# Combinatorial Optimization in Bioinfo

## Lecture 4 – Graph algorithms and assembly

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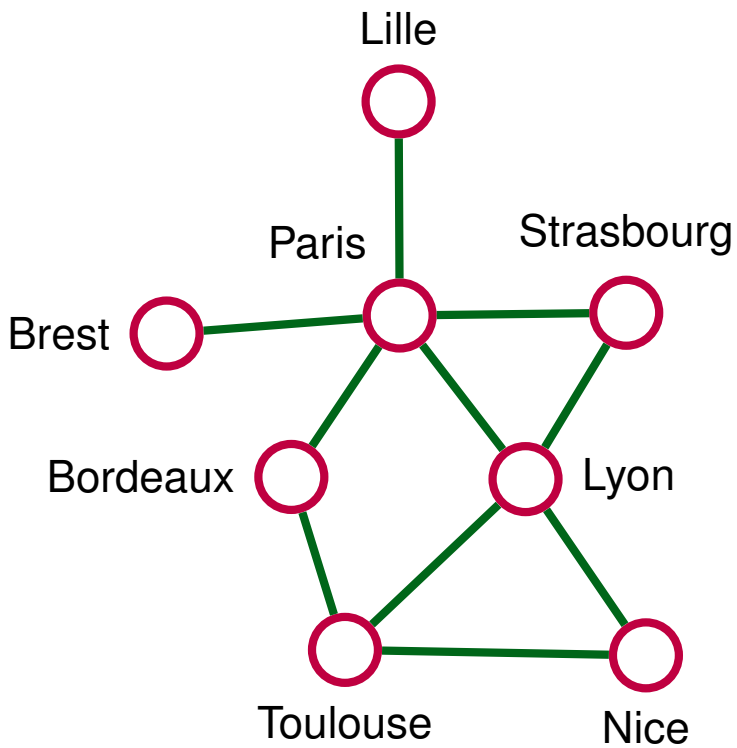
AMIBio Team
CNRS & École Polytechnique

$$G = (V, E)$$

where $V \rightarrow$ vertices/nodes, and $E \rightarrow$ edges.

**What for?** Graphs model entities, and the way they are connected



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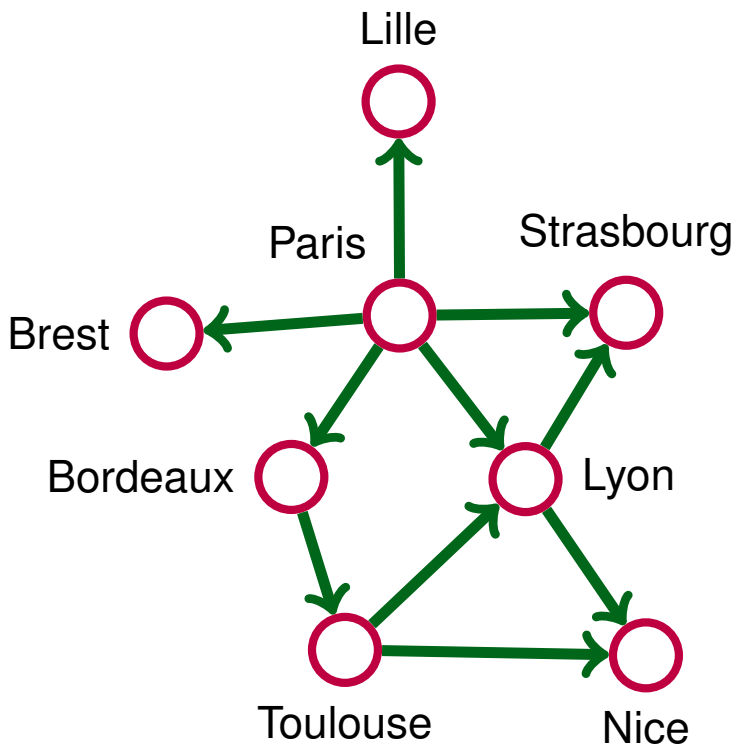

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- Shortest path between two nodes (GPS)
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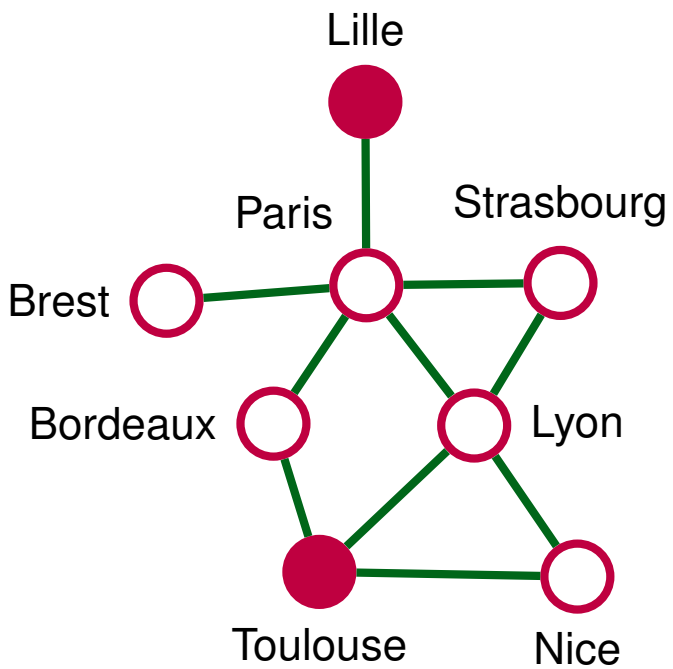


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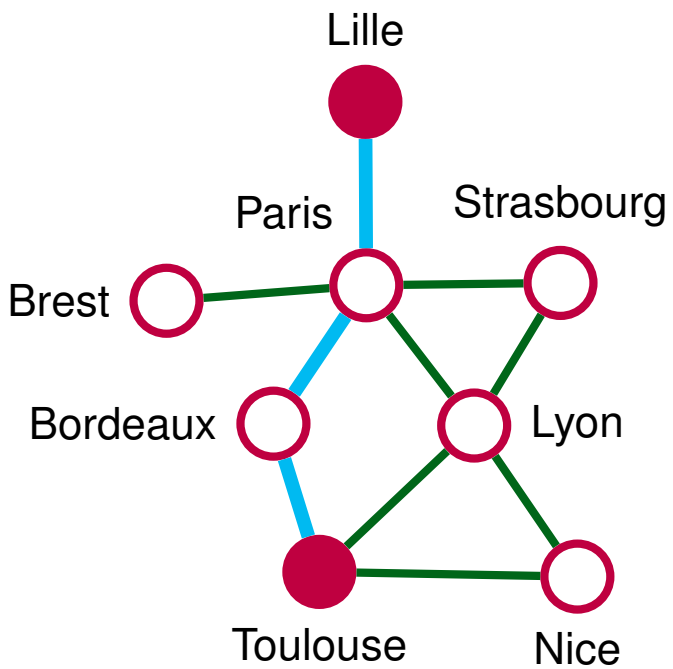


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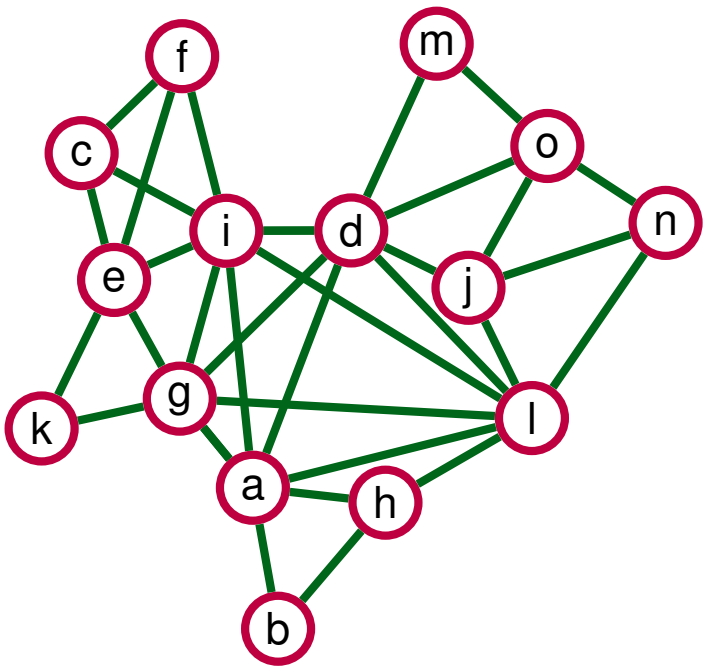


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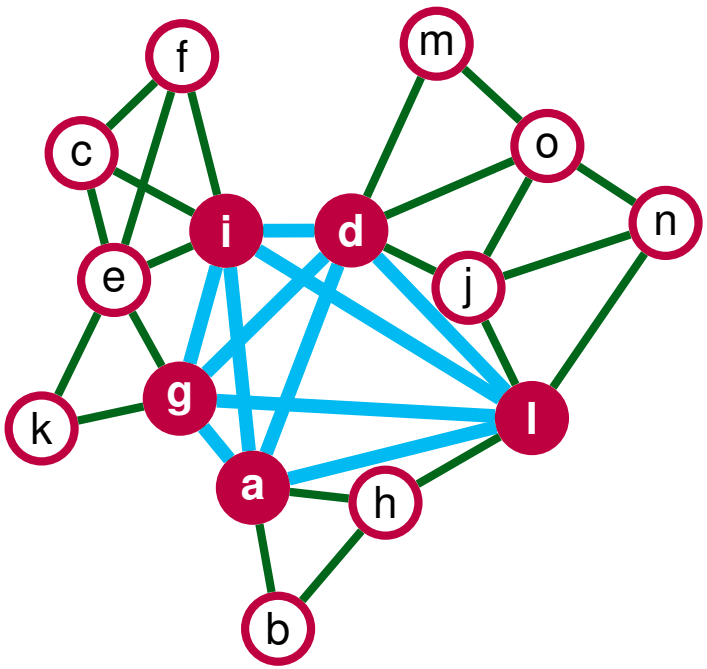


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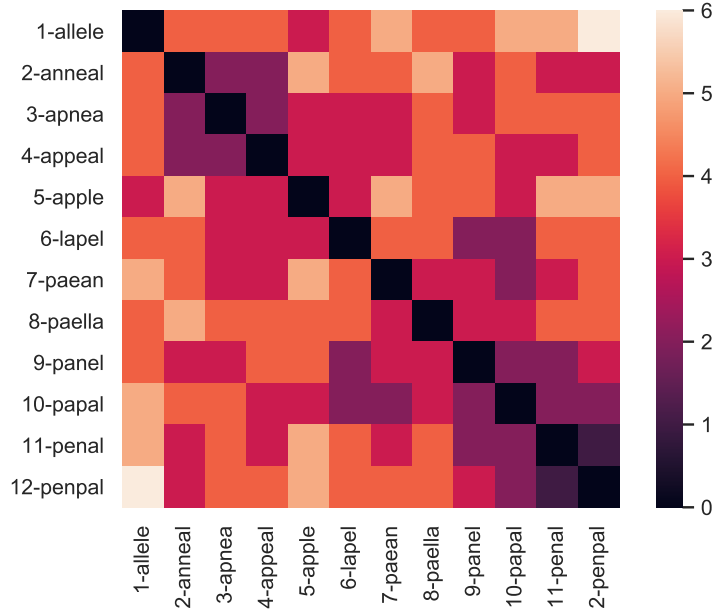


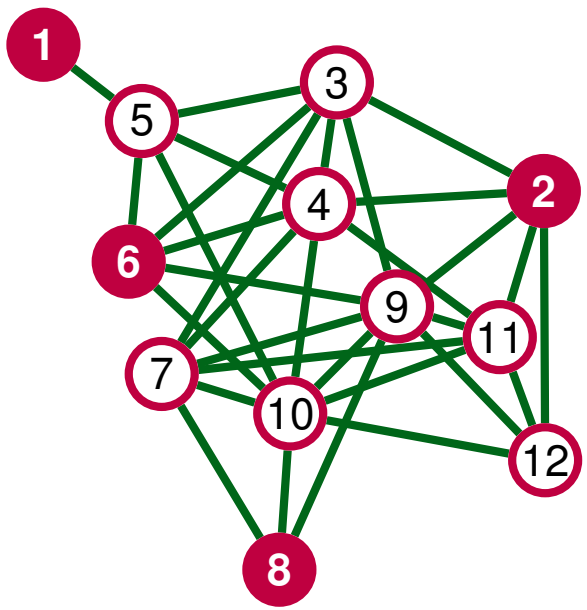


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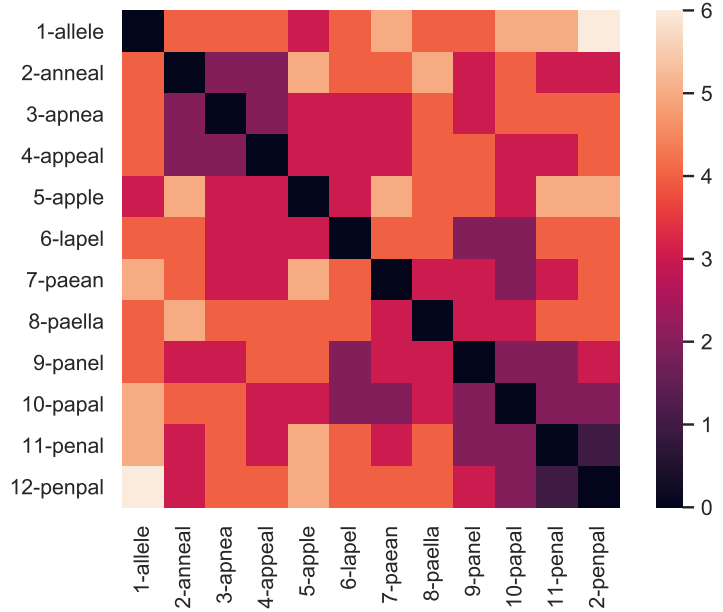


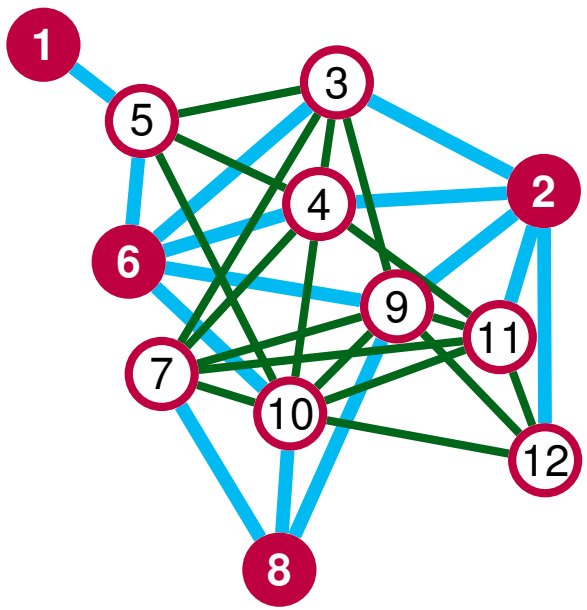


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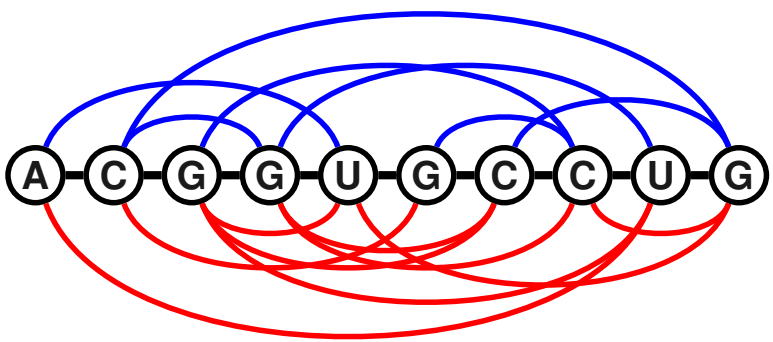


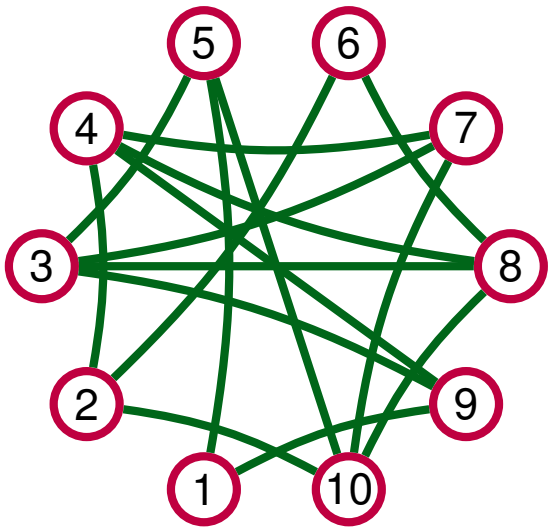


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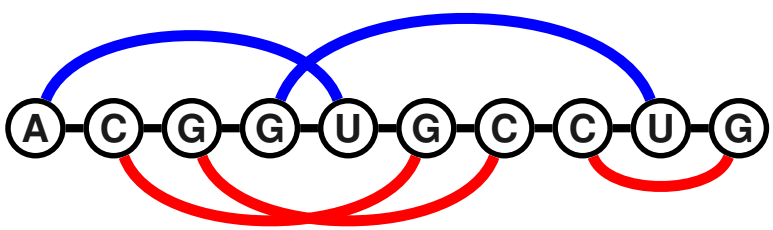


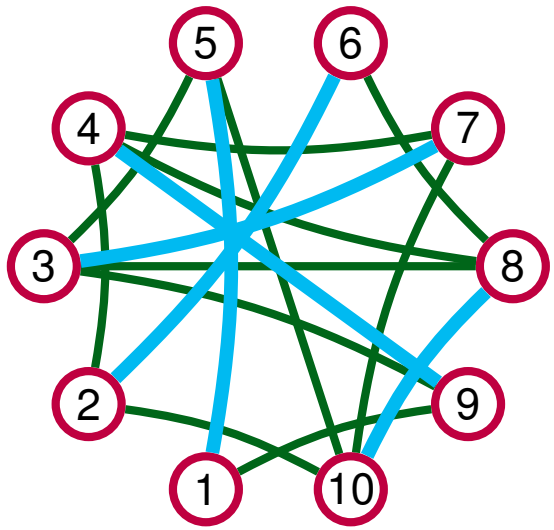


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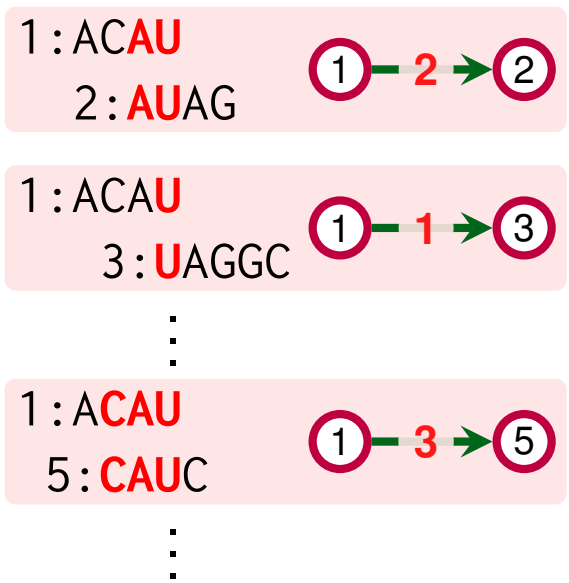


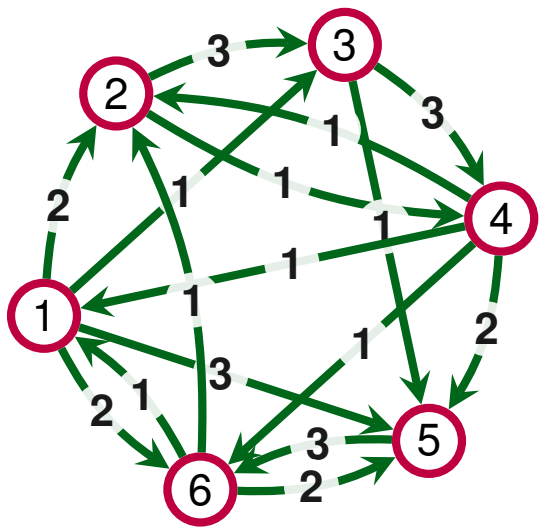


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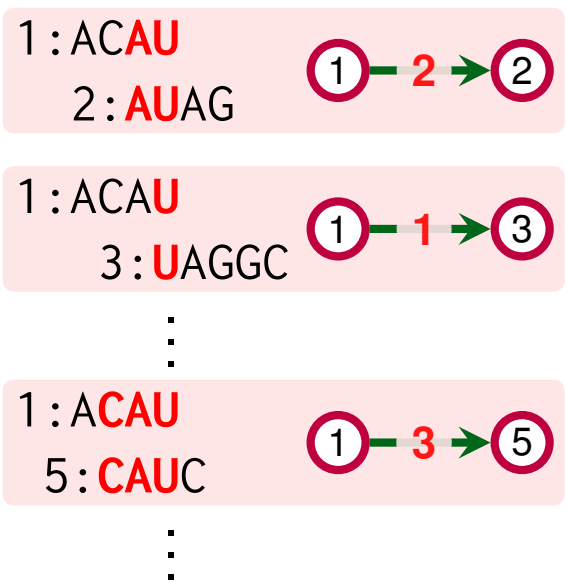


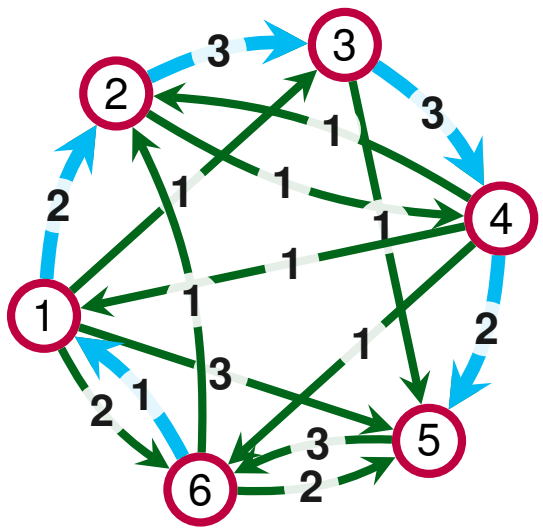


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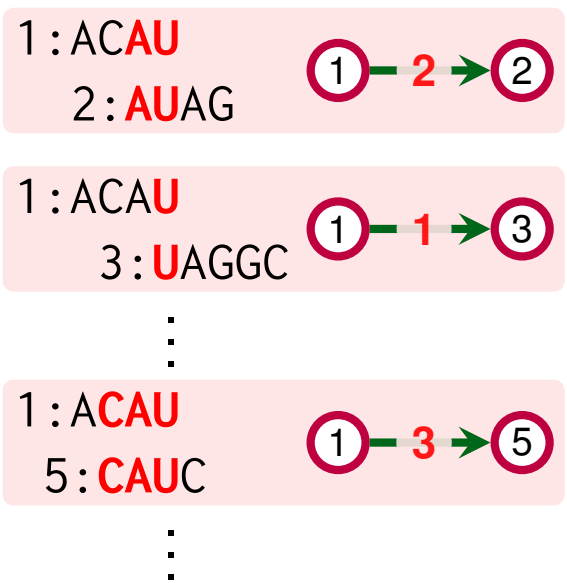


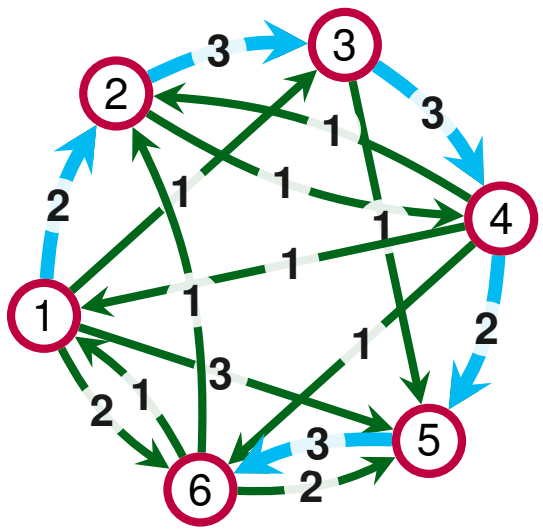


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**Input:** (Di)graph $G = (V, E)$; Origin $s \in E$ and Destination $t \in E$; Distance function $\delta : E \to \mathbb{R}^+$

**Output:** Minimal distance path from $s$ to $t$, *i.e.* $p^\star$ such that

$$p = \underset{\substack{p=(u_1,u_2\dots u_k)\\ u_1=s,u_k=t}}{\operatorname{argmin}} \sum_{i=1}^{k-1} \delta(u_i, u_{i+1})$$

- Easy problem $\Leftrightarrow$ Poly-time algo.
- **Idea (Dijkstra):**
  - **Flood** from $s$
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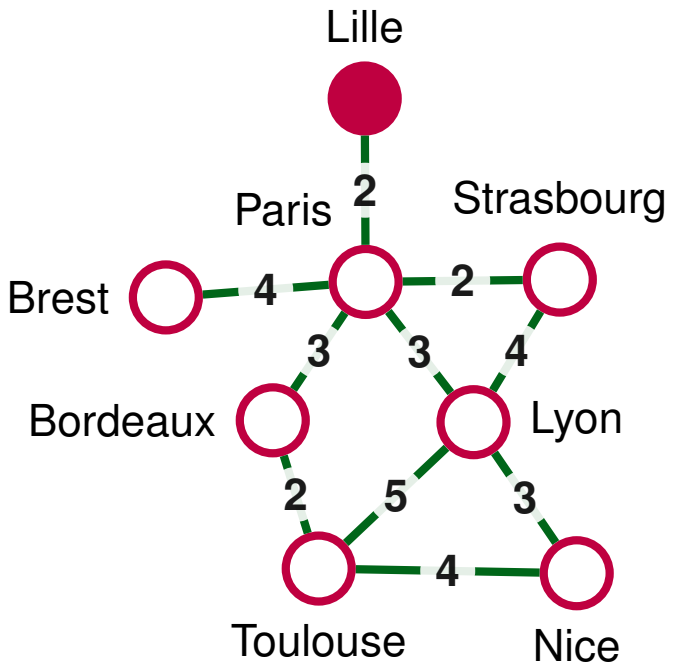

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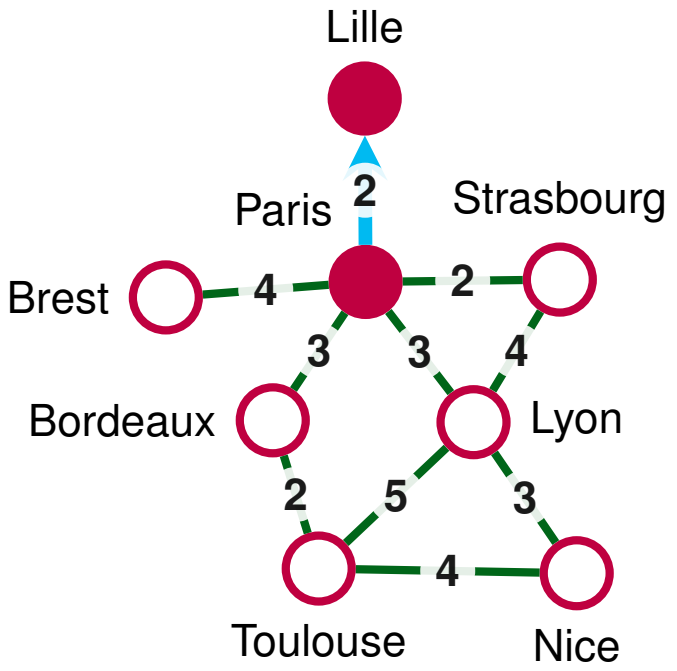

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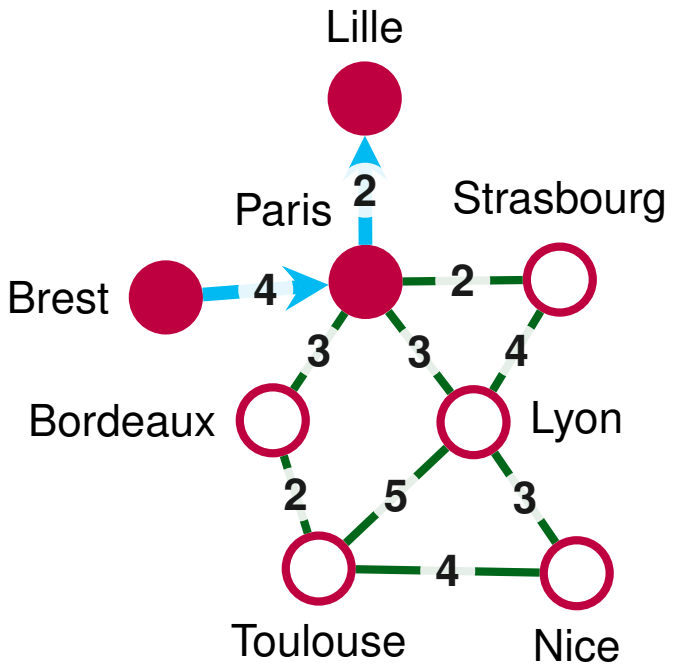

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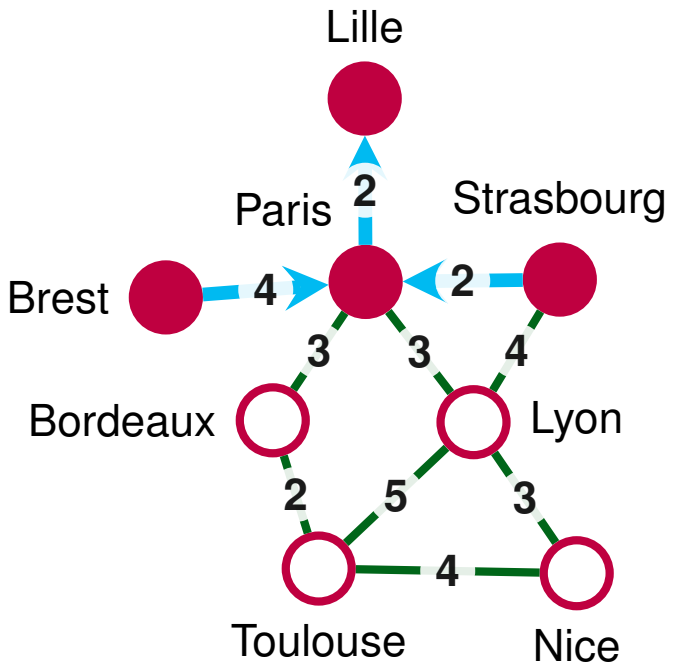

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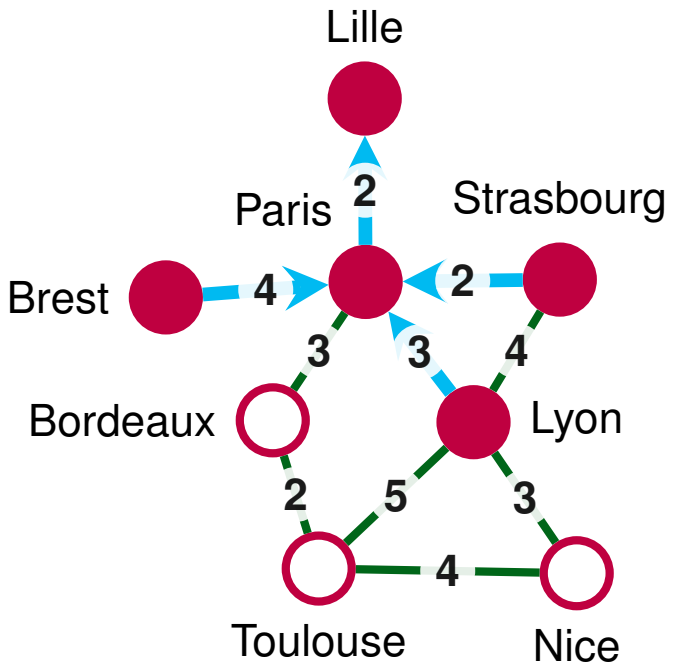

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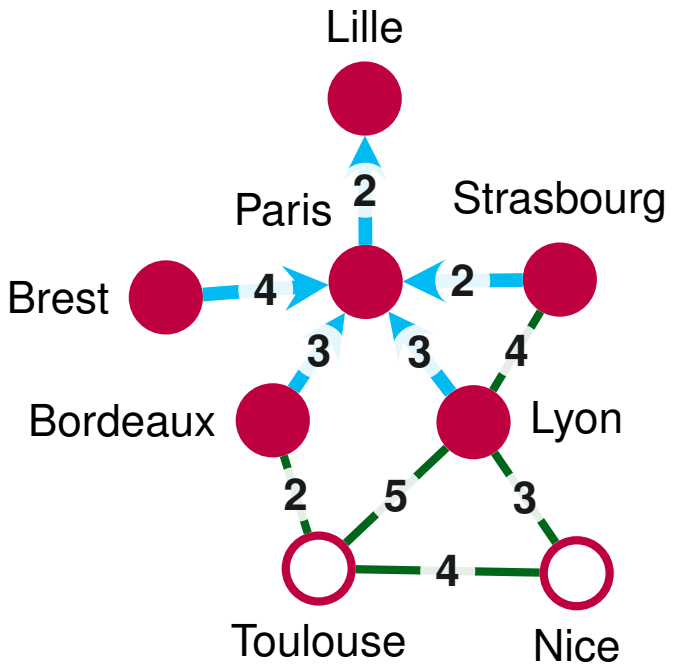

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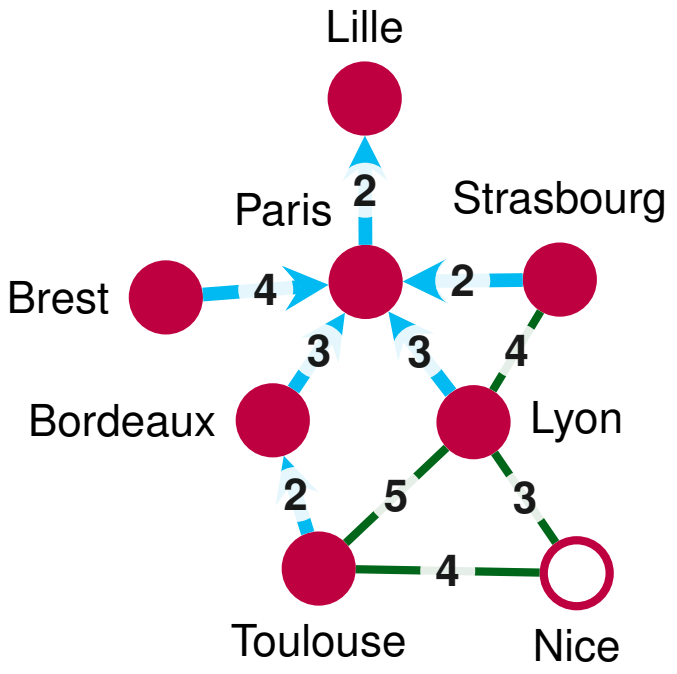
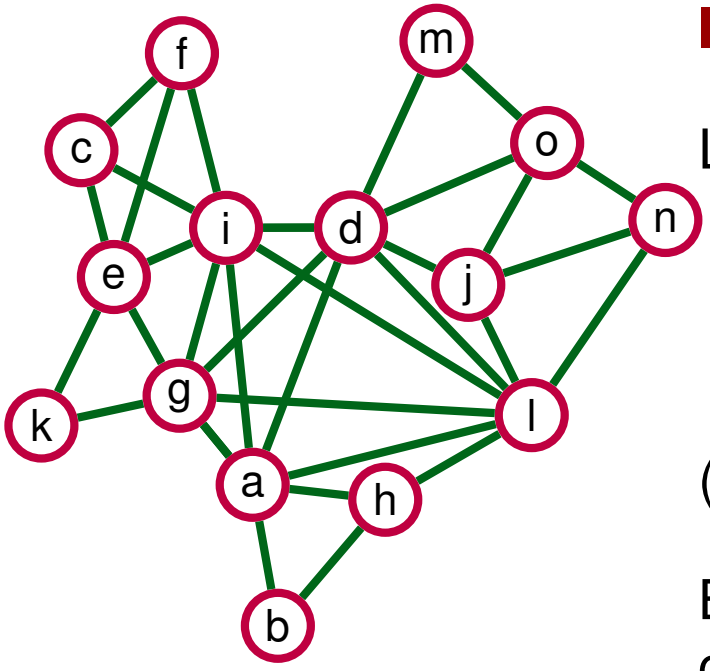


MAX CLIQUE **problem**
**Input:** Graph $G = (V, E)$
**Output:** Largest set of **pairwise connected** vertices.

Useful when trying to detect a group of highly interconnected elements (*e.g.* molecules)




**In a nutshell:** A **hard** problem!

Let $n = |V|+|E|$ & $k$ max size of clique:

- NP-hard: No $\mathcal{O}(P(n))$ algo
- Not FPT (W[1]): No $\mathcal{O}(\alpha^k.P(n))$ algo
- XP: Trivial algo in $\mathcal{O}(n^k)$

(unless P=NP)

But many heuristic solutions, so still worth considering if natural (last resort)

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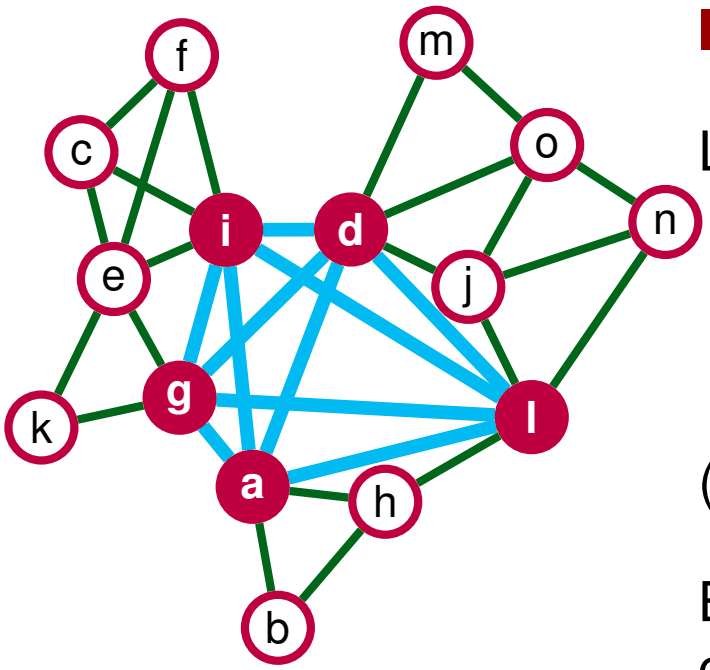


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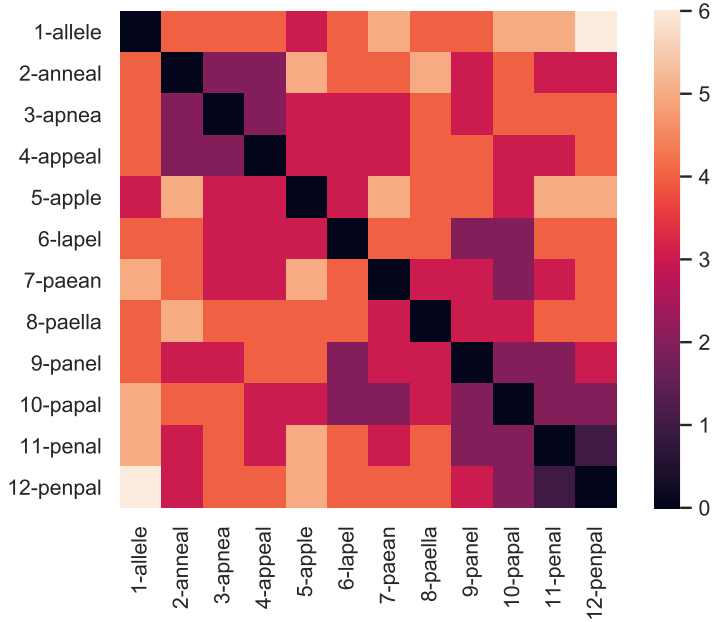


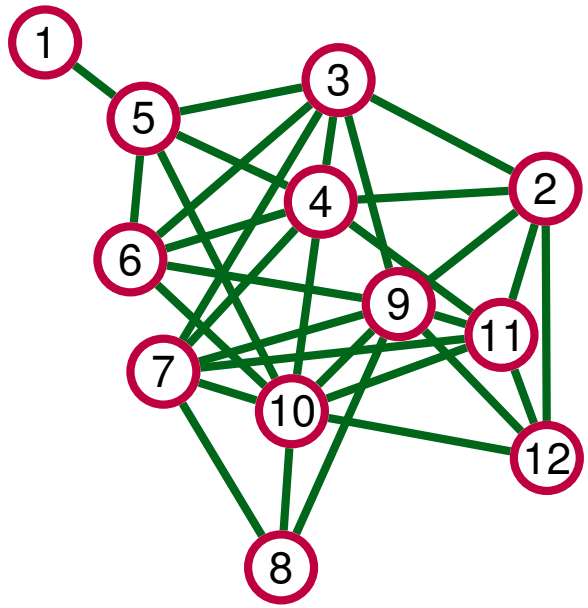


Unfortunately, NP-hard (again), but can be solved in $\mathcal{O}(2^t.|V| + |E|)$ time, *i.e.* efficiently for input graphs of low **tree-width** $t$.

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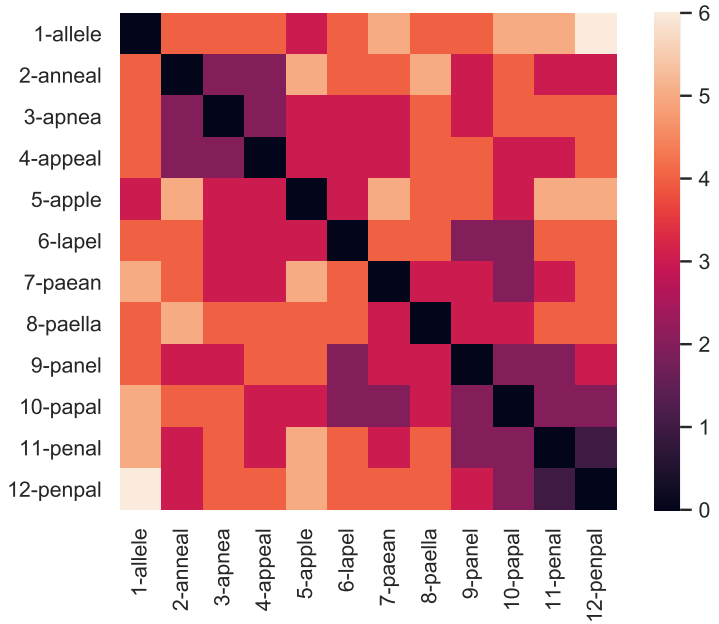
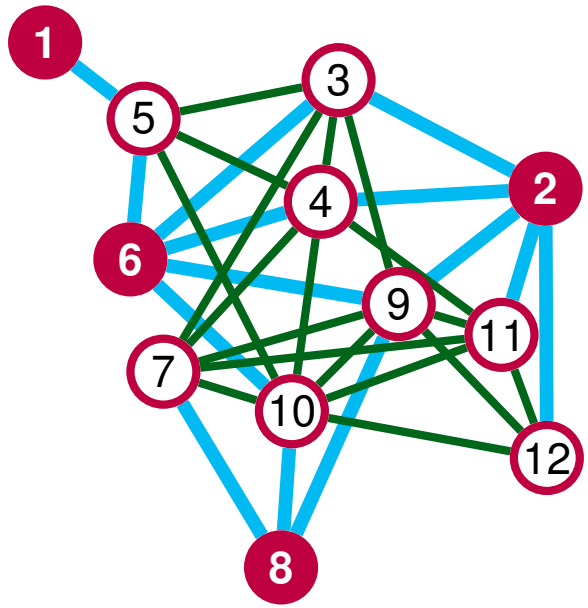



Unfortunately, NP-hard (again), but can be solved in $\mathcal{O}(2^t.|V| + |E|)$ time, *i.e.* efficiently for input graphs of low **tree-width** $t$.

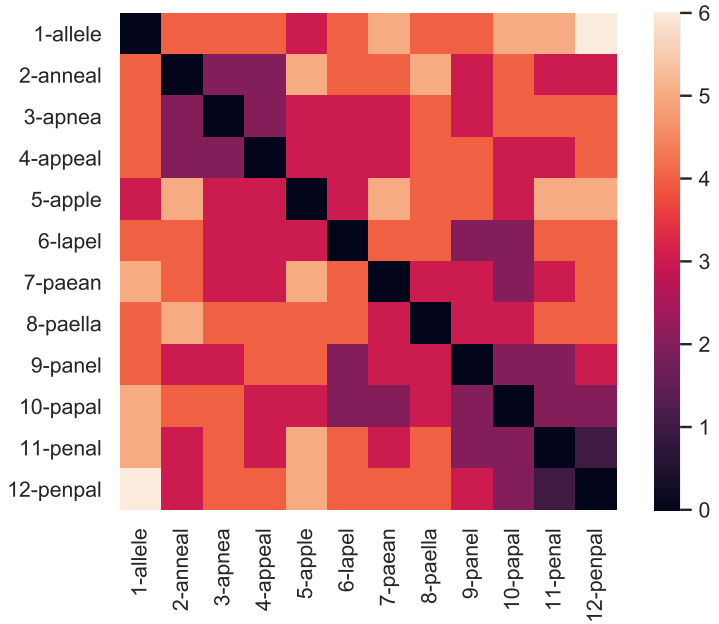
**MAX INDEPENDENT SETS problem**

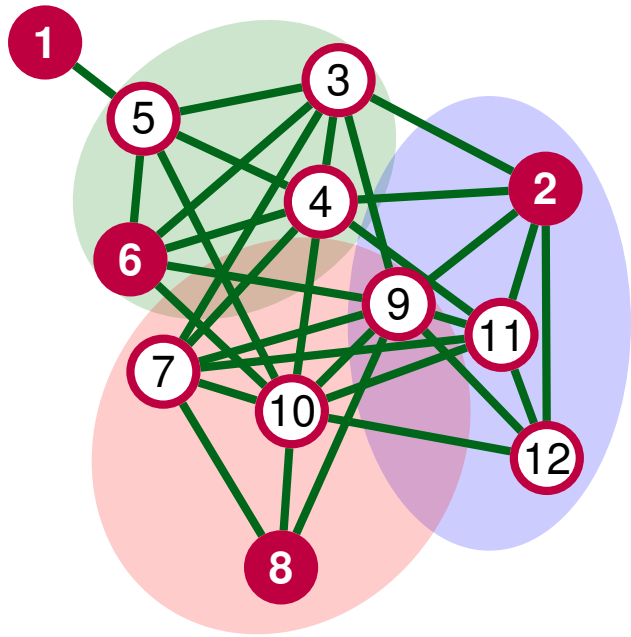
**Input:** Graph $G = (V, E)$

**Output:** Largest set of **pairwise disconnected** vertices.

Very natural while producing conflict-free collections of objects.

1-allele
2-anneal
3-apnea
4-appeal
5-apple
6-lapel
7-paean
8-paella
9-panel
10-papal
11-penal
12-penpa

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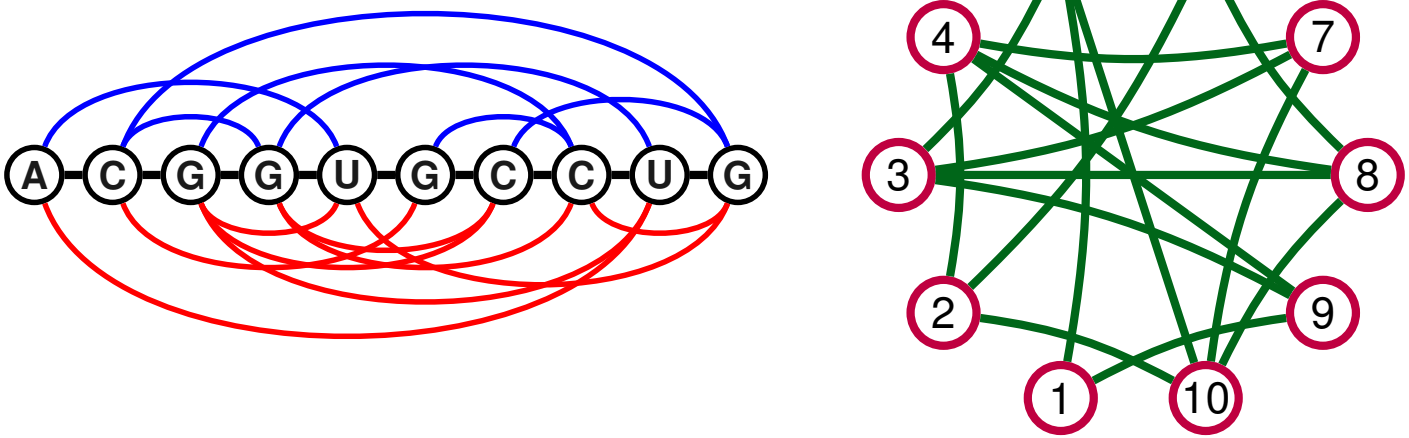
MAX MATCHING **problem**

**Input:** Graph $G = (V, E)$

**Output:** Largest set of edges such that each vertex is represented in $\leq 1$ edge.

**Typical use-case**: Simplify a $n$-body problem into a 2-body problem
$\rightarrow$ Useful for approximate solutions (guaranteed approx ratio)

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**Idea (Edmunds): Greedy** optim. by swapping **augmenting paths**
Yields **global** max. in $\mathcal{O}(|E|\sqrt{|V|})$ from Micali and Vazirani

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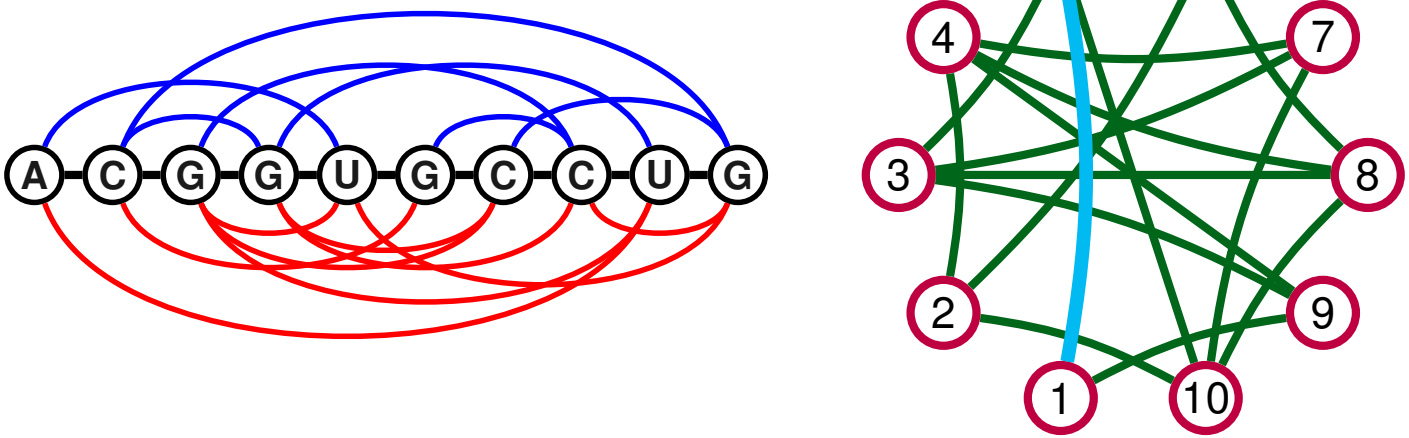


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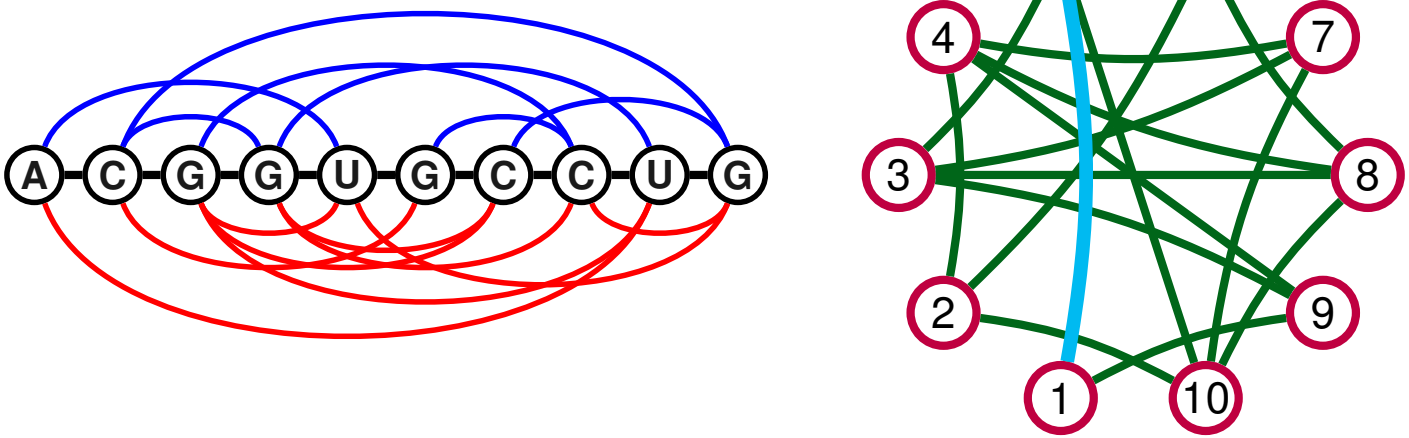


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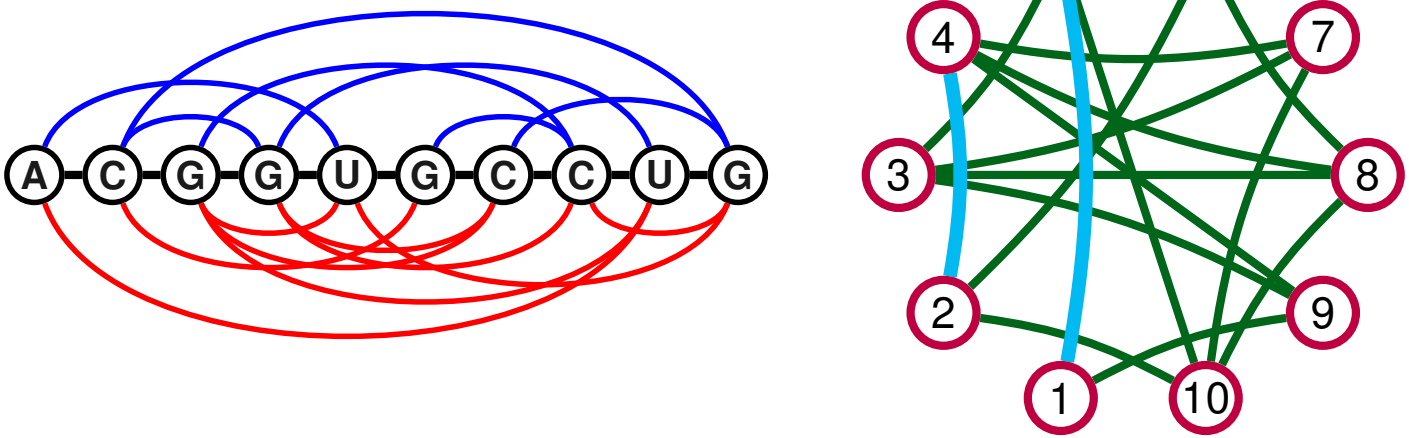


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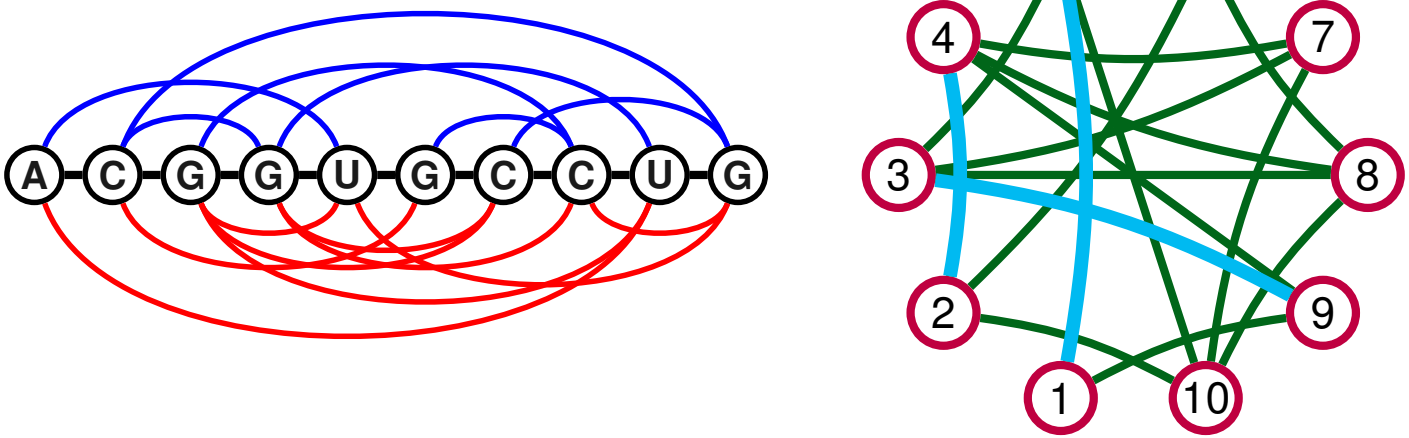


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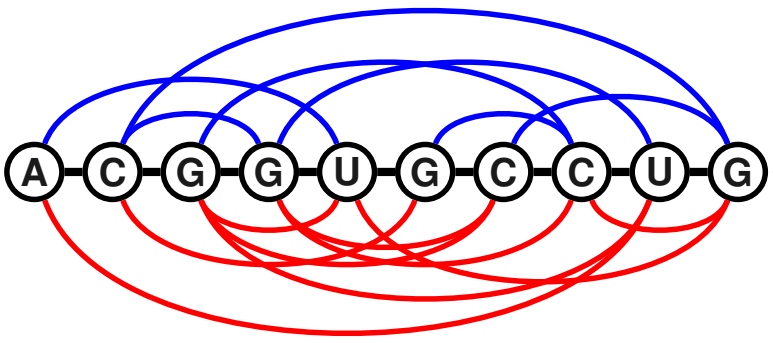


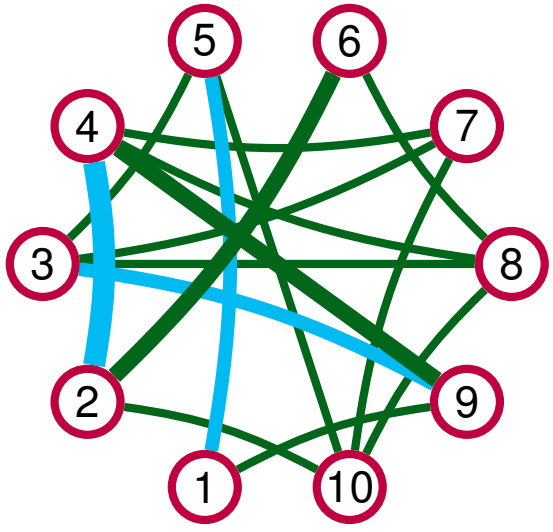


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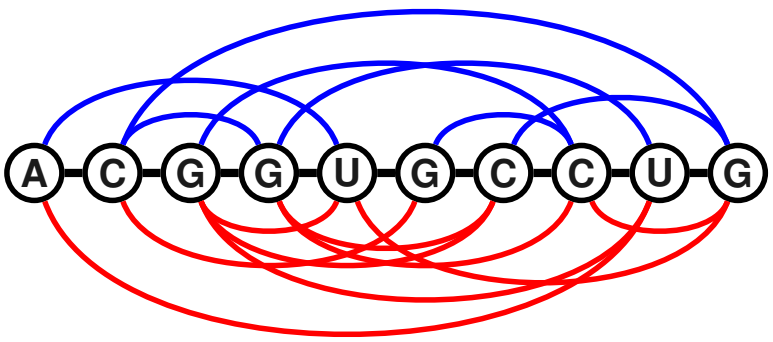


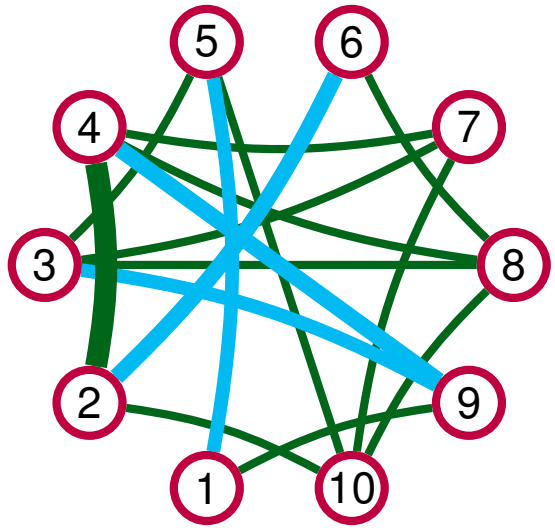


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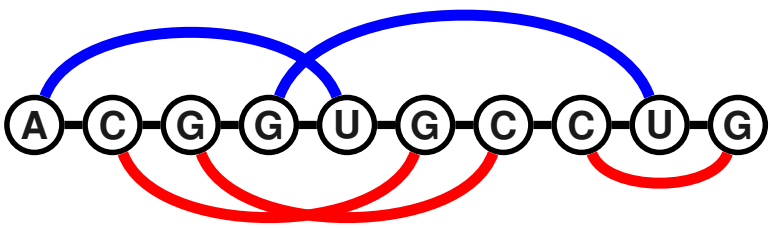


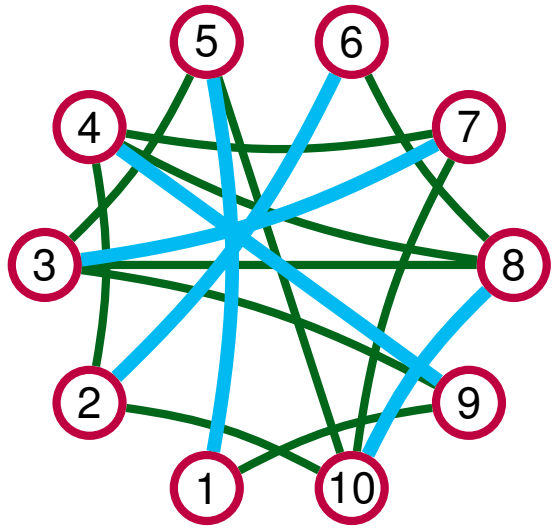


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HAMILTONIAN PATH **problem**

**Input:** (Di)graph $G = (V, E)$

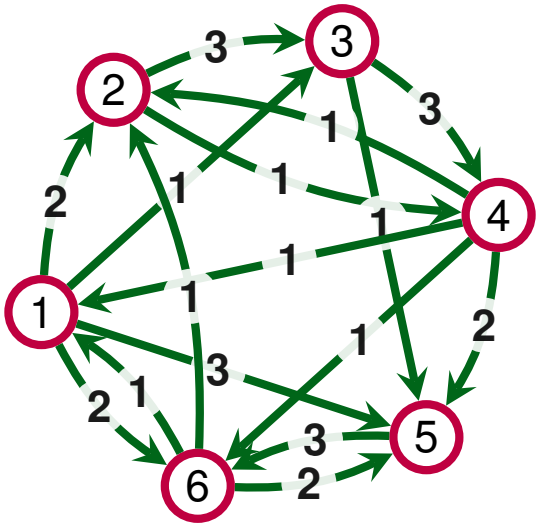
**Output:** Path of $G$ passing through vertex of $V$ **exactly once**

NP-hard along with its **optimization** version

TRAVELING SALESPERSON (TSP) **problem**

**Input:** (Di)graph $G = (V, E)$; Reward function $\rho : E \to \mathbb{R}$

**Output:** Hamiltonian path $p$ maximizing **reward** $\sum_{e \in p} \rho(e)$



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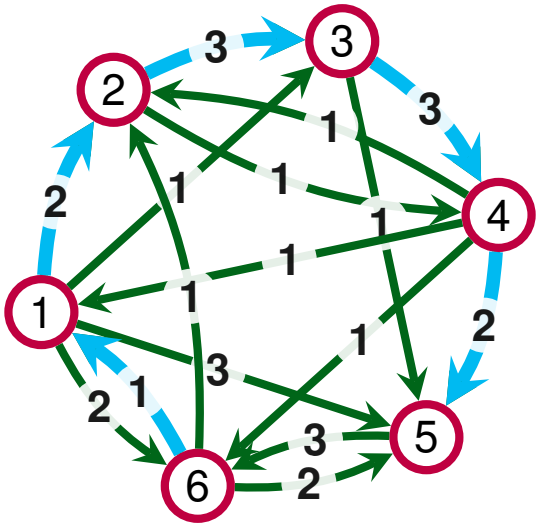


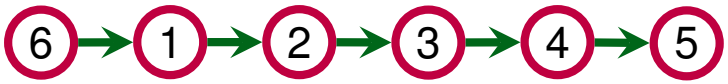


Reward: 11

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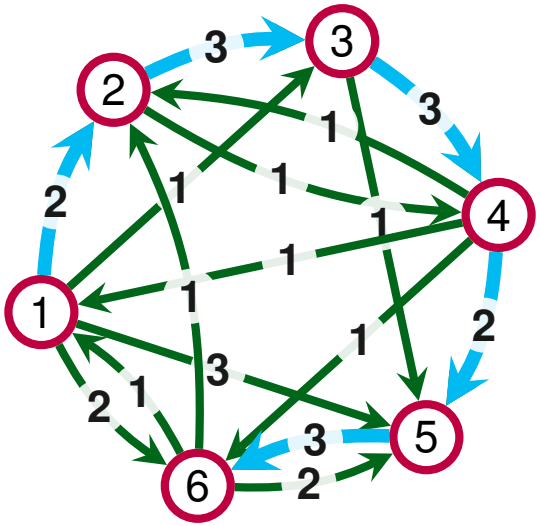


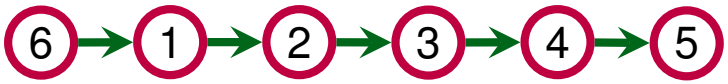


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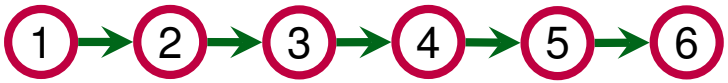


Reward: 13

**Assembly**: Given set of **NGS reads**, find **smallest** (parsimonious) genome/transcript that **explains** presence of each read in dataset

> SUPERSTRING **problem**
> **Input:** Strings $w_1, w_2, \ldots w_k$
> **Output:** String $w$ of min. length, where each $w_i$ occurs as motif

Again a **hard** problem, but highly similar to TSP.

NGS Reads

1 : ACAU
2 : AUAG
3 : UAGGC
4 : GGCA
5 : CAUC
6 : AUCA

Concatenation always possible but **costly**

ACAU AUAG UAGGC GGCA CAUC AUCA (len=25)

Compacting overlaps may be beneficial

ACAUAGGCAUCA (len=12)

but savings depends on **order**.

**Idea:** Find order that maximizes overlaps

$\text{len}(w_1, w_2 \ldots) = \sum_i \text{len}(w_i) - \sum_i \text{ov}(w_i, w_{i+1}))$

**Rem:** Assumes no read contained into another

NGS Reads

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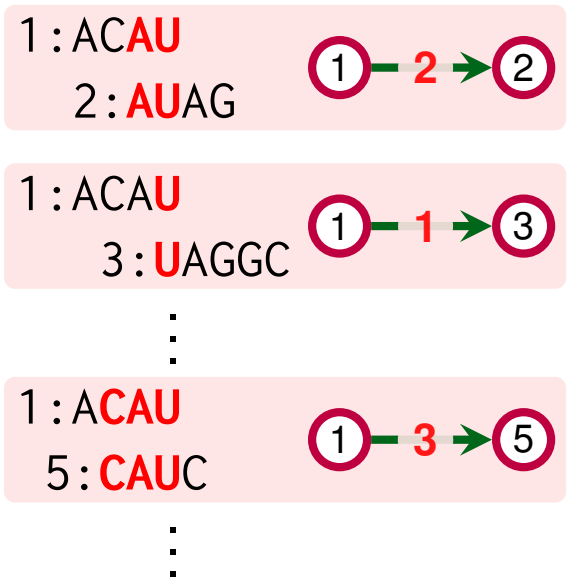


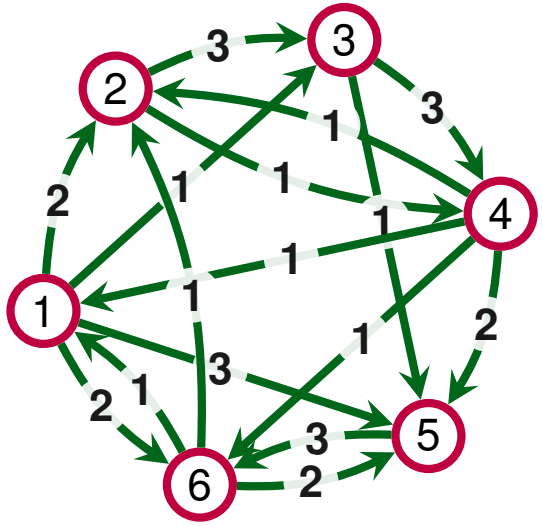

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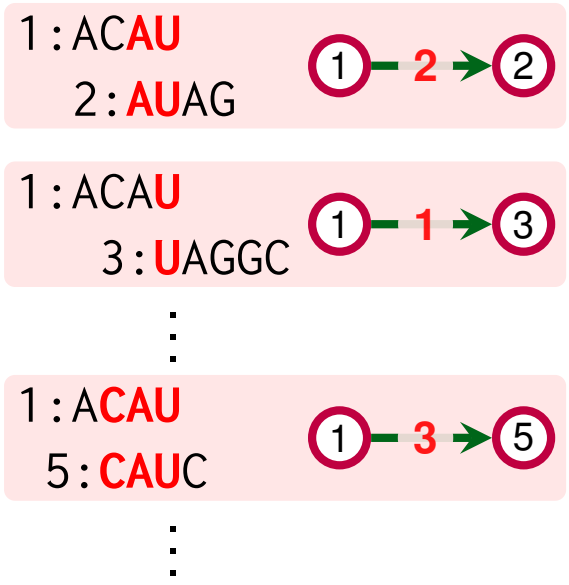


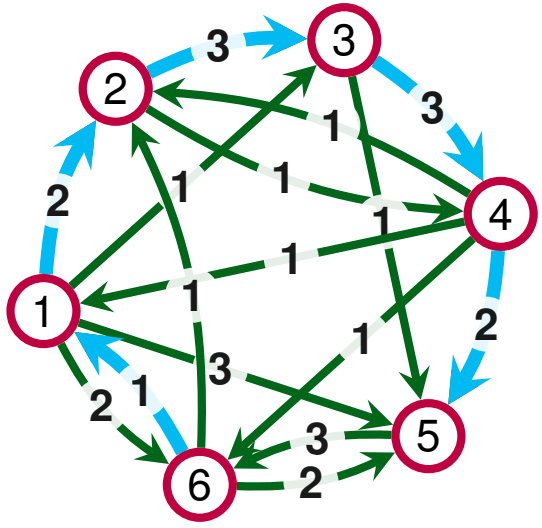


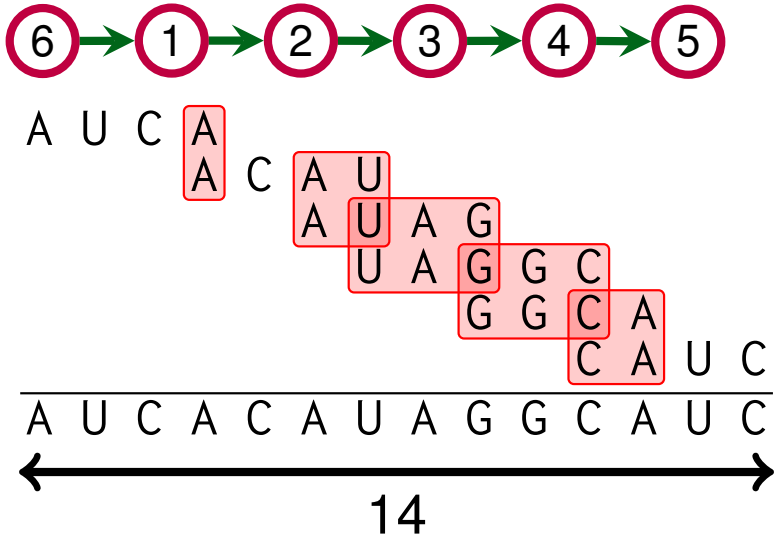

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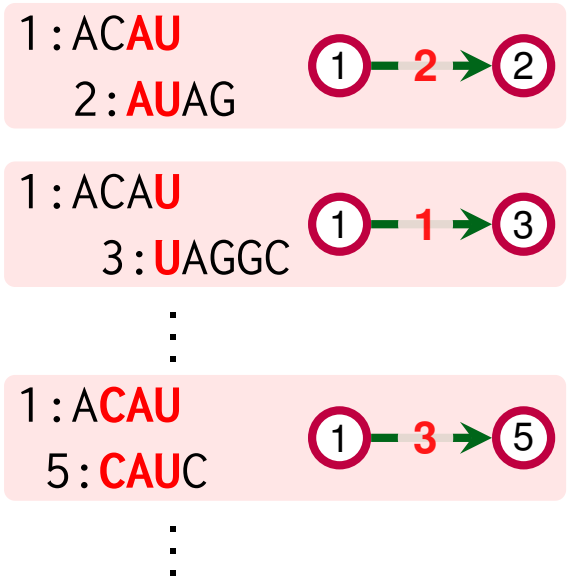


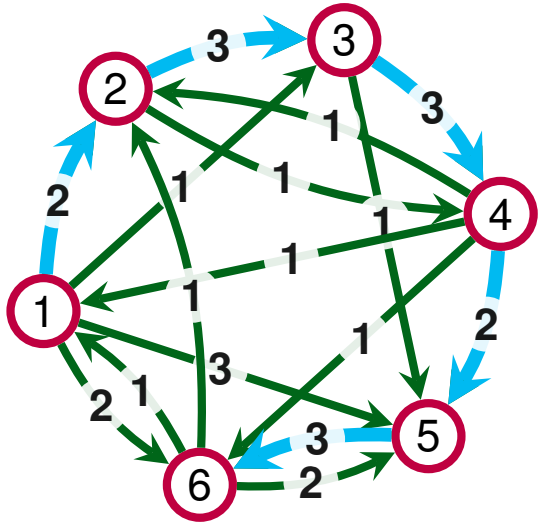


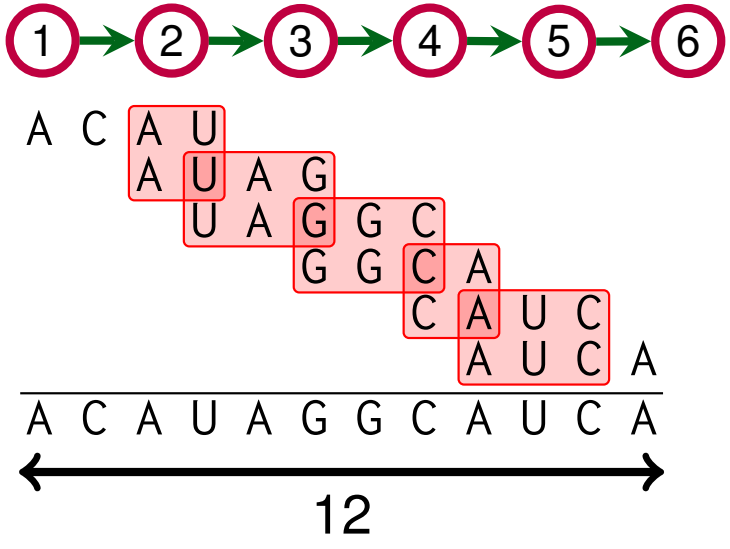

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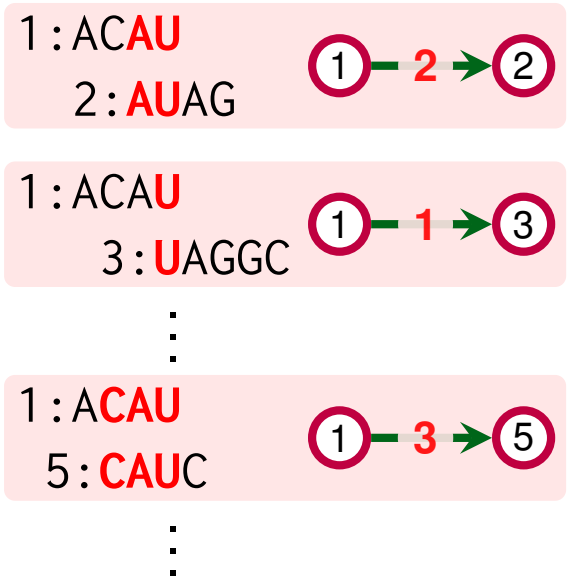
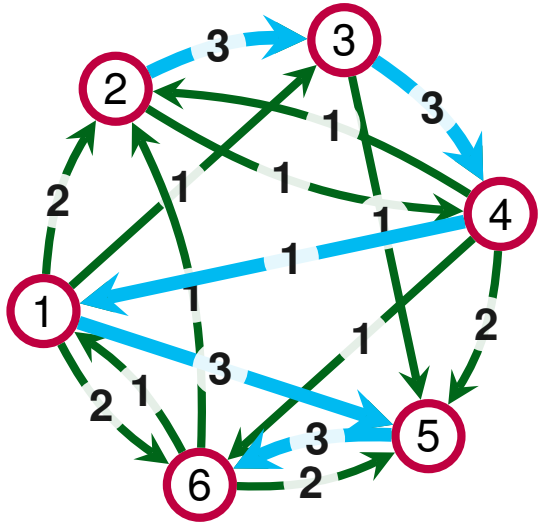
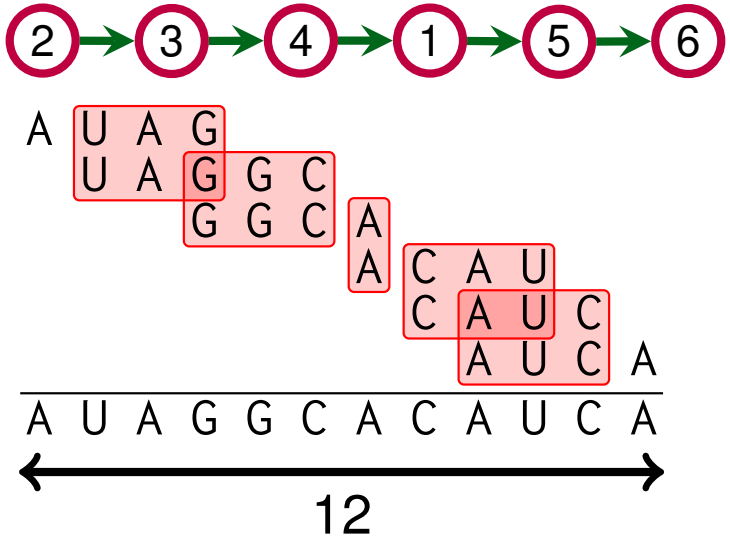


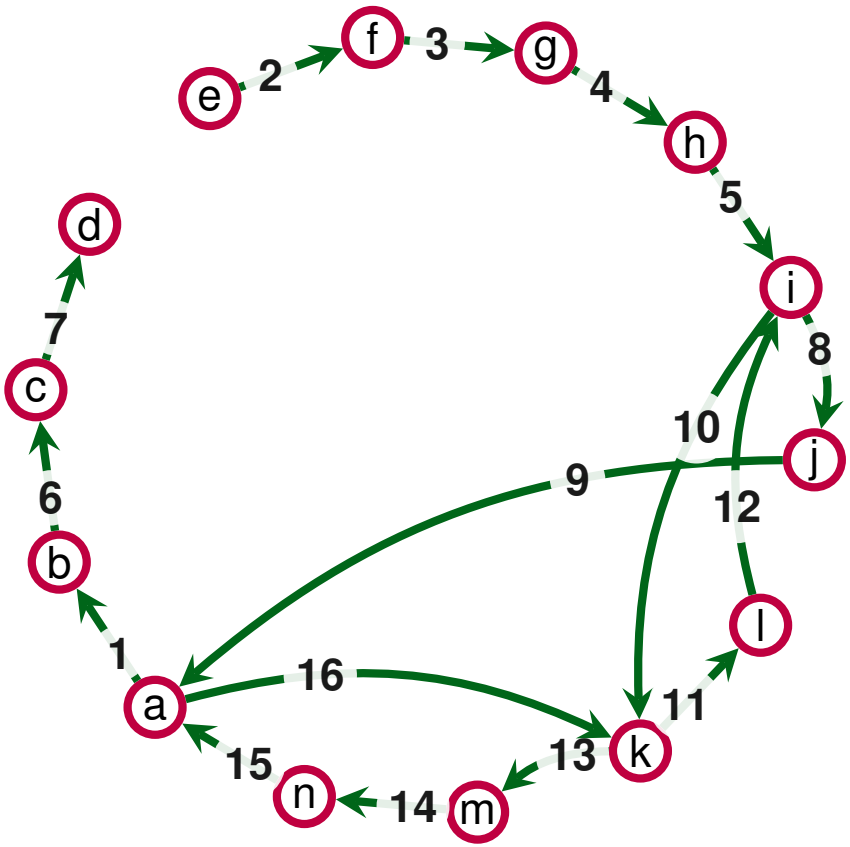



EULERIAN PATH **problem**

**Input:** Graph $G = (V, E)$

**Output:** Path $p$ traversing **every edge** of $E$ **exactly once**




Possible **only if** vertices **balanced**
(except possibly start & end)

**Algo**: Build start→end **greedy** path, extending until **deadend**
While edge(s) remain, iterate:
build cycle and insert it

Build edge sequence from cycles
(any order→ Possibly many!)

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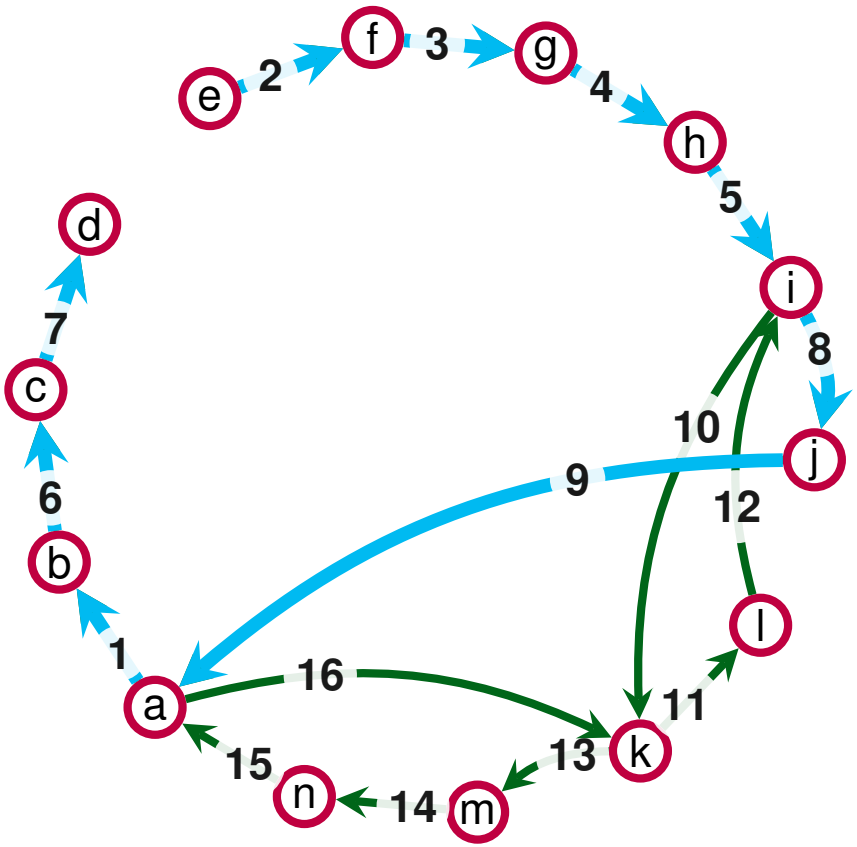


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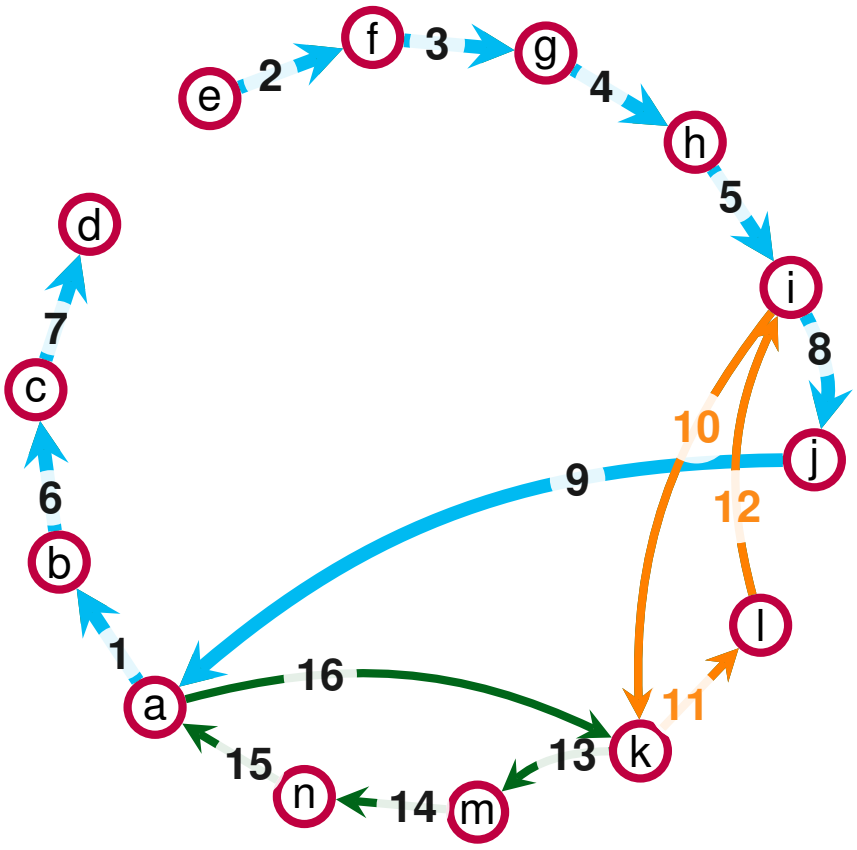


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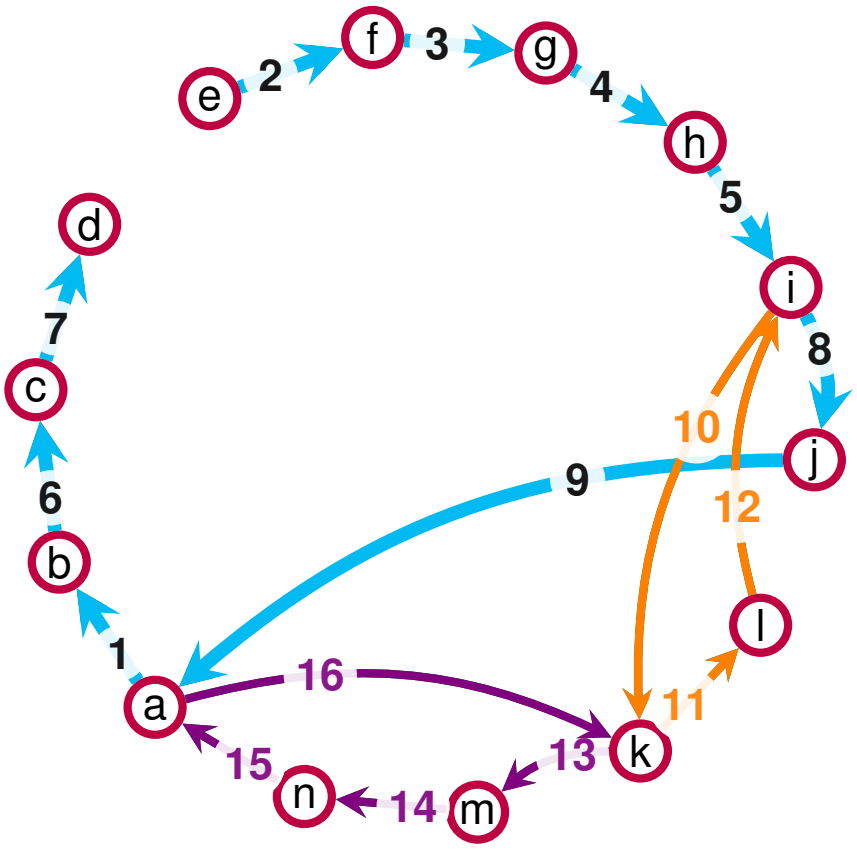


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4: AGGC
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13: CAGA
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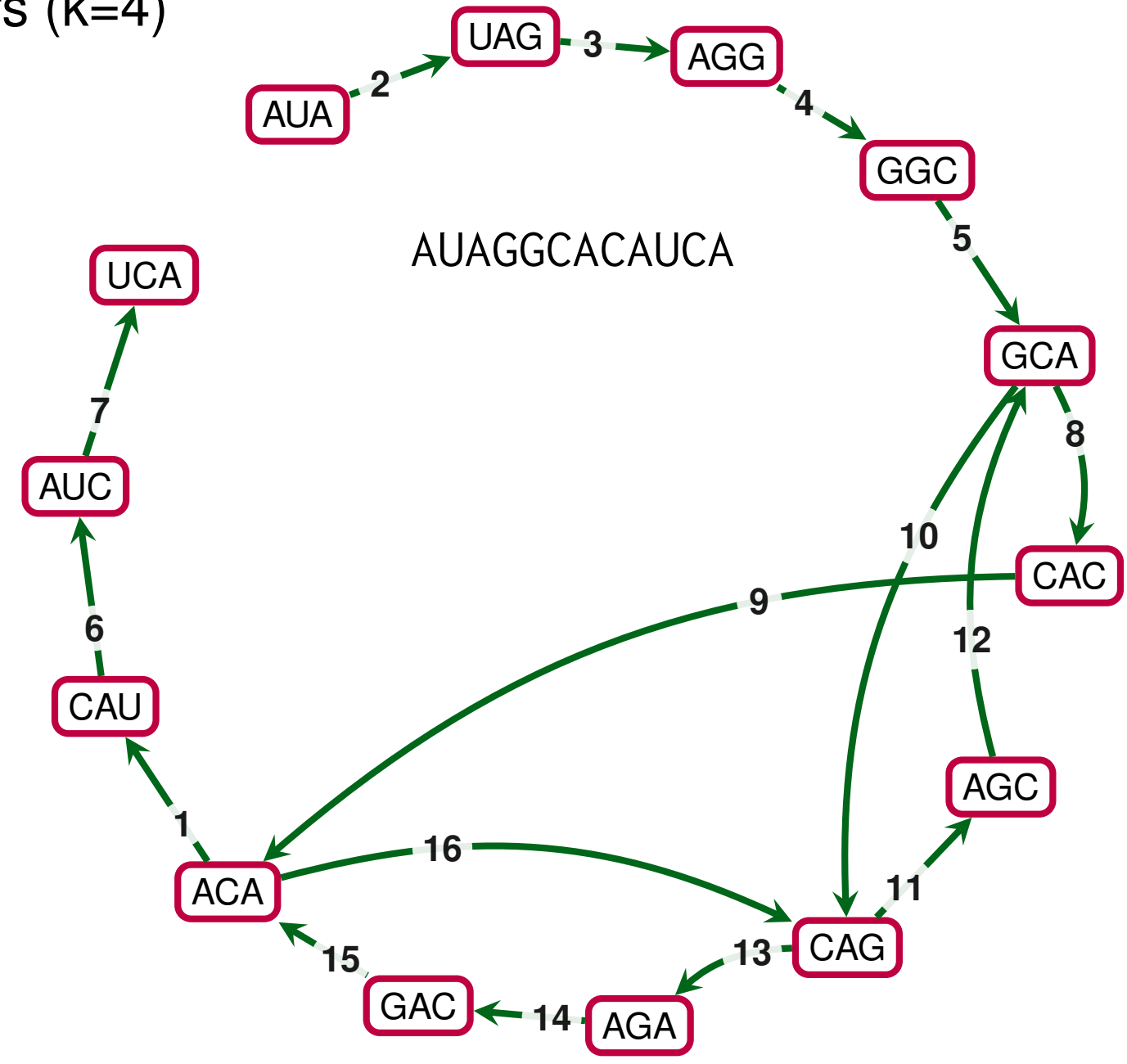
16: ACAG



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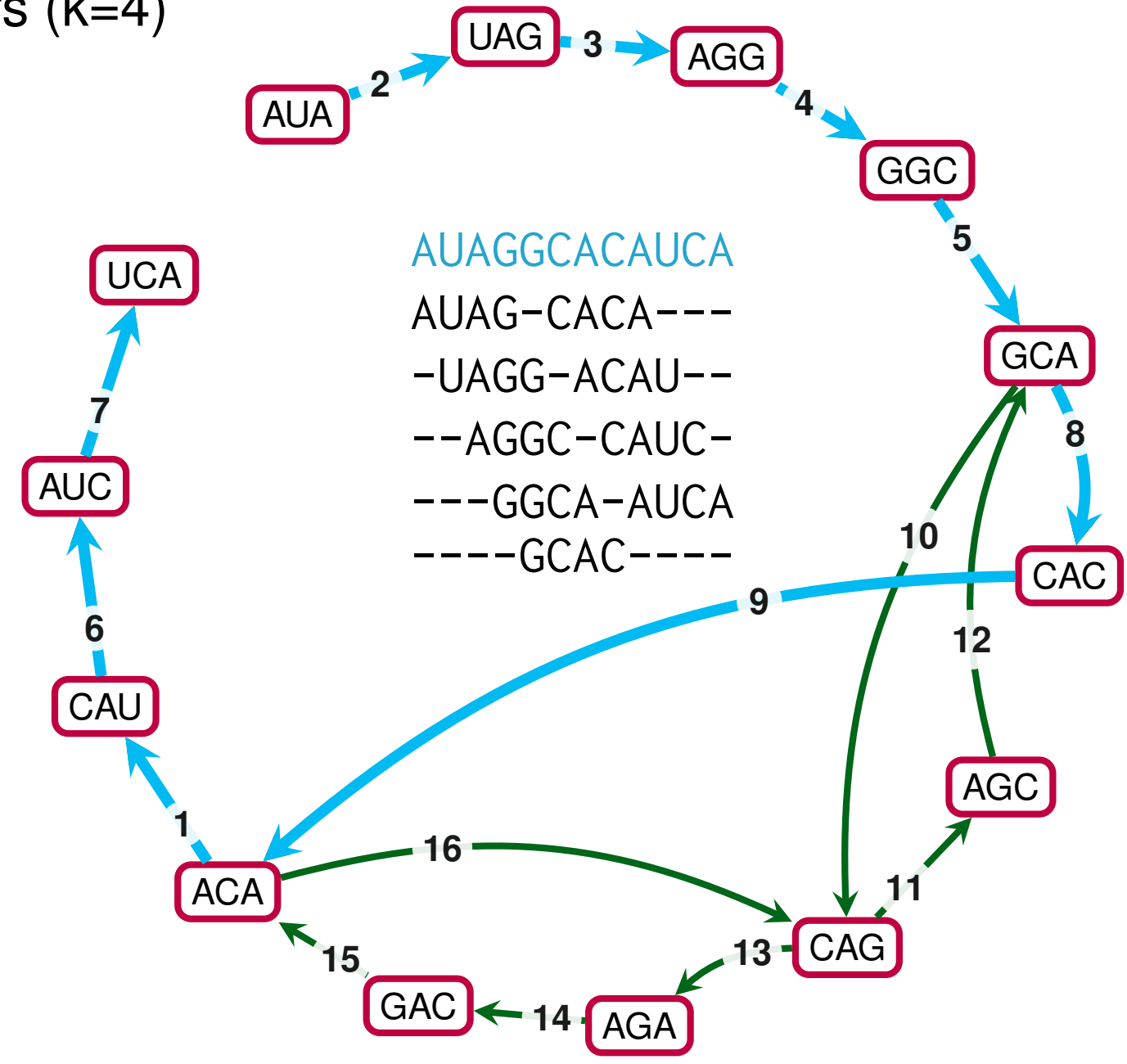
16: ACAG



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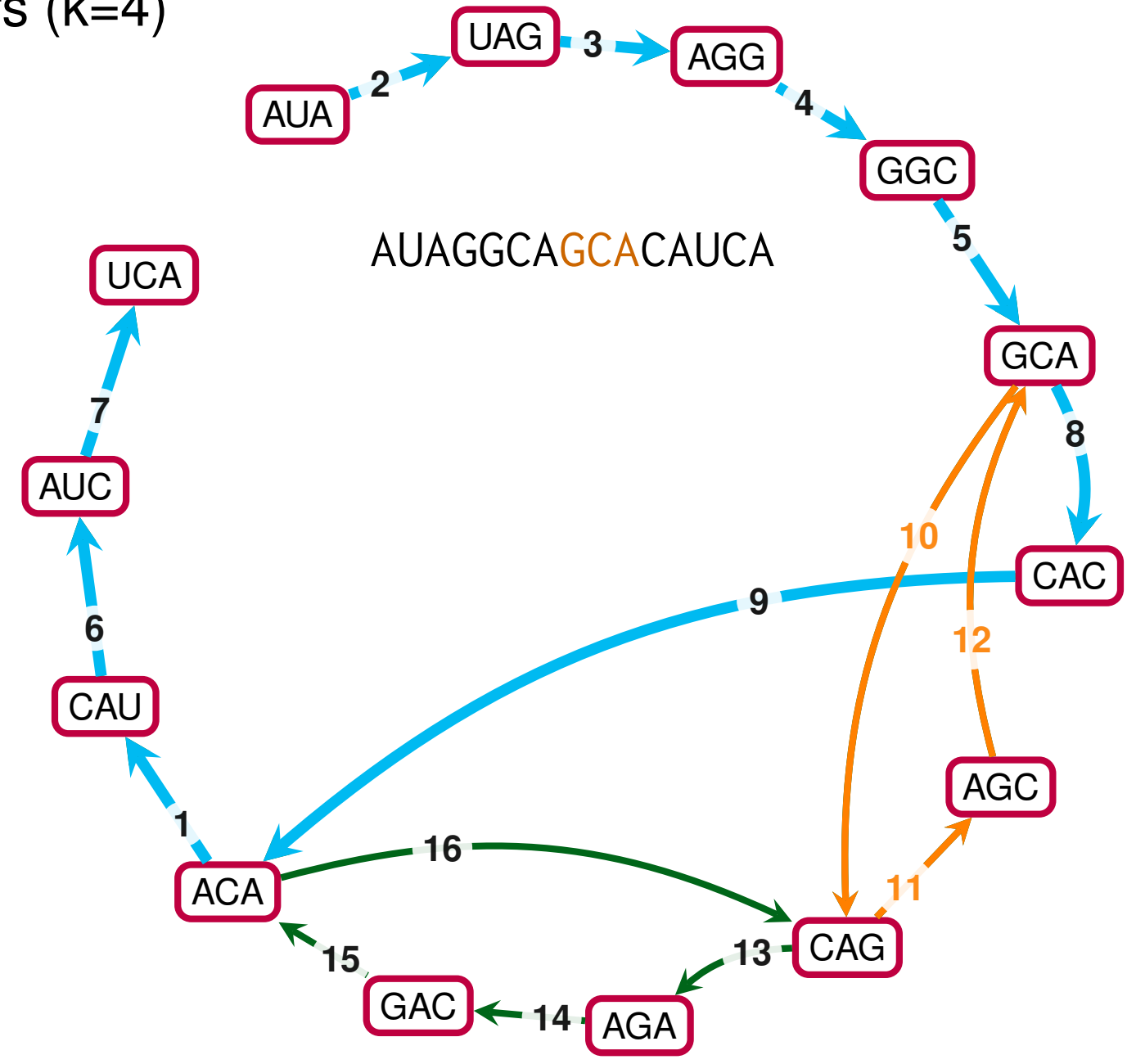
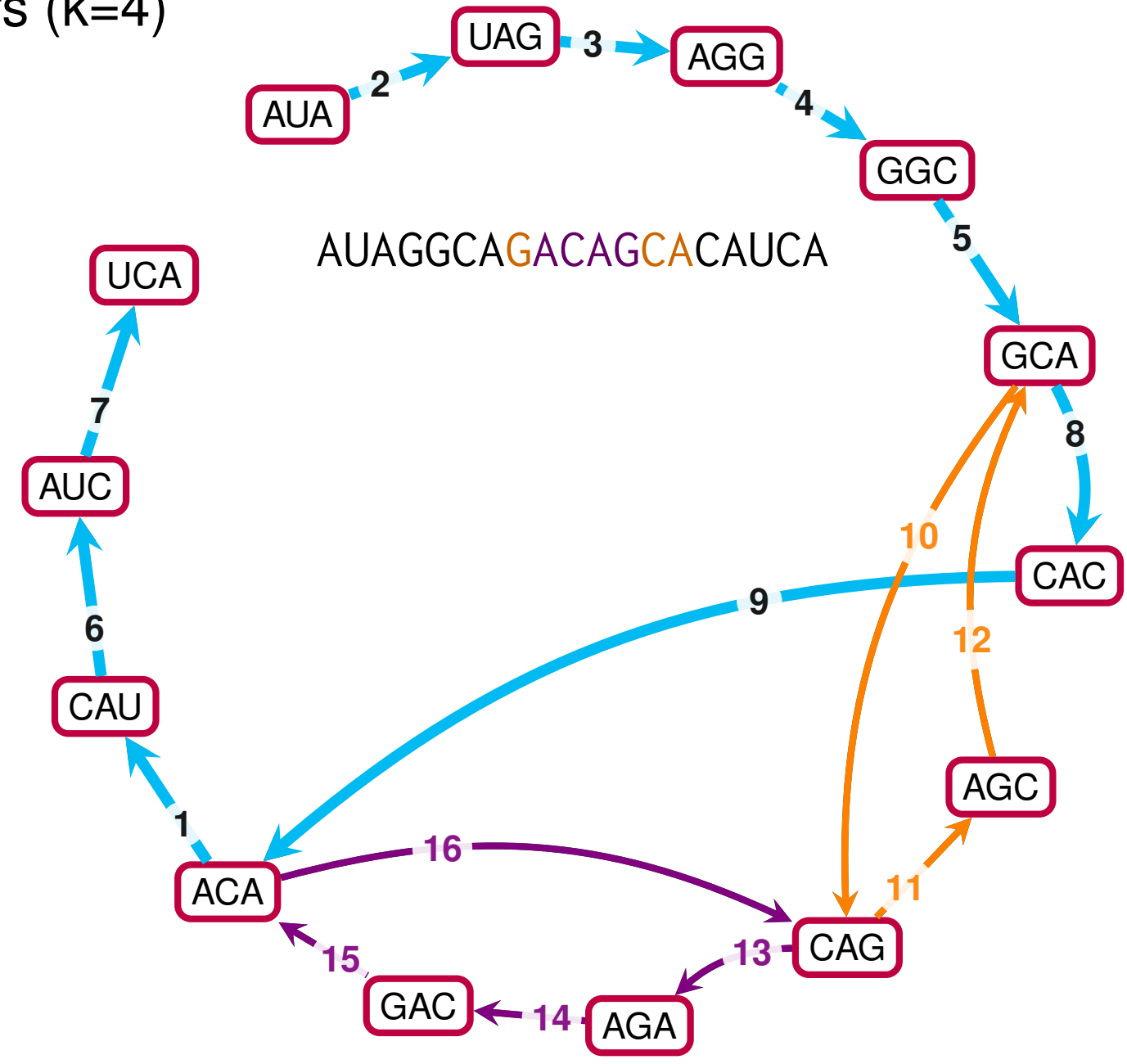
3: UAGG
4: AGGC
5: GGCA
6: CAUC
7: AUCA
8: GCAC
9: CACA
10: GCAG
11: CAGC
12: AGCA
13: CAGA
14: AGAC
15: GACA
16: ACAG



NGS k-mers (k=4)

1: ACAU
2: AUAG
3: UAGG
4: AGGC
5: GGCA
6: CAUC
7: AUCA
8: GCAC
9: CACA
10: GCAG
11: CAGC
12: AGCA
13: CAGA
14: AGAC
15: GACA
16: ACAG



- **Graphs** are awesome, and **ubiquitous** in Bioinformatics
- Faced with a **new problem**, finding formulation as **graph problem** allows to tap into centuries of algorithmic design...
- ... to find **efficient** (poly time) algorithms ...
- ... or identify **workarounds** for **hardness results** (FPT, approx, heuristics)
- It also enables **laziness** through reuse of implementations of algorithms and data structure $\rightarrow$ Lab work
- Knowing graphs algorithms informs choice of model/objective during method development, to achieve good **tradeoff** between **expressivity** and **tractability**

**But beware** of using graphs just for the sake of using them[2].

[2] From a Hammer's perspective, everything looks like a nail... Don't be a Hammer!