question 2 views

Daily Challenge 23.1

(**Due: Wednesday 2/27 at 12:00 noon Eastern**)

Today you will derive and test *Stirling's approximation*, an important result involving the gamma function (or equivalently the factorial) which appears repeatedly in statistical mechanics and thermodynamics (and thus in physical chemistry).

We wish to find an approximation to $n! = \Gamma(n+1)$ when n is very big (like Avogadro's number). Assume n is so large that $n \approx n+1$, that is, assume the fractional error $\frac{(n+1)-n}{n} = \frac{1}{n}$ can be neglected.

Our strategy will be to approximate $\log(n!)$ by computing an integral in two ways -- one exact, and one approximate using the trapezoidal rule -- and setting the two expressions equal. We then exponentiate both sides to approximate $n!$ itself.

(a) Evaluate the integral $\int_1^n \log(x)\,dx$ exactly (using integration by parts). You should find $n\log(n) - n + 1$

(b) Next approximate the integral using the trapezoidal rule, namely

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{N} \frac{f(x_{k-1}) + f(x_k)}{2}\,\Delta x_k$$

with integer steps. That is, approximate

$$\int_1^n \log(x)\,dx \approx \sum_{k=1}^{n-1} \frac{\log(k) + \log(k+1)}{2}$$

Compute the sum explicitly using the sum-of-a-logs rule to show that $\int_1^n \log(x)\,dx \approx \log((n-1)!) + \frac{1}{2}\log n$ Explain why we can re-write this as $\log(n!) - \frac{1}{2}\log n$.

(c) Set your two results in (a) and (b) equal to find

$$\log(n!) \approx n\log(n) + \frac{1}{2}\log(n) - n + C,$$

where I have added a constant C to signal that we have made an approximation that will have some error term. Then exponentiate both sides to find

$$\Gamma(n+1) = n! \approx e^C n^n \sqrt{n} e^{-n}.$$

(d) Find the constant e^C using Python. That is, solve the above equation for the constant factor,

$$e^C \approx \frac{n!}{n^n \sqrt{n} e^{-n}},$$

do `import math`, and then use `math.factorial` and `math.sqrt` and `math.exp` appropriately to compute the ratio on the right side when n is large. You should find $e^C \approx \sqrt{2\pi}$. Thus we have found *Stirling's approximation*,

$$\Gamma(n+1) = n! \approx \sqrt{2\pi n} n^n e^{-n}.$$

You will use this approximation frequently when studying ideal gases in more advanced courses.

daily_challenge

Updated 1 month ago by Christian Ferko

the students' answer, *where students collectively construct a single answer*

I shall send the scan and put my code on GitHub

Updated 1 month ago by Logan Pachulski

the instructors' answer, *where instructors collectively construct a single answer*

Click to start off the wiki answer

followup discussions *for lingering questions and comments*