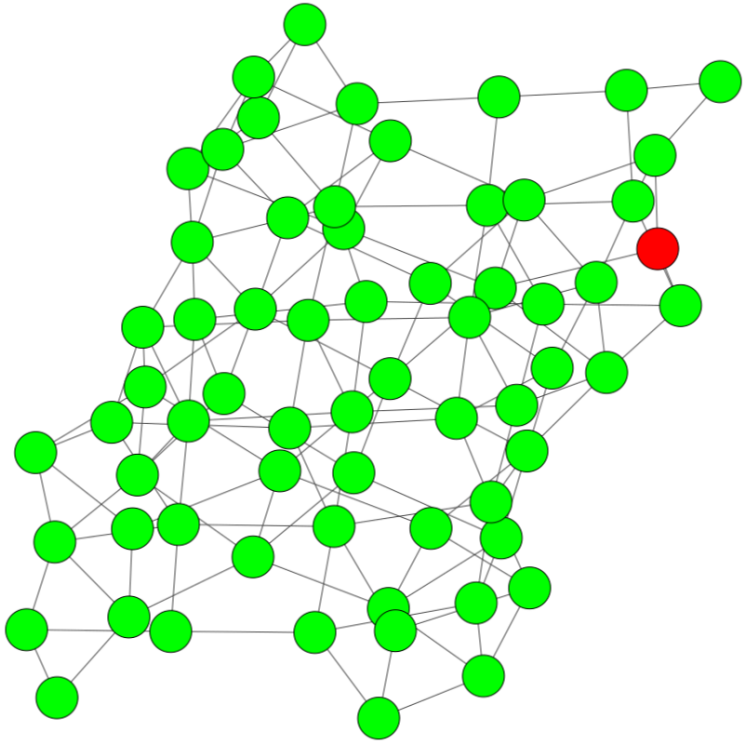
Report 2

Stoichiometric Space and Reaction Space

Cycles

- Catalytic Point is fixed
- Layouts won’t chage the number of cycles



Stoichiometric Space

- We consider an arbitrary Stoichiometry (NnHh) and assign it zero (Catalytic Point)
- CP = [0,0]
  CP + N2 = [2,0]
  CP +NH3 = [1,3]

$$S = \{(x,y) : -n-1 < x < n+1, -h-1 < y < h+1\}$$

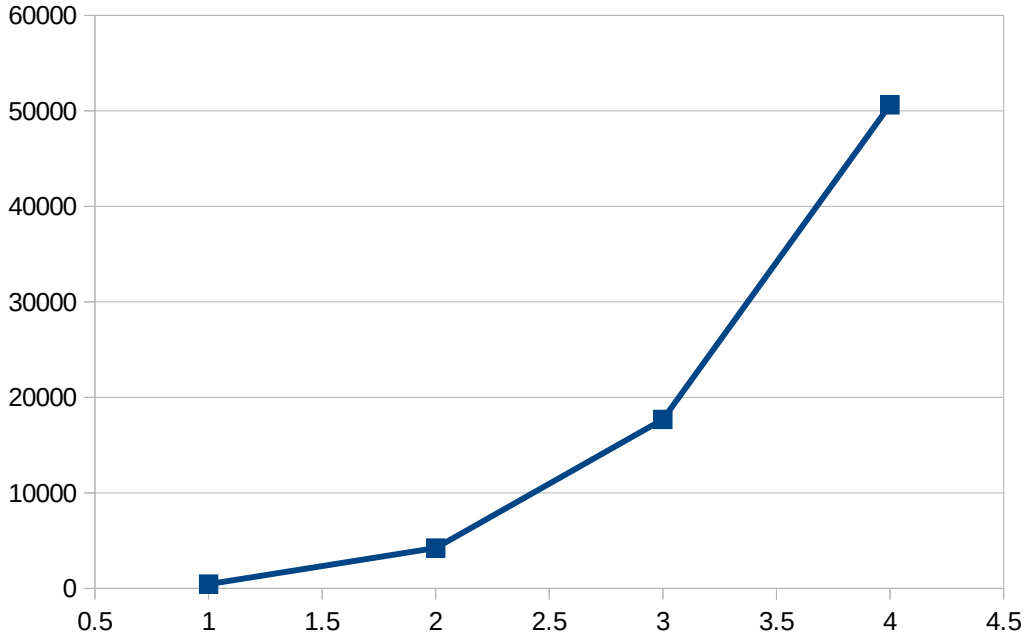
$$R = \{f : S \xrightarrow{f} S\}$$

R is reaction space

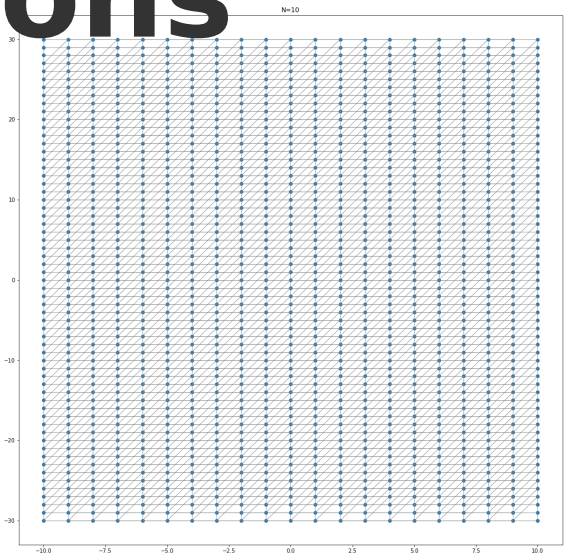
Reaction Space

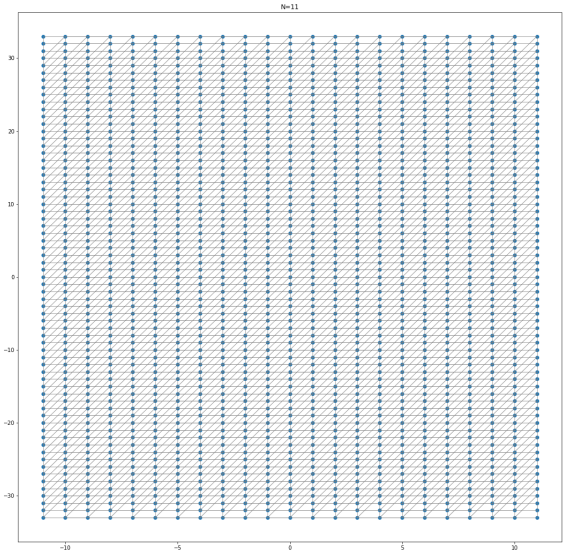
For n nitrogen atoms
| S | = (2n+1)(6n+1)
| R | =| S |^2

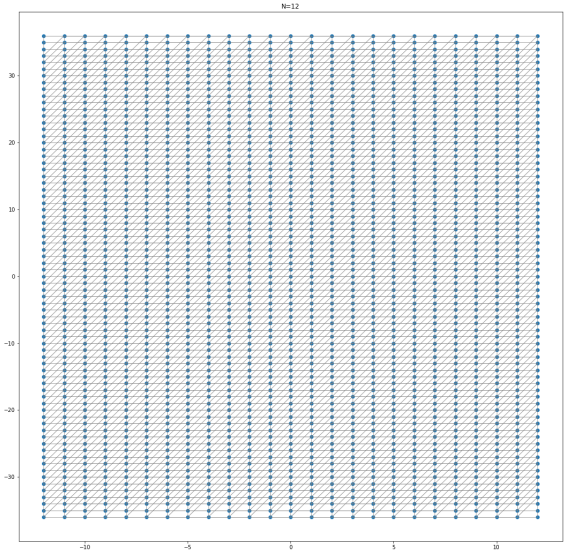
- Reaction space grows as n^4

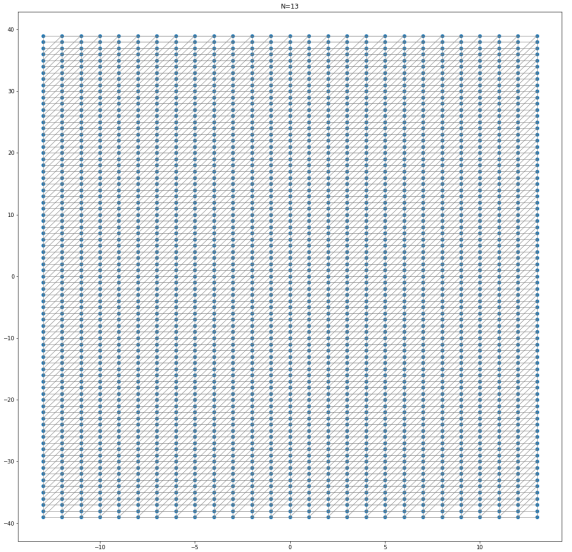


Illustrations

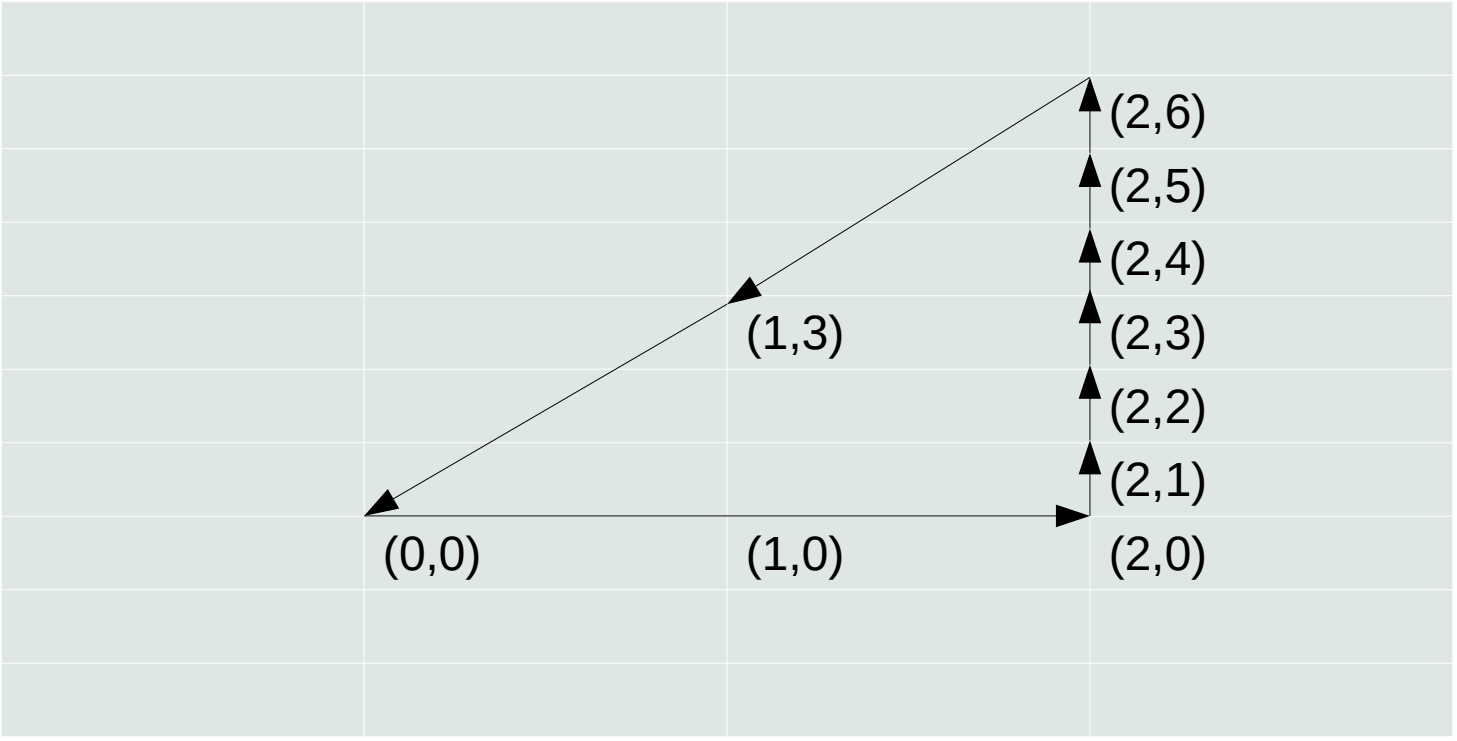








Closed Subgraphs



Search Algorithms

- Reading Graph Algorithms from Cormen
- Is there any other book?

Memory Problems

- While working with larger values of n (n=20, |R| > 24 million)
  Computer couldn’t process.
- Running out of RAM