

Homework5

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1 Problem1: five-point formula for $f''(x)$

1.1 problem description

Derive the five-point formula for the second-order derivative $f''(x)$.

1.2 Proof

with centered difference method, we have:

$$\begin{cases} f(x+2h) + f(x-2h) - 2f(x) &= 4h^2 f''(x) + \frac{16h^4}{24} f^{(4)}(x) + O(h^6) \\ f(x+h) + f(x-h) - 2f(x) &= h^2 f''(x) + \frac{h^4}{24} f^{(4)}(x) + O(h^6) \end{cases} \quad (1)$$

In order to eliminate $f^{(4)}(x)$, we multiply the second equation by -16 and add it to the first equation, which gives:

$$f(x+2h) - 16f(x+h) + 30f(x) - 16f(x-h) + f(x-2h) = -12h^2 f''(x) + O(h^6) \quad (2)$$

so we have the five-point formula for the second-order derivative:

$$f''(x) = \frac{-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} + O(h^4) \quad (3)$$

2 Problem2: Romberg Integration

2.1 problem description

Compute integration of $f(x) = \exp(-x^2)$ from 0 to 1 using Romberg Integration, using at least 4 layers of extrapolation to compute and analyze the error.

2.2 algorithm description

Romberg integration computes a sequence of trapezoidal approximations with equal 2^k subdivisions of the integration interval, and then use Richardson extrapolation to eliminate leading-order error terms.

$$\int_a^b dx f(x) \approx R(i, 0) = \frac{b-a}{2^{i+1}} \left[f(a) + f(b) + 2 \sum_{n=1}^{2^i-1} f\left(a + n \frac{b-a}{2^i}\right) \right] \quad (4)$$

and we can compute higher-order estimates recursively :

$$R(i, k) = \frac{4^k R(i, k-1) - R(i-1, k-1)}{4^k - 1} \quad (5)$$

where $R(i, k)$ is the k-th extrapolated value at level i.

2.3 output

run problem2.py

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Romberg table (rows i, columns k):
0.6839397206  0.0000000000  0.0000000000  0.0000000000  0.0000000000
0.7313702518  0.7471804289  0.0000000000  0.0000000000  0.0000000000
0.7429840978  0.7468553798  0.7468337098  0.0000000000  0.0000000000
0.7458656148  0.7468261205  0.7468241699  0.7468240185  0.0000000000
0.7465845968  0.7468242574  0.7468241332  0.7468241326  0.7468241331

Absolute error table:
6.288e-02
1.545e-02   3.563e-04
3.840e-03   3.125e-05   9.577e-06
9.585e-04   1.988e-06   3.710e-08   1.143e-07
2.395e-04   1.246e-07   4.172e-10   1.650e-10   2.827e-10

Relative error table:
8.420e-02
2.069e-02   4.771e-04
5.142e-03   4.184e-05   1.282e-05
1.283e-03   2.662e-06   4.967e-08   1.531e-07
3.207e-04   1.669e-07   5.586e-10   2.210e-10   3.785e-10

Final approximation R(4,4): 0.746824133095
True value: 0.746824132812
Absolute error: 2.827e-10
Relative error: 3.785e-10
```

Figure 1: output of Romberg Integration

3 Problem3:

3.1 problem description

Radial wave function of the 3s orbital is:

$$R_{3s}(r) = \frac{1}{9\sqrt{3}} (6 - 6\rho + \rho^2) Z^{3/2} e^{-\rho/2} \quad (6)$$

1. r = radius expressed in atomic units (1 Bohr radius = 52.9 pm)
2. e = 2.71828 approximately.
3. Z = effective nuclear charge for that orbital in that atom.

4. $\rho = 2\frac{Zr}{n}$, where n is the principal quantum number (3 for the 3s orbital)

Compute $\int_0^{40} |R_{3s}(r)|^2 r^2 dr$ for Si atom ($Z=14$) with Simpson's rule using two different radial grids:

(1) Equal spacing grids: $r[i] = (i - 1)h; i = 1, \dots, N$ (try different N)

(2) A nonuniform integration grid, more finely spaced at small r than at large r: $r[i] = r_0(e^{t[i]} - 1); t[i] = (i - 1)h; i = 1, \dots, N$ (One typically choose $r_0 = 0.0005$ a.u., try different N).

(3) Find out which one is more efficient, and discuss the reason.

3.2 algorithm description

(1) For uniform grid $r[i] = (i - 1)h; i = 1, \dots, N$, we use Simpson's rule, so N must be odd:

$$\int_a^b f(x)dx \approx \frac{h}{3} \sum_{i=1}^{N-2} [f(x_i) + 4f(x_{i+1}) + f(x_{i+2})], \quad h = \frac{b-a}{N-1} \quad (7)$$

we can thus compute the integral directly.

(2) For non-uniform grid $r[i] = r_0(e^{t[i]} - 1); t[i] = (i - 1)h; i = 1, \dots, N$, notice that $t[i] = (i - 1)h$ is uniform, we can use the change of variable to convert the integral:

$$\int_0^{40} |R_{3s}(r)|^2 r^2 dr = \int_{t(1)}^{t(N)} |R_{3s}(r(t))|^2 r(t)^2 \frac{dr}{dt} dt \quad (8)$$

where $\frac{dr}{dt} = r_0 e^t$. we can then use Simpson's rule (equation (7)) to compute the integral over t, since t is a uniform grid.

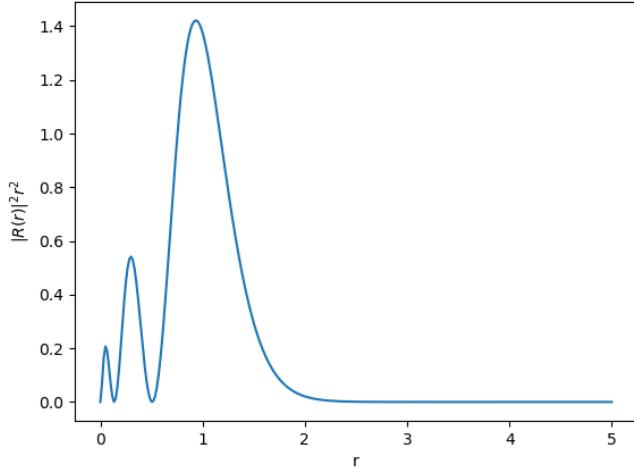


Figure 2: Integral function $|R_{3s}(r)|^2 r^2$

3.3 output

run problem3.py

$N = 201$	Uniform: 0.961099	Nonuniform: 1.000000
$N = 501$	Uniform: 1.002767	Nonuniform: 1.000000
$N = 1001$	Uniform: 1.000698	Nonuniform: 1.000000
$N = 2001$	Uniform: 1.000056	Nonuniform: 1.000000
$N = 4001$	Uniform: 1.000004	Nonuniform: 1.000000

Figure 3: output of uniform and non-uniform grid integration

Analysis: By comparing the results of the two methods with different N , we can find out nonuniform method is more efficient.

This is because the radial wave function changes rapidly at small r in $[0,2]$ (shown in Figure 2) and slowly at large r , so using a nonuniform grid that is more finely spaced at small r can capture the behavior of the function more accurately, leading to better integration results than uniform grid with the same N points.