TransProof: Computer assisted graph transformations

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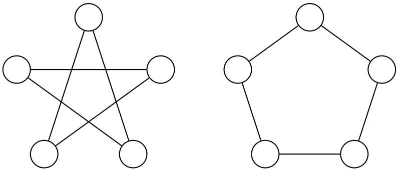
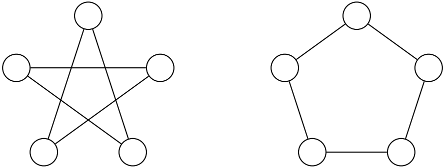
Isomorphism

- We work on simple undirected graphs.
- For a graph $G = (V, E)$, we denote
  - its order $|V|$ by n,
  - its size $|E|$ by m.
- We consider two graphs as equivalent if they are isomorphic.



Graph invariants

- A graph invariant is a function on graphs constant by isomorphism.
- Examples : average distance ($\overline{d}$), diameter (D), chromatic number (χ), planarity, ...



$$\overline{d} = 1.5, D = 2, \chi = 3, \textit{planarity} = \textit{true}, \ldots$$

This talk

- Context : Computer-assisted Proofs in Extremal Graph Theory.
- Objective of this talk :
  - Presentation of TransProof, a module of PHOEG
  - use of an illustrative problem (EMD).
- Remarks :
  - TransProof is currently a prototype
  - The problem about EMD is still open

Conjectures

- Extremal Graph Theory tries to define bounds on these invariants with respect to some constraints.
- The constraints are usually of two forms :
  - restricting to a class of graphs,
  - fixing or restricting some other invariant.
- Since tight bounds are even better, we search for graphs that realize these bounds : the extremal graphs.

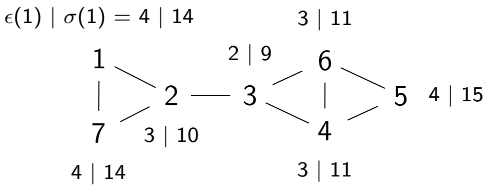
Distances

Definition

The eccentricity *of a vertex u ($\epsilon(u)$) is the maximal distance between u and any other vertex.*

Definition

The transmission *of a vertex u ($\sigma(u)$) is the sum of the distances between u and all the other vertices.*



Average eccentricity - average distance

- We denote by $(\overline{\epsilon} - \overline{d})(G)$ the difference between the average eccentricity and the average distance (EMD).

$$(\overline{\epsilon} - \overline{d})(G) = \frac{\sum\limits_{v \in V(G)} \epsilon(v)}{n} - \frac{\sum\limits_{v \in V(G)} \sigma(v)}{n \cdot (n-1)}$$

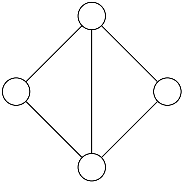
$$= \frac{1}{n \cdot (n-1)} \cdot \left(\sum_{v \in V(G)} (n-1) \cdot \epsilon(v) - \sigma(v) \right)$$

Conjecture (Aouchiche, 2006)

Let $\mathcal{G}$ be the set of connected graphs of order n,

$$\forall G \in \mathcal{G}, (\overline{\epsilon} - \overline{d})(G) \leq (\overline{\epsilon} - \overline{d})(P_n)$$

Proofs by Transformation



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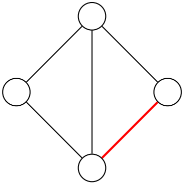
Proofs by Transformation



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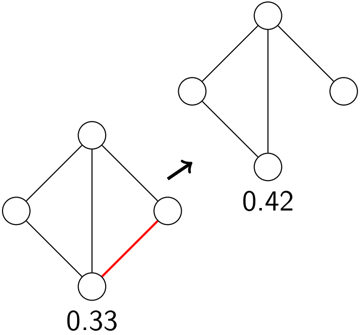
Proofs by Transformation



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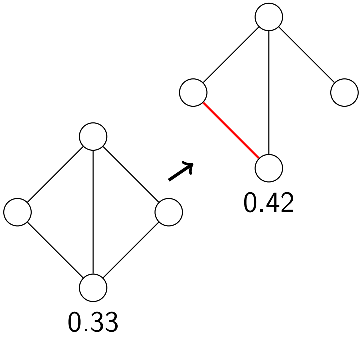

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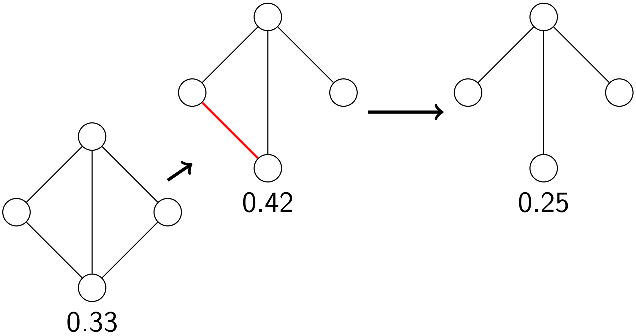
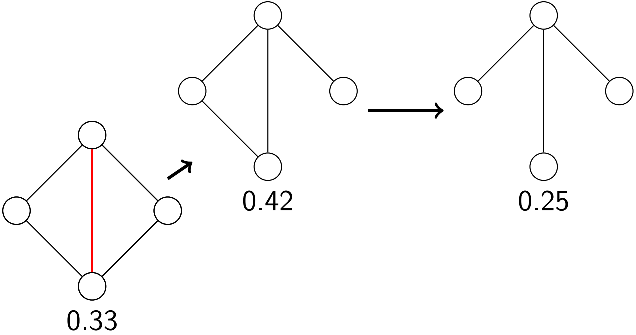
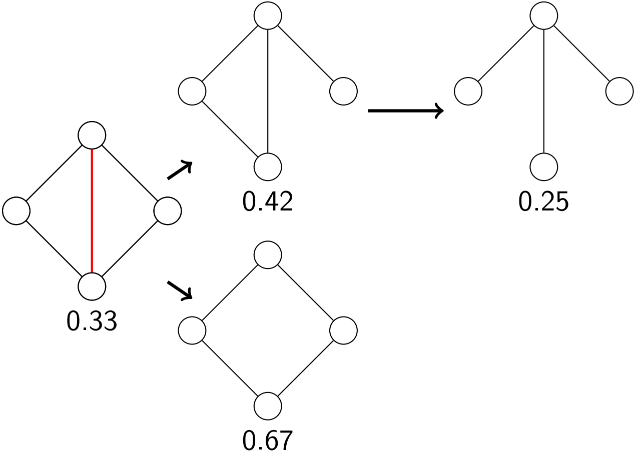


Proofs by Transformation



Proofs by Transformation



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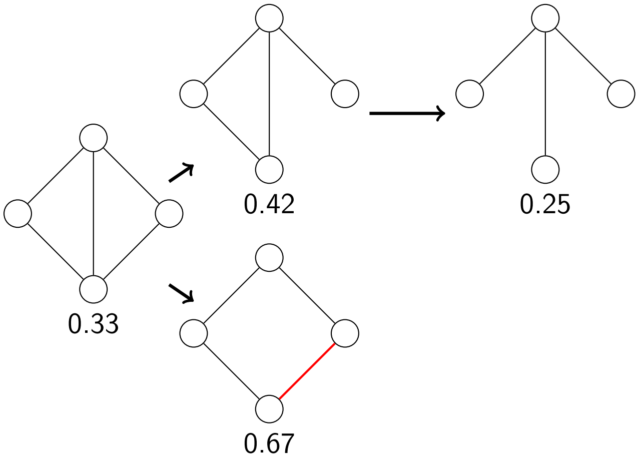
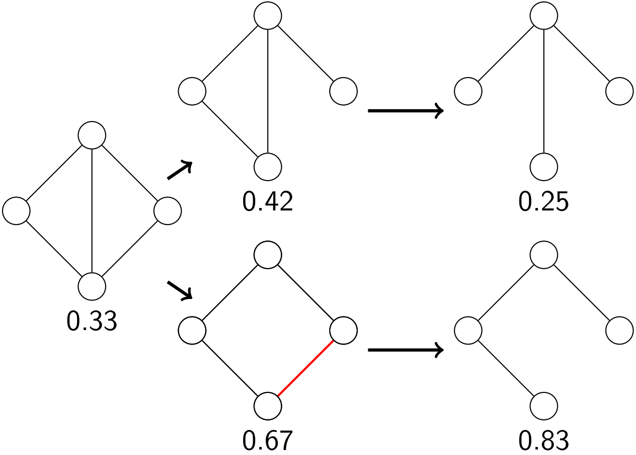
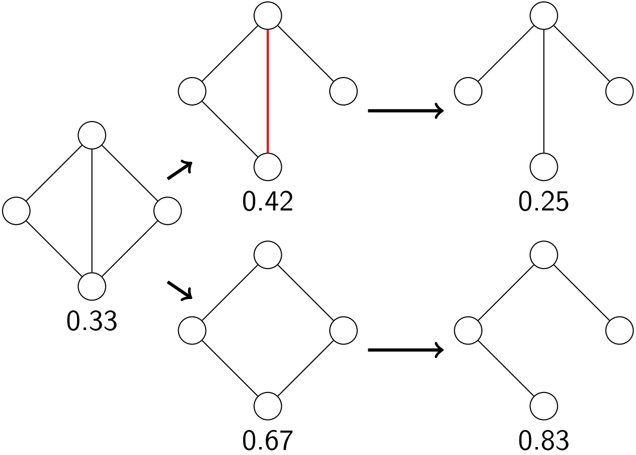


Proofs by Transformation



Proofs by Transformation



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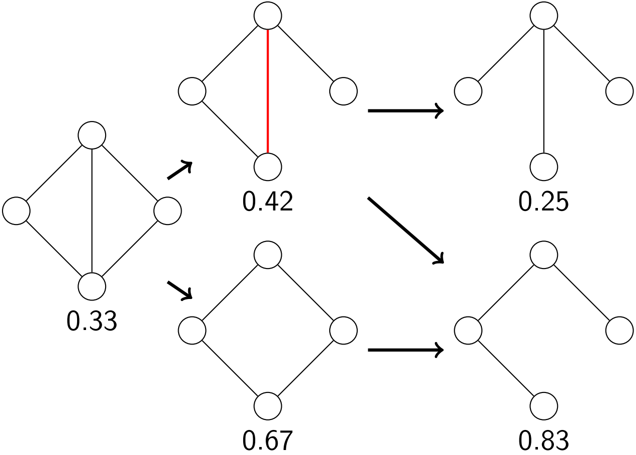
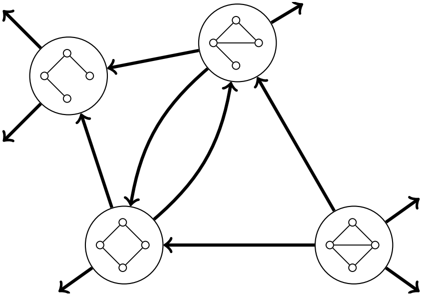


Metagraph of Transformations

- The idea of a proof by transformation can be represented as a directed multi graph.
- We call this graph the metagraph of transformations.
- It can be used to study transformations but also to help define proofs by transformation.



Graph Database

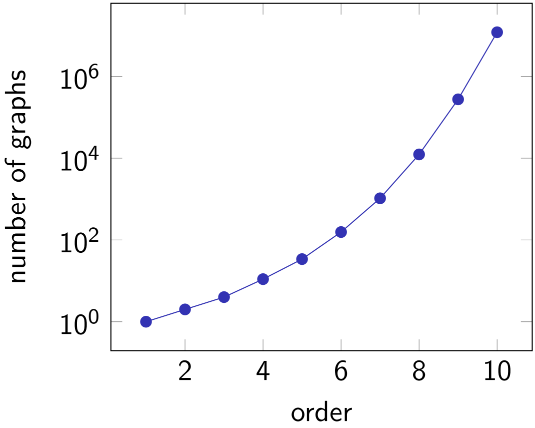
- TransProof can compute the metagraph and store it in a graph database.
- This database allows for easy queries about the transformations.

```
MATCH (n)-[r:edgeRemove]->(m) where n.invariant <
m.invariant return n,r,m;
```

```
MATCH (n id:42)-[r:edgeRemove*..]->(m id:65536) return r;
```

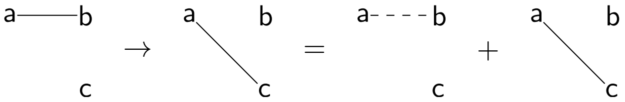
Limitations

- The number of graphs of some order n increases exponentially.
- The number of possible transformations is even bigger.

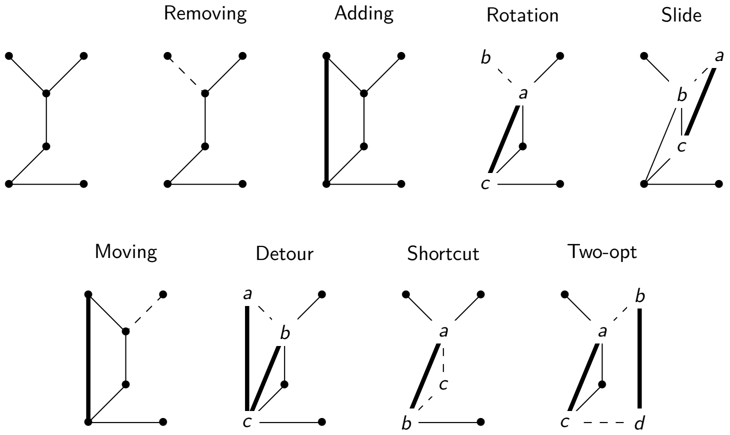


Basis of Transformations

- Most transformations can be described as combination of simpler transformations.
- Why not use a subset of simple transformation to generate more complex ones?



Commonly used transformations



Specific language

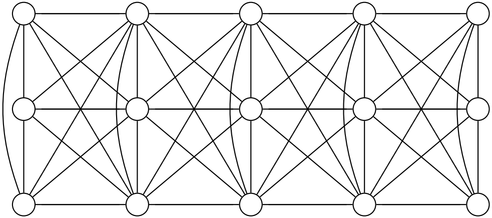
- To help with the writing of queries, we could define a specific language.
- This language could also provide some optimization.

```
MATCH (n)-[r:rotation]->(m) where
not edge(n.sig,r.b,r.c) with n,r,m
match (m)-[s:addEdge]->(o)
where s.a = r.b && and s.b = r.c
return n,r,m,s,o;
```

```
rotation(a,b,c):
  !edge(b,c);
addEdge(b,c);
```

Still Incomplete

- This language is not yet complete.
- It cannot describe transformations with unfixed number of edges
- As an example, consider a set of cliques joined to form a path.



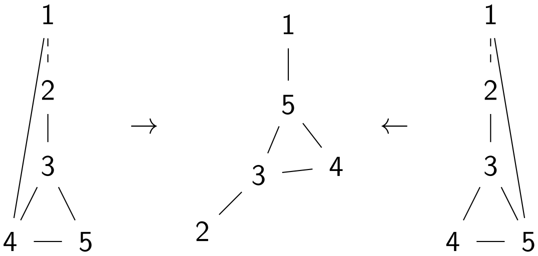
Some Numbers

- The problem is that only considering simple transformations still produces a huge amount.

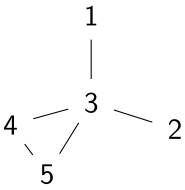
order	# graphs	# arcs
1	1	0
2	2	4
3	4	36
4	11	362
5	34	3 188
6	156	34 376
7	1 044	468 936
8	12 346	10 143 824
9	274 668	380 814 904

Symmetries

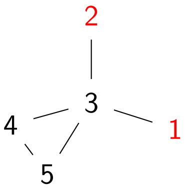
- Some of these transformations are symmetries.
- They actually come from automorphisms.



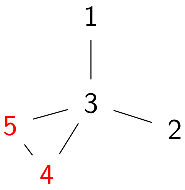
Automorphisms



(1, 2, 3, 4, 5)



(2, 1, 3, 4, 5)



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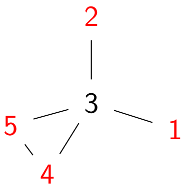
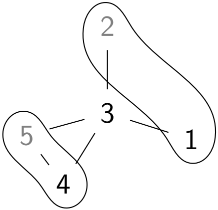


(2, 1, 3, 5, 4)

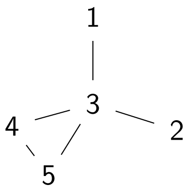
(1 2)(3)(4 5)

Using automorphisms

- To avoid these automorphisms, we have to :
  - Compute the orbits of the automorphism group.
  - Order them based on the lowest index.
  - Simply take one vertex from each.
  - When a vertex is fixed, the orbits can change.



Avoiding Symmetries



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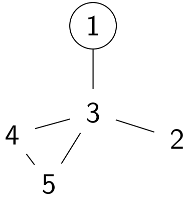

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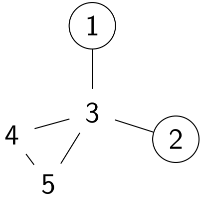

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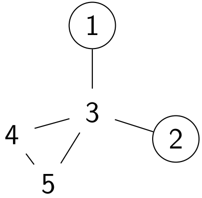

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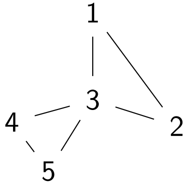

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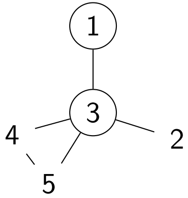

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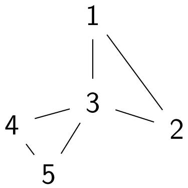

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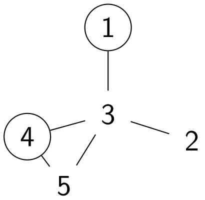

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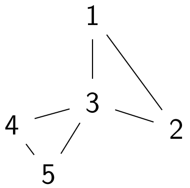

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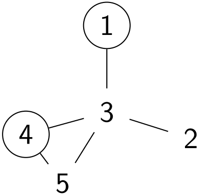

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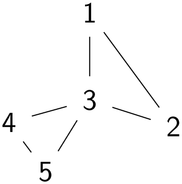

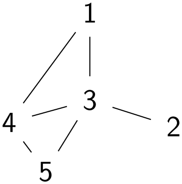

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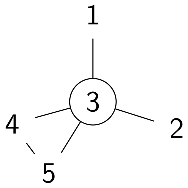

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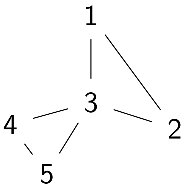

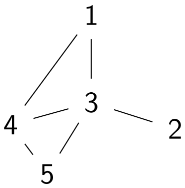

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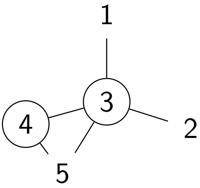

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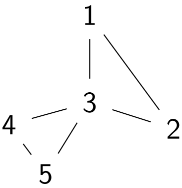

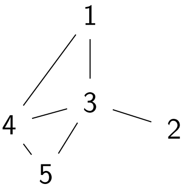

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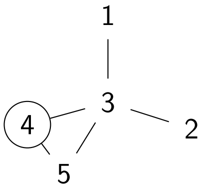

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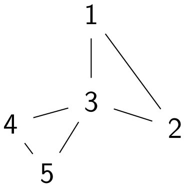

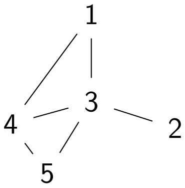

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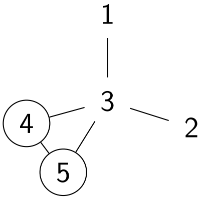

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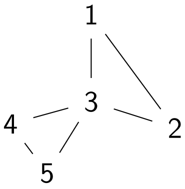

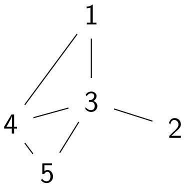

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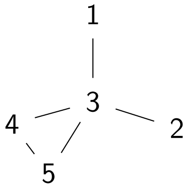

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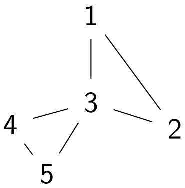
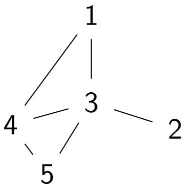




Effect of symmetries

- Without symmetries, we greatly reduce the size of the metagraph.

order	# graphs	# arcs	now
1	1	0	0
2	2	4	2
3	4	36	12
4	11	362	78
5	34	3 188	617
6	156	34 376	6 717
7	1 044	468 936	108 022
8	12 346	10 143 824	2 776 023
9	274 668	380 814 904	119 430 801

Using TransProof

- Now, we can try to use this metagraph for the EMD conjecture.

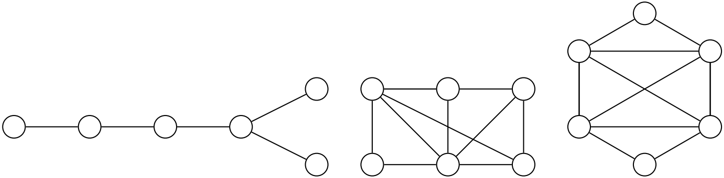
Conjecture (EMD)

Let $\mathcal{G}$ be the set of connected graphs of order n,

$$\forall G \in \mathcal{G}, (\overline{\epsilon} - \overline{d})(G) \leq (\overline{\epsilon} - \overline{d})(P_n)$$

Example of use of TransProof

- For our problem, we could try removing an edge.



- Some problematic graphs appear because of some "symmetry".
- These graphs have (almost) twin nodes.

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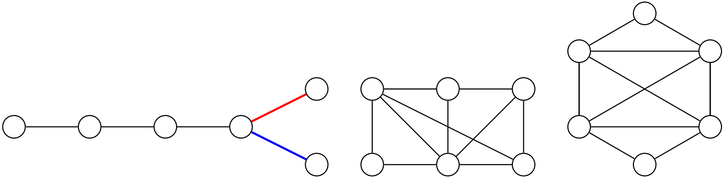

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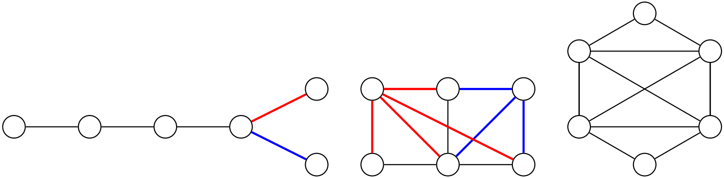

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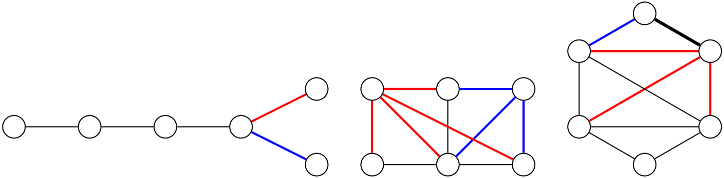
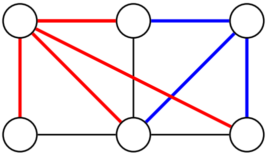


- Some problematic graphs appear because of some "symmetry".
- These graphs have (almost) twin nodes.

A more complex transformation

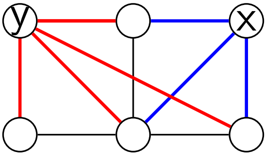
- Choose two vertices x and y such that y has at least the same neighbors as x.
- Choose a vertex z with maximal transmission.
- Make x a pending vertex to z.



$$(\overline{\epsilon} - \overline{d})(G) = 0.5$$

A more complex transformation

- Choose two vertices x and y such that y has at least the same neighbors as x.
- Choose a vertex z with maximal transmission.
- Make x a pending vertex to z.



$$(\overline{\epsilon} - \overline{d})(G) = 0.5$$

A more complex transformation

- Choose two vertices x and y such that y has at least the same neighbors as x.
- Choose a vertex z with maximal transmission.
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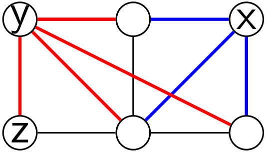

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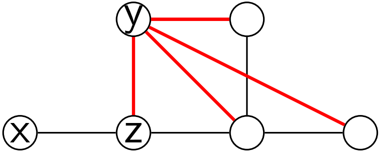
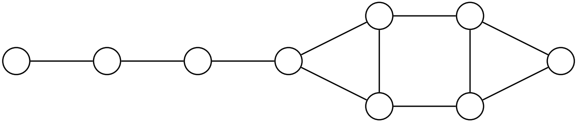


$$(\bar{\epsilon} - \bar{d})(G) = 0.9$$

Remaining graphs

- There are still situations where this transformation does not apply.



$$(\bar{\epsilon} - \bar{d})(G) = 2.1666\ldots$$

- Choose an edge xy and remove all vertices between x and all other vertices that are parts of a cycle.
- These two transformations are sufficient for all connected graphs up to order 10.

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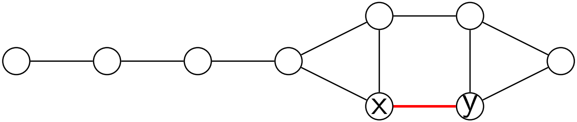

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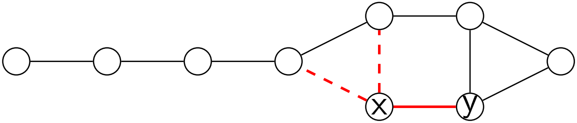

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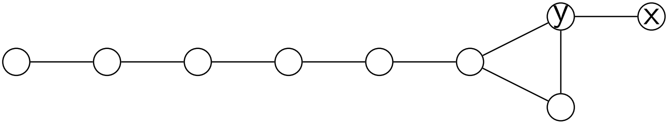

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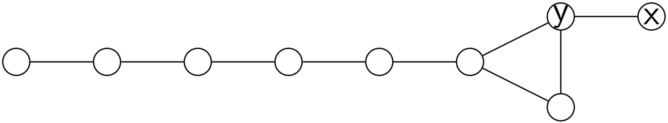

$$(\bar{\epsilon} - \overline{d})(G) = 2.5555\ldots$$

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Adding Constraints

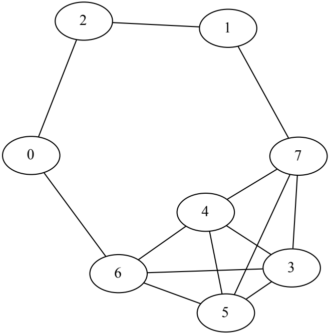
- While these transformations works on more than a million of graphs, there is no formal proof.
- There are still some cases where they do not increase the invariant.

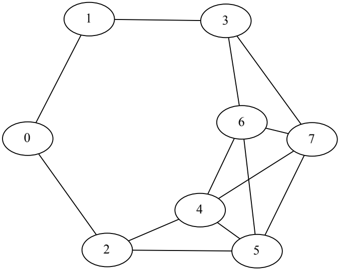
Problem

Among all connected graphs of order n and diameter D, what are the graphs maximizing the difference between the average eccentricity and average distance ?

New extremal graphs (when $2 \cdot D(G) \leq n$)

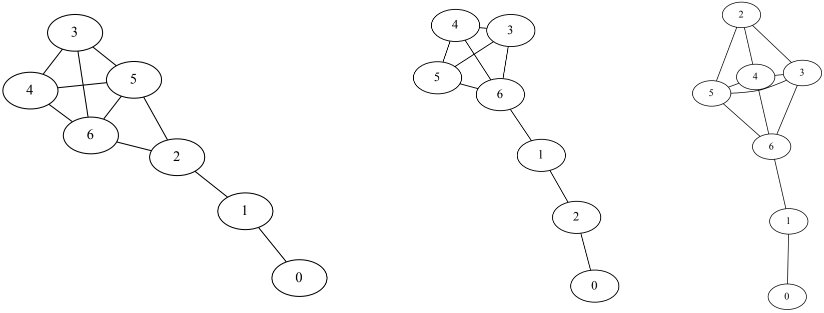
- When there is enough vertices, build a cycle of size $2 \cdot D(G)$.
- Add remaining nodes as twins to adjacent nodes of the cycle.





New extremal graphs (when $2 \cdot D(G) > n$)

- If there is not enough nodes, simply build a diametral path.
- Again, add remaining nodes as twins but to the node of index $p = \frac{2 \cdot d - n + 1}{4}$.



Notes

- If the diameter is 2, extremal graphs are complement of matchings.
- The cube is also extremal but not the square or other hypercubes.
- For a given n, the invariant strictly increases between extremal graphs when diameter increases.
- If $D(G) = n - 1$, the extremal graph is P_n.

Conclusion

- We are developing a system able to compute the metagraph
- It allows exploring the metagraph and testing proofs by transformations
- We use some ideas to tackle the problem of the amount of data.
- It could be used to speed up metaheuristics
- It is helpfull to define transformations.
- Sometimes, adding constraints can give some insight.

Conclusion

- We are developing a system able to compute the metagraph
- It allows exploring the metagraph and testing proofs by transformations
- We use some ideas to tackle the problem of the amount of data.
- It could be used to speed up metaheuristics
- It is helpfull to define transformations.
- Sometimes, adding constraints can give some insight.

Questions ?

Vertex index when $2 \cdot D(G) > n$

- Let G be a graph with n vertices and diameter d composed of a path $P = p_0, p_1, \ldots, p_d$ and $n - d$ vertices $(R = r_0, r_1, \ldots, r_{n-d-1})$ each twin to a vertex of the path.
- We want to find the vertex p_p which, if used as a twin to the vertices r_i, would maximise the invariant.
- We can suppose that vertices r_i form a clique (or we could increase the invariant).

$$(\overline{\epsilon} - \overline{d})(G) = \frac{1}{n \cdot (n-1)} \cdot \left(\sum_{v \in V(G)} (n-1) \cdot \epsilon(v) - \sigma(v) \right)$$

$$= \frac{1}{n \cdot (n-1)} \cdot \sum_{v \in V} W(v)$$

Vertex index when $2 \cdot D(G) > n$

- For the vertex of index p in the path :

$$W_P(p) = (n-1) \cdot \epsilon(p) - \sum_{u \in V} dpu$$

$$= (n-1) \cdot \max(d-p, p) - \left(\frac{(d-p) \cdot (d-p+1)}{2} + \frac{p \cdot (p+1)}{2} \right)$$

- For a twin node to the vertex of index p :

$$W_R(p) = (n-1) \cdot \max(d-p, p)$$

$$-2 \cdot \left(\frac{(d-p) \cdot (d-p+1)}{2} + \frac{p \cdot (p+1)}{2} \right) - 2 - (n-d-1)$$

$$= -2 \cdot p^2 + (2 \cdot d - n + 1) \cdot p - d^2 + (n-2) \cdot d$$

- This polynomial of degree 2 is maximal when $p = \frac{2 \cdot d - n + 1}{4}$