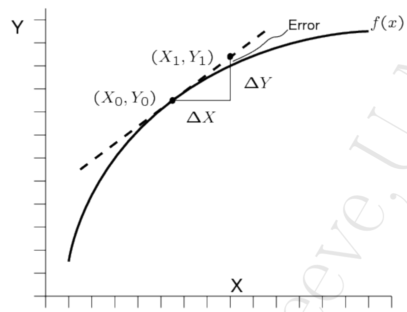
Intro to the Taylor Series

- method for estimating the value of a function based on the derivatives at another point (including the 'zeroth derivative').
- simple example is linear interpolation: knowing the value of a function and its first derivative at one point allows values of the function to be estimated at other points.

$$x = 0; y = 10$$
$$\frac{dy}{dx} = .1$$
$$y \approx .1x + 10$$



- If the interpolation is performed on a function that is not linear, the interpolation will be in error.
- If the distance between the known and interpolated point is small, the error should also be small.

Taylor Series Derivation

The Taylor series can be derived by considering a polynomial. Consider a second order polynomial:

$$f(x) = a \cdot x^2 + b \cdot x + c$$

Evaluating this function and its derivatives at a point x_0.

$$f(x_0) = a \cdot x_0^2 + b \cdot x_0 + c$$
$$f^{'}(x_0) = 2a \cdot x_0 + b$$
$$f^{''}(x_0) = 2a$$

Taking a function evaluated at x_0 and substituting back into the original equation:

$$f(x) = a \cdot x^2 + b \cdot x + c$$
$$f(x) = a \cdot x^2 + b \cdot x + \left(f(x_0) - a \cdot x_0^2 - b \cdot x_0\right)$$
$$\begin{aligned} f(x) =& a \cdot x^2 + x \left(f^{'}(x_0) - 2a \cdot x_0\right) \\ &+ \left(f(x_0) - a \cdot x_0^2 - x_0 \left(f^{'}(x_0) - 2a \cdot x_0\right)\right) \end{aligned}$$
$$f(x) = f(x_0) + f^{'}(x_0)(x - x_0) + a\left(x^2 - 2xx_0 - x_0^2 + 2x_0^2\right)$$
$$f(x) = f(x_0) + f^{'}(x_0)(x - x_0) + a\left(x^2 - 2xx_0 + x_0^2\right)$$
$$f(x) = f(x_0) + f^{'}(x_0)(x - x_0) + \frac{f^{''}(x_0)}{2}(x - x_0)^2$$

This gives the first three terms of the Taylor series. If a cubic equation had been used as the starting point, the first four terms of the Taylor series would have resulted.

$$f(x_0 + \Delta x) = \sum_{n=0}^{\infty} f^n(x_0)\frac{\Delta x^n}{n!}$$

- basis for many numerical methods
- used to evaluate errors
- when reference point is zero, get Maclauren Series.

The Taylor series is also applicable to multivariate problems.

$$f(x,y) = f(x_0,y_0) + \frac{1}{1!}\left(\Delta x\frac{\partial}{\partial x} + \Delta y\frac{\partial}{\partial y}\right) f(x_0,y_0) + \frac{1}{2!}\left(\Delta x\frac{\partial}{\partial x} + \Delta y\frac{\partial}{\partial y}\right)^2 f(x_0,y_0)\ldots$$

How well does the Taylor Series work? Lets consider some functions that are easy to differentiate with x_0=0, $\Delta x = \frac{\pi}{2}$:

$$f(x) = cos(x)$$
$$f^{'}(x) = -sin(x)$$
$$f^{''}(x) = -cos(x)$$
$$f^{'''}(x) = sin(x)$$
$$f(\frac{\pi}{2}) \approx f(0) + f^{'}(0)\frac{\frac{\pi}{2}}{1} + f^{''}(0)\frac{(\frac{\pi}{2})^2}{2!} + f^{'''}(0)\frac{(\frac{\pi}{2})^3}{3!}$$
$$f(\frac{\pi}{2}) \approx 1. + 0 - \frac{(\frac{\pi}{2})^2}{2!} + 0 + \frac{(\frac{\pi}{2})^4}{4!}$$

We can evaluate this infinite series using a programing language or spreadsheet software, to get some sense for how good the Taylor Series is.

The Taylor Series can be used to make good approximations. Remember the sin rule? When an angle is small:

$$sin(\theta) \approx \theta$$

Lets consider this using a Taylor Series:

$$f(x) = sin(x)$$
$$f^{'}(x) = cos(x)$$
$$f^{''}(x) = -sin(x)$$
$$f^{'''}(x) = -cos(x)$$
$$sin(x) \approx sin(0) + cos(0)\frac{x}{1!} - sin(0)\frac{x^2}{2!} - cos(0)\frac{x^3}{3!}$$
$$sin(x) \approx x - \frac{x^3}{3!}$$

$$\frac{x^3}{3!} \approx x - sin(x)$$

- For an angle x, the error in the approximation is a function of x cubed (x in radians).
- The sin rule can be expressed as a truncated Taylor Series , with the truncated term representing the error.
- This rule is second order accurate...terms higher than the second order term in the Taylor Series are ignored.

Error Propagation

- Taylor Series used to estimate the error propagation in calculations.
- If an independent variable has a known (or estimated) uncertainty, its error will propagate to the dependent variable.

$$f(x \pm e) = f(x) + \frac{(\pm e)^1}{1!} f^{'}(x) + \frac{(\pm e)^2}{2!} f^{''}(x) + \frac{(\pm e)^3}{3!} f^{'''}(x) \ldots$$
$$f(x \pm e) - f(x) \approx \frac{(\pm e)^1}{1!} f^{'}(x) + \frac{(\pm e)^2}{2!} f^{''}(x)$$
$$E \approx \frac{(\pm e)^1}{1!} f^{'}(x) + \frac{(\pm e)^2}{2!} f^{''}(x)$$

- Error of a function is roughly equal to the product of its derivative and error of independent variable.
- For functions with more curvature, the second term needed to estimate error properly.

Example: You determine that sediment is deposited at a rate (R)of 10cm/yr. At a poorly exposed outcrop, you estimate the thickness of the sediment (b)to be $57\,m \pm 5\,m$. What is your estimate for the time (t) it took to deposit the sediment?

Simple answer:

$$t = \frac{b}{R} = \frac{57}{.1} = 570\,yrs$$

Answer with error:

$$t = \frac{b \pm e}{R} \approx \frac{b}{R} \pm \frac{e}{R} \approx 570\,yrs \pm 50yrs$$

Error Propagation- Addition

Error Propagation in functions with more than one variable can also be evaluated using the Taylor Series.

$$\begin{aligned} f(x, y) &= x + y \\ f(x \pm e_x, y \pm e_y) &= f(x, y) + \left(\pm e_x \frac{\partial}{\partial x} + \pm e_y \frac{\partial}{\partial y} \right) \frac{f(x, y)}{1!} \\ &\quad + \left(\pm e_x \frac{\partial}{\partial x} + \pm e_y \frac{\partial}{\partial y} \right)^2 \frac{f(x, y)}{2!} \ldots \\ f(x \pm e_x, y \pm e_y) - f(x, y) &\approx \left(\pm e_x \frac{\partial (x + y)}{\partial x} + \pm e_y \frac{\partial (x + y)}{\partial y} \right) \\ E &\approx \pm e_x + \pm e_y = \pm(e_x + e_y) \end{aligned}$$

Results are identical for subtraction

Error propagation continued...Multiplication

$$\begin{aligned}
f(x,y) &= x\cdot y\\
f(x\pm e_x, y\pm e_y) =& f(x,y) + \left(\pm e_x\frac{\partial}{\partial x} + \pm e_y\frac{\partial}{\partial y}\right)\frac{f(x,y)}{1!}\\
&+ \left(\pm e_x\frac{\partial}{\partial x} + \pm e_y\frac{\partial}{\partial y}\right)^2\frac{f(x,y)}{2!}\dots
\end{aligned}$$

$$\begin{aligned}
E =& \left(\pm e_x\frac{\partial(x\cdot y)}{\partial x} + \pm e_y\frac{\partial(x\cdot y)}{\partial y}\right)\\
&+ \left((\pm e_x)^2\frac{\partial^2}{\partial x^2} + 2(\pm e_y)(\pm e_x)\frac{\partial^2}{\partial y\partial x} + (\pm e_y)^2\frac{\partial^2}{\partial y^2}\right)\frac{(x\cdot y)}{2!}\dots\\
E &\approx \pm e_x\cdot y + \pm e_y\cdot x + 0 + (\pm e_y)(\pm e_x) + 0\\
\frac{E}{x\cdot y} &\approx \frac{\pm e_x}{x} + \frac{\pm e_y}{y} + \frac{(\pm e_y)(\pm e_x)}{x\cdot y}
\end{aligned}$$

Error propagation continued...Division

$$\begin{aligned}
f(x,y) &= \frac{x}{y}\\
E =& \left(\pm e_x\frac{\partial(\frac{x}{y})}{\partial x} + \pm e_y\frac{\partial(\frac{x}{y})}{\partial y}\right)\\
&+ \left((\pm e_x)^2\frac{\partial^2}{\partial x^2} + 2(\pm e_y)(\pm e_x)\frac{\partial^2}{\partial y\partial x} + (\pm e_y)^2\frac{\partial^2}{\partial y^2}\right)\frac{(\frac{x}{y})}{2!}\dots\\
E =& \left(\pm e_x\frac{1}{y} + \pm e_y\frac{-x}{y^2}\right)\\
&+ \left(0 + 2(\pm e_y)(\pm e_x)\frac{-1}{y^2} + (\pm e_y)^2\frac{2\cdot x}{y^3}\right)\frac{1}{2!}\dots\\
E &\approx \frac{\pm e_x}{y} + \frac{\pm e_y(-x)}{y^2} + \frac{-(\pm e_y)(\pm e_x)}{y^2} + \frac{(\pm e_y)^2 x}{y^3}
\end{aligned}$$

The maximum value will at $+e_x, -e_y \to f(x+e_x, y-e_y) = \left(\frac{x+e_x}{y-e_y}\right)$:

$$E \approx \frac{e_x}{y} + \frac{e_y\cdot x}{y^2} + \frac{(e_y)(e_x)}{y^2} + \frac{(e_y)^2 x}{y^3}$$

similarly, the function is at its minimum when:

$$E \approx \frac{-e_x}{y} + \frac{-e_y\cdot x}{y^2} + \frac{(e_y)(e_x)}{y^2} + \frac{(e_y)^2 x}{y^3}$$

therefore:

$$E \approx \pm\left(\frac{e_x}{y} + \frac{e_y\cdot x}{y^2}\right) + \frac{(e_y)(e_x)}{y^2} + \frac{(e_y)^2 x}{y^3}$$

Divide by $\frac{x}{y}$ to turn this expression into a relative error.

$$\frac{E}{x/y} \approx \pm\left(\frac{e_x}{x} + \frac{e_y}{y}\right) + \frac{(e_y)(e_x)}{x\,y} + \frac{(e_y)^2}{y^2}$$

As a first order approximation,

- absolute errors add when adding and subtracting

$$E \approx \pm(e_x + e_y)$$

- relative errors add when multiplying and dividing

$$\frac{E}{f(x,y)} \approx \pm\left(\frac{e_x}{x} + \frac{e_y}{y}\right)$$

Example: Sedimentation problem revisited-the sedimentation rate has uncertainty associated with it. You determine that sediment is deposited at a rate (R)of 10cm/yr with an uncertainty of 2 cm/yr. How good is the estimate for time required to deposit the $57\,m \pm 5\,m$ of sediment?

$$t = \frac{b \pm e_b}{R \pm e_R}$$
$$E \approx \pm \left(\frac{5}{.1} + \frac{.02 \cdot 57}{.01} \right) = 50 + 114 = 164$$
$$t \approx 570 \pm 164 yrs$$

- higher order terms needed to accurately estimate the error
- this estimate of uncertainty clearly shows how poorly constrained the value is.

Numerical Differentiation

- Numerical methods commonly use Taylor Series to estimate derivatives.
- Based on set of equations based on Taylor Series
- combine equations (so terms cancel) and truncate
- provides estimate of error

Forward and backwards approximations, to fourth-order term:

$$f(x+\Delta x) = f(x) + \Delta x \frac{d}{dx}(f(x)) + \frac{1}{2}\Delta x^2 \frac{d^2}{dx^2}(f(x)) + \frac{1}{6}\Delta x^3 \frac{d^3}{dx^3}(f(x)) + \frac{1}{24}\Delta x^4 \frac{d^4}{dx^4}(f(x))$$
$$f(x-\Delta x) = f(x) - \Delta x \frac{d}{dx}(f(x)) + \frac{1}{2}\Delta x^2 \frac{d^2}{dx^2}(f(x)) - \frac{1}{6}\Delta x^3 \frac{d^3}{dx^3}(f(x)) + \frac{1}{24}\Delta x^4 \frac{d^4}{dx^4}(f(x))$$

What are estimates for $\frac{d}{dx}(f(x))$ and $\frac{d^2}{dx^2}(f(x))$?

$$f(x+\Delta x) - f(x-\Delta x) = 2\Delta x \frac{d}{dx}(f(x)) + \frac{1}{3}\Delta x^3 \frac{d^3}{dx^3}(f(x))$$
$$\frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} \approx \frac{d}{dx}(f(x))$$

$$f(x+\Delta x) + f(x-\Delta x) = 2f(x) + \Delta x^2 \frac{d^2}{dx^2}(f(x)) + \frac{1}{12}\Delta x^4 \frac{d^4}{dx^4}(f(x))$$
$$\frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} \approx \frac{d^2}{dx^2}(f(x))$$

Notice that we are shifting the focus from calculating values of a function based on knowledge at a single point to using known points to calculate derivatives.

Example
A geologist collects samples every 1000 m along a 3 km transect. She measures the following Reevium concentration, a shiny and very valuable metal, from south to north: 10, 40, 50, and 10 ppm. Estimate the Reevium concentration along the transect.

Plan of attack

- Estimate derivatives at points along transect
- Construct Taylor Series

$$\frac{dC}{dx}_{1000} = \frac{50-10}{2000} = 0.02$$
$$\frac{d^2C}{dx^2}_{1500} = \frac{\frac{10-40}{2000} - \frac{50-10}{2000}}{1000} = -3.5 \cdot 10^{-5}$$
$$\frac{d^2C}{dx^2}_{1000} = \frac{50 - 2 \cdot 40 + 10}{1000^2} = -2 \cdot 10^{-5}$$
$$\frac{d^3C}{dx^3}_{1250} = \frac{\frac{d^2C}{dx^2}_{1500} - \frac{d^2C}{dx^2}_{1000}}{500} = -3 \cdot 10^{-8}$$

$$C(1000 + \Delta x) \approx 40 + 0.02 \cdot \Delta x + -2 \cdot 10^{-5}\frac{\Delta x^2}{2} + -3 \cdot 10^{-8}\frac{\Delta x^3}{6}$$

Finite Diff. based on polynomials

An alternative way of estimating derivatives based on known values at different locations and fitting a polynomial to the data.

- pick simplest polynomial that fits data perfectly
- set up equation at each data point and solve for unknown coefficients
- take derivative of polynomial equation and substitute in coefficients

Two-point example

- pick simplest polynomial that perfectly fits data (linear for two points, quadratic for three, etc.)

$$f(x) = A_0 + A_1 \cdot x$$

- write equations for points:

$$f(\Delta x) = A_0 + A_1 \cdot \Delta x$$
$$f(-\Delta x) = A_0 - A_1 \cdot \Delta x$$

- calculate derivatives:

$$f'(x) = A_1$$

Two-point example Cont.

- combine equations:

$$f(\Delta x) - f(-\Delta x) = 2 \cdot A_1 \cdot \Delta x$$
$$f(\Delta x) - f(-\Delta x) = 2 \cdot f'(x) \;\cdot \Delta x$$
$$f'(x) = \frac{f(\Delta x) - f(-\Delta x)}{2 \cdot \Delta x}$$

- a similar approach can be used with higher order polynomials and a greater number of 'known' data points.

Three-point example

2nd order Polynomial fits 3 data points,set x=0 (approx. not dependent on position):

$$f(x) = a \cdot x^2 + b \cdot x + c$$
$$f(x + \Delta x) = a \cdot (x + \Delta x)^2 + b \cdot (x + \Delta x) + c$$
$$f(x - \Delta x) = a \cdot (x - \Delta x)^2 + b \cdot (x - \Delta x) + c$$

$$f'(x) = 2 \cdot a \cdot x + b$$
$$f''(x) = 2 \cdot a$$

$$f(0 + \Delta x) - f(0 - \Delta x) = 2 \cdot b \cdot \Delta x$$
$$f(0 + \Delta x) - f(0 - \Delta x) = 2 \cdot (f'(0) - 2 \cdot a \cdot (0)) \cdot \Delta x$$
$$f'(x) = \frac{f(0 + \Delta x) - f(0 - \Delta x)}{2 \cdot \Delta x}$$

Three-point example

$$f(0 + \Delta x) + f(0 - \Delta x) = 2 \cdot a \cdot \Delta x^2 + 2 \cdot c$$
$$f(0 + \Delta x) + f(0 - \Delta x) = 2 \cdot a \cdot \Delta x^2 + 2 \cdot f(x)$$
$$f(0 + \Delta x) + f(0 - \Delta x) = 2 \cdot \left(\frac{f''(x)}{2}\right) \cdot \Delta x^2 + 2 \cdot f(x)$$
$$f''(x) = \frac{f(x + \Delta x) - 2 \cdot f(x) + f(x - \Delta x)}{\Delta x^2}$$

This method is useful for defining forward/backward approx. and approx. with telescoping grid spacing.

Miscellaneous Comments

- differential is an infinitely small amount
- derivative is a rate of change