**Differentials and Changes along Different Paths**

1. Let us recap some of the properties of differentials. Fill in the missing pieces below:

The general form for a differential in two variables is:

* describes the change of quantity as we take an infinitesimal step (\_\_\_) along the x-direction plus an infinitesimal step (\_\_\_) along the y-direction.
* and are the \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ of along the x- and y-direction.
* The differential is called *exact*, if:
* If is exact, then the change obtained by summing up *does / does not* depend on the path.
* If is exact, then *can / cannot* be represented as a function.
* The differential is called *inexact*, if:
* If is *in*exact, then the change obtained by summing up *does / does not* depend on the path.
* If is *in*exact, then *can / cannot* be represented as a function.

1. **Critical thinking question:** Can you think of a simple explanation why the sum over an *in*exact differential depends on the path, whereas the sum over an exact differential does not depend on the path? You could, for example, use the following information:

for an *in*exact differential

for an exact differential

*Now we’re going to investigate several differentials for (in)exactness and we’ll calculate changes along different pathways. We’ll use the MoCChA online tool to calculate sums over differentials.*

**Differential #1:**

1. Is this an exact or inexact differential?
2. Do you expect the sum of to depend on the path? Explain your answer.
3. Go to <https://hub-dev.crc.pitt.edu> -> run Chem1000/differentials.ipynb. This notebook calculates by summing up along a path.
   1. Calculate , i.e. the sum over , along the path from to .   
        
        
      Result:
   2. Calculate along the path from to .   
        
        
      Result:
   3. Compare the results for both pathways. Are and equal? Explain your finding.
   4. Repeat (a) and (b) with step size 0.01. Are and equal?

**Differential #2:**

1. Is this an exact or inexact differential?
2. Do you expect the sum of to depend on the path? Explain your answer.
3. Go to <https://hub-dev.crc.pitt.edu> -> run Chem1000/differentials.ipynb. This notebook calculates by summing up along a path.
   1. Calculate , i.e. the sum over , along the path from to . Use a step size of 0.1.  
        
        
      Result:
   2. Calculate along the path from to . Use a step size of 0.1.  
        
        
      Result:
   3. Compare the results for both pathways. Are and equal? Explain your finding.
   4. Repeat (a) and (b) with step size 0.01. Are and equal?

1. How could you improve the numerical simulation to achieve agreement with the expected result?

**Differential #3:**

1. Is this an exact or inexact differential?
2. Do you expect the sum of to depend on the path? Explain your answer.
3. Go to <https://hub-dev.crc.pitt.edu> -> run Chem1000/differentials.ipynb. This notebook calculates by summing up along a path.
   1. Calculate , i.e. the sum over , along the path from to . Use a step size of 0.1.  
        
        
      Result:
   2. Calculate along the path from to . Use a step size of 0.1.  
        
        
      Result:
   3. Compare the results for both pathways. Are and equal? Explain your finding.
   4. Repeat (a) and (b) with step size 0.01. Are and equal?

**Differential #4:**

1. Is this an exact or inexact differential?
2. Do you expect the sum of to depend on the path? Explain your answer.
3. Go to <https://hub-dev.crc.pitt.edu> -> run Chem1000/differentials.ipynb. This notebook calculates by summing up along a path.
   1. Calculate , i.e. the sum over , along the path from to . Use a step size of 0.1.  
        
        
      Result:
   2. Calculate along the path from to . Use a step size of 0.1.  
        
        
      Result:
   3. Compare the results for both pathways. Are and equal? Explain your finding.
   4. Repeat (a) and (b) with step size 0.01. Are and equal?