2023/24
Science Society
Newsletter
October 2023

Rat's Monthly Science Quest

1) There are n rats in a field in circle shape. Find the probability p_n such that the rats lie on a semicircle. Assume that the rats are points.
2) Generally, consider $0° < \theta < 360°$ and find the probability that the n rats lie in a sector with an angle θ.

Junior form students need to at least answer question 1. Senior form students need to attempt question 2. Submit your answer (Steps are optional but recommended) to the collection box outside the staff room or email your answer to s201901056@ccchwc.edu.hk.

From Combinatorics to Combinatorial Chemistry

(Disclaimer: Don't play Sudoku during the lesson.)

I believe that a lot of you love doing Sudoku in Sound of Science. Basic rule of Sudoku is to search for the missing 1 out of the 9 numbers in each row, column or sub square. Today, let's play some special - some variant of Sudoku.

- Anti-Knight Sudoku - Chess in Sudoku

	5				1			
							5	
					2			
	2							
1			9					
		9					8	
			2	7	6			
	4		8					

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Normal Sudoku rules apply but, in addition, the same number cannot appear in cells linked by a single knight's move in chess.

For example, x in the following figures mean that 1 cannot be put in those boxes.

	×		×	
×				×
		1		
×				×
	×		×	

There are some techniques in solving anti-knight Sudoku [1]:

- L shape technique: When there are only three cell possibilities remaining for a particular number (say A) which forms L shape then extend this L backwards two

steps back in both the direction forming + with original L shape. These two cells cannot have number A.

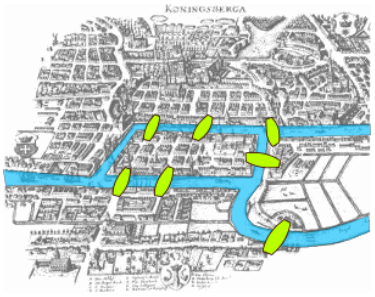
- Corners Box Technique: For any box, the central number in the next box touching the edge in the original box can lie only on the corners of the original box.
- Edge touching numbers: If in a box there are only two possibilities of a number (say B) which lies on the edge of the box and these two possibilities are one cell apart then number B cannot be in the immediately next cell in the touching box.

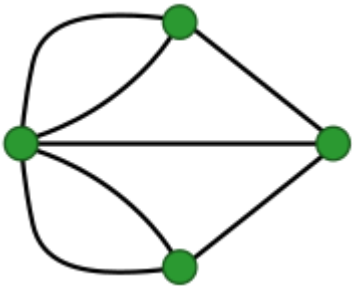
In fact, when solving the basic Sudoku, have you ever thought of some problems like “How many puzzles have exactly one solution?”, “How many puzzles with exactly one solution?”, “What is the maximum number of givens for a minimal puzzle?”. In fact, these questions related to combinatorics, a field of mathematics that studies counting.

In Chemistry, isomers are compounds that have the same formula but different arrangements of atoms. For instance, $C_{14}H_{10}$ and C_5H_{12} are isomers. However, have you ever considered the number of isomers a compound can have based on its molecular formula?

Combinatorial chemistry is distinct from typical combinatorics and counting problems found in math textbooks or Olympiad competitions. This is because isomers must abide by numerous chemical regulations that have many exceptions. Some arrangements are theoretically possible but cannot exist in reality due to electrostatic or packing restrictions. Therefore, enumerating all possibilities is a challenging and arduous task.

There is no general formula for calculating the number of isomers. To do isomer counting, we have to use the concept of graph theory.

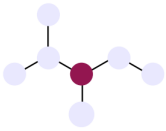




(Image from Wikipedia)

Seven Bridges of Königsberg, a famous question in graph theory

Is it possible to cross every bridge exactly once and start and end at the same spot? Picture on the right is the equivalent **graph** to the Seven Bridges of Königsberg.



Caylee Approach

Recursive approach: Counted the number of centric and bicentric trees centric tree bicentric tree Developed methods for counting

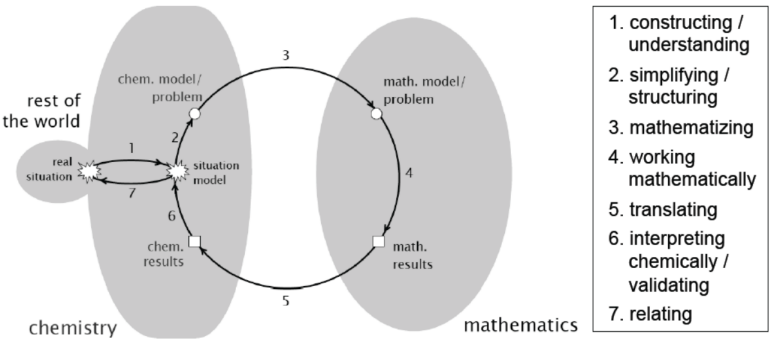
rooted and unrooted trees and then limited them to 4 vertices Successfully counted the number of C1-C11 alkanes Rather tedious process Gave incorrect answers for C12 and C13 alkanes.

In graph theory, a tree is an undirected graph in which any two vertices are connected by exactly one path.
A rooted tree is a tree in which one vertex has been designated the root.

Actually, Math is useful in Chemistry. One example is the rate equation. Consider a chemical reaction $mA + nB \rightarrow C$. The rate of reaction r is given by $r = -\frac{1}{m}\frac{d[A]}{dt}$ where $[A]$ is the activity of the reagent A.

Note: 1) A reagent is a substance or compound added to a system to cause a chemical reaction. If you want to understand activity of a substance, you can think about the metal: The activity of sodium is higher than gold.
2) You can think $\frac{d[A]}{dt}$ as the rate of change of the activity of the reagent A with respect to the time.

How can we solve a Chemistry problem with Math?



Source:
https://conference.pixel-online.net/NPSE/files/npse/ed0003/FP/0099-SSE94-FP-NPSE3.pdf

Math in Quantum Chemistry & Physical Chemistry
Quantum chemistry is a subfield of chemistry that applies the principles of quantum mechanics to the study of chemical systems. It involves the use of mathematical models and computational methods to describe the behavior of atoms, molecules, and other chemical systems at the quantum level.

At the heart of quantum chemistry is the Schrödinger equation, a fundamental equation in quantum mechanics that describes how the wavefunction of a physical system evolves over time. In quantum chemistry, the Schrödinger equation is used to calculate the electronic structure of atoms and molecules, which determines their chemical and physical properties.

By solving the Schrödinger equation for a given chemical system, we can predict a wide range of properties, such as the electronic energy levels, the geometry of the molecule, and the reactivity of the system. These predictions can be compared to experimental data to test the accuracy of the model and improve our understanding of chemical systems.

Quantum chemistry has numerous applications in chemistry, materials science, and other fields. For example, it can be used to design new materials with specific properties, such as conductivity or catalytic activity. It can also be used to study chemical reactions and reaction mechanisms, which is important for understanding how reactions occur and designing new synthetic routes.

Summary

To summarize, when we study Science, we may face a number of complex problems. To work on these, models and modelling are of great importance. Mathematical models, like equations or graphs, describe scientific facts or data by the means of mathematical terms. We also need to have an idea of interdisciplinary learning to have a completely different idea.

Resources

[1] https://www.funwithpuzzles.com/2017/01/anti-knight-sudoku-puzzles-index.html

[2] Diocesan Boys' School Mathematics Club "Why Chemistry Students Should Learn Mathematics?"

[3] https://macmillan.princeton.edu/wp-content/uploads/Graph-Theory-copy.pdf

Comic Zone

(Source: https://www.explainxkcd.com/wiki/index.php/465:_Quantum_Teleportation)

2023-2024 Science Society

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