PHYSNET

MISN-0-4

TAYLOR'S POLYNOMIAL APPROXIMATION FOR FUNCTIONS

$$f(x \pm \Delta)$$

$$= f(x) \pm \frac{f'(x)}{1\,!}\Delta + \frac{f''(x)}{2\,!}\Delta^2 \pm \cdots$$

$$= 1.000 \pm 0.100 + 0.005 \pm \cdots$$

Project PHYSNET Physics Bldg. Michigan State University East Lansing, MI

TAYLOR'S POLYNOMIAL APPROXIMATION FOR FUNCTIONS

by
Peter Signell

Title: **Taylor's Polynomial Approximation for Functions**

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Input Skills:

1. Formally differentiate polynomial, transcendental, and exponential functions (MISN-0-1).

Output Skills (Knowledge):

K1. Use the Taylor Series to derive the formal expressions for the finite difference approximations to the first and second derivatives.

Output Skills (Rule Application):

R1. Use the Taylor Series to expand any given common function in a power series about any given point.

R2. Evaluate the first and second derivatives of any given function by numerical techniques.

Post-Options:

1. "Relativistic Energy: Thresholds for Particle Reactions, Binding Energies" (MISN-0-23).
2. "Small Oscillation Techniques" (MISN-0-28).
3. "Numerov Computer Algorithm for the Damped Oscillator" (MISN-0-39).
4. "Numerov Computer Algorithm in Two Dimensions for Satellite Orbits" (MISN-0-104).
5. "The Runge-Kutta Computer Algorithm in Two Dimensions for Trajectories in Magnetic Fields" (MISN-0-128).

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New authors, reviewers and field testers are welcome.

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1. Introduction

1a. Simplifying a Complicated Function. We frequently encounter some complicated mathematical function, $f(x)$, which is valid over a wide range of x, in a situation where we would prefer a simpler polynomial even if it were a good approximation only over a limited region. For example, the force holding two atoms together in a diatomic molecule is an exceedingly complicated function of the interatomic distance. If we attempt to use this function directly, we find it almost impossible to calculate the vibrational motions of the atoms. Even if we succeed through the use of heroic computer calculations, we get little insight. However, if we replace the complicated function by a simple best-match polynomial, the approximate atomic motions can be easily obtained. Such approximate solutions are very important in applied mechanics and in molecular chemistry and physics. In this module we show you how to obtain the best-match polynomial for any given (complicated) function.

1b. The Goal of This Module. Technically, this module explains how to make a power series expansion of a function using the Taylor series method, and how to check the validity of the expansion. No attempt is made to give the mathematical basis for the method. The module also uses such expansions to derive handy approximations for the derivatives of a function.

2. The Expansion of a Function

2a. The Taylor Series Method. Suppose we have a complicated function $f(x)$ and that we know or can find its value and the value of each of its derivatives at some point x_0. We can put that value and those derivatives into the Taylor Series and use it to evaluate $f(x)$ at any other point x that is in neighborhood of x_0:

$$f(x) = f(x_0) + \frac{f'(x_0)}{1!}(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \ldots \qquad (1)$$

The complete definition of the Taylor Series is:

$$f(x) = \sum_{n=0}^{n=\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n\,, \qquad (2)$$

where $f^{(n)}(x_0)$ is the n^{th} derivative of $f(x)$, evaluated at x_0. The quantity $n!$ is the factorial ($n! = 1 \cdot 2 \cdot 3 \cdots (n-1) \cdot n$).

2b. Truncating the Series. The Taylor series is an infinite series, but if x is near to x_0, the series can usually be truncated (cut-off) after a few terms and this leaves a simple polynomial.

2c. Example of a Taylor Series Expansion. Here is a specific example: Suppose you wish to have a power series expansion of $f(x) = \sin x$ about the point $x_0 = 0$, where x is in radians. To make the power series we evaluate the terms of the Taylor Series:

$$\begin{aligned} f(x) &= +\sin x \Longrightarrow f(0) = 0 \\ f'(x) &= +\cos x \Longrightarrow f'(0) = 1 \\ f''(x) &= -\sin x \Longrightarrow f''(0) = 0 \\ f'''(x) &= -\cos x \Longrightarrow f'''(0) = -1 \\ f''''(x) &= +\sin x \Longrightarrow f''''(0) = 0 \end{aligned} \qquad (3)$$

Putting these and further derivatives into Eq. (1) gives us the power series:

$$\sin x = x - \frac{x^3}{6} + \frac{x^5}{120} - \ldots \qquad (4)$$

For cases where x is much smaller than 1, x^3 is much smaller than x and hence x^5 is much much smaller than x. Then we can truncate the series after the first term:

$$\sin x \simeq x \qquad (x^2 \ll 1)\,. \qquad (5)$$

2d. Convergence of the Series. How rapidly does the series approach the correct answer? Technically, this question is phrased: "How rapidly does the series converge?" As an example, suppose $x = \pi/6 = 30°$ so that $\sin x = 0.500$. Then various truncations of the series for the expansion of $\sin x$ about the origin gives:

TERMS	APPROXIMATION	SUM	ERROR	% ERROR
1	x	0.523599	+0.023599	+5
2	$x - x^3/6$	0.499674	−0.000326	−0.07
3	$x - x^3/6 + x^5/120$	0.500002	+0.000002	+0.0004

Since the series rapidly approaches the exact answer, it is said to "converge rapidly" for $x = \pi/6$.

2e. Always Check For Convergence. A check for convergence should always be made: the range of Δ for which the series converges may be unexpectedly small.[1] The usual method of checking is to calculate the next term or two and see whether the additional contribution to the sum is or is not significant at the desired level of accuracy.

3. Approximations for Derivatives

3a. Rewriting the Expansion. In order to work with finite difference equations we usually write Taylor's series in an especially convenient notation. First we substitute $x = x_0 + \Delta$ into Eq. (1):

$$f(x_0 + \Delta) = f(x_0) + \frac{f'(x_0)}{1!}\Delta + \frac{f''(x_0)}{2!}\Delta^2 + \ldots \qquad (6)$$

A similar expression is written with $x = x_0 - \Delta$. The subscript on x_0 is then dropped and the two equations are written as one:

$$f(x \pm \Delta) = f(x) \pm \frac{f'(x)}{1!}\Delta + \frac{f''(x)}{2!}\Delta^2 \pm \frac{f'''(x)}{3!}\Delta^3 + \ldots \qquad (7)$$

We say "f at x plus or minus delta equals f at x plus or minus f prime at x over one factorial times delta plus ..."

3b. A Finite Difference Approximation for $f'(x)$. An approximation for $f'(x)$ can be obtained by subtracting $f(x - \Delta)$ from $f(x + \Delta)$:

$$f(x + \Delta) - f(x - \Delta) = 2\frac{f'(x)}{1!}\Delta + 2\frac{f'''(x)}{3!}\Delta^3 + \ldots \qquad (8)$$

[1] This would be due to a nearby singularity in the complex plane. See "Some Simple Functions in the Complex Plane" (MISN-0-59) for some highly visual examples.

For small Δ, the Δ^3, Δ^5, etc. terms will be much smaller than the Δ term . Truncating and solving for $f'(x)$ gives:[2]

$$f'(x) \simeq \frac{f(x + \Delta) - f(x - \Delta)}{2\Delta}\,. \qquad (9)$$

3c. Approximations for Higher Derivatives. An approximation for $f''(x)$ can be obtained by adding $f(x + \Delta)$ to $f(x - \Delta)$. Truncating and solving for $f''(x)$ gives:

$$f''(x) \simeq \frac{f(x + \Delta) - 2f(x) + f(x - \Delta)}{\Delta^2}\,. \qquad (10)$$

Approximations for higher derivatives can be developed by similar techniques. You might wish to verify that: *Help: [S-1]*

$$f'''(x) \simeq \frac{f(x + 2\Delta) - 2f(x + \Delta) + 2f(x - \Delta) - f(x - 2\Delta)}{2\Delta^3} \qquad (11)$$

3d. A Handy Check of Formal Derivatives. Equations (9), (10), and (11) offer a quick calculator method for checking your work when formally differentiating complicated functions. Merely choose some convenient point x and a small value for Δ and use them to evaluate the finite difference derivative. Then evaluate your formal derivative at the same point x and compare the two answers.

3e. A Calculator Caution. Truncation and rounding errors may lead to incorrect results if Δ is too small. For example, in Eq. (9) the numerator is small through almost exact cancellation of its two terms. If Δ is too small, the terms will be the same to as many significant digits as the calculator carries. The net result for the numerator is then zero! A slightly larger Δ will result in a non-zero numerator but one with little accuracy. Watch out for this effect whenever using the finite difference equations.

Acknowledgments

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[2] Note the similarity of this approximate result to the precise definition of the derivative:

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

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PROBLEM SUPPLEMENT

Note: There is a Table of Derivatives in the *Model Exam.* Problems 9 and 10 (below) also occur in the *Model Exam.*

1. Obtain the power series expansion of $\cos x$ about the point $x = 0$, obtaining at least the first three terms. [C]

2. Do the same as in problem 1, but for the function e^x. [B]

3. Obtain the power series expansion for $\ell n\, x$ about the point $x = 1$. Note that you must go back to the full Taylor Series, and you must evaluate the derivatives of $\ell n\, x$ at $x = 1$. When you have finished, ask yourself why we chose $x = 1$ for this expansion rather than, say, $x = 0$. [D]

4. Obtain the power series expansion of $(x^2+4)^{-1}$ about the point $x = 0$. Show, by numerical evaluation of the first few terms, that the series converges rapidly for $x = 1$, does not converge for $x = 2$, and diverges (goes away from the exact value as more terms are added) for $x = 3$. [A]

5. Differentiate the power series expansion of e^x and see that all the derivatives of e^x are equal to itself.

6. If $z = x + iy$, the exponential function of z is defined by its power series:
$$e^z = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \ldots$$
By substituting $z = iy$, show that $e^{iy} = \cos y + i \sin y$.

7. By substituting the first two terms of the power series for $\sin x$ into the first three terms of the power series for $(1-x^2)^{1/2}$, determine the first three terms of the power series for $\cos x$.

8. Given $f(x) = (x^2 + 4)^{-1}$, find $f'(1)$ and $f''(1)$:

   a. by formal differentiation *Help: [S-2]*

   b. by numerical differentiation (using finite difference approximations). [E] *Help: [S-3]*

9. Determine the first three terms of the power series expansion, about the origin, of the function: $f(x) = (1 + x^2)^{-1/2}$. [F]

10. Use numerical differentiation to determine $f''(x)$ at $x = 0.5$ where:

$$f(x) = (x^2 - 8x + 25)^{-1}. \qquad \text{[G]}$$

Brief Answers:

A. $(x^2 + 4)^{-1} = 1/4\left[1 - (x/2)^2 + (x/2)^4 - (x/2)^6 + \ldots\right]$

B. $e^x = 1 + x + x^2/2! + x^3/3! + x^4/4! + \ldots$ (see module's cover for $x = 0.1$)

C. $\cos x = 1 - x^2/2! + x^4/4! - x^6/6! + \ldots$

D. $\ell n\, x = (x - 1) - (x - 1)^2/2 + (x - 1)^3/3 - \ldots$

E. $f'(1) = -0.0800$

$f''(1) = -0.0160$

F. $(1 + x^2)^{-1/2} = 1 - \frac{1}{2}x^2 + \frac{3}{8}x^4 - \frac{5}{16}x^6 + \ldots$

G. $f''(0.5) = .00578$

SPECIAL ASSISTANCE SUPPLEMENT

S-1 *(from TX-3c)*

Evaluate Eq.(4) with one more term, so you include f''', substituting these values successively for Δ: (2Δ, Δ, $-\Delta$, and -2Δ). This gives you four equations that you can properly substitute into the right side numerator of Eq. (9). You should find the terms up through the second derivative canceling and just the proper quantity remaining.

S-2 *(from PS, problem 8a)*

$f'(x) = -2x(x^2 + 4)^{-2}$ hence $f'(1) = -2/25$.

S-3 *(from PS, problem 8b)*

Students have asked: "What are x and Δ when $x = 1$?"
Answer: if $x = 1$ and, say, $\Delta = 0.01$, then in equations such as Eq. (7): $x + \Delta = 1.01$ and $x - \Delta = 0.99$. You have to evaluate some particular problem's $f(x)$ at some such values of x. The smaller the value of Δ you use, the better your numerical approximation to the true value of $f'(1)$, but see Sect. 3e in the *text*.

MODEL EXAM

1. See Output Skill K1 in this module's *ID Sheet*.

2. Determine the first three terms of the power series expansion, about the origin, of the function: $f(x) = (1 + x^2)^{-1/2}$.

3. Use numerical differentiation to determine $f''(x)$ at $x = 0.5$ where:

$$f(x) = (x^2 - 8x + 25)^{-1}\,.$$

Table of Derivatives

Combinations of Functions	Specific Functions
$\frac{d}{dx}(f(u)) = \frac{df(u)}{du} \cdot \frac{du}{dx}$	$\frac{d}{dx}(x^n) = nx^{n-1}$
$\frac{d}{dx}(f \pm g) = \frac{df}{dx} \pm \frac{dg}{dx}$	$\frac{d}{dx}(e^x) = e^x$
$\frac{d}{dx}(fg) = f\frac{dg}{dx} + g\frac{df}{dx}$	$\frac{d}{dx}(\ell n\, x) = 1/x$
$\frac{d}{dx}(f/g) = \left(g\frac{df}{dx} - f\frac{dg}{dx}\right)/g^2$	$\frac{d}{dx}(\sin x) = \cos x$
	$\frac{d}{dx}(\cos x) = -\sin x$

Brief Answers:

1. See this module's *text*.

2. See this module's *Problem Supplement*, problem 9.

3. See this module's *Problem Supplement*, problem 10.