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:

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

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

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

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

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

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.

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

and we can compute higher-order estimates recursively :

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

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

2.3 output

run `problem2.py`

```
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:

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

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,...,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, ..., 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,...,N , we use Simpson's rule, so N must be odd:

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

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, ..., N , notice that $t[i] = (i-1)h$ is uniform, we can use the change of variable to convert the integral:

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

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.

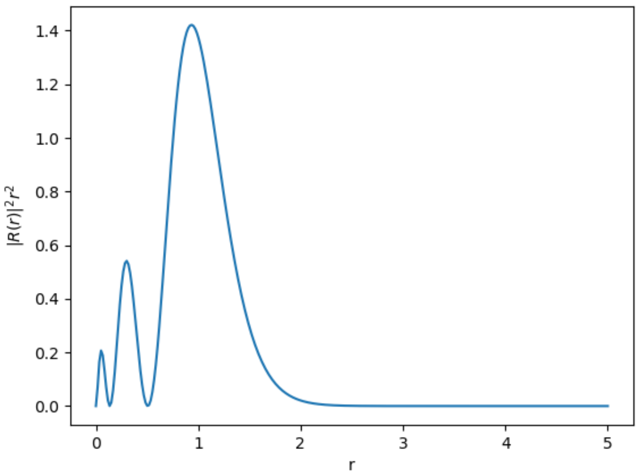

Figure 2: Integral function $|R_{3s}(r)|^2 r^2$

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.