Numerical Integration II

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Numerical Methods,
31 October, 2016

Reminder

⇛ On the last lecture with prof. van Dyk :P we learned how to do numerical integration.

⇛ The standard solution is to use the Newton-Coates Quadrature:

$$I^{\mathrm{NC}} = \sum_{k=0}^{K} \omega_k f(x_k), \quad x_k = a + (b-a)\frac{k}{K}$$

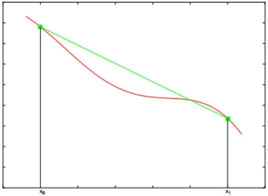
⇛ In practical application we use low order quadratures:

- Simplicity.
- Not easy to calculate high order differentials.
- Rundge effect.
- It's more effective to use the composite quadratures.

Practical information

⇛ There are 4 closed Newton-Cotes methods you need to remember (no more nor less):

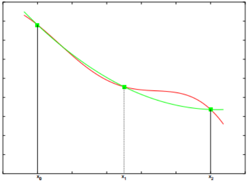
⇛ Trapezoid rule:



$$\int_a^b f(x)\,dx \simeq \frac{b-a}{2}(f_0+f_1)$$

$$E = -\frac{1}{12}(b-a)^3 f''(\zeta)$$

⇛ Simpson rule:



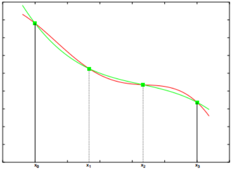
$$\int_a^b f(x)\,dx \simeq \frac{b-a}{6}(f_0+4f_1+f_2)$$

$$E = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\zeta)$$

Practical information

⇛ There are 4 closed Newton-Cotes methods you need to remember (no more nor less):

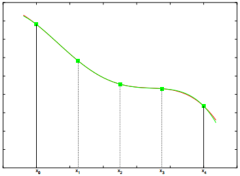
⇛ 3/8 rule:



$$\int_a^b f(x)\,dx \simeq \frac{b-a}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

$$E = -\frac{3}{80}\left(\frac{b-a}{3}\right)^5 f^{(4)}(\zeta)$$

⇛ Boole rule:



$$\int_a^b f(x)\,dx \simeq \frac{b-a}{90}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4)$$

$$E = -\frac{8}{945}\left(\frac{b-a}{4}\right)^7 f^{(6)}(\zeta)$$

Composite quadratures

$\Rrightarrow$ In practice instead of using high order interpolating polynomial it's beneficial to divide the domain $[a, b]$ into smaller domains and use lower order Newton-Cotes method.

$\Rrightarrow$ The procedure can be iterated $\mapsto$ more divisions.

$\Rrightarrow$ When dividing we can re-use the old points $\mapsto$ evaluating function is the most expensive part of the calculation.

$\Rrightarrow$ To re-use the points we need the close versions of the Newton-Cotes methods.

Error reduction

⇛ Division of the integration domain leads towards reduction of the error of the integral.

⇛ For example let's say we calculate the integral with trapezoid rule. We are getting an error:

$$\hat{E} = -\frac{1}{12}(b-a)^3 f^{(2)}(\xi_0)$$

⇛ Now let's divide the domain in two:

$$I = \int_a^b f(x)dx = \int_a^{(a+b)/2} f(x)dx + \int_{(a+b)/2}^b f(x)dx$$

⇛ And the error:

$$\hat{E} = -\frac{1}{12}(\frac{b-a}{2} - a)^3 f^{(2)}(\xi_1) - \frac{1}{12}(b - \frac{a+b}{2})^3 f^{(2)}(\xi_2) =$$
$$-\frac{1}{4}\frac{1}{12}(b-a)^3 f^{(2)} \frac{f^{(2)}(\xi_1) + f^{(2)}(\xi_2)}{2}$$

Error reduction

⇛ Now using the average value theorem:

$$\xi_1 \in [a,(a+b)/2]\,, \quad \xi_2 \in [(a+b)/2, b]$$
$$\frac{f^{(2)}(\xi_1)+f^{(2)}(\xi_2)}{2} = f^{(2)}(\xi_3)$$

⇛ We get in the end:

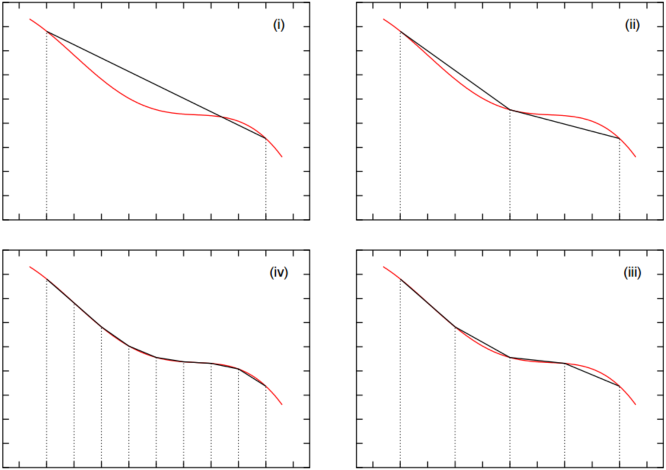
$$\hat{E} = -\frac{1}{4}\frac{1}{12}(b-a)^3 f^{(2)}(\xi_3)$$

⇛ We reduced the error by factor of 4!

⇛ In general for n divisions:

$$\hat{E} = \sum_{i=1}^{n}(-\frac{1}{12})\left(\frac{b-a}{2}\right)^n f^{(2)}(\xi_i) = -\frac{1}{12}\frac{(b-a)^3}{n^2}\frac{1}{n}\sum_{i=1}^{n} f^{(2)}(\xi_i) =$$
$$-\frac{1}{n^2}\frac{(b-a)^3}{12} f^{(2)}(\xi_i)$$

Error reduction



Error reduction

⇛ Remember for trapezoid formula we need to just to remember the sum when we will make the domain more dense:

$$I_N \sim h(\frac{1}{2}f_0 + f_1 + f_2 + ... + f_{N-1} + \frac{1}{2}f_N)$$

⇛ The division can be stopped when we reach the wanted precision:

$$\frac{|I_{k+1} - I_k|}{|I_k| + \epsilon'} < \epsilon$$

Richardson extrapolation

⇛ Using the composite quadratures we are getting sequence of numbers that will converge to the value of the integral.
⇛ Now in the "normal" composite quadrature we just use the final value, but in principle the previous calculated one might be also useful!
⇛ The simplest algorithm that uses them is the Richardson extrapolation:

- We divide the $[a, b]$ in the n and $2n$ divisions:

$$I = I_n - \frac{(b-a)^3}{12n^2} f^{(2)}(\xi_n)$$
$$I = I_{2n} - \frac{(b-a)^3}{12(2n)^2} f^{(2)}(\xi_{2n})$$

⇛ Now if we assume that $f^{(2)}(\xi_{2n}) \simeq f^{(2)}(\xi_{2n})$ we can calculate:

$$I \simeq \frac{4I_{2n} - I_n}{3}$$

Richardson extrapolation

$\Rrightarrow$ Now this will work only if the assumption is true: $f^{(2)}(\xi_{2n}) \simeq f^{(2)}(\xi_{2n})$.
$\Rrightarrow$ This is true if the sequence I_k is monotonically approaching the true value.

Richardson extrapolation

- $\Rightarrow$ Now this will work only if the assumption is true: $f^{(2)}(\xi_{2n}) \simeq f^{(2)}(\xi_{2n})$.
- $\Rightarrow$ This is true if the sequence I_k is monotonically approaching the true value.
- $\Rightarrow$ Aka. the function always underestimates the integral.

Richardson extrapolation

$\Rrightarrow$ Now this will work only if the assumption is true: $f^{(2)}(\xi_{2n}) \simeq f^{(2)}(\xi_{2n})$.
$\Rrightarrow$ This is true if the sequence I_k is monotonically approaching the true value.
$\Rrightarrow$ Aka. the function always underestimates the integral.
$\Rrightarrow$ Aka. Convex of the function doesn't change much.
$\Rrightarrow$ If the convex of teh function changes the application of Richardson extrapolation might now be a good idea.

Richardson extrapolation

⇛ For example let's try to calculate:

$$I = \int_1^2 \frac{dx}{x}$$

⇛ the exact solution is $I = \ln 2 = 0.69314718...$

⇛ now using the trapezoid method:

$$I_1 = \frac{1}{2}\left(f(1) + f(2)\right) = 0.75$$

⇛ making more dense domain:

$$I_2 = \frac{1}{2}\left(\frac{1}{2}f(1) + f(1.5) + \frac{1}{2}f(2)\right) = \frac{1}{2}\frac{17}{12} = 0.708333...$$

Richardson extrapolation

⇛ making more^2 dense domain:

$$I_4 = \frac{1}{4}\left(\frac{1}{2}f(1) + f(1.5) + \frac{1}{2}f(2)\right) + \frac{1}{4}\left(f(1.25) + f(1.75)\right) =$$

$$\frac{1}{4}\frac{17}{12} + \frac{1}{4}\left(\frac{4}{5} + \frac{4}{7}\right) = 0.69702381$$

⇛ The I_1, I_2, I_4 make a monotonic sequnce of integral approximations. Applying the Richardson extrapolation to I_4 and I_2:

$$\frac{4 \cdot 69702381 + 0.708333}{3} = 0.69325397$$

Romberg method

$\Rrightarrow$ There is a way to do better the Richardson extrapolation. The prove of this is non trivial but let's just see how this works.
$\Rrightarrow$ Let $A_{0,k}$ be trapezoid approximation with 2^k subdivisions.
$\Rrightarrow$ We know that:

$$\lim_{k \to \infty} A_{0,k} = I$$

$\Rrightarrow$ Now if we define the:

$$A_{n,k} = \frac{1}{4^n - 1} \left(4^n A_{n-1,k+1} - A_{n-1,k} \right)$$

Romberg method

$\Rrightarrow$ Now the order to calculate the $A_{n,k}$ is:

$$
\begin{array}{ccccccccccc}
A_{0,0} & & & & & & & & & & \\
A_{0,1} & \overset{\searrow}{\rightarrow} & A_{1,0} & & & & & & & & \\
A_{0,2} & \overset{\searrow}{\rightarrow} & A_{1,1} & \overset{\searrow}{\rightarrow} & A_{2,0} & & & & & & \\
A_{0,3} & \overset{\searrow}{\rightarrow} & A_{1,2} & \overset{\searrow}{\rightarrow} & A_{2,1} & \overset{\searrow}{\rightarrow} & A_{3,0} & & & & \\
A_{0,4} & \overset{\searrow}{\rightarrow} & A_{1,3} & \overset{\searrow}{\rightarrow} & A_{2,2} & \overset{\searrow}{\rightarrow} & A_{3,1} & \overset{\searrow}{\rightarrow} & A_{4,0} & & \\
\dots & \overset{\searrow}{\rightarrow} & \dots & \overset{\searrow}{\rightarrow} & \dots & \overset{\searrow}{\rightarrow} & \dots & \overset{\searrow}{\rightarrow} & \dots & \overset{\searrow}{\rightarrow} & \dots
\end{array}
$$

$\Rrightarrow$ Arrows indicate which elements are needed to calculate the next one.

$\Rrightarrow$ In practice we don't need to remember all of them, but the last row.

Romberg method

⇛ One can show:

$$\begin{pmatrix} A_{00} \\ A_{10} \\ A_{20} \\ \dots \\ A_{k0} \end{pmatrix} = \begin{pmatrix} c_{00} & 0 & 0 & \dots & 0 \\ c_{11} & c_{10} & 0 & \dots & 0 \\ c_{22} & c_{21} & c_{20} & \dots & 0 \\ \dots & & & & \\ c_{kk} & c_{k,k-1} & c_{k,k-2} & \dots & c_{k,0} \end{pmatrix} \begin{pmatrix} A_{00} \\ A_{01} \\ A_{02} \\ \dots \\ A_{0,k} \end{pmatrix}$$

⇛ If it is true: $\lim_{k\to\infty} A_{0,k} = I$ then $\lim_{k\to\infty} A_{k,0} = I$

⇛ Now the numbers $A_{k,0}$ are the extrapolation of the extrapolation :) Yes I know how this sounds :P

⇛ The convergence of $A_{k,0}$ is much faster then $A_{0,k}$

Romberg method, in practice

⇛ The algorithm works as follows: we start from calculating the $A_{0,k}$ and our current estimator of the integral is $A_{k,0}$. (remember we have 2^k divisions)
⇛ Now we calculate the $A_{0,k+1}$ using the trapezoid method with 2^{k+1} divisions.
⇛ We calculate the whole row using eq. from two slides up.
⇛ The whole procedure is finished when the $A_{k,0}$ and $A_{k+1,0}$ are similar.

Warning:

There is not guarantee that the algorithm will converge! One has to set a maximum number of steps. If the algorithm doesn't converge since then the method might not be converging.

⇛ If the method converges the convergence is much faster then the trapezoid method.

Romberg method, example

$\Rrightarrow$ Lest calculate the integral:

$$I = \int_1^{1.5} \frac{dx}{1 + 2x^2 - 0.25\sin(9x)}$$

with 10^{-8} accuracy.

$k = 0$	0.13347528					
$k = 1$	0.12398581	0.12082265				
$k = 2$	0.12173305	0.12098214	0.12099277			
$k = 3$	0.12118491	0.12100220	0.12100353	0.12100370		
$k = 4$	0.12104904	0.12100375	0.12100385	0.12100386	0.12100386	
$k = 5$	0.12101515	0.12100385	0.12100386	0.12100386	0.12100386	0.12100386
$k = 6$	0.12100668	...				
$k = 7$	0.12100456	...				
$k = 8$	0.12100403	...				
$k = 9$	0.12100390	...				
$k = 10$	0.12100387	...				
$k = 11$	0.12100386	...				
$k = 12$	0.12100386	...				

$\Rrightarrow$ To reach the required precision we need $2^5 + 1 = 33$ function evaluations. If we use classical Romberg method we would need $2^12 + 1 = 4097$.

$\Rrightarrow$ This numbers are just an example. This is hugely case dependent.

Romberg method, example 2

⇛ Lest calculate the integral from previous example:

$$I = \int_1^2 \frac{dx}{x} = \ln 2$$

⇛ We get:

$$\begin{array}{lll} k=0 & I_1 = 0.75 & & \\ k=1 & I_2 = 0.70833333 & 0.69444444 & \\ k=2 & I_4 = 0.69702381 & 0.69325397 & 0.69317461 \end{array}$$

⇛ Now we see that evaluating the function 5 times we got precision of $3 \cdot 10^{-5}$

Integrals with ∞ boundary

$\Rrightarrow$ What if we want to find an integral (we know it exists):

$$\int_0^{\infty} f(x)dx$$

$\Rrightarrow$ To do so we use an old trick:

$$\int_0^{\infty} f(x)dx = \int_0^{A} f(x)dx + \int_A^{\infty} f(x)dx$$

$\Rrightarrow$ With the information that the function has to approach 0 very fast at ∞.

$\Rrightarrow$ in practice we need to choose A to be large.

$\Rrightarrow$ The A we choose in a way that for $x > A$ the function $|f(x)| \leqslant Bg(x)$, where $g(x)$ is fastly converging to 0 and $\int g(x)dx$ can be calculated analytically.

Multidimensional integrals

⇛ Most of the time we need to calculate integrals like:

$$\int_{a_1}^{b_1} dx_1 \int_{a_2}^{b_2} dx_2 ... \int_{a_n}^{b_n} dx_n f(x_1, x_2, ..., x_n)$$

⇛ For $n \leqslant 3$ use Monte Carlo methods to calculate this!

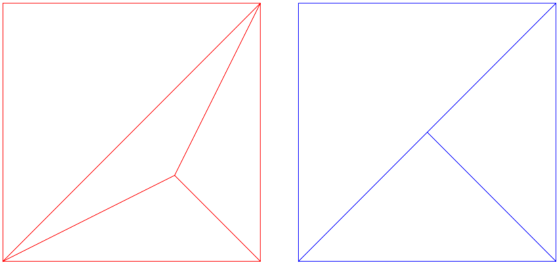
⇛ So in practice we need to know how to calculate this in 2D.

Triangularization

Any multidimensional polygon can be covered by triangles Ω_i such that:

- $D = \cup_i \Omega_i$
- $\Omega_i \cap \Omega_j$, $i \neq j$ is :
  - empty
  - common vertex
  - common edge

Triangularization example



⇛ Which is correct which is not correct?

Multidimensional integral, algorithm

⇛ After we do triangulation of the domain.
⇛ Calculate the integral using Prism volume.
⇛ Do the traingularization again and calculate the next iteration of the integral.
⇛ Stop when the improvement is getting small.

Backup