MathCad Functions

Examples of built-in functions

- Trigonometry: \( \sin(x), \cos(x), \tan(x), \arcsin(x), \arccos(x), \arctan(x) \), …
- Truncation and rounding: \( \text{floor}(x), \text{ceil}(x), \text{trunc}(x), \text{mod}(x,y) \), …
- Log and exponential: \( \exp(x), \ln(x), \log(x), \log(x, [b]) \)
- Root finding and solving: \( \text{root}, \text{polyroot}, \text{lsove} \), …
- Statistics: \( \text{mean}, \text{median}, \text{stdev} \), …
- Regression: \( \text{linfit}, \text{expfit}, \text{genfit} \), …
- Boolean operations: \( \text{if}(\text{condition}, \text{TrueValue}, \text{FalseValue}) \), …
- Complex number functions: \( \text{Re}(z), \text{Im}(z), \text{arg}(z) \), …
- File access: \( \text{READFILE}, \text{READ_IMAGE} \), …
- String and text: \( \text{strlen}(S), \text{search}(S, \text{SubS}, x), \text{num2str}(x) \), …

User-defined functions

- You can define fairly complex functions in MathCAD using a combination of operators, logical statements, and built-in functions
- Once defined, the functions can be used in your worksheet multiple times

<table>
<thead>
<tr>
<th>Define function</th>
<th>MyFunction (x) := 3x^4 - 2x^2</th>
</tr>
</thead>
<tbody>
<tr>
<td>And use it in a calculation</td>
<td>MyFunction (4) = 736</td>
</tr>
<tr>
<td>And again ...</td>
<td>MyFunction (3) = 225</td>
</tr>
<tr>
<td>And again ...</td>
<td>MyFunction (8) = 1.216 \times 10^4</td>
</tr>
</tbody>
</table>
Inserting Built-In Functions

1. From the Calculator Window
   - The simplest functions such as square root, inverse, etc.
   \[
   \sqrt{\frac{356 - 24}{13}} = 5.054 \quad \frac{100!}{93! \cdot 7!} = 1.601 \times 10^{10} \quad \sqrt[3]{e^\pi} = 2.85
   \]
   \[
   3^3 = 7.626 \times 10^{12} \quad \ln(e^{10}) = 10 \quad \log_{10}(1024, 2) = 10
   \]
   \[
   \left(1 - \frac{1}{1000}\right)^{1000} = 0.368 \quad \left|(-18)^3\right| = 5.832 \times 10^{3}
   \]

2. From the "Insert Function" menu
   - Called by "Ctrl-E" or from "Insert" menu
   - Displays a list of functions
   
   **Very useful:** Pressing the "?" sign brings up the help window with information about this function.
Remember that:

- The default unit for the angle is rad (radian). If you do not specify a unit for the angle, MathCAD will assume it is in radians. Another unit you can use is deg (degrees).
- Inverse trigonometric functions will return the angle in radians by default.
  - 90 deg = π/2 rad (quarter circle)
  - 180 deg = π rad (half circle)
  - 360 deg = 2π rad (full circle)
  - etc.

Example of use

Convert into radians in your head if you are used to radians:

\[
\text{Length}_1 := 7\text{cm} \cdot \sin \left( \frac{\pi}{6} \right) \quad \text{Length}_1 = 3.5\text{cm}
\]

Or use the "deg" unit

\[
\text{Length}_2 := 7\text{cm} \cdot \sin(30\text{deg}) \quad \text{Length}_2 = 3.5\text{cm}
\]
Rounding Functions

It is often necessary to round real numbers to their closest integer values in calculations. MathCAD functions that do this include:

- **floor**(x) – rounds x to the closest integer value that is smaller or equal than x.
  - floor(5.61) = 5
  - floor(-3.17) = -4

- **ceil**(x) – rounds x to the closest integer value that is greater or equal than x.
  - ceil(5.61) = 6
  - ceil(-3.17) = -3

- **round**(x, n) – rounds x to n decimal places. If n is omitted, x is rounded to the nearest integer. If n < 0, x is rounded to the left of the decimal point.
  - round(33.456, 2) = 33.46
  - round(33.456, -1) = 30
  - round(33.456) = 33

**Example:** Calculate the number of NaCl molecules on a 2.3 nm x 2.3 nm surface of NaCl(001) crystal. The surface density of ion pairs for the NaCl(001) surface is $S_{NaCl} = 6.4 \times 10^{14}$ cm$^{-2}$.

\[
S_{NaCl} := 6.4 \times 10^{14} \cdot \frac{1}{\text{cm}^2}
\]

\[
\text{Area} := (2.3\text{nm})^2
\]

\[
N_{NaCl} := S_{NaCl} \cdot \text{Area} = 33.856
\]

\[
\text{answer} := \text{round}(N_{NaCl}) = 34
\]
User-Defined Functions

- Defined similar to a variable but has a list of dummy (undefined) arguments
- The right side of the equation contains mathematical manipulations on the arguments
  \[ \text{MyFunky}(x) := \left( \frac{x}{5} \right)^2 + \frac{\sin(3x)}{x} \]
- Once defined, the function can be used in calculations…
  \[ \text{MyFunky}(3) = 0.497 \]
- Or in plot:

![Graph of MyFunky(x) plot](Image)
Plotting Multiple Functions

- Multiple functions can appear in the same graph. Simply separate them with commas when entering them in the Y-axis placeholder.
- Practice: define and plot functions corresponding to radial wavefunctions of hydrogen atom for $\rho = 0-20$:

\[ H \text{- atom wavefunctions ( } \rho=2Zr/a_0) \]

\[
\Psi_{1s}(\rho) := 2 \exp\left(\frac{-\rho}{2}\right)
\]

\[
\Psi_{2s}(\rho) := \frac{1}{2\sqrt{2}} \left( 2 - \frac{\rho}{2} \right) \exp\left(\frac{-\rho}{4}\right)
\]

\[
\Psi_{3s}(\rho) := \frac{1}{9\sqrt{3}} \left( 6 - 2 \cdot \rho + \frac{\rho^2}{9} \right) \exp\left(\frac{-\rho}{6}\right)
\]
Rotational Energy Distribution

- Rotational energy levels of a diatomic
  
  \[ E_{\text{rot}} = BJ_{\text{rot}}(J_{\text{rot}} + 1) \]
  
  \[ B = \frac{\hbar^2}{8\pi^2 I} \quad \text{where} \quad I = \frac{m_1m_2}{m_1 + m_2} R^2 \]

- Probability for a molecule to be found in a given rotational state

  \[ Q = \text{rotational partition function} \]
  
  \[ k = 1.38 \times 10^{-23} \text{J/K} \quad \text{Boltzmann constant} \]

- Task

  Assume \( B=3.0 \times 10^{-23} \text{J} \)
  
  Assume \( T=300 \text{K} \)
  
  Define and plot the following functions using \( J_{\text{rot}} \) as a variable:
  - \( E(J_{\text{rot}}) \) – energy of a given rotational quantum state
  - \( P(J_{\text{rot}}) \) – probability to find the molecule in a given rotational quantum state
Things to watch out for: (1) MathCad selects the ranges for variables in plots automatically. Oftentimes, the MathCAD's choice is far from ideal. In such cases, you have to reset the scale manually. (2) Most MathCAD functions do not accept arguments with units. If you want to avoid problems it is safer to do your calculation without using units explicitly.
Conditional Statements

It is often necessary to assign a different value to a function depending on the value of a previous calculation. **IF** function is used for this purpose

\[
\text{if(condition, truevalue, falsevalue)}
\]

- Practice: define a function that is:
  \[
  = x \text{ for } |x| < 1 \\
  = 1 \text{ for } x \geq 1 \\
  = -1 \text{ for } x \leq -1
  \]

- Plot both functions to make sure they do what you expect. Select appropriate x,y-scales to make the functions clearly visible.

\[
F_2(x) := \text{if}(|x| < 1, 1, 0) \quad F_1(x) := \text{if}(|x| < 1, x, \text{sign}(x))
\]

Additional practice: define and plot a function that is:

\[
= x^2 \text{ for } |x| < 1 \\
= 1 \text{ for } x \geq 1
\]
Example of Using IF: Titration

Problem: titrate a given volume \( V_{\text{acid}} = 50 \text{ mL} \) containing a strong acid with concentration \( C_{\text{acid}} = 0.1 \text{ M} \) using a strong base with concentration \( C_{\text{base}} = 0.1 \text{ M} \)

The total volume during the titration:

\[ V_{\text{total}} = V_{\text{acid}} + V_{\text{base added}} \]

The initial number of moles of acid:

\[ n_{\text{acid}} = C_{\text{acid}}^0 \times V_{\text{acid}}^0 \]

The number of moles of base added:

\[ n_{\text{base}} = C_{\text{base}}^0 \times V_{\text{base added}} \]

An IF function is going to be necessary to decide whether to calculate \([H^+]\) or \([OH^-]\) during different points in the titration:

**BEFORE** the end-point \((n_{\text{acid}} > n_{\text{base}})\):

\[ [H^+] = \frac{(n_{\text{acid}} - n_{\text{base}})}{V_{\text{total}}} \]

**AT** the end-point \((n_{\text{acid}} = n_{\text{base}})\):

\[ [H^+] = [OH^-] = \sqrt{K_w} = 10^{-7} M \]

**AFTER** the end-point \((n_{\text{acid}} < n_{\text{base}})\):

\[ [OH^-] = \frac{(n_{\text{base}} - n_{\text{acid}})}{V_{\text{total}}} \quad [H^+] = \frac{K_w}{[OH^-]} \]
We define the known values of volumes and concentrations as the first step. The units are going to be implicit: L for volumes and mol/L for concentrations.

\[
V_{\text{acid}} := 0.050 \quad C_{\text{acid}} := 0.1 \quad C_{\text{base}} := 0.1 \quad K_w := 10^{-14}
\]

Now we can calculate the initial amount of acid in the solution (in mol)

\[
n_{\text{acid}} := V_{\text{acid}} \cdot C_{\text{acid}} = 5 \times 10^{-3}
\]

The added volume of base is going to be our variable in this example \((V_{\text{base}})\)

\[
V_{\text{solution}}(V_{\text{base}}) := V_{\text{acid}} + V_{\text{base}} \quad n_{\text{base}}(V_{\text{base}}) := C_{\text{base}} \cdot V_{\text{base}}
\]

At this point, we are ready to do the calculation using if functions. It is convenient to define some intermediate functions first.

before\((V_{\text{base}})\) := \(\frac{n_{\text{acid}} - n_{\text{base}}(V_{\text{base}})}{V_{\text{solution}}(V_{\text{base}})}\)

after\((V_{\text{base}})\) := \(\frac{K_w \cdot V_{\text{solution}}(V_{\text{base}})}{n_{\text{base}}(V_{\text{base}}) - n_{\text{acid}}}\)

\(a(V_{\text{base}}) := (K_w)^{0.5}\)

The first if statement calculates \([H^+]\) in different ways depending on whether we are before or after the equivalence point

\[
C_H(V_{\text{base}}) := \text{if}(n_{\text{acid}} > n_{\text{base}}(V_{\text{base}}), \text{before}(V_{\text{base}}), \text{after}(V_{\text{base}}))
\]

The second if is necessary in order to avoid discontinuities at the equivalence point

\[
C_{H\text{mod}}(V_{\text{base}}) := \text{if}(C_H(V_{\text{base}}) = 0, a(V_{\text{base}}), C_H(V_{\text{base}}))
\]

We are now ready to calculate the pH value as a function of the added volume of base

\[
pH(V_{\text{base}}) := -\log(C_{H\text{mod}}(V_{\text{base}}))
\]
Random Numbers

Random numbers are required in many calculations, e.g., Monte-Carlo simulations of molecular motion. MathCAD provides several useful random number generators. We will practice with the simplest one:

Function \( \text{rnd}(x) \) produces uniformly distributed random number between 0 and \( x \):

- Use \( \text{rnd}(1) \) repeatedly and see what you get each time
- Now define the function \( \text{Uniform}(\text{dummy}):=2*\text{rnd}(1)-1 \)
- Plot it over the y-range range of -1 to 1
- The result is so called "white noise" (the Fourier transform of white noise is a constant; all frequencies are equally represented)

\[
\text{Uniform}(\text{dummy}) := 2 \times \text{rnd}(1) - 1
\]

\[
\begin{align*}
\text{rnd}(1) &= 0.925 & \text{rnd}(1) &= 0.63 & \text{rnd}(1) &= 0.106
\end{align*}
\]
Application: Adding Noise to Waveforms

Sine wave parameters
Amplitude := 3
Frequency := 10
Phase := $\frac{\pi}{2}$

Sine wave using t (=time) as the independent variable

\[ \text{sine}(t) := \text{Amplitude} \cdot \sin(\text{Frequency} \cdot t + \text{Phase}) \]

Noise parameters

\[ \text{Noise} := \frac{\text{Amplitude}}{2} \]

Noisy sine function

\[ \text{noisy}(t) := \text{sine}(t) + \text{Noise} \cdot (\text{rnd}(1) - 0.5) \]
Plotting Two-Dimensional Functions

Functions of two variables can be plotted in three dimensions.

- Define the function $\text{Test}(x,y):=x^2-y^2$ (function that looks like a "saddle")
- Generate a surface plot of Test over the x and y range of -6 to 6
- Set rotation to 0, tilt to 30, and twist to 30
- Rotate it manually to view the plot from all angles
- Now generate a contour plot of Test with a color map

\[
\text{Test}(x,y) := x^2 - y^2
\]
Practice: 3D plotting

• Define/plot function:

$$\Psi(x, y) = \frac{1}{\sqrt{\pi}} e^{-\frac{x^2 + y^2}{2}}$$

• Define function and generate its contour and surface plots:

$$\Omega(x, y) = \sin(\sqrt{x^2 + y^2})$$