THE APPLICATIONS OF INFINITE SERIES TO THE PHYSICAL AND LIFE SCIENCES

An Honors Thesis (ID 499)

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BACKGROUND AND DEFINITIONS

In many mathematical endeavors in pure and applied mathematics, it often happens that a result cannot be directly obtained as in $3 + X = 5$. When this situation occurs, one tries to calculate the result with a sequence of approximations. For example, in calculating the $\sqrt{2}$ one might first estimate this value to be 1. A better approximation would be 1.4, then 1.41. This kind of work would eventually lead to the following sequence of numbers:

$$1, 1.4, 1.41, 1.414, \ldots$$

Sequences, however, are not as important to the mathematician as the series they generate.

Definition 1: If A is a function whose domain is the set of positive integers, then A is called an Infinite Sequence.

Definition 2: If $\{a_n\} = a_1, a_2, \ldots, a_n, \ldots$ is an infinite sequence, the sequence $\{s_n\}$ defined by

$$s_n = a_1 + a_2 + \ldots + a_n \quad n = 1, 2, \ldots$$

is called an infinite series and is symbolized by $\sum_{i=1}^{\infty} a_i$. The numbers $a_1, a_2, \ldots, a_n$ are called terms, and $s_1, s_2, \ldots$ are called the partial sums of the series.

An infinite series will be of very little help in solving a problem if it does not converge to a limit point, L. To determine whether or not a series converges we must look at its sequence of partial sums, $\{s_n\}$.

s_n is formed as follows:

$s_1 = a_1;\ s_2 = a_1 + a_2;\ \ldots;\ s_n = a_1 + a_2 + \ldots + a_n$

Definition 3: If $\{s_n\}$ is convergent and has the limit S, the infinite series $\sum_{n=1}^{\infty} a_n$ is called convergent, and S is called the sum of the series.(for more details see [5].)

A necessary condition for a series, $\sum_{n=1}^{\infty} a_n$, to converge is that the $\lim_{n\to\infty} a_n = 0$. If this does not occur, the series is said to be divergent. Merely satisfying this condition does not necessarily imply the series will converge. For example, the Harmonic series, 1, 1/2, 1/3, . . ., has the limit point S = 0, yet is a known divergent series.

There are many tests available to determine the behavior of a series. For example, given a series, $\sum_{n=1}^{\infty} a_n$, if there exists a known convergent series $\sum_{n=1}^{\infty} c_n$, such that $0 \leq a_n \leq c_n$, for all n, then by comparison, $\sum_{n=1}^{\infty} a_n$ is also convergent. Two other tests for series convergence are the integral test and the ratio text.

Once we have a convergent series, $\sum_{n=1}^{\infty} a_n$, we can add or subtract a finite number of terms, and the new series, $\sum_{n=1}^{\infty} a_n^*$, will also be convergent. Also, given a convergent series, $\sum_{n=1}^{\infty} a_n$, multiplication by a non-zero, real constant will not affect its convergence pattern.

BASIC USES OF SERIES

Infinite series are used for two basic reasons: 1) they can be useful in approximating an unknown value; and 2) they can be used to transform an equation into a more workable form.

The best approximation to a given function is provided by the series originally developed in the nineteenth century by Tchebychev. Tchebychev's series has the following form:

$$f(x) = a_o + a_1T_1(x) + a_2T_2(x) + \ldots$$

for $|x| < 1$, and where $T_r(x) = \cos(r\cos^{-1}x)$, $r = 1, 2, \ldots$ The first three polynomials are:

$$T_1(x) = \cos(\cos^{-1}x) = x$$

$$T_2(x) = \cos(2\cos^{-1}x) = 2\cos^2(\cos^{-1}x) - 1$$

$$T_3(x) = \cos(3\cos^{-1}x) = 4x^3 - 3x$$

Note that the function $T_r(x)$ is odd if r is odd and even if r is even. The terms of the series also have the property of orthogonality. This implies that the terms are independent of each other.

To find the coefficients, a_i, we take successive derivatives of f(x) and solve the resulting system of equations at the point x = 0. This method is similar to that used by Fourier.

With the growing use of computers, Tchebychev's series are especially useful in estimating functions. They enable a function to be stored with a minimum number of coefficients for a given degree of accuracy.

Sometimes, however, a series will need to be adapted into a more suitable form before it can be used to evaluate a problem. This can be accomplished through a series transformation from one convergent series to another.

To accomplish a series transformation we take an arbitrary series $\sum_{n=0}^{\infty} a_n$ and introduce a matrix $T = \{t_{mn}\}$ and under the assumption of convergence of the series that appear, set

$$\sum_{n=0}^{\infty} t_{mn} a_n = \alpha_m, \qquad m = 0, 1, 2, \ldots$$

We then say that the series $\sum_{n=0}^{\infty} a_n$ has been transformed into the series $\sum_{n=0}^{\infty} \alpha_n$ by means of the transformation T. From this we get the following theorem:

Let $T = \{t_{mn}\}$ be a matrix such that

$\sum_{p=0}^{M} t_{pn} = T_{mn}$ satisfies the following

(1) There exists an $M > 0$ such that $\sum_{i=0}^{\infty} |T_{mi} - T_{m(i+1)}| \leq M$ for all $m = 0, 1, 2, \ldots$

(2) $\lim_{m \to \infty} T_{mn} = \sum_{n=0}^{\infty} t_{mn} = 1$ for every $n = 0, 1, 2, \ldots$

Then, if $\sum_{n=0}^{\infty} a_n$, with partial sums s_n, is an arbitrary convergent series,

$\alpha_m = \sum_n t_{mn} a_n$ for all m = 0, 1, 2,... exists and $\sum_{n=0}^{\infty} \alpha_n$ is a convergent series such that $\sum_{n=0}^{\infty} \alpha_n = \sum_{n=0}^{\infty} a_n$ (for a proof of this theorem, see [4, p. 141].)

Series transformations provide an especially effective means for evaluating series. For example, if $\sum_{n=0}^{\infty} a_n$ is a convergent series, the $\sum_{n=0}^{\infty} \alpha_n$ where $\alpha_n = 1/2^{n+1}\left[\binom{n}{0}a_0 + \binom{n}{1}a_1 + \dots + \binom{n}{n}a_n\right]$ is also convergent and has the same sum as $\sum_{n=0}^{\infty} a_n$. This is known as an Eulerian transformation.

One application of the Eulerian transformation is to obtain a better representation of a convergent series. For example, let

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

Calculating the first four terms we get the following:

$$1 - 1/2 + 1/3 - 1/4 = .5833$$

By applying Euler's transformation we get

$$\ln 2 = 1/1\cdot 2^1 + 1/2\cdot 2^2 + \dots$$

Calculating the first four terms here we have ln 2 = .6823. Note that the value of ln 2 is approximately .6931. Thus, we can see that by applying Euler's transformation to the series we obtained a better representation of ln 2, for it will converge more quickly to the actual value.

Eulerian transformations can also be used to change a divergent series into a convergent series. For instance, if we take the divergent series:

$$\sum_{n=0}^{\infty} a_n = \sum_{n=0}^{\infty} (-1)^n$$

By applying Euler's transformation we get a new series

$$1/2 + 0 + 0 + 0 + \dots = \sum_{n=0}^{\infty} \alpha_n$$

Now $\sum_{n=0}^{\infty} \alpha_n$ is a convergent series and its sum is 1/2.

If we want to evaluate a series $\sum_{n=0}^{\infty} a_n$, sometimes we are able to choose a convergent series $\sum_{n=0}^{\infty} c_n = C$ such that the terms c_n are asymptotically proportional to the a_n. That is,

$$\frac{a_n}{c_n} \to \gamma \neq 0$$

This produces the following series:

$$S = \sum_{n=1}^{\infty} a_n = \gamma C + \sum_{n=0}^{\infty} \left(1 - \gamma \frac{c_n}{a_n}\right) \cdot a_n$$

The form of the series on the right is called Kummer's transformation. The beauty of this transformation is that the new series converges much more rapidly, because

$$\left(1 - \gamma \frac{c_n}{a_n}\right) \to 0$$

Thus, if we take the series $\sum_{n=1}^{\infty} 1/n^2$ and associate with it the convergent series $\sum_{n=1}^{\infty} 1/n(n + 1) = 1$, we get

$$S = 1 + \sum_{n=1}^{\infty} 1/n^2(n + 1)$$

Furthermore, if we associate the new series with the series $\sum_{n=1}^{\infty} 1/n(n+1)(n+2) = 1/4$, we find that

$$S = 1 + 1/4 + 2\sum_{n=1}^{\infty} 1/n^2(n+1)(n+2)$$

This process continues until the desired level of precision is obtained.

Transformations like Kummer's and Euler's are especially useful for research conducted in conjunction with a computer. They allow for faster and more accurate evaluation of otherwise slowly converging series.

POWER SERIES SOLUTIONS

Often in scientific problems we encounter series of the form $\sum_{n=0}^{\infty} a_n x^n$ where x is unrestricted within a determined interval. The series $\sum_{n=0}^{\infty} a_n(x - x_0)$ is called a power series, and if the series is convergent for $|x - x_0| < r$, then r is called the radius of convergence.

Power series are usually employed if a summary of a set of accurate experimental measurements y at various x-values is required. For example, if no theoretical relation between x and y is known and x and y form a smooth curve, when plotted, then infinite series may be used to determine the equation of the curve.

The simple power series method is used to describe the variations of thermal properties such as specific heat or latent heat with temperature. That is, let

$$Q = Q_0 + Q_1 t + Q_2 t^2 + \ldots ,$$

where t = temperature, and Q_0 = the value of Q at t = 0. We can evaluate this series by direct substitution or repeated graphical differentiation, thereby determining valuable information about the thermal properties in question.

On the whole, the simple power series method is adequate for most ideal cases. Sometimes, however, when a relationship is known for two variables in the ideal case, more complex series can be used to express the results for the non-ideal case.

The Claussius-Clapeyron equation is a differential equation which expresses the rate of change of the vapor pressure of a pure liquid with absolute temperature. It was deduced from thermodynamic theory. The equation is as follows:

(1) $$\frac{dp}{dT} = \frac{Qp}{RT^2}$$

Where p = vapor pressure at absolute temperature T, R = a gas constant, and Q = latent heat of evaporation of the liquid.

The ideal case expresses Q as independent of temperature, but over a wide range of temperatures this is inaccurate. More precisely, Q can be expressed as a power series in T:

(2) $$Q = Q_0 + AT + BT^2 + CT^3.$$

(Note that for our purposes a cubic term provides sufficient accuracy. Theoretically, it may be extended infinitely.) Substituting this value of Q into equation (1) gives:

(3) $$\frac{dp}{p} = \frac{(Q_0 + AT + BT^2 + CT^2)dT}{RT^2}$$

Hence, by integrating both sides of eq. (3) we get

$$\ln p = \frac{-Q_0}{RT} + \frac{A}{R}\ln T + \frac{B}{R}T + \frac{C}{2R}T^2 + C_0$$

where C_0 is the constant of integration.

This provides us with a means for evaluating p over a wide range of values of T. (For more information on the applications of the Claussius Clapeyron equation, see [3].)

Another biological application of power series is the determination of virial coefficients (See, [3].) The virial series is used to express pressure-p, molar volume-v relations for an imperfect gas at a constant temperature. The ideal gas equation is:

$$pv = RT \iff p = RT(1/v)$$

If the gas is not ideal, the pressure may be expressed as a power series in 1/v:

$$p = RT(1/v + A(1/v)^2 + B(1/v)^3 + \ldots)$$

Thus,

$$pv = RT(1 + A(1/v) + B(1/v)^2 + \ldots)$$

Where the coefficients A, B, ... are called the second, third, ... virial coefficients of the gas.

A special application of power series is Taylor's theorem. It provides us with a method to generate infinite sums from a given function.

The development of a given function f(x) by Taylor's expansion can be denoted by:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^n(x_o)}{n!} (x - x_o)^n$$

Taylor's series are especially useful in approximating values of logarithmic and trigonometric functions with great accuracy. Computer technology has simplified the evaluating process. Some of the more important expansions using Taylor's theorem are as follows:

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

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

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

$$\ln x = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n!} , \quad -1 < x \leq 1$$

Oftentimes in physics or chemistry a differential equation will arise that can be solved using a Taylor's series expansion. An example of one such differential equation is:

(1) $$y'' = xy$$

To solve eq. (1) we assume $x_0 = 0$. By differentiating we get

$$y''' = x'y + y$$
$$y^{(iv)} = xy'' + 2y'$$
$$y^{(v)} = xy''' + 3y''$$
$$y^{(vi)} = xy^{(iv)} + 4y'''$$

Let $y = C_1$ and $y' = C_2$ at $x = 0$.

This gives

$$y''(0) = 0$$
$$y'''(0) = C_1$$
$$y^{(iv)}(0) = 2C_2$$
$$y^{(v)}(0) = 0$$

and so forth.

Hence, the Taylor's series generated is

$$y = C_1 + C_2x + C_1\frac{x^3}{3!} + 2C_2\frac{x^4}{4!} + 4C_1\frac{x^6}{6!} + \ldots$$

or by associating the C_1's and C_2's,

$$y = C_1\left[1 + \frac{x^3}{3!} + \frac{4x^6}{6!} + \ldots\right] + C_2\left[x + \frac{2x^4}{4!} + \frac{10x^7}{7!} + \ldots\right]$$

If we have a Taylor's series with $x_0 = 0$, i.e.

$$\sum_{n=0}^{\infty} \frac{f^n(0)}{n!}x^n$$

we call this special case a Maclaurin's series.

Maclaurin's theorem has proven to be very useful in physical chemistry. For example, an equation like

$$y = A + Bx + Cx^2 + Dx^3 + \ldots$$

can be used to describe the relationship between pressure-volume (pv) under the condition of constant temperature. This may be conveniently represented by equations of the form

$$pv = A + Bp + Cp^2 + Dp^3 + \ldots$$

where A, B, C, ... are constants. The value of these constants can be determined by applying Maclaurin's theorem. Thus,

$$f(0) = A$$

$$f'(0) = B$$

$$\frac{f''(0)}{2!} = C \quad \text{, and so forth.}$$

There are many opportunities in physical chemistry to use power series in the analysis of a problem. For further examples, see [2].

FOURIER SERIES

The use of power series can be summarized as follows:

> If a summary of a set of accurate experimental measurements y at various values of x is required, a series can be used.

As a generality, this concept is fine, but cases will occur in which no simple series can be found that can satisfy the conditions of the problem. For example, in the early nineteenth century Fourier posed the following problem, while studying heat conduction:

Given an insulated bar of length L which is initially at 100° C and has its ends kept at a temperature of 0° C, find the bar's heat conductivity.

Solution:

We have the following boundary value problem.

(1) $$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}$$

(2) $$U(0,t) = 0,\ U(L,t) = 0,\ U(x,0) = 100$$

where x = the position on the bar, t = temperature at position x and U = the bar's conductivity at temperature t.

Assuming that position can be represented in terms of x only and temperature in terms of t only, we desire a solution of the form:

$$U(x,t) = X(x)T(t)$$

Substituting into eq. (1) we get

(3) $$\frac{T'}{kT} = \frac{X''}{X}$$

Thus, it follows that since the right side of (3) is dependent only on X and the left side of the equation is dependent only on T, each side is constant. Let c be this constant.

Then,

Case I; $c = 0$

We have from (3) $\frac{T'}{kT} = c = 0$

$$\Rightarrow T' = 0$$

$$\Rightarrow T = c^*, \text{ where } c^* \text{ is constant}$$

$$\frac{X''}{X} = 0$$

$$\Rightarrow X' = A^*$$

$$\Rightarrow X = A^*X + B^*$$

$$U(x,t) = X(x)T(t) = c^*(A^*X + B^*) = AX + B$$

using the boundary conditions in eq. (2) we have

$$U(0,t) = 0 \Rightarrow B = 0, \; U(L,t) = 0 \Rightarrow AL = 0$$

Now, if $L = 0$ we have the trivial case, therefore we assume $L \neq 0$. This implies that $A = 0$. Yet if $A = 0$, then we cannot fulfill the last boundary condition $U(x,0) = 100$. Thus, the case $c = 0$ fails.

Case II; $c > 0$

Let $c = \lambda^2$ where $\lambda \in R$. Then we have

$\frac{X''}{X} = \lambda^2$ which becomes $X'' - \lambda^2 X = 0$, and

$\frac{T'}{kT} = \lambda^2$ which becomes $T' - \lambda^2 kT = 0$.

Solving we get

$$T = C_1e^{\lambda^2 kt}$$

$$X = A_1\cos\lambda x - B_1\sin\lambda x$$

And, $$U(x,t) = e^{\lambda^2 kt}(A\cos\lambda x - B\sin\lambda x)$$

By methods similar to those in case I, we find that $c > 0$ also fails to meet the boundary requirements. Logically, this makes sense. For as $t \to \infty$ the temperature will be unbounded if $c > 0$ which violates a fundamental law of nature. Also, if $c = 0$, the assumption that temperature and time are dependent is violated.

Case III; $c < 0$

Let $c = -\lambda^2$ where $\lambda \in R$.

Then solving for X and T in the usual manner we get

$$T = C_1e^{-\lambda^2 kt}$$

$$X = A_1\cos\lambda x + B_1\sin\lambda x$$

$$U(x,t) = e^{-\lambda^2 kt}(A\cos\lambda x + B\sin\lambda x)$$

Now, we will examine the boundary conditions:

$$U(0,t) = e^{-\lambda^2 kt}A = 0 \Rightarrow A = 0$$

Thus, the solution so far is

$$U(x,t) = Be^{-\lambda^2 kt}\sin\ x$$

The second condition gives

$$U(L,t) = Be^{-\lambda^2 kt}\sin L\lambda = 0$$

This implies either $B = 0$ or $\sin L\lambda = 0$.

If B = 0, we have the trivial solution. Therefore,

$$\sin L\lambda = 0 \quad \Rightarrow \quad L\lambda = n\pi \qquad n = 0, \pm 1, \pm 2, \ldots$$

$$= \frac{n\pi}{L}.$$

Thus, $U(x,t) = Be^{-kn^2\pi^2 t/L^2}\sin\frac{n\pi x}{L}$

But if we take the last boundary condition

$U(x,0) = B\sin\frac{n\pi x}{L} = 100$ we are stuck!

That is, B is a constant, yet it would be represented in terms of x which is a variable. Thus, it is impossible to solve for B directly.

To solve this problem Fourier used an extension of the principle of superposition and reasoned that an infinite number of terms might yield the proper result.

This led to

$$100 = U(x,0) = b_1\sin\frac{\pi x}{L} + b_2\sin\frac{2\pi x}{L} + \ldots + b_n\sin\frac{n\pi x}{L} + \ldots \quad *$$

By inspection we can see that this equation can only hold in the open interval (0,L).

Now, Fourier was faced with determining the constants b_1, b_2, ... such that this equation was true. His results were:

Consider the generalization of the right side of *

$$f(x) = \frac{a_0}{2} + a_1\cos\frac{\pi x}{L} + a_2\cos\frac{2\pi x}{L} + \ldots + b_1\sin\frac{\pi x}{L} + b_2\sin\frac{2\pi x}{L} + \ldots \quad **$$

To find a_0, integrate both sides of ** over (-L,L).

$$\int_{-L}^{L} f(x)dx = \int_{-L}^{L}(a_0/2)\,dx + \int_{-L}^{L} a_1\cos\frac{\pi x}{L}\,dx + \ldots + \int_{-L}^{L} b_1\sin\frac{\pi x}{L}\,dx + \ldots$$

This becomes $\int_{-L}^{L} f(x)dx = 2L(a_o/2) + 0$

$$\Longrightarrow \quad a_o = (1/L)\int_{-L}^{L} f(x)dx$$

To determine the a_k's simply multiply both sides of ** by $\cos(k\pi x/L)$ and integrate over $(-L,L)$.

It is easy to show that for $n,\ k \in Z$

$$\int_{-L}^{L}\cos(n\pi x/L)\cos(k\pi x/L)dx = \begin{cases} 0 \text{ if } n \neq k \\ L \text{ if } n = k \end{cases}$$

and

$$\int_{-L}^{L}\sin(n\pi x/L)\cos(k\pi x/L)dx = 0$$

Thus, we find that

$$a_k = (1/L)\int_{-L}^{L} f(x)\cos(k\pi x/L)dx \qquad k = 1,\ 2,\ \ldots$$

Similarly, to determine the b_k's, we multiply both sides of ** by $\sin(k\pi x/L)$ and integrate over $(-L,L)$.

This gives $b_k = (1/L)\int_{-L}^{L} f(x)\sin(k\pi x/L)dx,\ k = 1,\ 2,\ \ldots$

Fourier series are an essential part of mathematical physics. They have provided the means of analysis in many areas. One well-known application of the Fourier series is the mathematical analysis of the patterns produced when x-rays are diffracted by crystals. It can be shown that at any position in the diffraction pattern the intensity is a periodic function of position (for further description of the diffraction pattern, see [1].) By evaluating the Fourier coefficients representing this effect, we can elucidate important information about the molecular structure of the crystalline compounds.

SERIES SOLUTIONS

Another application of series is Picard's method. This method is used for obtaining solutions of first-order differential equations. It is possible, however, to generalize to higher orders (see [6]). The method can best be illustrated by an example:

Consider the first order differential equation

$$(1) \qquad y' = x + y + 1$$

To solve by Picard's method, first assume that y = c when x = 0. Integrating both sides of eq. (1) with respect to x then yields

$$(2) \qquad y = C + \int_0^x (x + y + 1)dx$$

Now, since we have no information about how y depends on x, the integral cannot be solved directly.

Picard's method provides us with a tool to approximate this integral.

As a first approximation to y assume $y_1 = C$. Substituting this value into the integrand we can integrate eq. (2):

$$y_2 = C + \int_0^x (x + y + 1)dx = C + \int_0^x (x + C + 1)dx = C + \frac{x^2}{2} + Cx + x$$

Repeating this procedure yields:

$$y_3 = C + (C+1)x + \frac{(C+1)x^2}{2!} + \frac{x^3}{3!}$$

This leads to the general case where

$$y_n = C + (C+1)x + \frac{(C+1)x^2}{2!} + \ldots + \frac{(C+1)x^{n-1}}{(n-1)!} + \frac{x^n}{n!}$$

If we allow $n \to \infty$ we find that this is truly the solution of eq. (1). Thus, the sequence of approximations can be shown to converge to the required solution.

Sometimes in solving an equation, it is obvious that a simple series like

$$y = a_0 + a_1 x + a_2 x^2 + \ldots \qquad \text{(i)}$$

will not suffice. In this case, one option available is the method of Frobenius (For further explanation of Frobenius' method, see [6].) Frobenius assumed that the solution would take the general shape

$$y = x^r(a_0 + a_1 x + a_2 x^2 + \ldots) \qquad \text{(ii)}$$

where r is any real number. Note that (i) is merely the special case of (ii) where r = 0.

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