]$ until the above inequality of equipartition of errors is satisfied. If the inequality is not satisfied, those subintervals must be further subdivided and the entire process repeated.

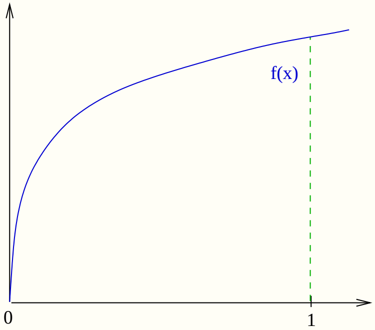
Adaptive quadrature

- Example

$$I(f) = \int_0^1 \sqrt{x}dx$$

and the error $\epsilon = 0.0005$.

- Sketch of function $f(x) = \sqrt{x}$



The curve is very steep in the vicinity of 0 while it is fairly flat as $x \to 1$.

Adaptive quadrature

- Step 1: Divide the interval $[0,1]$ into $[0,\frac{1}{2}]$ and $[\frac{1}{2},1]$.

$$S[\frac{1}{2},1] = 0.43093403$$

$$\bar{S}[\frac{1}{2},1] = 0.43096219$$

then

$$E[\frac{1}{2},1] = \frac{1}{15}(\bar{S} - S) = 0.0000018775 < \frac{1/2}{1}(0.0005) = 0.00025$$

The error criterion is satisfied, we accept the value $\bar{S}[\frac{1}{2},1]$.

- Step 2: Compute the integral in $[0,\frac{1}{2}]$:

$$S[0,\frac{1}{2}] = 0.22449223$$

$$\bar{S}[0,\frac{1}{2}] = 0.23211709$$

and

$$E[0,\frac{1}{2}] = 0.00043499 > 0.00025$$

The error criterion is not satisfied, we must subdivide $[0,\frac{1}{2}]$ again.

Adaptive quadrature

- Step 3: Compute the integral in $[\frac{1}{4}, \frac{1}{2}]$:

$$S[\frac{1}{4}, \frac{1}{2}] = 0.15235819$$

$$\bar{S}[\frac{1}{4}, \frac{1}{2}] = 0.15236814$$

  and

$$E[\frac{1}{4}, \frac{1}{2}] = 0.664 \cdot 10^{-6} < \frac{1/4}{1}(0.0005) = 0.000125$$

  The error criterion is satisfied, we accept the value $\bar{S}[\frac{1}{4}, \frac{1}{2}]$.

- Step 4: Compute the integral in $[0, \frac{1}{4}]$:

$$S[0, \frac{1}{4}] = 0.07975890$$

$$\bar{S}[0, \frac{1}{4}] = 0.08206578$$

  and

$$E[0, \frac{1}{4}] > \frac{1/4}{1}(0.0005) = 0.000125$$

  The error criterion is not satisfied, we must subdivide $[0, \frac{1}{4}]$ again.

Adaptive quadrature

- Step 5: We repeat the procedure above again and again until all of the subintervals satisfies the condition. The subintervals are

$$[0, \frac{1}{8}], \ [\frac{1}{8}, \frac{1}{4}], \ [\frac{1}{4}, \frac{1}{2}], \ [\frac{1}{2}, 1],$$

- So we have the approximate integration values

$$P = \sum_i \bar{S}_i = 0.66621524$$

We have $I(f) = \frac{2}{3}$, so

$$|P - F(f)| = 0.00045142 < 0.0005$$

- The subroutine for adaptive quadrature is very complicate in general. But it is very useful for large scale computations.