Complexity of enumeration and a practical example in cheminformatics

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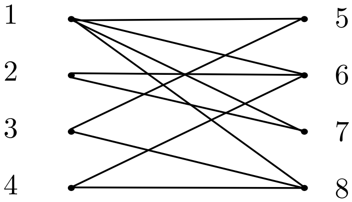
Enumeration problems

- Enumeration problems: list all solutions rather than just deciding whether there is one.

Perfect matchings:



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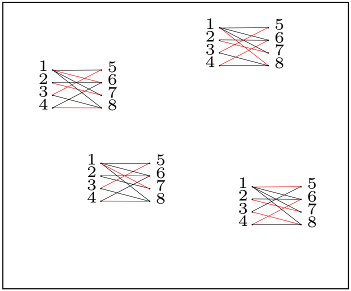

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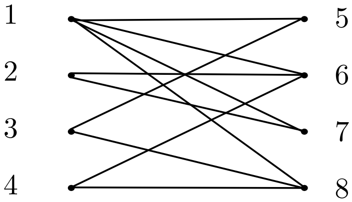

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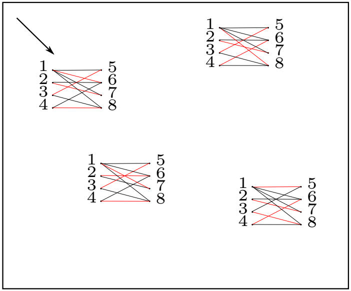

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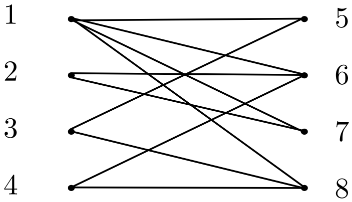

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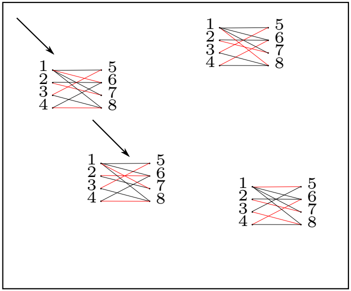

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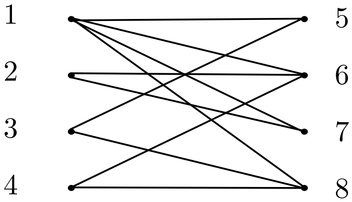

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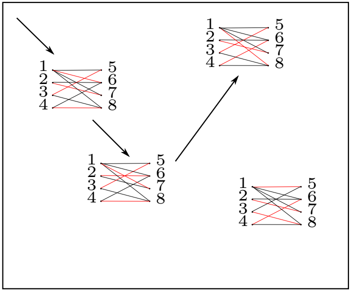

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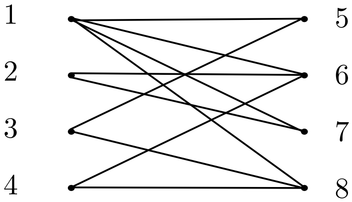

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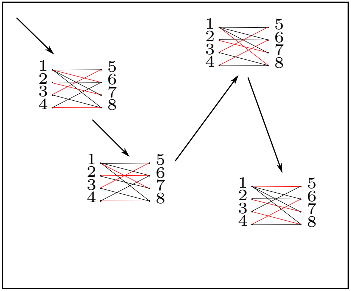

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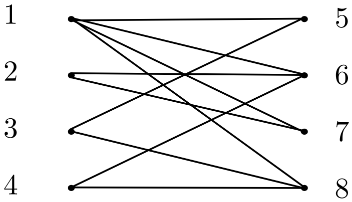

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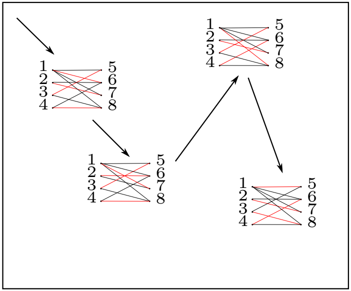

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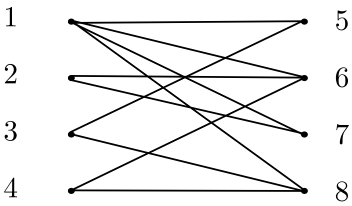

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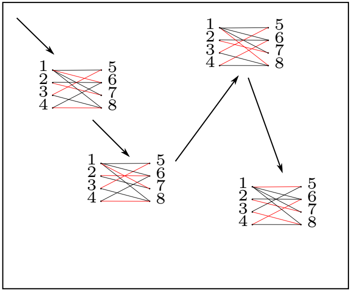

Enumeration Complexity

- Theoretical framework
- Methods for enumeration

A practical enumeration problem from cheminformatics

- Enumeration of planar maps with constraints
- Our algorithm: Kékulé

Framework

Polynomially balanced predicate $A(x, y)$, decidable in polynomial time.

- $\exists ? y A(x, y)$: decision problem (class NP)
- $\sharp\{y \mid A(x, y)\}$: counting problem (class $\sharp\mathrm{P}$)
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    - constant amortized time: CAT (Tree enumeration)
2. The delay
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Relation between classes

- $\mathrm{SDelayP}$: produce the next solution from the last one only in polynomial time
- QueryP: produce the i^{th} solution in polynomial time

Proposition

Conditional separation under $\mathsf{P} \neq \mathsf{NP}$ *hypothesis:*

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1. We can allow some randomization in our algorithms. They must satify that all solutions are enumerated correctly with probability $1 - \epsilon$.
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Uniform generation + space implies efficient enumeration

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If A has a polytime almost uniform random generator, then $\textsc{Enum}{\cdot}A \in \textsc{Inc}\mathrm{PP}$.

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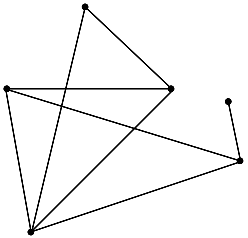

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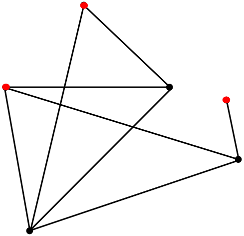

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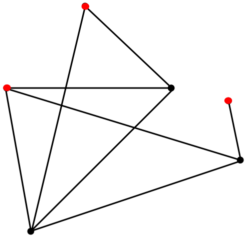

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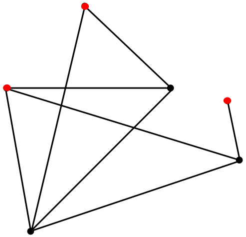

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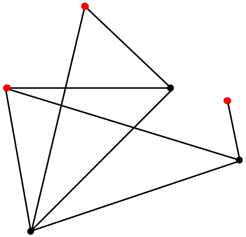

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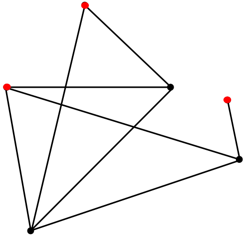

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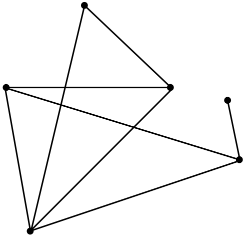

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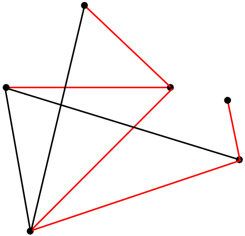

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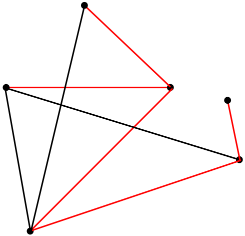

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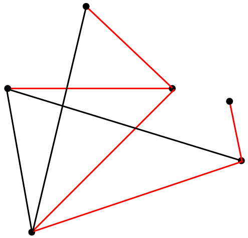

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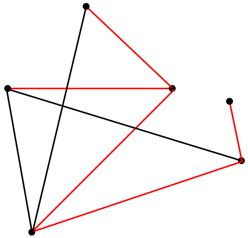

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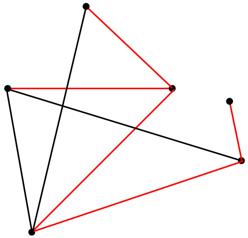

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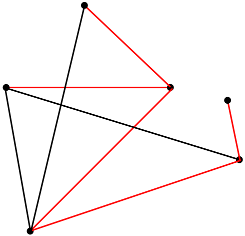

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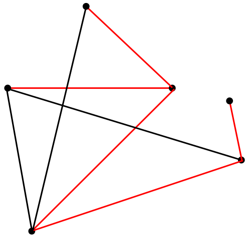

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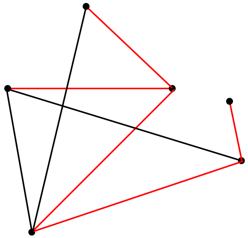

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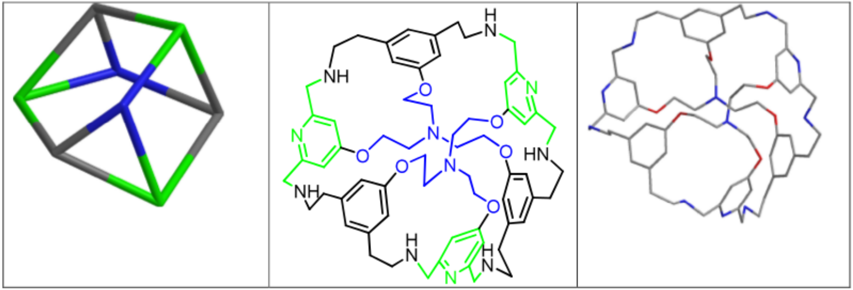
- Our algorithm: Kékulé

Nice pictures to impress the layman

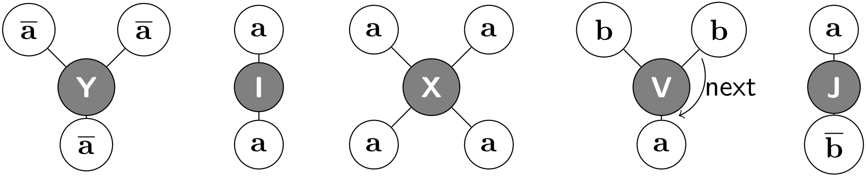


The motifs

Definition

A map $G = (V_{\mathsf{c}}, V, E, \text{next})$ is a **motif** if

1. V_{c} contains only one vertex c called the center
2. each vertex in V is colored with a color in $\mathcal{A}$ a fixed alphabet
3. $E = \{(c, u),\ u \in V\}$
4. next gives an order on the edges of c



Map of motifs

Definition

A connected planar map $G = (V_c, V, E, \text{next})$ is a **map of motifs** based on $\mathcal{M}$ if,

1. each vertex in V is connected to at most one vertex in V, which is of the complementary colour.
2. when all edges between vertices in V are removed, the remaining connected components must all be motifs of $\mathcal{M}$

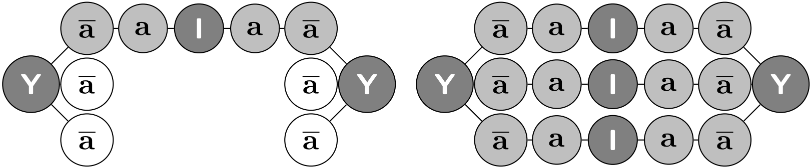


Figure : Example of two maps of motifs based on $\mathcal{M} = \{\mathbf{Y}, \mathbf{I}\}$, the first map is unsaturated while the second map is saturated.

Molecular map

Definition

Let $G = (V_{\mathsf{c}}, V, E_G, \mathsf{next}_G)$ be a saturated map of motifs based on $\mathcal{M}$, we define the **molecular map** $M = (V, E_M, \mathsf{next}_M)$:

1. $V = V_{\mathsf{c}}$
2. $(c_1, c_2) \in E_M$ if it exists a path (c_1, u, v, c_2) in G
3. $\mathsf{next}_M((c, c_1)) = (c, c_2)$ if it exists two paths (c, u_1, v_1, c_1) and (c, u_2, v_2, c_2) in G and $\mathsf{next}_G((c, u_1)) = (c, u_2)$

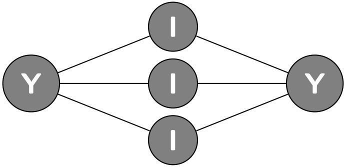


Figure : The molecular map corresponding to the saturated map of motifs in Fig. 1

The indices

Why is a molecular map a good representation of a molecula ?

1. Constraint on the edges: possible chemical connections
2. The *size* of a cut $S = (S_1, S_2)$ is the number of edges with one end in S_1 and the other in S_2.

$$sparsity(S) = \frac{size(S)}{\min(|S_1|, |S_2|)}$$

Sound molecula have high minimum sparsity.

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4. A large face in the graph $\equiv$ an entrance in the cage

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The problem

Enumeration problem

We want to generate, given a set of motifs $\mathcal{M}$ and a size n, all molecular maps based on $\mathcal{M}$ and of size n.

The number of maps is exponential in n. We would like an algorithm in $\textsc{DelayP}$ or at least in linear total time.

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Fold and outline

The fold operation on the vertices u and v is adding the edge (u, v) to G. Valid when u and v are:

1. free
2. of complementary colors
3. in the same face of G

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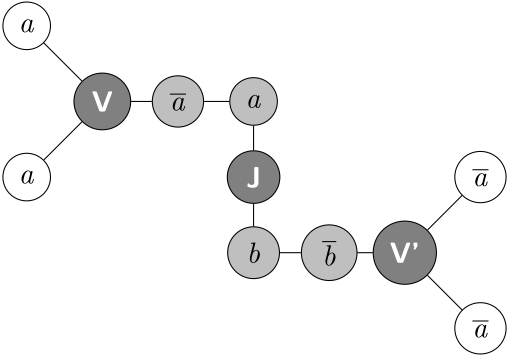

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Figure : A map of three motifs on $\mathcal{A}_M = \{\mathbf{V}, \mathbf{V}', \mathbf{J}\}$ and its outline before a fold operation.

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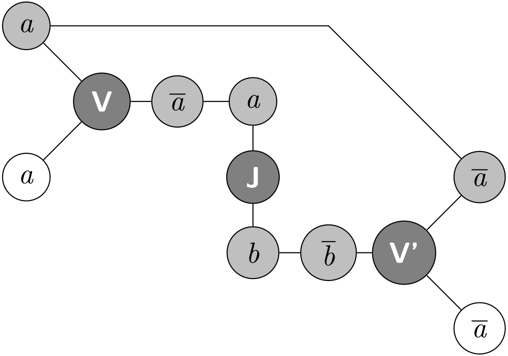

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The outline is a circular sequence of vertices. The fold remove two vertices of compatible colours.

Enough to work with the sequence of colours of the vertices. In the previous example $a\bar{a}\bar{a}a$.

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A map is almost foldable if for every letter in $a \in \mathcal{A}$, there are as many vertices labeled with a and $\bar{a}$.

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Dynamic programming algorithm:
k is the number of positive letters in $\mathcal{A}$.
We generate a k-dimensional array which allows to decide whether a path can be extended by l motifs and be almost foldable.

Takes $O(n^{k+1})$ but there are about C^n paths and it reduces their number by a large factor.

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Some hidden costs:

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Let's all do enumeration

Open Questions

Enumeration:

1. Separate DelayP from IncP modulo ETH
2. Design a reduction compatible with low enumeration classes.

Cheminformatics:

1. A CAT algorithm to generate maps of motifs which are trees
2. A smaller family of backbones which still make the generation exhaustive.
3. A better fold algorithm (constant delay, linear precomputation).
4. A way to avoid some foldings.