CHEM 3PC3 - Mathematical Tools for Chemical Problems

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Limits

- The function $1/x$ is not defined everywhere. It blows up at $x = 0$ where we divide by zero.
- Sometimes we can save a function from being undefined at some point.
- A silly example is $f(x) = x^2/x$. Which is initially not defined at $x = 0$.
- But we can see that $f(x) = x$.
- This is done by dividing by a common factor. We can see some examples.

Limits

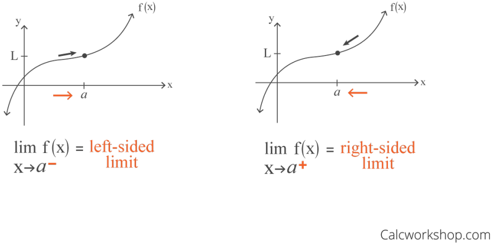
- The function $f(x) = (x^3 - 1)/(x - 1)$ is not defined at $x = 1$.
- But for x really close to 1 nothing bad happens.
- We can evaluate the function at points closer and closer to 1 and get closer and closer to a value.
- Using the difference of two cubes $(x^3 - 1^3) = (x - 1)(x^2 + x + 1)$.

$$f(x) = \frac{(x-1)(x^2+x+1)}{(x-1)} = x^2 + x + 1 \tag{1}$$

- And now when $x = 1$, there is a natural value associated with the function.
- Definition: We write $x \to a$ to indicate that x approaches a.

Limits

- Why do we worry about limits ? We will define derivatives and integrals using limits.
- The limit can be from either side, from the left $x \to a^-$ or from the right $x \to a^+$.



- A function $f(x)$ has a limit at a point a if exists a unique b such that:

$$\lim_{x \to a} f(x) = b \tag{2}$$

Rate of Change

- Given a function f and a constant $h > 0$, we can look at a new function:

$$Df(x) = \frac{f(x+h) - f(x)}{h}. \tag{3}$$

- Is the average rate of change of the function with step size h.
- When we take the limit $h \to 0$ we have the instantaneous rate of change.
- And we can derive important formulas: $\frac{d}{dx}x^n = nx^{n-1}$, $\frac{d}{dx}\exp(ax) = a\exp(x)$, $\frac{d}{dx}sin(ax) = acos(ax)$, $\frac{d}{dx}cos(ax) = -asin(ax)$.
- Definition: If the limit $\frac{d}{dx}f(x) = \lim_{h\to 0}\frac{f(x+h)-f(x)}{h}$ exist, we say f is differentiable at point x.

Continuity

- A function f is continuous at a point x_0 if a value of $f(x_0)$ can be found such that $f(x) \to f(x_0)$ for $x \to x_0$.
- Intuitively, a function is continuous if one can draw the graph of the function without lifting the pencil.
- Why do we like continuity ?
- Continuity also will be useful when finding maxima and minima.
- Finding discontinuities and plotting it is a work we can do in Python.

Graphs

- In Python, common practice is to use matplotlib for graphics.
- In matplotlib, a plot consists of a figure and one or more axes.
- Example: Determine for the function $f(x) = \log(|x^2 - 1|)$ where the discontinuities appear.
- This can be found by knowing that the log is only defined for positive values $x > 0$.
- So the discontinuities will show up when we evaluate log at zero i.e. $|x^2 - 1 = 0$.
- Which leads to two solutions $x = 1$ and $x = 1$.
- We can actually plot the function to see if our analysis hold.

Exercises

- Determine for each of the following functions, where discontinuities appear:
  - $f(x) = sin(cos(\pi/x))$
  - $f(x) = cot(x) + tan(x) + x^4$
  - $f(x) = (x^2 + 2x + 1)/(x + 10 + (x-1)^2/(x-1))$
  - $f(x) = (x^2 - 4x)/x$
- Evaluate:
  - $\lim_{z \to 8} \frac{2z^2 - 17z + 8}{8 - z}$
  - $\lim_{x \to 0} \frac{x}{3 - \sqrt{x+9}}$

1. Given the function

$$f(x) = \begin{cases} 7 - 4x, & x < 1, \\ x^2 + 2, & x \geq 1. \end{cases}$$

   Evaluate the following limits, if they exist.

   (a) $\lim\limits_{x \to -6} f(x)$

   (b) $\lim\limits_{x \to 1} f(x)$