This week we're finishing the first unit

Last Wednesday:

- Trees
- Started Chemistry at very end

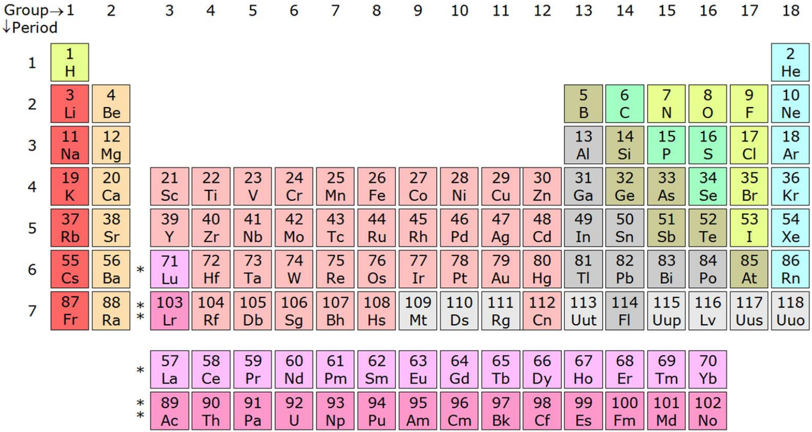
Today:

- Chemistry
- Eulerian + semi-Eulerian graphs

Wednesday

- Hamiltonian graphs

Chemical formulas encode degree sequences



Group→ ↓Period	1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
			*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb		
			**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No		

Atom	C	N	O	H
Degree	4	3	2	1

Shortcuts around Carbon and Hydrogen

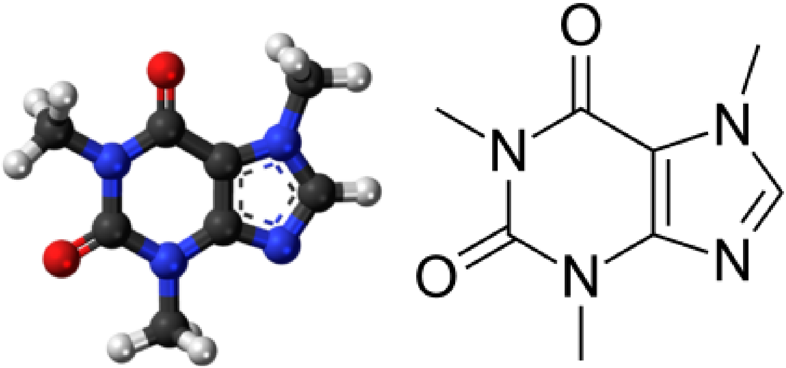


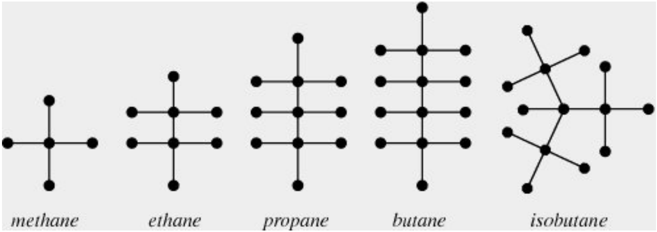
Figure: Two pictures of Caffeine

- Unlabelled vertices are Carbon
- Hydrogen not drawn; inferred to make degrees correct

Isomers are graphs with the same degree sequence

Definition

An *Alkane* is a molecule with formula $C_n H_{2n+2}$



Definition (Isomer)

Two different molecules are *isomers* if they have the same chemical formula.

Lemma: Any alkane is a tree.

Proof: Handshaking.

Question: How many isomers does $C_5 H_{12}$ have?

Bridges of Konigsberg: birth of graph theory

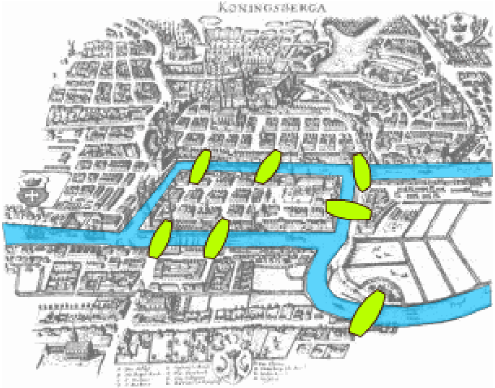
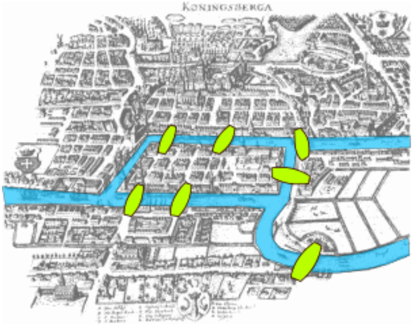


Figure: The city of Konigsberg

A puzzle:

Cross every bridge exactly once and return to where you started.

The puzzle has no solution



Suppose there was a walk:

- Stand on far bank
- Watch friend do walk
- Comes by one bridge
- Leaves by another bridge
- When they cross third bridge they're stuck with you

Generalizing with graph theory

Definition

- A walk is *closed* if it starts and ends at the same point.
- A graph is *Eulerian* if it has a closed walk that uses every edge exactly once

Lemma:

If G is Eulerian, then every vertex has even degree.

Proof.

Every time the walk visits v, pair the edge it arrives by with the edge it leaves by. $\square$

The first theorem in graph theory

Theorem (Euler)

A connected graph G is Eulerian if and only if every vertex of G has even degree.

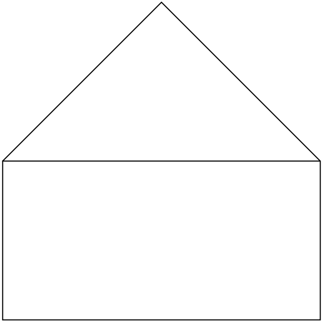
Proof.

We proved Eulerian $\implies$ even degree in last lemma.
For other direction:

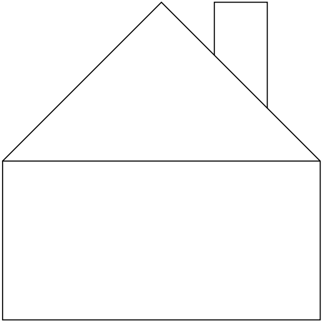
- Walking randomly will eventually get back to where we started (why?)
- Remove edges we used to get a smaller graph
- By induction, each connected piece is Eulerian
- Glue the cycles back together

$\square$

What can you draw without lifting your pen or retracing?



A house?



A house with a chimney?

Formalizing our observations

Definition

A graph G is *semi-Eulerian* if it has a (not necessarily closed) walk that uses every edge exactly once.

Theorem

A connected graph G is semi-Eulerian if and only if it has at most two vertices of odd degree

One proof: tweak the original proof

Easy direction: every point but start and end needs even degree.
Hard direction:

- Start walk at one odd degree point
- Walking randomly can only end at other odd degree point
- Delete this path, then use induction + gluing as before

A devious trick to avoid doing work

Mathematicians are lazy

- It's unsatisfying to "redo" the work of the proof
- Slicker to reduce it to a problem we've already solved

The tricky/easy proof:

- Let $u, v \in G$ be the two vertices of odd degree
- Add an edge e from u to v to get G'
  (this may make G non-simple, that's okay)
- In G', every vertex has even degree, so it has Eulerian cycle
- Delete e from the eulerian cycle to get an Eulerian walk from u to v

A preview of next lecture

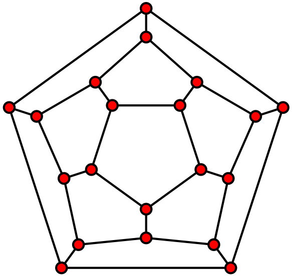
Definition

A graph G is *Hamiltonian* if there is a closed walk that visits every vertex exactly once. G is *semi-Hamiltonian* if there is a not necessarily closed walk that visits every vertex exactly once.

- It was Easy to tell if a graph was Eulerian (Edges)
- It's Hard to tell if a general graph is Hamiltonian (Vertices)

Question to lead into it:

- Is D_{20} Hamiltonian?
- Is the Petersen graph?
- If we remove a vertex from D_{20} is it Hamiltonian? How about Petersen?



Dodecahedron graph D_{20}