## Approximating Functions

Consider the geometric series (a=1, r=x)

$$1+x+x^2+x^3+x^4+\ldots+x^{n-1}=\frac{1-x^n}{1-x}$$

But, written the other way round, this is a *polynomial expansion* of a function;

$$\frac{1-x^n}{1-x}=1+x+x^2+x^3+x^4+\ldots+x^{n-1}$$

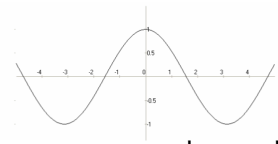
## Power Series - Maclaurin

In general a function may be *expanded* in a *power series* defined as;

$$f(x)=c_0+c_1x+c_2x^2+c_3x^3+\ldots+c_nx^n+\ldots$$

Here, all of the polynomial terms are centred on x=0, it is and *expansion about the point x=0* or a *Maclaurin Series.*

## For example : cos($x$)

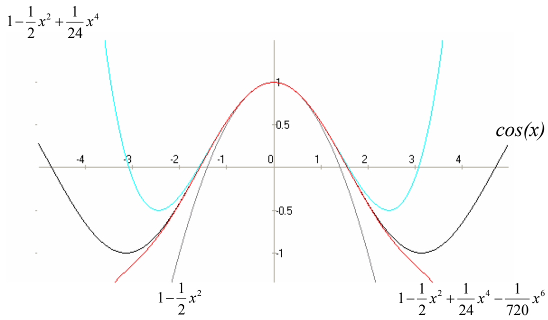



Note: $x$ measured in radians

$$\cos(x)=1-\frac{1}{2}x^2+\frac{1}{24}x^4-\frac{1}{720}x^6+\ldots$$

- We'll see why this is the expansion later
- More terms → the power series becomes more accurate for a wider range of values of $x$

$$\cos(x)=1-\frac{1}{2}x^2+\frac{1}{24}x^4-\frac{1}{720}x^6+\ldots$$




## Why bother ?

- Approximating an analytic function by its series expansion often helps us to visualise and understand its behaviour – eg: <E>(T) in the problem class.
- Series can be used to represent experimental data when you don't know the analytic form (eg: curve fitting, drawing a straight line…).

## Finding the coefficients: Maclaurin

***$c_0$***

$$f(x)=c_0+c_1x+c_2x^2+c_3x^3+\ldots$$

$$f(0)=c_0+c_1\times 0+c_2\times 0+c_3\times 0+\ldots=c_0$$

***$c_1$***

$$\frac{df}{dx}=c_1+2c_2x+3c_3x^2+4c_4x^3+\ldots$$

$$\left.\frac{df}{dx}\right|_{x=0}=c_1$$

$c_2$

$$\frac{d^2f}{dx^2} = 2c_2 + 2\times3c_3 + 3\times4c_4x^2 + \ldots$$

$$\left.\frac{d^2f}{dx^2}\right|_{x=0} = 2!c_2$$

$c_3$

$$\frac{d^3f}{dx^3} = 2\times3c_3 + 2\times3\times4c_4x + \ldots$$

$$\left.\frac{d^3f}{dx^3}\right|_{x=0} = 3!c_3$$

## The coefficients are the derivatives

$$c_0 = f(0)$$

$$c_1 = \left.\frac{df}{dx}\right|_{x=0}$$

$$c_2 = \frac{1}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=0}$$

$$c_3 = \frac{1}{3!}\left.\frac{d^2f}{dx^2}\right|_{x=0}$$

$$\ldots$$

$$c_n = \frac{1}{n!}\left.\frac{d^nf}{dx^n}\right|_{x=0}$$

That's it - you can now expand any function !

## The Maclaurin Series - Summary

$$f(x) = f(0) + \left.\frac{df}{dx}\right|_{x=0} x + \frac{1}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=0} x^2 + \frac{1}{3!}\left.\frac{d^3f}{dx^3}\right|_{x=0} x^3 + \ldots$$

Knowledge of all of the derivatives at one point completely determines any well behaved function (eventually)

## Maclaurin for cos(x)

$$\cos(0) = 1$$

$$\left.\frac{d}{dx}\cos(x)\right|_{x=0} = -\sin(0) = 0$$

: All odd derivs 0

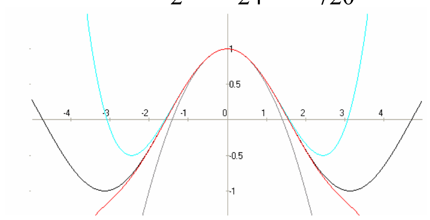
$$\left.\frac{d^2}{dx^2}\cos(x)\right|_{x=0} = -\cos(0) = -1$$

: Even derivs alternate -1, +1, -1, +1 etc..

$$\ldots$$

$$\cos(x) = 1 - \frac{1}{2!}x^2 + \frac{1}{4!}x^4 - \frac{1}{6!}x^6 + \ldots$$

$$\cos(x) = 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 - \frac{1}{720}x^6 + \ldots$$




It works well for small $x$ – how many terms would we need to approximate a whole cycle of cos($x$) ?

## Power Series - Taylor

It may be convenient to expand about some other point, eg: x=a, then the power series is;

$$f(x) = c_0 + c_1(x-a) + c_2(x-a)^2 + c_3(x-a)^3 + \ldots$$

Expansion about the point x=a is a *Taylor Series*.

## Taylor Series

The analysis is very similar to the Maclaurin series leading to;

$$f(x) = f(a) + \left.\frac{df}{dx}\right|_{x=a}(x-a) + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x=a}(x-a)^2 + $$
$$+\frac{1}{3!}\left.\frac{d^3 f}{dx^3}\right|_{x=a}(x-a)^3 + \ldots$$

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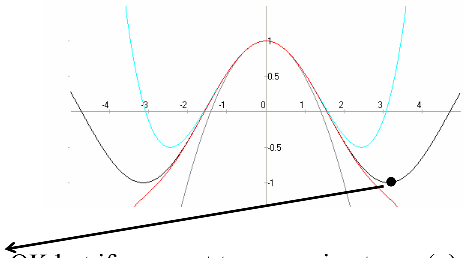
$$\cos(x) = 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 + \frac{1}{720}x^6 + \ldots$$




OK but if we want to approximate cos(x) at x=π we will need a lot of terms – better to expand about x= π using a Taylor expansion.

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## cos(x) : Taylor Series

$\cos(\pi) = -1$

$\frac{d}{dx}\cos(x)\Big|_{x=\pi} = -\sin(\pi) = 0$ : All odd derivs 0

$\frac{d^2}{dx^2}\cos(x)\Big|_{x=\pi} = -\cos(\pi) = +1$ : Even derivs alternate +1, -1, +1, -1 etc..

…

So …

$$\cos(x) = -1 + \frac{1}{2!}(x-\pi)^2 - \frac{1}{4!}(x-\pi)^4 + \frac{1}{6!}(x-\pi)^6 - \ldots$$

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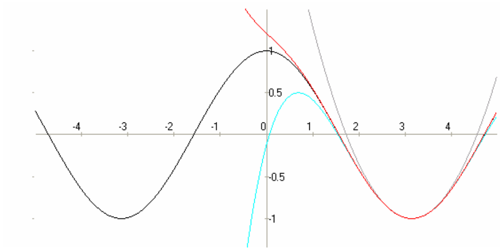
$$\cos(x) = -1 + \frac{1}{2!}(x-\pi)^2 - \frac{1}{4!}(x-\pi)^4 + \frac{1}{6!}(x-\pi)^6 - \ldots$$




Now an excellent approximation at x=π with a few terms.

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## Summary

- Knowledge of the derivatives of a function can be used to make a polynomial expansion which, if you use enough terms, reproduces the function exactly
- A Maclaurin series achieves this by expansion about x=0
- Faster convergence can be achieved away from x=0 by using a Taylor series which expands about any point, eg: x=a.

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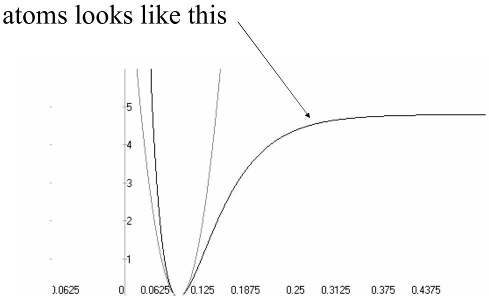
## Potential Energy of a Diatomic Molecule

In $H_2$ the potential energy of interaction of the atoms looks like this



## The Morse Potential

To a good approximation the potential energy is give by the Morse form which is;

$$E(r) = D_e \left\{1 - e^{-\alpha(r-a)}\right\}^2$$

with, De=4.79eV, a = 0.074 nm and α=19.3 nm$^{-1}$.

## Problem Class 2

Compute an Harmonic approximation to the Morse potential for $H_2$ and thus compute the vibrations of the molecule.