Sequences

A sequence is:

1. A list of numbers
   \[ a_1, a_2, a_3, a_4, \ldots, a_n \]
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, ….
\[ 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} + \frac{1}{6} + \ldots \]

Example 1

\[ a_n = \frac{1}{n} \]

\[ n \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad \ldots \]
\[ a_n \quad \frac{1}{2} \quad \frac{1}{3} \quad \frac{1}{4} \quad \frac{1}{5} \quad \ldots \]

More Examples

\[ a_n = \left\{ (-1)^n \right\}_{n \geq 1} \]

\[ 1, \frac{1}{4}, \frac{1}{9}, \ldots, \frac{1}{n^2} \]

Recursive Definition of a Sequence

\[ a_1 = 2 \]
\[ a_{n+1} = a_n + \frac{1}{a_n} \]

\[ n \quad 1 \quad 2 \quad 3 \quad 4 \quad \ldots \]
\[ a_n \quad 2 \quad 3/2 \quad 17/12 \quad 577/408 \quad \ldots \]

The Limit of a Sequence

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

\[ L = \lim_{n \to \infty} \{a_n\} \]

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

A sequence may be convergent, divergent or conditionally convergent.
Limits - Examples

\[
\lim_{n \to \infty} \left\{ \frac{1}{n} \right\} = 0
\]

\[
\lim_{n \to \infty} \frac{(-1)^n}{\sqrt{n}} = 0
\]

Finding Limits…

Sometimes the limit is not obvious:

\[
\lim_{n \to \infty} \frac{5n^2 - 10n + 2}{2n^2 + 1}
\]

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

Series

A series is a summed list of numbers:

\[
S_n = a_1 + a_2 + a_3 + a_4 + \ldots + a_n
\]

\( S_n \) 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
  \[
  Z = \sum_{i=1}^{\infty} e^{-\frac{E_i}{kT}}
  \]

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

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

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:

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

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

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

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

Add the two series term by term,

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

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

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

The Geometric Series

\[ S_n = a + ar + ar^2 + \ldots + ar^{n-1} \]

\[ S_n = \sum_{i=1}^{n} ar^{i-1} \]

For example with \(a=1\) and \(r=2\):

\[ S_6 = 1 + 2 + 4 + 8 + 16 + 32 \]

Summing the Geometric Series

\[ S_n = a(1-r^n) \]

\[ rS_n = a(1-r^{n+1}) \]

\[ S_n - rS_n = a - ar^n \]

\[ S_n (1-r) = a(1-r^n) \]

\[ S_n = a \frac{(1-r^n)}{(1-r)}, \quad (\text{for } r \neq 1) \]

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

\[ S_n = a + ar + ar^2 + \ldots \]
\[ = \sum_{i=1}^{\infty} ar^{i-1} \]
\[ \lim_{n \to \infty} S_n = \lim_{n \to \infty} a \frac{(1-r^n)}{(1-r)} = a \frac{1}{1-r}, \text{ if } |r| < 1 \]

Infinite GS: power series expansion

\[ \frac{1}{(1-r)} = 1 + r + r^2 + r^3 + \ldots, \text{ for } |r| < 1 \]

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!

\[ S = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} + \frac{1}{6} + \frac{1}{7} + \frac{1}{8} + \frac{1}{9} + \frac{1}{10} + \frac{1}{11} + \frac{1}{12} + \frac{1}{13} + \frac{1}{14} + \frac{1}{15} + \frac{1}{16} + \ldots \]

\[ S = 1 + \frac{1}{2} + s_1 + s_2 + s_3 + \ldots + s_n \]

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,

\[ S > 1 + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \ldots \]

which, diverges

The Harmonic Series

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

\[ S = 1 + \frac{1}{2} + s_1 + s_2 + s_3 + \ldots + s_n \]

The Alternating Harmonic Series

\[ E = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \ldots = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \]

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:

\[
E = -\frac{2q^2}{4\pi\varepsilon_0a}\left(1 - \frac{1}{2} - \frac{1}{3} - \frac{1}{4} - \frac{1}{5}\right) \quad \text{Joules/ion}
\]

This is the alternating harmonic series....
So – what is the energy of rocksalt NaCl?  

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

\[
\begin{align*}
1 + \frac{1}{3} + \frac{1}{5} + & \ldots + \frac{1}{15} = 2.021800422 \\
& - \frac{1}{2} = 1.521800422 \\
& + \frac{1}{17} + \frac{1}{19} + \frac{1}{21} + & \ldots + \frac{1}{41} = 2.004063454 \\
& - \frac{1}{4} = 1.754063454 \\
& + \frac{1}{43} + \frac{1}{45} + & \ldots + \frac{1}{69} = 2.009446048 \\
\end{align*}
\]
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!!