Sequences

A sequence is:

1. A list of numbers

$$a_1, a_2, a_3, a_4, \ .... \ , a_n$$

2. A function whose domain is the set of all positive integers ie: $a_n = a(n)$

Sequences and Series

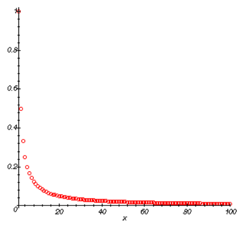
1, 3, 5, 7, 9, 11, …..

-999, 807, 54, 1, -10, -50, ….

1 + ½ + 1/3 + ¼ + 1/5 + 1/6 +…..

Example 1

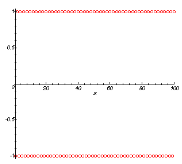
$$a_n = \frac{1}{n}$$



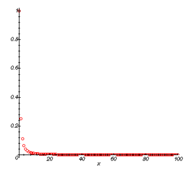
n	1	2	3	4	5	…
a_n	1	½	1/3	¼	1/5	…

More Examples

$$a_n = \{(-1)^n\}_{n \geq 1}$$



$$1, \frac{1}{4}, \frac{1}{9}, ... \frac{1}{n^2}$$



Recursive Definition of a Sequence

$$a_1 = 2$$

$$a_{n+1} = \frac{a_n}{2} + \frac{1}{a_n}$$

n	1	2	3	4	…
a_n	2	3/2	17/12	577/408	…

The Limit of a Sequence

The limit, L, of the sequence $\{a_n\}$ is;

$$L = \lim_{n \to \infty} \{a_n\}$$

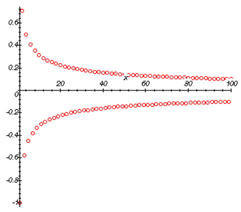
If an n exists such that $|L - a_n| < \varepsilon$ for any $\varepsilon > 0$.

A sequence may be *convergent*, *divergent* or *conditionally convergent*

Limits - Examples

$$\lim_{n\to\infty}\{1/n\}=0$$

$$\lim_{n\to\infty}\left\{\frac{(-1)^n}{\sqrt{n}}\right\}=0$$

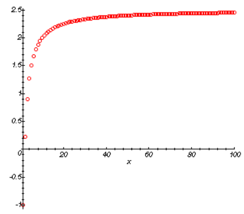


Finding Limits…

Sometimes the limit is not obvious:

$$\lim_{n\to\infty}\left\{\frac{5n^2-10n+2}{2n^2+1}\right\}$$

For large n the n^2 term dominates.. L=5/2



Series

A series is a summed list of numbers:

$$S_n = a_1 + a_2 + a_3 + a_4 + \;....\; + a_n$$

S_n is a number – the partial sum of n-terms of the series. This is usually written:

$$S_n = \sum_{i=1}^{n} a_i$$

Convergence of a Series

The infinite series, $\sum_{i=1}^{\infty} a_i$

Is *convergent* if,

$$\lim_{n\to\infty} S_n = \lim_{n\to\infty}\sum_{i=1}^{n} a_i = L$$

and *divergent* if the sequence of its partial sums S_n does not converge

The n^{th} term test

The series, $\sum_{i=1}^{n} a_i$

Will converge if,

$$\lim_{n\to\infty} a_n = 0$$

and will diverge otherwise.

Series in Chemistry

Many problems require series:

- The partition function $Z = \sum_{i=1}^{\infty} e^{-\varepsilon_i/kT}$

- Solutions of differential equations
- Huckel theory / LCAO
- Fourier analysis
- Bond energy sums

The Arithmetic Series

$$S_n = a + [a+d] + [a+2d] + \ldots + [a+(n-1)d]$$
$$= \sum_{i=1}^{n} \left[a + d(i-1)\right]$$

For example with a=1 and d=1;

$$S_6 = 1+2+3+4+5+6$$

Summing The Arithmetic Series

This series is sufficiently simple for its partial sum to be written in closed form:

$$S_n = \frac{n}{2}\left[2a + (n-1)d\right]$$

So the sum of the first n integers is:

$$S_n = 1+2+3+\ldots+n = \frac{1}{2}n(n+1)$$

Proof !

Just write the series out forward and backwards

$$S_n = a + [a+d] + \ldots. + [a+(n-1)d]$$
$$S_n = [a+(n-1)d] + [a+(n-2)d] + \ldots.. + a$$

Add the two series term by term,

$$2S_n = [2a+(n-1)d] + [2a+(n-1)d] + \ldots.. + [2a+(n-1)d]$$
$$2S_n = n\left[2a+(n-1)d\right]$$
$$S_n = \frac{n}{2}\left[2a+(n-1)d\right]$$

The Geometric Series

$$S_n = a + ar + ar^2 + \ldots + ar^{n-1}$$
$$= \sum_{i=1}^{n} ar^{i-1}$$

For example with a=1 and r=2;

$$S_6 = 1+2+4+8+16+32$$

Summing the Geometric Series

$$S_n = a + ar + ar^2 + \ldots + ar^{n-1}$$
$$rS_n = ar + ar^2 + \ldots + ar^{n-1} + ar^n$$
$$S_n - rS_n = a - ar^n$$
$$S_n(1-r) = a(1-r^n)$$
$$S_n = a\frac{(1-r^n)}{(1-r)}, \qquad (for, r \neq 1)$$

GS is a Polynomial Expansion

$$a + ar + ar^2 + \ldots + ar^{n-1} = a\frac{(1-r^n)}{(1-r)}$$

Eg: for a=1;

$$\frac{(1-r^n)}{(1-r)} = 1 + r + r^2 + \ldots + r^{n-1}$$

The Infinite Geometric Series

$$S_n = a + ar + ar^2 + ...$$
$$= \sum_{i=1}^{\infty} ar^{i-1}$$

$$\lim_{n\to\infty} S_n = \lim_{n\to\infty} a\frac{(1-r^n)}{(1-r)} = a\frac{1}{1-r},\ if\ |r| < 1$$

Infinite GS: power series expansion

$$\frac{1}{(1-r)} = 1 + r + r^2 + r^3 + ...,\quad for\,|\,r\,| < 1$$

The geometric series with a=1 is the power series expansion of $(1-r)^{-1}$.

This series converges for |r|<1 and diverges otherwise.

The Convergence of Series…

The convergence of a series is not always immediately apparent from inspection ?

Example: The *harmonic series* looks at first sight as if it should converge !

$$S = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} +$$

The Harmonic Series

$$S = 1 + \frac{1}{2} + \left(\frac{1}{3} + \frac{1}{4}\right) + \left(\frac{1}{5} + \frac{1}{6} + \frac{1}{7} + \frac{1}{8}\right) +$$
$$+ \left(\frac{1}{9} + \frac{1}{10} + \frac{1}{11} + \frac{1}{12} + \frac{1}{13} + \frac{1}{14} + \frac{1}{15} + \frac{1}{16}\right)$$

$$S = 1 + \frac{1}{2} + s_1 + s_2 + s_3 + ... + s_n$$

The Harmonic Series II

Each of the partial sums, s_n, contains 2^n terms each of which has a smallest term $1/2^{n+1}$.

So, each $s_n > 2n.(1/2^{n+1}) = 1/2$.

So,

$$S > 1 + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + ...$$

which, diverges

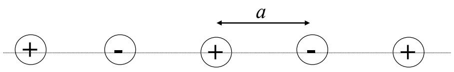
The Alternating Harmonic Series

$$E = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - ... = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n}$$

This series is *conditionally convergent* in short we can make it converge to *any answer* we want…

so what ?

Ionic Bonding !



The energy of a chain of ions of alternating charge (*q*) separation *a* is;

$$E = -\frac{2q^2}{4\pi\varepsilon_0 a}\left(1-\frac{1}{2}+\frac{1}{3}-\frac{1}{4}+\frac{1}{5}-\right) \quad \text{Joules/ion}$$

This is the alternating harmonic series….

So – what is the energy of rocksalt Na^+Cl^- ?

Conditional Convergence

The limit of the alternating harmonic series depends on how we arrange the sum of the terms, so…

We can make it converge to any number - for example 2.0000

Note: There are an infinite number of terms and we can add them in *any order* – however we decide to do that we will never run out of positive or negative terms.

Alternating Harmonic Series = 2.000

Strategy:

- Sum just positive terms to get a sum > 2
- Subtract a single negative term
- Add more positive terms until > 2
- Subtract a single negative term
- Repeat for ever

And… it must converge to 2.

Alternating Harmonic Series = 2.000

$$1+\frac{1}{3}+\frac{1}{5}+....+\frac{1}{15}=2.021800422$$

$$-\frac{1}{2}=1.521800422$$

$$+\frac{1}{17}+\frac{1}{19}+\frac{1}{21}+.....+\frac{1}{41}=2.004063454$$

$$-\frac{1}{4}=1.754063454$$

$$+\frac{1}{43}+\frac{1}{45}+.....+\frac{1}{69}=2.009446048$$

Etc…

How odd is that ?

This may seem very strange.

But..

We have an infinite number of +ve and –ve terms – it doesn't matter that we are using more +ve ones than –ve ones…

The sum, and thus the energy of a rocksalt crystal, converges to any number you want !!

The Energy of NaCl !!