## **The Taylor Expansion**

The Taylor Expansion of a function f(x) about a point x = a is a scheme of successive approximations of this function, in



UNIVERSITY OF

**ROCHESTER** 

the neighborhood of x = a, by a power series or polynomial. The successive terms in the series involve the successive derivatives of the function. As an example, one can consider the distance d(t) covered by a slow particle in times *t* not too far from time t=0.

DEPARTMENT OF CHEMISTRY

W. Udo Schröder

To zeroth order approximation,

$$f(x) \approx f(a) \tag{1}$$

for values of  $x \approx a$ . In the example, the distance  $d(t) \approx d(0)$ . This approximation is exact only, as long as f(x) is a constant and good enough, if the rate of change  $(\partial f / \partial x) \approx 0$ . In the example, the particle velocity is very small, i.e.,  $v(t) = (\partial d / \partial t) \approx 0$ . The next better approximation to f(x) in the vicinity of x = a involves the rate of change of the function,

$$f(x) \approx f(a) + \left(\frac{\partial f}{\partial x}\right)_{x=a} \cdot (x-a)$$
 (2)

where the partial derivative  $(\partial f / \partial x)$  should be evaluated for x = a (*insert a for every x in the expression for this deriva-tive*). In the example, the calculation of the distance traveled

1

Tutorial

UNIVERSITY OF DEPARTMENT OF CHEMISTRY **Tutorial** W Udo Schröder **ROCHESTER** 

finite velocity of particle: includes the the now  $d(t) = d(0) + v(0) \cdot t$ .

The first-order Taylor approximation (2) is exact, as long as the derivative of f does not change, i.e., as long as  $\left(\partial^2 f / \partial x^2\right) \approx 0$ . In the example, this requires that  $(\partial v / \partial t) = (\partial^2 d / \partial t^2) \approx 0$ . The next better approximation accounts for the change in the first derivative, i.e., the second derivative. In the example, the latter accounts for the finite acceleration. Then, one has in second order,

$$f(x) \approx f(a) + \left(\frac{\partial f}{\partial x}\right)_{x=a} \cdot (x-a) + \frac{1}{2} \left(\frac{\partial^2 f}{\partial x^2}\right)_{x=a} \cdot (x-a)^2 \quad (3)$$

The distance traveled in time t by the particle in the example can now be written as

$$d(t) \approx d(0) + v(0) \cdot t + \frac{1}{2}a(0) \cdot t^{2}$$
(4)

where a(0) is the acceleration at t = 0. One can continue this scheme to higher and higher order in the difference in the argument, until the desired accuracy is reached. The general expression for the Taylor series up to a power of N in the difference is

$$f(x) \approx \sum_{n=0}^{N} \frac{1}{n!} \left( \frac{\partial^{n}}{\partial x^{n}} \right)_{x=a} \cdot (x-a)^{n}$$
 (5)

The uncertainty in this approximation is the of the order N+1and higher.

2