Mathematics Methods and Thermodynamics

Mathmatics - Functions, Transformations and Deltas

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September 13, 2017

Class Overview

- Integral Ranges
- Kronecker Delta
- Orthogonality
- Recursion Relations
- Dirac Delta
- Fourier Transform

Review

- Last week we discussed special ODE
- These are useful ODE solved in a general way with special functions
- Some of the more useful functions that come from these special ODEs for chemistry are:
  - Laguerre Polynomial
  - Legendre Polynomial
  - Hermite Polynomial
- Fourier Series is a method of approximating any function into an expansion of trigonometric functions
- Fourier series is different from Fourier transform in that it is discreet while Fourier transform is continuous

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Integral Range

- One of the questions from the previous week asked for you to transform the integral range from $\int_0^3$ to $\int_{-\pi}^{\pi}$
- But how is this actually done?

Integral Range

- First lets consider what happens when you change the coordinate via $x = u + 1$

$$\int_{x=0}^{x=10} F(x) = \int_{u+1=0}^{u+1=10} F(u+1)$$

$$\int_{u=-1}^{u=9} F(u+1)$$

Integral Range

- When you write the integrals in this form $\int_x$ it becomes much easier to see how it transforms more generally if you have some function that transform x to u lets call this $u(x)$ then the integral range transform as

$$\int_a^b F(x)\ dx = \int_{u(a)}^{u(b)} F(u(x))\ du$$

Integral Range

- In the case where we are trying to transform to known limits, for example transforming to $\int_c^d$, we need to find an appropriate function that will convert x to u $(X(u))$ if we lay out the question as follows we can see how we might find such a function

$$\int_{x=a}^{x=b} F(x)\ dx = \int_{X(c)=a}^{X(d)=b} F(X(u))\ du$$

Integral Range

- For this unknown function we have two known points

$$X(c) = a$$
$$X(d) = b$$

- So for this function when we put in the new lower limit we get the old lower limit and similarly for the upper limit

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- Ideally it would have 2 unknowns (that can be solved with our two knowns) and not warp our function i.e. linear

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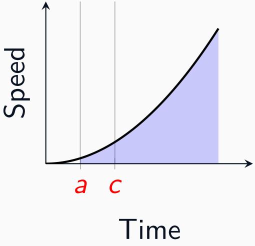
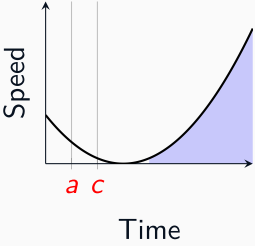
Integral Range

- If for a moment we ignore our upper limit you should know how to translate a function by some about along the axis Δx

$$F(x) \to F(x - \Delta x)$$



$f(x)$



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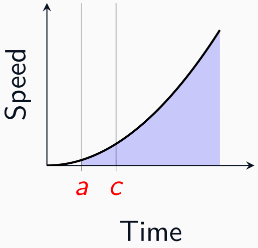
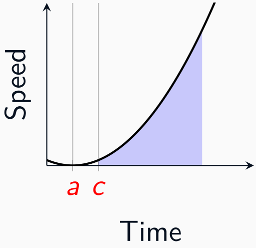


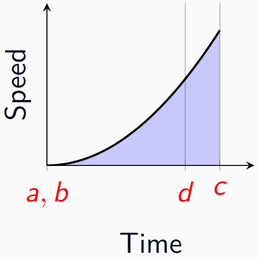
$f\,(x)$



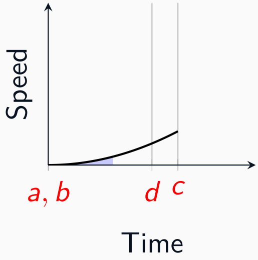
$f\,(x - (b - a))$

Integral Range

- To also set the upper limit we must scale the coordinate



$f\left(x\right)$



$f\left(\frac{1}{2}x\right)$

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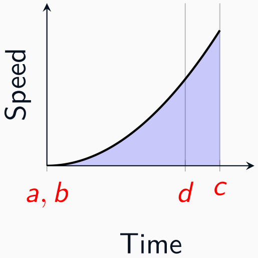
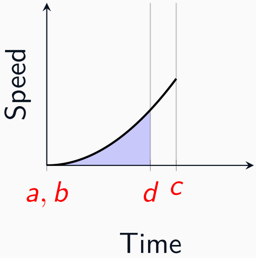


$f(x)$



$$f\left(\frac{d-c}{b-a}x\right)$$

Integral Range

- The general form of $X(u)$ must therefore contain an addition and a multiplication.
- Generally we can write this as

$$X(u) = Au + B$$

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Integral Range

- Now that we have a general form we can go about using our knowns to solve our unknowns

$$X(c) = Au + B \qquad = a$$
$$X(d) = Au + B \qquad = b$$

- Solving first equation for A

$$A = \frac{a - B}{c}$$

- Substituting into the second equation then solving for B

$$B = \frac{bc - ad}{c - d}$$

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Integral Range

- Finally substituting B into A

$$A = \frac{a - b}{c - d}$$

Integral Range

- One last thing to remember is that since we are applying a coordinate transformation then we need to use the same rules we do for integration by substitution. As in w need to apply the change in size of an infinitely small chunk of dx to du

$$\int_a^b F(x)\ dx = \int_c^d F(Au+B)\,\frac{dAu+B}{du}\,du$$

Where

$$A = \frac{a-b}{c-d}$$

$$B = \frac{bc-ad}{c-d}$$

$$\frac{dAu+B}{du} = A = \frac{a-b}{c-d}$$

Kronecker Delta

- Last week we came across the Kronecker Delta
- This is given the definition

$$\delta_{n,m} = \begin{cases} 1 & \text{If } n = m \\ 0 & \text{else} \end{cases}$$

- It is the mathematical form of an on off switch and is often used in orthogonality relationships
- The Kronecker Delta only works with integers. Meaning it is discrete

Kronecker Delta

- How would these Kronecker Delta´s behave?

$$\sum_{i=0}^{5} i\delta_{i,3} = 3$$

$$\sum_{i=0}^{5} i\delta_{i,7} = 0$$

$$\sum_{i=0}^{5}\sum_{j=0}^{5} jx^i\delta_{i,3} = \sum_{j=0}^{5} jx^3$$

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Orthogonality

- A lot of the polynomials from ODEs have a property called orthogonality
- This property can be useful to avoid integration under certain conditions
- The general form for orthogonality for some indexed function like a ODE function $F_n(x)$ is

$$\int_a^b G(x) F_n(x) F_m(x)\, dx = k\delta_{n,m}$$

- Where $G(x)$ is some function (sometimes called the weighting function) that makes $F_n(x)$ orthogonal. This is sometimes just $G(x) = 1$. It depends upon what $F_n(x)$ is. For example with Laguerres it is $G(x) = \mathrm{e}^{-x}$.

ORTHOGONALITY

- Here are the orthogonality relationships for the three ODEs we mentioned last week

  Generalised Laguerre

$$\int_0^\infty x^\alpha e^{-x} L_n^\alpha(x)\, L_m^\alpha(x)\, dx = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{n,m}$$

  Laguerre

$$\int_0^\infty e^{-x} L_n L_m = \delta_{n,m}$$

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Legendre

$$\int_{-1}^{1} P_n(x)\, P_m(x)\; dx = \frac{2}{2n+1}\delta_{n,m}$$

Hermite

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2} H_n(x)\, H_m(x)\; dx = \sqrt{\pi}2^n n!\delta_{n,m}$$

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Using Orthogonality

- Orthogonality can be quite useful consider the following

$$\int_0^\infty \sum_{i=0}^{10} \sum_{j=0}^{10} C_{i,j} \mathrm{e}^{-x} L_i(x) L_j(x)\, dx = \sum_{i=0}^{10} C_{i,i}$$

- This sort of expression can turn up quite often in places where we use approximate functions

Recursion Relations

- In addition to orthogonality these polynomials also typically have recursion relations
- These are relations that link a polynomial of one degree to another degree
- For Example with Laguerre polynomials we have the recursion relations

$$xL_n(x) = -(n+1)L_{n+1}(x) + (2n+1)L_n(x) - nL_{n-1}(x)$$
$$xL_n'(x) = nL_n(x) - nL_{n-1}(x)$$
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$$

The Dirac Delta

- We saw that the Kronecker delta is discrete and is a picking function for a discrete sum

$$\sum_{i=0}^{20} C_i F_i(x)\, \delta_{i,3} = C_3 F_3(x)$$

- What about the continuous case?
- What is a continuous sum?
- An integral is the continuous alternative of a discrete sum

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The Dirac Delta

- The the Dirac delta is the continuous version of the Kronecker delta

$$\int_{-10}^{10} F(x)\delta(x)\, dx = F(0)$$

- For the Dirac delta $\delta(G(x))$ the function is picked where the value from the function is equal to zero
- This means it could "pick" more that one value if there is more than one root for $G(x)$, in this case the answer is the sum of the values

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The Dirac Delta

- The Dirac delta has the definition that it is 0 everywhere except at the origin
- At the origin its value is *undefined*
- However at the origin its *area* is defined as 1
- As a result the Dirac delta has no meaning in contexts without an area so without an integral the results are *undefined*

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The Dirac Delta

- Given this information have a go at the bonus question from a previous worksheet

$$\int_0^2 \left(\sin\,(x)\,x^3 \mathrm{e}^{-x} + \ln\,(x)\,x^2\right)\delta(x-1)\,dx$$

$$\left(\sin\,(1)\,1^3 \mathrm{e}^{-1} + \ln\,(1)\,1^2\right)$$

$$\left(\sin\,(1)\,\mathrm{e}^{-1} + \ln\,(1)\right)$$

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Fourier Series

- Last week we discussed the real coefficients Fourier series
- This series allows us to approximate a function as a series of sinusoid functions

$$f\left(x\right) = f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(nx\right) + \sum_{n=1}^{\infty} b_n \sin\left(nx\right)$$

- Where we can calculate the coefficients as the following

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\,dx$$
$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos\left(nx\right)\,dx$$
$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin\left(nx\right)\,dx$$

Fourier Series

- We can extend Fourier series to complex coefficients using the relationship

$$e^{\pm ix} = \cos(x) \pm i\sin(x)$$

Which is Euler's identity

- We extend Fourier series to the complex coefficient domain by using the following function

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{-inx}$$

Complex Numbers

- Complex numbers are an integral part to the Fourier transform
- We can describe a complex number in two parts

$$z = x + iy$$

- Where x is the real part, y is the imaginary part and i is the imaginary number $i = \sqrt{-1}$. This is square or standard notation

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Complex Numbers

- Addition is done by adding each part

$$z_1 + z_2 = (x_1 + x_2) + i\,(y_1 + y_2)$$

- Multiplication is done like bracket expansion

$$z_1 z_2 = (x_1 + iy_1)\,(x_2 + iy_2)$$

$$z_1 z_2 = x_1 x_2 + ix_1 y_2 + iy_1 x_2 + i^2 y_1 y_2$$

$$z_1 z_2 = x_1 x_2 + ix_1 y_2 + iy_1 x_2 - y_1 y_2$$

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Complex Numbers

- Division is best done using polar notation
- In polar notation a complex number is

$$z = |z| \, e^{i\theta}$$

$$|z| = \sqrt{zz^*} = \sqrt{(x + iy)(x - iy)}$$

$$|z| = \sqrt{zz^*} = \sqrt{x^1 + y^1}$$

$$x = |z| \cos(theta)$$

$$y = |z| \sin(theta)$$

$$\theta = \begin{cases} \text{arctan} \frac{x}{y} & x \geq 0 \\ \text{arctan} \frac{x}{y} + 180^\circ & x < 0 \end{cases}$$

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$$z_1 z_2 = |z_1|\,|z_2|\,\mathrm{e}^{i(\theta_1+\theta_2)}$$

- Division in polar notation is

$$\frac{z_1}{z_2} = |z_1|\,|z_2|\,\mathrm{e}^{i(\theta_1-\theta_2)}$$

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Fourier Series

- For the Fourier series with complex coefficient

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{inx}$$

- To calculate the coefficients we evaluate the integral multiplied by the complex term, e^{-imx}

$$\int_{-\pi}^{\pi} f(x) e^{-imx}\, dx = \int_{-\pi}^{\pi} \left(\sum_{n=-\infty}^{\infty} A_n e^{inx} \right) e^{-imx}\, dx$$

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Fourier Series

$$\sum_{n=-\infty}^{\infty} A_n \int_{-\pi}^{\pi} \mathrm{e}^{i(n-m)x}\,dx$$

$$\sum_{n=-\infty}^{\infty} A_n \int_{-\pi}^{\pi} \left(\cos\left(\left(n-m\right)x\right) + i\sin\left(\left(n-m\right)x\right)\right)\,dx$$

$$\sum_{m=-\infty}^{\infty} A_n 2\pi\delta_{n,m} = 2\pi A_m$$

Fourier Series

- Therefore

$$\int_{-\pi}^{\pi} f(x)\,\mathrm{e}^{-inx}\,dx = 2\pi A_n$$

$$A_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\,\mathrm{e}^{-inx}\,dx$$

Fourier Series

- The Fourier series we have discussed is for a function in the range $-\pi$ to π
- If we have a periodic function that repeats around the origin with a period of L we can represent it via a coordinate transform as:

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{i\left(\frac{2\pi nx}{L}\right)}$$

$$A_n = \frac{1}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} f(x)\, e^{i\left(\frac{2\pi nx}{L}\right)}\, dx$$

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- Now for the *Fourier Transform*
- This is an incredible useful transformation that breaks down a wave (or any well behaved function) into all of its component sinusoidal functions
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Fourier Transform

- From the complex Fourier Series

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{i\left(\frac{2\pi nx}{L}\right)}$$

- We extend to the Fourier transform which works for non periodic (as in not discrete, but instead continuous) by extending $L \to \infty$
- When we extend to infinity we replace the discrete parts continuous parts:
  - $A_n \to F(k)$
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- The Fourier transform is therefore

$$f(x) = \mathcal{F}^{-1}[F(k)] = \int_{-\infty}^{\infty} F(k)\, \mathrm{e}^{2\pi ikx}\, dk$$

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$$F(k) = \mathcal{F}[f(x)] = \int_{-\infty}^{\infty} f(x)\, \mathrm{e}^{-2\pi ikx}\, dx$$

- The later equation is the Fourier transform $\mathcal{F}[f(x)]$, while the former is the inverse $\mathcal{F}^{-1}[F(k)]$

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- We usually represent the Fourier transform in the frequency ν and time domains t

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- In terms of ODEs the most important relation is that Fourier transform of a derivative is given by

$$\mathcal{F}\left[\frac{d^n f(t)}{dt^n}\right] = (i2\pi\nu)^n F(\nu)$$

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- The Fourier transform is a linear transformation

$$\mathcal{F}[f(t)+g(t)] = \mathcal{F}[f(t)] = \mathcal{F}[g(t)]$$

- We can use these two properties on the following ODE

$$y''(t) - y(t) = -g(t)$$

- First take the Fourier transform of the equation

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- We can now solve for Y in the frequency domain easier than in the time domain

$$Y(\nu) = \frac{G(\nu)}{1 + 4\pi^2\nu^2}$$

- Then apply the inverse transform

$$y(t) = \mathcal{F}^{-1}[Y(\nu)] = \mathcal{F}^{-1}\left[\frac{G(\nu)}{1 + 4\pi^2\nu^2}\right]$$

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$$\mathcal{F}[g(t)h(t)] = G(\nu) * H(\nu)$$

$a * b$ is a convolution no multiplication

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- We can use the Fourier transform to solve ODE under certain conditions

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Summary

- We covered how integral ranges transform with the coordinates and how you can obtain a specific integral range
- The Kronecker delta, which is a discrete picking function
- The orthogonality and recursion relations of special functions
- The Dirac delta which is a continuous picking function
- The Fourier transform and its application in ODEs