Mathematical Methods for the Physical Sciences. Lecture 1.

1 Operators

Operators: We start treating *operators* as just a fancy name for a rule (a recipe, a 'black box') that takes a function and produces another function. The rule can be as simple as a multiplication by a constant, or very complicated (the sky is the limit). Few examples of operators:

Operator	'Input'		'Output'
Multiplication by a constant **c**:	$f(x) = x^2$	$\longrightarrow$	$g(x) = cx^2$
	$f(x) = \sin(x)$	$\longrightarrow$	$g(x) = c\sin(x)$
	$f(x) = \sqrt{x}$	$\longrightarrow$	$g(x) = c\sqrt{x}$
Multiplication by the independent variable **x**:	$f(x) = x^2$	$\longrightarrow$	$g(x) = x^3$
	$f(x) = \sin(x)$	$\longrightarrow$	$g(x) = x\sin(x)$
	$f(x) = \sqrt{x}$	$\longrightarrow$	$g(x) = x\sqrt{x}$
Differentiation $\frac{\mathrm{d}}{\mathrm{d}x}$:	$f(x) = x^2$	$\longrightarrow$	$g(x) = 2x$
	$f(x) = \sin(x)$	$\longrightarrow$	$g(x) = \cos(x)$
	$f(x) = \sqrt{x}$	$\longrightarrow$	$g(x) = \frac{1}{2\sqrt{x}}$

Powers of operators: Let's use the notations

$$\hat{D} \equiv \frac{\mathrm{d}}{\mathrm{d}x}, \quad \hat{D}f(x) = \frac{\mathrm{d}f}{\mathrm{d}x} \equiv f'(x). \tag{1}$$

What is $\hat{D}^2$, $\hat{D}^3$, $\ldots \hat{D}^n$?

$$\hat{D}^2 f(x) = \hat{D}\hat{D}f(x) = \hat{D}\left(\hat{D}f(x)\right) = \hat{D}f'(x) = f''(x) = \frac{\mathrm{d}^2 f}{\mathrm{d}x^2}, \tag{2}$$

i.e.

$$\hat{D}^2 \equiv \frac{\mathrm{d}^2}{\mathrm{d}x^2}. \tag{3}$$

$$\hat{D}^3 f(x) = \hat{D}\hat{D}^2 f(x) = \hat{D}\left(\hat{D}^2 f(x)\right) = \hat{D}f''(x) = f'''(x) = \frac{\mathrm{d}^3 f}{\mathrm{d}x^3}, \tag{4}$$

i.e.

$$\hat{D}^3 \equiv \frac{\mathrm{d}^3}{\mathrm{d}x^3}. \tag{5}$$

In general,

$$\hat{D}^n f(x) = f^{(n)}(x) = \frac{\mathrm{d}^{\mathrm{n}} f}{\mathrm{d}x^n}, \tag{6}$$

i.e.

$$\hat{D}^n \equiv \frac{\mathrm{d}^{\mathrm{n}}}{\mathrm{d}x^n}. \tag{7}$$

We consider n for the time being as a non-negative integer.

Operator polinomials: Let $p(x)$ be a quadratic polynomial

$$p(x) = a_2 x^2 + a_1 x + a_0. \tag{8}$$

What is $p(\hat{D})$?

$$p(\hat{D}) = a_2 \hat{D}^2 + a_1 \hat{D}^1 + a_0 \hat{D}^0. \tag{9}$$

Since we know what is a power of operator,

$$p(\hat{D}) = a_2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + a_1 \frac{\mathrm{d}}{\mathrm{d}x} + a_0, \tag{10}$$

We can 'construct' the differential operator $p(\hat{D})$.

Operator functions: Lef $f(x)$ be a function represented by the following Taylor series:

$$f(x) = \sum_n a_n x^n. \tag{11}$$

What is $f(\hat{D})$? Using the approach we used for polynomials,

$$f(\hat{D}) = \sum_n a_n \hat{D}^n = \Sigma_n a_n \frac{\mathrm{d}^{\mathrm{n}}}{\mathrm{d}x^n} \tag{12}$$

Operator of translation: Let's consider the operator $\hat{T}_a$:

$$\hat{T}_a \equiv e^{a\hat{D}}. \tag{13}$$

What is $\hat{T}_a f(x)$? Recall that the Taylor series for e^a is as following:

$$e^a = 1 + a + \frac{1}{2!}a^2 + \frac{1}{3!}a^3 + \ldots \frac{1}{n!}a^n + \ldots = \sum_{n=0}^{\infty} \frac{1}{n!}a^n. \tag{14}$$

and the Taylor series for $f(x+a)$ is

$$f(x+a) = f(x) + a\frac{\mathrm{d}f}{\mathrm{d}x} + \frac{1}{2!}a^2 \frac{\mathrm{d}^2\mathrm{f}}{\mathrm{d}x^2} + \frac{1}{3!}a^3 \frac{\mathrm{d}^3\mathrm{f}}{\mathrm{d}x^3} + \ldots \frac{1}{n!}a^n \frac{\mathrm{d}^{\mathrm{n}}\mathrm{f}}{\mathrm{d}x^n} + \ldots \tag{15}$$

$$f(x+a) = \sum_{n=0}^{\infty} \frac{1}{n!} a^n \frac{\mathrm{d^n f}}{\mathrm{d}x^n} = \sum_{n=0}^{\infty} \frac{1}{n!} a^n \hat{D}^n f(x) \tag{16}$$

From the definition of an operator function above,

$$\hat{T}_a f(x) = e^{a\hat{D}} f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} a^n \hat{D}^n f(x) \tag{17}$$

Comparing Eqs. (16) and (17),

$$\hat{T}_a f(x) = f(x+a). \tag{18}$$

2 Summation of series. Euler-Maclaurin formula.

Series: Consider the following sum.

$$S = \sum_{n=N_0}^{N_1} f(n) = f(N_0) + f(N_0+1) + \ldots + f(N_1-1) + f(N_1), \tag{19}$$

where $f(n)$ is an arbitrary function $f(x)$ and n is an integer summation index.

A particular example of series Eq. (19) that we will keep in mind is

$$S = \sum_{n=2}^{\infty} \frac{1}{n\log(n)^2}, \quad f(x) = \frac{1}{n\log(n)^2}. \tag{20}$$

S in Eq. (19) can be calculated exactly in analytic form only in exceptional cases. Our goal is to find a usable approximate analytic form for the sum Eq. (19).

Using operator of translation: Each term in the sum Eq. (19) can be rewritten in the following form:

$$f(N_0+n) = \hat{T}_1 f(N_0+n-1) = \hat{T}_1^2 f(N_0+n-2) = \ldots = \hat{T}_1^n f(N_0) \tag{21}$$

The whole sum Eq. (19) can therefore be rewritten as

$$S = f(N_0) + \hat{T}_1 f(N_0) + \hat{T}_1^2 f(N_0) + \ldots = \sum_{n=N_0}^{N_1} \hat{T}_1^n f(N_0) = \left(\sum_{n=N_0}^{N_1} \hat{T}_1^n\right) f(0). \tag{22}$$

The sum in Eq. (22) is a geometric series, thus

$$\begin{aligned} S &= \frac{\hat{T}_1^{N_0} - \hat{T}_1^{N_1+1}}{1-\hat{T}_1} f(0) = \frac{1}{1-\hat{T}_1} f(N_0) - \frac{1}{1-\hat{T}_1} f(N_1+1) && (23) \\ &= s(N_0) - s(N_1+1) && (24) \end{aligned}$$

Lets consider the first term in Eq. (24):

$$s(N_0) = \frac{1}{1-\hat{T}_1} f(N_0) = \left(-\frac{1}{\hat{D}} + \frac{1}{2} - \frac{\hat{D}}{12} + \frac{\hat{D}^3}{720} - \frac{\hat{D}^5}{30240} + \ldots\right) f(N_0). \tag{25}$$

Negative powers of the differential operator

$$\frac{1}{\hat{D}}g(x) = h(x). \tag{26}$$

Applying operator $\hat{D}$ to both sides of Eq. (26), we obtain:

$$g(x) = \hat{D}h(x), \quad \text{i.e.} \quad \frac{\mathrm{d}h(x)}{\mathrm{d}x} = g(x). \tag{27}$$

Integrating Eq. (27), we get

$$h(x) = \int g(x)\mathrm{d}x. \tag{28}$$

Therefore,

$$\frac{1}{\hat{D}}g(x) = \int g(x)\mathrm{d}x, \quad \frac{1}{\hat{D}} \equiv \int, \tag{29}$$

which make sence since the operation inverse to diffrentiation is indeed integration.

Substituting Eq. (29) into Eq. (25), obtain:

$$\begin{aligned} s(N_0) &= -\int_{\infty}^{N_0} f(x)\mathrm{d}x + \frac{1}{2}f(N_0) - \frac{1}{12}f'(N_0) + \frac{1}{720}f'''(N_0) - \ldots \\ &= \int_{N_0}^{\infty} f(x)\mathrm{d}x + \frac{1}{2}f(N_0) - \frac{1}{12}f'(N_0) + \frac{1}{720}f'''(N_0) - \ldots \end{aligned} \tag{30}$$

Combining Eq. (19), (24), and (30),

$$\begin{aligned} \sum_{n=N_0}^{N_1} f(n) &= s(N_0) - s(N_1+1) \\ &= \int_{N_0}^{N_1+1} f(x)\mathrm{d}x + \frac{1}{2}\left(f(N_0) - f(N_1+1)\right) - \frac{1}{12}\left(f'(N_0) - f'(N_1+1)\right) \\ &\quad + \frac{1}{720}\left(f'''(N_0) - f'''(N_1+1)\right) + \ldots \end{aligned} \tag{31}$$

To make the expression Eq. (31) more symmetric let's add $f(N_1+1)$ to both sides of the equation:

$$\begin{aligned} \sum_{n=N_0}^{N_1+1} f(n) &= \int_{N_0}^{N_1+1} f(x)\mathrm{d}x + \frac{1}{2}\left(f(N_0) + f(N_1+1)\right) - \frac{1}{12}\left(f'(N_0) - f'(N_1+1)\right) \\ &\quad + \frac{1}{720}\left(f'''(N_0) - f'''(N_1+1)\right) + \ldots \end{aligned} \tag{32}$$

Finally, renaming $N_1 + 1 \to N_1$,

$$\begin{aligned} \sum_{n=N_0}^{N_1} f(n) &= \int_{N_0}^{N_1} f(x)\mathrm{d}x + \frac{1}{2}\left(f(N_0) + f(N_1)\right) - \frac{1}{12}\left(f'(N_0) - f'(N_1)\right) \\ &\quad + \frac{1}{720}\left(f'''(N_0) - f'''(N_1)\right) + \ldots \end{aligned} \tag{33}$$

Consistency check To have some trust in Eq. (33), let's consider few simple cases:

- $N_0 = N_1$: in this case the sum on the left reduces to one term - $f(N_0)$; the integral is equal to zero; $\frac{1}{2}\left(f(N_0) + f(N_1)\right) = f(N_0)$; all terms on the right containing derivatives are zero. Eq. (33) reduces to $f(N_0) = f(N_0)$ which is correct.
- $f(x) = 1$: in this case the sum on the left is equal to $N_1 - N_0 + 1$; the integral on the right is $N_1 - N_0$; $\frac{1}{2}\left(f(N_0) + f(N_1)\right) = 1$; all terms on the right containing derivatives are zero. Eq. (33) reduces to $N_1 - N_0 + 1 = N_1 - N_0 + 1$ which is correct.
- arithmetic progression — $f(x) = x$, $N_0 = 1$, $N_1 = N$. $\sum_{n=1}^{N} n \equiv \frac{1}{2}N(N+1)$: the integral on the right $\int_1^N x\mathrm{d}x = \frac{1}{2}(N^2 - 1)$; $\frac{1}{2}\left(f(1) + f(N)\right) = \frac{1}{2}(1 + N)$; the contribution of all terms containing the difference of derivatives is 0; therefore the expression on the right is $\frac{1}{2}(N^2 - 1) + \frac{1}{2}\left(1 + N\right) = \frac{1}{2}N(N+1)$ which is the correct answer.
- the sum of squares — $f(x) = x^2$, $N_0 = 1$. $\sum_{n=1}^{N} n^2 \equiv \frac{1}{6}N(N+1)(2N+1)$: the integral on the right $\int_1^N x^2\mathrm{d}x = \frac{1}{3}(N^3 - 1)$; $\frac{1}{2}\left(f(1) + f(N)\right) = \frac{1}{2}(1 + N^2)$; the term containing the first derivatives $\frac{1}{12}\left(f'(N) - f'(1)\right) = \frac{1}{6}(N-1)$. Collecting allterms on the right arrive to the following expression $\frac{1}{6}\left(2N^3 - 2 + 3N^2 + 3 + N - 1\right) = \frac{1}{6}N(N+1)(2N+N)$ which is the correct answer.