Applications of Taylor Series

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(Completed 1st October, 2008; submitted 23rd October, 2008)

Polynomial functions are easy to understand but complicated functions, infinite polynomials, are not obvious. Infinite polynomials are made easier when represented using series: complicated functions are easily represented using Taylor's series. This representation make some functions properties easy to study such as the asymptotic behavior. Differential equations are made easy with Taylor series. Taylor's series is an essential theoretical tool in computational science and approximation. This paper points out and attempts to illustrate some of the many applications of Taylor's series expansion. Concrete examples in the physical science division and various engineering fields are used to paint the applications pointed out.

INTRODUCTION

Taylors series is an expansion of a function into an infinite series of a variable x or into a finite series plus a remainder term[1]. The coefficients of the expansion or of the subsequent terms of the series involve the successive derivatives of the function. The function to be expanded should have a nth derivative in the interval of expansion. The series resulting from Taylors expansion is referred to as the Taylor series. The series is finite and the only concern is the magnitude of the remainder. Given the interval of expansion $a \leqq \xi \leqq b$ the Lagrangian form of the remainder is given as follows:

$$R_n = \frac{(x-a)^n}{n!} f^{(n)}(\xi) \tag{1}$$

a, is the reference point. The $f^{(n)}(\xi)$ is the nth derivative at a. When the expanding function is such that:

$$\lim_{n\to\infty} R_n = 0, \tag{2}$$

the Taylors series of the expanding function becomes

$$f(x) = \sum_{n=0}^{\infty} \frac{(x-a)^n}{n!} f^{(n)}(a). \tag{3}$$

Taylor series specifies the value of a function at one point, x. Setting the derivative operator, D = d/dx, the Taylor expansion becomes:

$$f(x+h) = \sum_{n=0}^{\infty} \frac{h^n D^n}{n!} f(x) = e^{hD} f(x) \text{ [2]} \tag{4}$$

Taylor series could also be written in the context of a complex variable

EVALUATING DEFINITE INTEGRALS

Some functions have no anti-derivative which can be expressed in terms of familiar functions. This makes evaluating definite integrals of these functions difficult because the fundamental theorem of calculus cannot be used. However, a series representation of this function eases things up. Suppose we want to evaluate the definite integral

$$\int_0^1 \sin\left(x^2\right)\, dx \tag{5}$$

this integrand has no anti-derivative expressible in terms of familial functions. However, we know how to find its Taylor series:

$$\sin t = t - \frac{t^3}{3!} + \frac{t^5}{5!} + \frac{t^7}{7!} + \dots \tag{6}$$

if, we substitute t = x^2 , then

$$\sin\left(x^2\right) = x^2 - \frac{x^6}{3!} + \frac{x^{10}}{5!} + \frac{x^{14}}{7!} + \dots \tag{7}$$

The Taylor series can then be integrated:

$$\int_0^1 \sin\left(x^2\right)\, dx = \frac{x^3}{3} + \frac{x^7}{7\times 3!} + \frac{x^{11}}{11\times 5!} + \frac{x^{15}}{15\times 7!} + \dots \tag{8}$$

This is an alternating series and by adding all the terms, the series converges to 0.31026 [1].

UNDERSTANDING ASYMPTOTIC BEHAVIOR

Sometimes the Taylor series is used to describe how a function behaves in a sub domain [2]. The electric field obeys the inverse square law.

$$E = \frac{kq}{r^2} \tag{9}$$

Where E is the electric field, q is the charge, r is the distance away from the charge and k is some constant of proportionality. Two opposite charges placed side by side, setup an electric dipole moment such that we can

consider the electric field far away from the dipole moment. Taylor's series is used to study this behavior.

$$E = \frac{kq}{(x-r)^2} + \frac{kq}{(x+r)^2} \tag{10}$$

An electric field further away from the dipole is obtained from (10) after expanding the terms in the denominator.

$$E = \frac{kq}{x^2\left(1-\frac{r}{x}\right)^2} - \frac{kq}{x^2\left(1+\frac{r}{x}\right)^2}. \tag{11}$$

Taylor's series can be used to expand the denominators if (x≫r)

$$\frac{kq}{\left(1-\frac{r}{x}\right)^2} = 1 + \frac{2r}{x} + \frac{3r^2}{x^2} + \frac{4r^3}{x^3} \tag{12}$$

$$\frac{kq}{\left(1+\frac{r}{x}\right)^2} = 1 - \frac{2r}{x} + \frac{3r^2}{x^2} - \frac{4r^3}{x^3}. \tag{13}$$

One now obtain:

$$E \approx \frac{4rq}{x^3}. \tag{14}$$

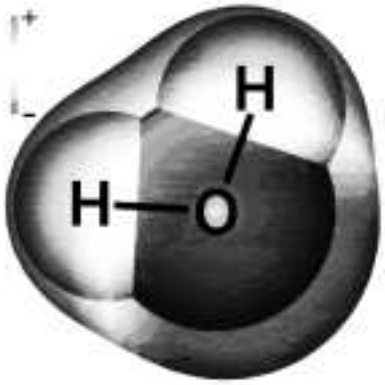
In the field of physics and chemistry, there is a great need for geometric optimization of physical systems. In chemistry, as an example, the quasi-newton method make use of a two variable Taylor's series to approximate the equilibrium geometry of a cluster of atoms [3]. Consider U,the geometry of a molecule, and assume it is a function of only two variables, x and y, let x_1 and y_1 be the initial coordinates, if terms higher than the quadratic terms are neglected then the Taylor series is as follows:

$$\begin{aligned} U(x,y) &\approx U(x_1,y_1) + \frac{\partial U}{\partial x}|_{(x_1,y_1)}(x-x_1) \\ &+ \frac{\partial U}{\partial y}|_{(x_1,y_1)}(y-y_1) + \frac{1}{2}\frac{\partial^2 U}{\partial x^2}|_{(x_1,y_1)}(x-x_1)^2 \\ &+ \frac{1}{2}\frac{\partial^2 U}{\partial y^2}|_{(x_1,y_1)}(y-y_1)^2 + \frac{\partial^2 U}{\partial x \partial y}|_{(x_1,y_1)}(x-x_1)(y-y_1) \end{aligned} \tag{15}$$

The U(x, y) function fits well around the equilibrium position, the quadratic approximation works well around the minimum. If U were accurately a quadratic function of the coordinates in the region near (x_1, y_1), then the elements of the Hessian matrix (second partial derivatives) will be constant in this region. Accurate ab initio self consistent field calculation of the second derivatives is very time consuming, thus the optimization usually starts with an approximation of the Hessian and then proceeds to improve on this approximation. If U(x,y) is written in the form below then, the first approximation to the Hessian matrix element at (or near) the equilibrium geometry can be computed.

$$\begin{aligned} U(x,y) &\approx U_1 + U_{x,1}(x-x_1)U_{y,1}(y-y_1) \\ &+ \frac{1}{2}U^{(1)}_{x,x}(x-x_1)^2 + U^{(1)}_{x,y}(x-x_1)(y-y_1) \\ &+ \frac{1}{2}U^{(1)}_{y,y}(y-y_1)^2 \end{aligned} \tag{16}$$

FIG. 1: Dipole of optimized water molecule[8]



geometry autosym units angstrom			
O	0.00000	0.00000	0.00000
H	0.922641	0.652406	0.00000
H	-0.922641	0.652406	0.00000

TABLE I: Nwchem[9]cartesian coordinates of water molecule

The superscript denotes the first approximation to the Hessian matrix elements at or near the equilibrium geometry. The molecular geometry has a 3N-6 dimensional vector when internal coordinates are considered and by 3N when only cartesian coordinates are used. N is the number of atoms in the molecule. In cartesian coordinates, rotation and translation accounts for the six in 3N-6. Once the Hessian matrix elements are determined, the molecular properties can be extracted via the Taylor's series expansion.

The position of the atom in the molecule constantly shift from the equilibrium position. an overall atomic behavior , in the course of vibration, is modeled on the Lennard-Jones 6-12 potential. The dynamics of the vibrations can be study by expanding the potential in a Taylor's series. The second derivative of the Taylor's series expansion correspond to the gradient of the,(harmonic) potential curve of a short range vibration around the equilibrium position,r_e.

$$V(r) = 4\epsilon[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \tag{17}$$

EXAMPLES OF APPLICATIONS OF TAYLOR SERIES

The Gassmann relations of poroelasticity provide a connection between the dry and the saturated elastic moduli of porous rock and are useful in a variety of petroleum geoscience applications [4]. Because some uncertainty is usually associated with the input parameters, the propagation of error in the inputs into the final moduli estimates is immediately of interest. Two common approaches to error propagation include: a first-order Taylor's series expansion and Monte-Carlo methods. The Taylor's series approach requires derivatives, which are obtained either analytically or numerically and is usually limited to a first-order analysis. The formulae for analytical derivatives were often prohibitively complicated before modern symbolic computation packages became prevalent but they are now more accessible [4].

A numerical method for simulations of nonlinear surface water waves over variable bathymetry (study of underwater depth of third dimension of lake or ocean floor) and which is applicable to either two- or three-dimensional flows, as well as to either static or moving bottom topography, is based on the reduction of the problem to a lower-dimensional Hamiltonian system involving boundary quantities alone. A key component of this formulation is the Dirichlet-Neumann operator (used in analysing boundary conditions e.g fluid dynamics and crystal growth) which, in light of its joint analyticity properties with respect to surface and bottom deformations, is computed using its Taylor's series representation. The new stabilized forms for the Taylor terms, are efficiently computed by a pseudo spectral method using the fast Fourier transform [5].

The current-mode pseudo-exponential circuit based is optimized using the n-order Taylor's series expansion. The effect of this optimization is noticed in the circuit, wherein a smaller value of the total computing error (under 0.3 dB) is obtained. The maximum output range of the proposed function generator is greater than 40 dB. The total error could be very easily reduced by increasing the number of terms considered in the Taylor expansion [6].

In stochastic processes, generalized processes are expressed theoretically through the Gaussian random walk. The cumulants (some expectation value or variance of statistical data) are expressed in terms of Taylor series with coefficients that involve the Riemann Zeta function (special function that arises from definite integration and can give the asymptotic form for the prime counting function π (n),which count the number of primes less than some integer,)n. The method of obtaining the cumulate is systematized such as to yield Taylor series xpression for all cumulants. The Taylor series for the kth cumulants is then obtained [7].

The Galerkin Computational Fluid Dynamics (a robust and high accuracy methode that is use to study abitrary shapes) (CFD) algorithm is optimally made accurate for the unsteady Incompressible Navier-Stokes (INS) equation via Taylor series (TS) operation followed by pseudo-limit process. A spatially finite element democratization in the implementation of the INS termed Taylor Weak Statement (TWS) generates a CFD algorithm for analysis. The TWS algorithm phase velocity and amplification factor error function are then derived for linear and bi-linear basis implementations assembled at the generic node. The lower order error terms are affected as a result of a subsequent TS expansion in wave number space.

CONCLUSION

We have probe through the complexity of Taylor series and shown evidence of its extensive and very effective applications. The effectiveness in error determination, function optimization, definite integral resolution, and limit determination is evidence of the Taylor series being an enormous tool in physical sciences and in Computational science as well as an effective way of representing complicated functions.

ACKNOWLEDGMENTS

I want to acknowledge the original topic proposal by Dr. Adriana Moreo, her advice and her willingness to have me be not only a participant but a contributor to the success of this course. I again felt the pain of what it is to read, understand and communicate complex scientific information which is another step in my training as an independent thinker.

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