Chem237: Lecture 4

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More Series

The alternating series has some interesting convergence properties, it takes the form

$$\sum_{n=0}^{\infty} \frac{(-1)^{n+1}}{n} = \ln(1+1) = 2 \tag{1}$$

If we start to look at some of the explicit values of the series we see

$$1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots \tag{2}$$

With general numbers we know that addition and subtraction commute i.e. A + B = B + A, so we would expect that if we re-arrange the order in which we take our infinite summation we would still produce teh same result at the end. So consider a fancy summation scheme for the alternating series where we group terms

$$\left(1 + \frac{1}{3} + \frac{1}{5}\right) - \frac{1}{2} + \left(\frac{1}{7} + \frac{1}{9} + \frac{1}{11} + \frac{1}{13} + \frac{1}{15}\right) - \frac{1}{4} \cdots \tag{3}$$

So we bnreak the summation into positive and negative terms, defining a set of partial summations over the positive and then negative terms. If you numerically evaluate the summations in this way you will find that the summation appears to approach 1.5 as n goes to ∞. In fact it turns out that you can re-arrange the terms in any sort of pattern, and find the series converges to any value you want. This is a consequence of the series not being absolutely convergent! The commutation of terms applies to finite numbers, it is not true for an infinite series, meaning A + B $\neq$ B + A over an infinite interval, it is only true for finite numbers. If the series is absolutely convergent however, than the series converges to the same value no matter what, and changing the order of the summation will not effect the result.

Power Series

The purpose of the power series is to exapnd a function in terms of x.

$$\sum_{n=0}^{\infty} a_x x^n = f(x) \tag{4}$$

If we have a Taylor series of a known function x than things are simple for example

Geometric

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \tag{5}$$

Expotential

$$\sum_{n=0}^{\infty} \frac{x^n}{n!} = e^x \tag{6}$$

Sine

$$\sum_{n=0}^{\infty} \frac{x^{2k+1}(-1)^{k+1}}{(2k+1)!} = \sin(x) \tag{7}$$

Cosine

$$\sum_{n=0}^{\infty} \frac{x^{2k}(-1)^k}{(2k)!} = \cos(x) \tag{8}$$

Logarithm

$$\sum_{n=0}^{\infty}(-1)^{n+1}\frac{x^n}{n} = \ln(1+x) \tag{9}$$

If we are given a series we do not recognize, we can try applying a transformation to make it into a recognized form, such as taking a derivitive or an integral of the original series.

$$f(x) = \sum_{n=1}^{\infty} a_n x^n \tag{10}$$

We can write a new series, using the derivative.

$$f'(x) = \sum_{n=1}^{\infty} n a_n x^{n-1} \tag{11}$$

Now consider an integral

$$\int_1^x dx f(x) = \sum_{n=1}^{\infty} \frac{a_n}{n+1} x^{n+1} \tag{12}$$

Consider for example

$$\sum_{n=1}^{\infty} n x^n \tag{13}$$

This is similar to a geometric series in form.

$$\begin{aligned} \sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \Rightarrow \frac{d}{dx}\left(\sum_{n=0}^{\infty} x^n\right) = \frac{d}{dx}\left(\frac{1}{1-x}\right) \\ \sum_{n=0}^{\infty} n x^{n-1} = \frac{1}{(1-x)^2} \end{aligned} \tag{14}$$

To make this lase line look like our example we just need to multiple by x and cahnge the summation bounds

$$\sum_{n=1}^{\infty} n x^n = \frac{x}{(1-x)^2} \tag{15}$$

As another example this time consider

$$\sum_{n=1}^{\infty} \frac{x^n}{n} \tag{16}$$

This expression again looks similar to a geometric series. Consider what happens if we take an integral of a geometric series

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \Rightarrow \int dx \frac{1}{1-x} = \tag{17}$$

If we divide by x we reproduce the problem.

$$\begin{aligned} \sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \Rightarrow \int dx \frac{1}{1-x} \Rightarrow \\ \int dx \left(\frac{1}{1-x}\right)\left(\frac{1}{x}\right) = \int dx \sum_{n=0}^{\infty} x^n \left(\frac{1}{x}\right) = \sum_{n=1}^{\infty} \frac{x^{n+1}}{n}\left(\frac{1}{x}\right) \\ \sum_{n=1}^{\infty} \frac{x^n}{n} = \int dx \left(\frac{1}{1-x}\right)\frac{1}{x} \Rightarrow \ln(1-x) \Rightarrow \\ \sum_{n=1}^{\infty} \frac{x^n}{n} = \ln(1-x) \end{aligned} \tag{18}$$

Another example, we can start using power series, consider a function of x.

$$S(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^2} \tag{19}$$

Where S(1) would be evaluated as

$$S(1) = \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{20}$$

The solution of S(x) is related to the previous problem, consider takng a derivative.

$$\begin{aligned}
S(x) &= \sum_{n=1}^{\infty} \frac{x^n}{n^2} \\
S'(x) &= \sum_{n=1}^{\infty} \frac{x^{n-1}}{n} \\
xS'(x) &= \sum_{n=1}^{\infty} \frac{x^n}{n} \\
xS'(x) &= \ln(1-x) \\
S'(x) &= \int_0^x dx \frac{\ln(1-x)}{x}
\end{aligned} \tag{21}$$

The integral on the last line cannot be evaluated analytically, but we have converted an infinite series to an integral which a nuch simplier problem, and this is a solution.

Methods Of Integration

This is not a specific chapter in the book, we are just going to cover some simple classes of integrals and standard solutions. A common theme for this course, there is no general method for solving integrals, and most integrals cannot be solve in terms of elementary functions.

Integration By Parts

Integration By Parts is a common method for replacing one integral (you cannot solve) for another integral (that you can hopefully solvE). It is useful if your integrand is a product of functions, and one of the functions can be reduced in order by taking a derivative.

$$\int_a^b U(x)dV(x) = U(x)V(x)\Big|_a^b - \int_a^b V(x)dU(x) \tag{22}$$

We do know that any elementary function has a derivative that is also an elementary function, so you could go about making a database for easily solvable problems. Applying IBP then we want to solve for integrals that are the derivative of elementary functions.

As an example consider IBP of function I (containing parameter n).

$$\begin{aligned}
I(n) &= \int_a^b dx x^n d^x \\
&= e^x x^n\Big|_a^b - \int_a^b dx e^x n x^{n-1} \\
&= e^x x^n\Big|_a^b - nI(n-1) \\
&= \cdots \\
&= I(0) = \int_a^b dx e^x = e^x\Big|_a^b
\end{aligned} \tag{23}$$

So for this example we can continue evaluating until we reach the integral of a simple expotential. Therefore any expotential times a polynomial can be evalued using IBP.

If we can evaluate any polynomial times an expotential, consider another example.

$$\int dx x^n \cos(x) \tag{24}$$

We know that we can express cos(x) in terms of expotentials

$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2} \tag{25}$$

So we can really convert this problem into the same form and solve with IBP, let s = ix

$$\int ds x^n e^s \tag{26}$$

Gaussian Integrals

Another well known and useful integral we will want to evaluate is the Gaussian.

$$I = \int_{-\infty}^{\infty} dx e^{-x^2} \tag{27}$$

If the limits are not ∞ than you can get the special function known as the **Error Fucntion**. Basically a special function is a common or useful function that appears but cannot be evaluated using elementary functions, it is useful wso we give it a name. There is a well known trick for evaluating a Gaussian Integral. You instead consider the square of the integral, and convert to polar coordinates to see a nice simplification.

$$\begin{aligned} I &= \int_{-\infty}^{\infty} dx e^{-x^2} \Rightarrow \\ I^2 &= \left(\int_{-\infty}^{\infty} dx e^{-x^2}\right)\left(\int_{-\infty}^{\infty} dy e^{-y^2}\right) \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx dy e^{-x^2-y^2} \end{aligned} \tag{28}$$

We can now switch over to polar coordinates and re-define the integrals

$$\begin{aligned} I^2 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx dy e^{-x^2-y^2} \\ &= \int_0^{2\pi} d\theta \int_0^{\infty} dr e^{0r^2} r \\ &= 2\pi \int_0^{\infty} dr r e^{-r^2} \to [t = r^2] \\ I^2 &= 2\int_0^{\infty} dt e^{-t} = \pi \\ I &= \sqrt{\pi} \end{aligned} \tag{29}$$

Consider now a related example

$$I = \int dx e^x \sin(x) \tag{30}$$

We know that we can rewrite sin(x) as

$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i} \tag{31}$$

If we make the substitution we find integrals of the form

$$\int e^{ax} dx \tag{32}$$

Where a is potentially complex and we can work through the math. However, we can also just use integration by parts to evaluate this integral.

$$I = \int dxe^x \sin(x) = -e^x \cos(x) + \int dxe^x \cos(x) \rightarrow \text{[IBP Again]}$$
$$I = -e^x \cos(x) + e^x \sin)x) - I = I = \frac{-e^x \cos(x) + e^x \sin(x)}{2} \tag{33}$$

Integrals of Rational Functions

We can now consider anpother class of integrals. Take P(x) to be a polynomial of degree n: $P_0 + P_1x + \cdots P_nx^n$, and Q(x) to be a polynomial of degree m $Q_0 + Q_1x + \cdots Q_nx^n$.

$$\int dx \frac{P(x)}{Q(x)} \tag{34}$$

To evaluate we will assume n < m, which is always true because we can simply reduce by dividing by polynomials i.e. if m > n than just divid the polynomials.

It is always possible to find the roots of a polynomial, can be done analytically if degree 4 or less, numerically if higher degree polynomials are involved. SO it is safe to assume the roots exist, we will assume the roots are not degenerate for convenience. This means Q can be written as $Q(x) = (x-x_1) \cdots (x-x_m)$.

$$\frac{P(x)}{Q(x)} = \frac{P(x)}{(x-x_1)(x-x_2)\cdots(x-x_m)} = \frac{A_1}{x-x_1} + \cdots + \frac{A_m}{x-x_m} \tag{35}$$

Where the coefficients A_i can be found throughFor example

$$\frac{1}{(x-a)(x-b)} = \frac{A}{x-a}\frac{B}{x-b} \Rightarrow \frac{A(x-b)+B(x-a)}{(x-a)(x-b)} = 1 \tag{36}$$

Doing some algebra we find

$$A = \frac{1}{b-a}, \quad B = \frac{1}{b-a}, \quad \frac{1}{b-a}\left(\frac{1}{x-a} - \frac{1}{x-b}\right) \tag{37}$$

$\int \frac{A_k}{x-x_k} = A_k \ln(x-x_k)$

If we consider a different probelm with degenerate roots we find a similar result.

$$\frac{1}{(x-a)^2(x-b)} = \frac{A_1x + A_0}{(x-a)^2} + \frac{B}{(x-b)} \tag{38}$$

And go through the process to find our new constants. another example.

$$\frac{1}{(x-a)^2(x-b)^3} = \frac{A_1x + A_0}{(x-a)^2} + \frac{B_2x^2 + B_1x + B_0}{(x-b)^3} \tag{39}$$

And again we need to solve a system of equations to find the constants.

Consider a final strategy for evaluating integrals known as **Parameter Differentation**.

$$I_0(a) = \int_0^\infty dxe^{-ax^2} = \frac{1}{2}\sqrt{\frac{\pi}{4}} \tag{40}$$

$$I_1(a) = \int_0^\infty dxe^{-ax^2}x = \frac{1}{2a} \tag{41}$$

How do we solve $I_2(a)$? Consider a derivative

$$\frac{d}{da}I_0(a) = \int_0^\infty dx(-x^2)e^{-ax^2} \tag{42}$$

$$I_2(a) = \int dxx^2e^{-ax^2} = \frac{1}{4a}\sqrt{\frac{\pi}{a}} \tag{43}$$

$$I_{2n}(a) = \int dx x^{2n} e^{-ax^2} = \frac{1}{4a}\sqrt{\frac{\pi}{a}} \tag{44}$$

$$\frac{d}{da} I_{2n}(a) \Rightarrow_{2n+1} a \tag{45}$$

The above is for even powers, and for odd powers we would apply.

$$\frac{d}{da} I_1(a) \Rightarrow_{2n-1} a \tag{46}$$