

Structure generation

Generation of generalized cubic graphs

N. Van Cleemput



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Exhaustive isomorph-free structure generation

Create all structures from a given class of combinatorial structures without isomorphic copies

Combinatorial enumeration is not always sufficient.

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Exhaustive isomorph-free structure generation

- all graphs with 10 vertices
- all cubic multigraphs with 20 vertices
- all molecules for the formula $C_{20}H_{10}$
- all permutations of 12 elements
- all tilings of the plane with 2 face orbits
- all union-closed families of sets on a ground set with 5 elements

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Historic highlights of structure generation

- Theaetetus (± 400 BC): 5 platonic solids
- Narayana Pandit (14th century): all permutation of n elements (probably not for very large n)
- Jan de Vries (1889): all cubic graphs on up to 10 vertices
- Donald W. Grace (1965): all polyhedra with up to 11 faces
- Alexandru T. Balaban (1966): all cubic graphs on up to 10 vertices (1967: 12 vertices)

This list is not exhaustive!

Why is structure generation useful?

- test conjectures
- build intuition
- search for specific structures
- count structures

A case study

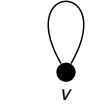


Generation of generalized cubic graphs

Which structures will be generated?

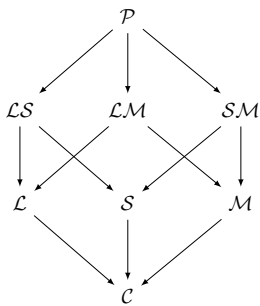
connected, cubic variety of

- simple graphs
- multigraphs
- graphs with loops
- graphs with semi-edges
- any combination of these

Which structures will be generated?

Name	Type	Counts as
Loop		2
Multi-edge		2
Semi-edge		1

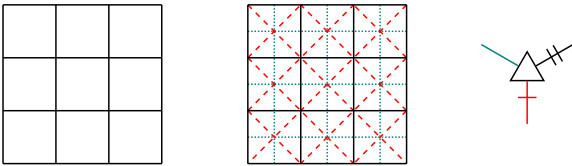
Which structures will be generated?



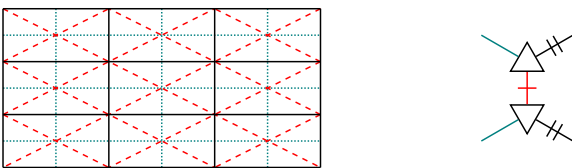
Motivation

- Study of maps
 - flag graphs of maps / hypermaps
 - symmetry type graphs / Delaney-Dress graphs
 - arc graphs of oriented maps
- Voltage graphs

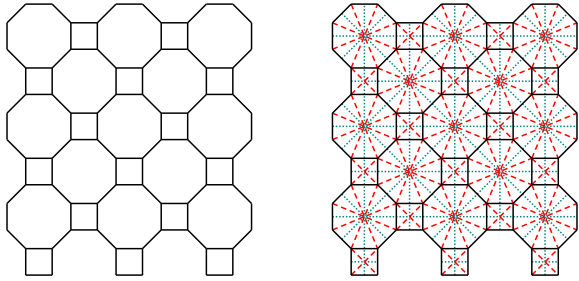
Motivation - Delaney-Dress graph



Motivation - Delaney-Dress graph

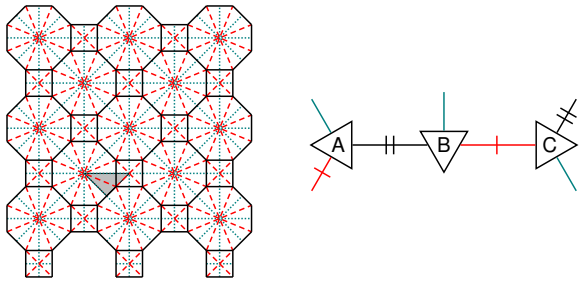


Motivation - Delaney-Dress graph



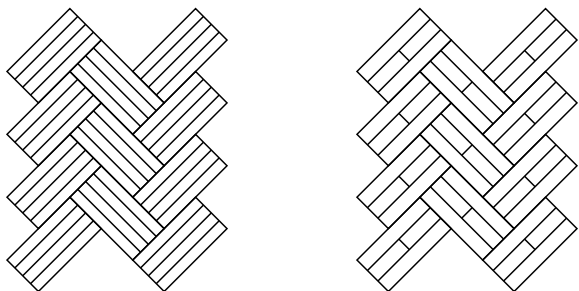
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Motivation - Delaney-Dress graph



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Motivation - Delaney-Dress graph



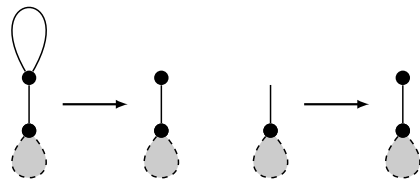
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Generation of pregraphs

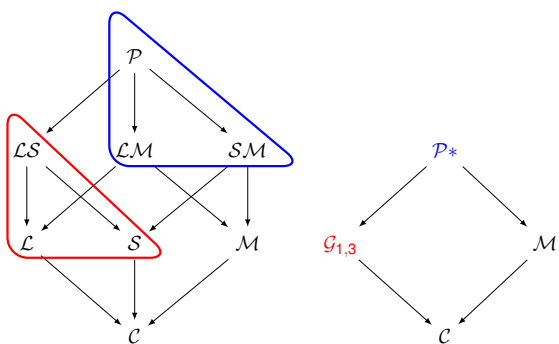
Translation to multigraphs

Pregraph primitives

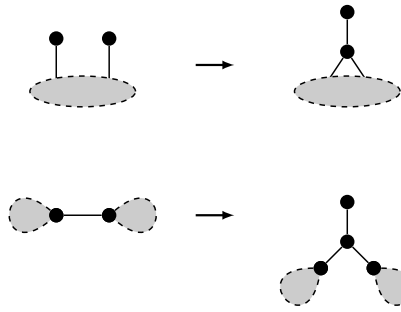
Translate cubic pregraphs to multigraphs with degrees 1 and 3.
 Notation: $*(G)$ is the primitive of G .



Translation to multigraphs

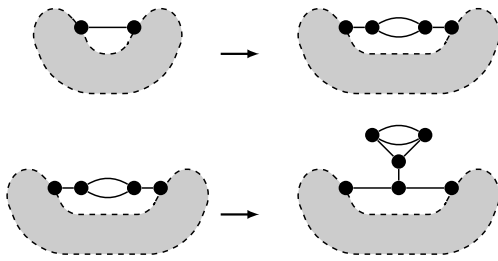


Which are the construction operations?



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Which are the construction operations?



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Exhaustive?

- Can we generate all structures with these operations?
- From which graphs should we start?

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Reductions

Look at the inverse of the construction operations.

- Prove that 'each' structure can be reduced
- Irreducible structures are the start graphs

Reductions

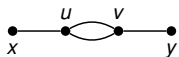
Each cubic pregraph primitive containing a parallel edge can be reduced by reduction 3 or 4 to a cubic pregraph primitive with fewer vertices, except when it is the theta graph or the buoy graph.



Reductions

There exists a parallel edge uv :

- u and v are adjacent to two different vertices x and y
- u and v are adjacent to one vertex x : x is adjacent to z
 - z is adjacent to two different other vertices z_1 and z_2
 - z is adjacent to one other vertex z_1



Reductions

There exists a parallel edge uv :

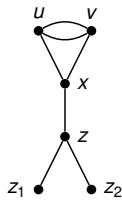
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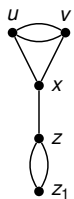
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Reductions

Number of vertices decreases in each step, so this process halts.

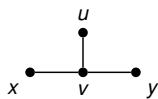
- theta graph
- buoy graph
- simple cubic pregraph primitives

Reductions

Each simple cubic pregraph primitive containing a vertex of degree 1 can be reduced by reduction 1 or 2 to a simple cubic pregraph primitive with fewer edges, except when it is K_2 .

Reductions

There exists a vertex u of degree 1, adjacent to a vertex v of degree 3. The vertex v is adjacent to two other different vertices x and y .



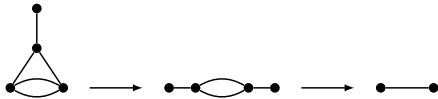
Reductions

Number of edges decreases in each step, so this process halts.

- K_2
- cubic graph

Reductions


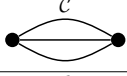
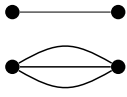
The buoy graph reduces to K_2 by applying reduction 1 and 3.



The irreducible graphs

Each pregraph primitive can be reduced to a cubic simple graph, K_2 or the theta graph.

The irreducible graphs

Target class	Irreducible graphs
\mathcal{C}	\mathcal{C}
$\mathcal{G}_{1,3}$	
\mathcal{M}	
\mathcal{P}^*	

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The irreducible graphs

- degree 1 vertices don't count towards the order of the graph when translating from $\mathcal{G}_{1,3}$ to \mathcal{S} (and similar)
- number of degree 3 vertices never decreases when applying the construction operations

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Structure generation

The irreducible graphs

- \mathcal{L} , \mathcal{M} , \mathcal{LM} with n vertices $\rightarrow \mathcal{C}$ with $\leq n$ vertices.
- \mathcal{S} , \mathcal{LS} , \mathcal{SM} , \mathcal{LSM} with n vertices $\rightarrow \mathcal{C}$ with $\leq n$ vertices, but intermediate $\mathcal{G}_{1,3}$ and \mathcal{P}^* with $\leq 2n + 2$ vertices

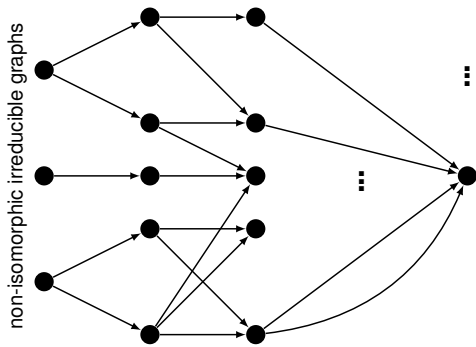
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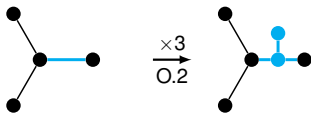
Avoiding isomorphic copies

- isomorphism rejection by list
- canonical representatives and Read/Faradzev-type orderly algorithms
- McKay's canonical construction path method
- homomorphism principle
- double coset method
- closed structures
- ...

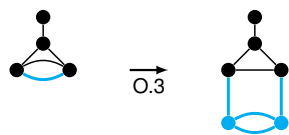
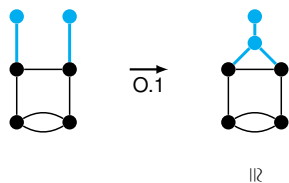
McKay's canonical construction path method



Avoid the same graph from the same parent

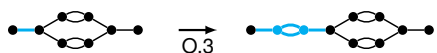
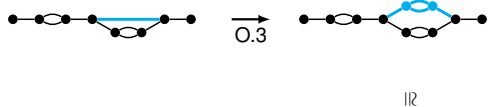


Avoid the same graph from different parents



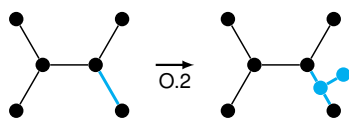
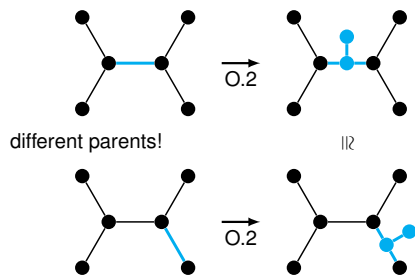
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Avoid the same graph from different parents



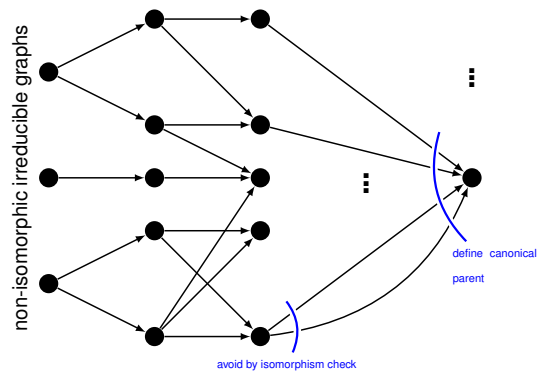
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Avoid the same graph from different parents



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McKay's canonical construction path method



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The canonical parent

For each cubic pregraph primitive:

- define canonical double edge
- define canonical vertex of degree 1

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The canonical parent

A cubic pregraph primitive G is constructed from its canonical parent if

- G contains a double edge
- last operation was operation 3 or 4
- new double edge is in the orbit of the canonical double edge

or

- G is a cubic simple pregraph primitive
- the new vertex of degree 1 is in the orbit of the canonical vertex of degree 1

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Canonicity

Let \mathcal{G} denote the set of all labelled graphs

- *Canonical representative function* c is a function $c : \mathcal{G} \rightarrow \mathcal{G}$
 - $\forall G \in \mathcal{G} : c(G) \cong G$
 - $\forall G, G' \in \mathcal{G} : G \cong G' \Rightarrow c(G) = c(G')$
- *Canonical representative* is the unique element in an isomorphism class that is fixed by c
- *Canonical labelling* is an isomorphism $\phi : G \rightarrow c(G)$

The canonical vertex of degree 1

Canonical vertex of degree 1 is the vertex of degree 1 with the smallest canonical label.

The canonical vertex of degree 1

Computing the canonical labelling is slow (although it is fast).

The canonical vertex of degree 1

Assign to each vertex v of degree 1 a pair of numbers $(n(v), l(v))$

- $n(v)$ is number of vertices at distance at most 4 of v
- $l(v)$ is canonical label of v

Canonical vertex of degree 1 is the vertex of degree 1 with the lexicographically smallest pair.

The canonical vertex of degree 1

Generation of all simple cubic pregraph primitives with 18 vertices

Total operation count	703 520	100%
only 1 vertex of degree 1	91 729	13%
rejected by colour	316 083	45%
accepted by colour	123 628	18%
rejected by <code>nauty</code>	56 911	8%
accepted by <code>nauty</code>	115 169	16%

The canonical double edge

Similar to canonical vertex of degree 1.

Exhaustive isomorph-free generation

If for one representative of each isomorphism class of simple cubic pregraph primitives on up to n vertices with $n_3 < n$ vertices of degree 3

- operation O_1 is applied to one pair of degree-1 vertices in each orbit of pairs of degree-1 vertices,
- operation O_2 is applied to one bridge in each orbit of bridges,

and the resulting graph is accepted if and only if

- it has at most n vertices
- the new vertex of degree 1 is in the orbit of the canonical vertex of degree 1

then exactly one representative of each isomorphism class of simple cubic pregraph primitives on up to n vertices with $n_3 + 1 < n$ vertices of degree 3 and $n_1 > 0$ vertices of degree 1 is accepted.

Isomorphism-free generation

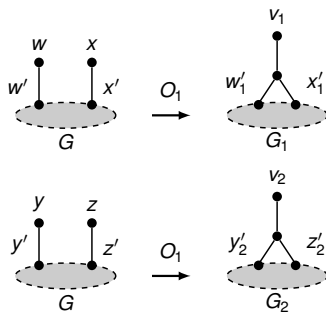
Two isomorphic graphs G_1 and G_2 with respective new vertices of degree 1 v_1 and v_2 .

Let γ be an isomorphism from G_1 to G_2 .

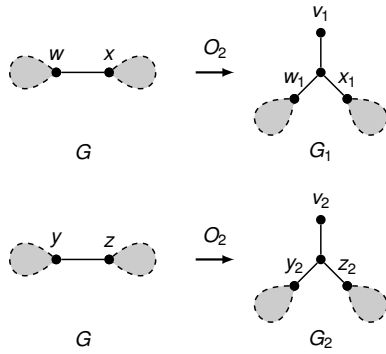
$\gamma(v_1)$ is in the same orbit as v_2 under the automorphism group of G_2 .

A vertex of degree 1 cannot be reduced by both O_1 and O_2 , so v_1 and v_2 were obtained by applying the same operation.

Isomorphism-free generation



Isomorphism-free generation



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Exhaustive generation

Each simple cubic pregraph primitive on up to n vertices with $n_3 + 1 < n$ vertices of degree 3 and $n_1 > 0$ vertices of degree 1 has a canonical vertex of degree 1 (and this vertex is reducible).

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Translation from $\mathcal{G}_{1,3}$ to \mathcal{L} , \mathcal{S} and \mathcal{LS}

- $\mathcal{G}_{1,3}(n)$ to $\mathcal{L}(n)$: there is always a unique pregraph in $\mathcal{L}(n)$.
- $\mathcal{G}_{1,3}(\leq 2n + 2)$ to $\mathcal{S}(n)$: if there are n vertices of degree 3, then there is a unique pregraph in $\mathcal{S}(n)$.
- $\mathcal{G}_{1,3}(\leq 2n + 2)$ to $\mathcal{LS}(n)$: if there are at least n vertices and at most n vertices with degree 3, then there exist pregraphs in $\mathcal{LS}(n)$ corresponding to this pregraph primitive. $n - |V_3(G)|$ vertices of degree 1 correspond to vertices with loops, rest corresponds to semi-edges

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Homomorphism principle

For a group Γ acting on a set M , let $R_\Gamma(M)$ be a set of orbit representatives.

For $m \in M$ let Γ_m denote the stabiliser group.

Given a group Γ acting on two sets M, M' and a surjective mapping $\phi : M \rightarrow M'$ so that $\phi(\gamma m) = \gamma(\phi(m)) \forall m \in M, \gamma \in \Gamma$, then $\cup_{m' \in R_\Gamma(M')} R_{\Gamma_{m'}}(\phi^{-1} m')$ is a set $R_\Gamma(M)$ of orbit representatives for the action of Γ on M .

Homomorphism principle

An isomorphism of 2 cubic pregraphs induces an isomorphism of the cubic pregraph primitives.

Isomorphic cubic pregraphs come from the same cubic pregraph primitive.

An isomorphism of 2 cubic pregraphs induces a nontrivial automorphism of the cubic pregraph primitive.

Homomorphism principle

Compute orbits of $(n - |V_3(G)|)$ -element subsets of the set of all vertices of degree 1.

For each orbit choose a representative.

For each representative, turn all vertices in that set into loops and the other vertices of degree 1 into semi-edges.

Homomorphism principle

If the cubic pregraph primitive has a trivial automorphism group, then each subset corresponds to a distinct cubic pregraph.

If the automorphism group acts trivially on the set of vertices of degree 1, then each subset corresponds to a distinct cubic pregraph.

In other cases some work needs to be done, but the group is often smaller.

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Results and timings

<i>n</i>	<i>C</i>	<i>L</i>	<i>S</i>	<i>M</i>	<i>LS</i>	<i>LM</i>	<i>SM</i>	<i>LSM</i>
1	0	0	1	0	2	0	1	2
2	0	1	1	1	3	2	3	5
3	0	0	2	0	4	0	4	7
4	1	2	6	2	12	5	12	22
5	0	0	10	0	22	0	22	43
6	2	6	29	6	68	17	68	141
7	0	0	64	0	166	0	166	373
8	5	20	194	20	534	71	534	1270
9	0	0	531	0	1589	0	1589	4053
10	19	91	1733	91	5464	388	5464	14671
11	0	0	5524	0	18579	0	18579	52826
12	85	509	19430	509	66320	2592	66320	203289
13	0	0	69322	0	255424	0	255424	795581
14	509	3608	262044	3608	1000852	21096	1000852	3241367
15	0	0	1016740	0	4018156	0	4018156	13504130
16	4060	31856	4101318	31856	16671976	204638	16671976	57904671
17	0	0	16996157	0	70890940	0	70890940	233656990
18	41301	340416	7256640	340416	308439942	2317172	308439942	1139231977
19	0	0	317558689	0	1381815168	0	1381815168	5219113084
20	510489	4269971	1424644848	4269971	6310880471	30024276	6310880471	24401837085
21	0	0	6536588420	0	29428287639	0	29428287639	116278408069
22	7319447	61133757	33647561117	61133757	140012980007	437469859	140012980007	564380686932
23	0	0	146647344812	0	0	0	0	0
24	117940535	978098997	0	978098997	7067109598	0	0	0

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Results and timings

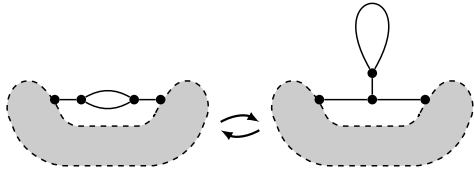
<i>n</i>	<i>C</i>	<i>L</i>	<i>S</i>	<i>M</i>	<i>LS</i>	<i>LM</i>	<i>SM</i>	<i>LSM</i>
10	0.0s	0.0s	0.0s	0.0s	0.1s	0.0s	0.1s	0.1s
11	0.0s	0.0s	0.1s	0.0s	0.2s	0.0s	0.3s	0.4s
12	0.0s	0.0s	0.6s	0.0s	0.8s	0.0s	1.3s	1.8s
13	0.0s	0.0s	2.2s	0.0s	3.5s	0.0s	5.4s	7.4s
14	0.0s	0.0s	9.1s	0.1s	14.9s	0.2s	22.6s	32.2s
15	0.0s	0.0s	37.3s	0.0s	64.1s	0.0s	97.2s	144.5s
16	0.0s	0.3s	158.3s	0.5s	290.1s	2.5s	427.1s	669.5s
17	0.0s	0.0s	695.9s	0.0s	1372.7s	0.0s	1931.5s	3192.3s
18	0.1s	3.0s	3182.2s	5.1s	6552.1s	31.0s	8933.5s	15725.4s
19	0.0s	0.0s	14398.5s	0.0s	32533.2s	0.0s	42194.7s	78738.8s
20	1.4s	39.0s	67781.7s	67.9s	164334.4s	441.9s	203152.1s	404351.9s
21	0.0s	0.0s	329875.5s	0.0s	853461.3s	0.0s	997604.8s	2128059.3s
22	18.6s	577.2s	1627712.4s	1044.1s	4549317.5s	7058.5s	4985448.0s	11440675.6s
23	0.0s	0.0s	8088214.3s	0.0s	0.0s	0.0s	0.0s	0.0s
24	298.4s	9620.6s	0	18022.4s	0	124630.6s	0	0

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Results and timings

n	\mathcal{L}	\mathcal{S}	\mathcal{M}	\mathcal{LS}	\mathcal{LM}	\mathcal{SM}	\mathcal{LSM}
20	109486.4/s	21018.1/s	62886.2/s	38402.7/s	67943.6/s	31064.8/s	60348.0/s
21		19815.3/s		34481.1/s		29498.9/s	54640.6/s
22	105914.3/s	18828.6/s	58551.6/s	30776.7/s	61977.7/s	28084.3/s	49331.1/s
23		18131.0/s					
24	101667.2/s		54271.3/s		56704.4/s		

Connection loops and multi-edges



Subclasses

3-edge-colourable pregraphs

Cubic pregraphs with loops are never 3-edge-colourable.

Other cubic pregraphs are 3-edge-colourable if and only if the corresponding cubic pregraph primitive is 3-edge-colourable.

3-edge-colourable pregraphs

G is not 3-edge-colourable $\Rightarrow O_1(G)$ is not 3-edge-colourable.

G is 3-edge-colourable $\Leftrightarrow O_2(G)$ is 3-edge-colourable.

G is 3-edge-colourable $\Leftrightarrow O_3(G)$ is 3-edge-colourable.

$\forall G: O_4(G)$ is not 3-edge-colourable.

3-edge-colourable pregraphs

3-edge-colourability is compatible with the construction operations.

Parent of 3-edge-colourable graph is 3-edge-colourable.

Never perform operation O_4 .

Check colourability after performing operation O_1 .

3-edge-colourable pregraphs

n	Cc	Sc	Mc	S,Mc
1	0	1	0	1
2	0	1	1	3
3	0	2	0	3
4	1	6	2	11
5	0	9	0	17
6	2	28	5	59
7	0	59	0	134
8	5	187	16	462
9	0	501	0	1332
10	17	1679	65	4774
11	0	5310	0	16029
12	80	18989	363	60562
13	0	67461	0	225117
14	475	257738	2588	898619
15	0	997460	0	3598323
16	3848	4052146	23702	15128797
17	0	16762252	0	64261497
18	39687	71905738	263952	283239174
19	0	314293531	0	1264577606
20	496430	1414799656	3438642	5817868002
21	0	6484967876	0	27138011161
22	7174735	30479739145	50763502	129848052113
23	0	145735267008	0	
24	116214038		831898577	

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3-edge-colourable pregraphs

n	Cc	Sc	Mc	S,Mc
10	0.0s	0.0s	0.0s	0.1s
11	0.0s	0.2s	0.0s	0.3s
12	0.0s	0.6s	0.0s	1.2s
13	0.0s	2.4s	0.0s	4.9s
14	0.0s	9.3s	0.0s	20.6s
15	0.0s	39.2s	0.0s	88.3s
16	0.0s	164.1s	0.3s	395.7s
17	0.0s	740.1s	0.0s	1794.5s
18	0.2s	3245.6s	3.4s	8245.1s
19	0.0s	15254.9s	0.0s	39076.4s
20	3.0s	70520.4s	48.3s	191074.5s
21	0.0s	349170.5s	0.0s	932273.4s
22	47.1s	1722625.2s	791.7s	4683143.7s
23	0.0s	8491130.8s	0.0s	
24	886.3s		14271.1s	

N. Van Cleemput Structure generation

3-edge-colourable pregraphs

n	Sc	Mc	S,Mc
20	20 062.3/s	71 193.4/s	30 448.2/s
21	18 572.5/s		29 109.5/s
22	17 693.8/s	64 119.6/s	27 726.7/s
23	17 163.2/s		
24		58 292.5/s	

N. Van Cleemput Structure generation

Bipartite pregraphs

Cubic pregraphs with loops are never bipartite.

Other cubic pregraphs are bipartite if and only if the corresponding cubic pregraph primitive is bipartite.

Bipartite pregraphs

G is bipartite and $d(v, w)$ is even $\Leftrightarrow O_1(G)$ is bipartite.

G is bipartite $\Leftrightarrow O_2(G)$ is bipartite.

G is bipartite $\Leftrightarrow O_3(G)$ is bipartite.

$\forall G: O_4(G)$ is not bipartite.

Bipartite pregraphs

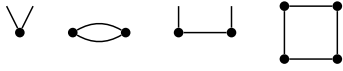
Being bipartite is compatible with the construction operations.

Parent of bipartite graph is bipartite.

Never perform operation O_4 .

Only perform operation O_1 for pairs of vertices in the same partition.

Quotients of a 4-cycle



C_4^q -markable cubic pregraphs

Cubic pregraphs admitting a 2-factor composed of quotients of C_4 .

Underlying graphs for Delaney-Dress graphs.

C_4^q -markable cubic pregraphs

Being C_4^q -markable is not compatible with the construction operations.

A linear time filtering algorithm was developed.

Timings and results

<i>n</i>	<i>Cq</i>	<i>Sq</i>	<i>Mq</i>	<i>SMq</i>
1		1		1
2		1	1	3
3		1		2
4	1	4	2	9
5		3		7
6	0	10	3	29
7		9		27
8	3	34	9	105
9		34		118
10	0	98	14	392
11		125		546
12	10	367	48	1722
13		526		2701
14	0	1352	95	7953
15		2234		13966
16	43	5710	331	40035
17		10187		75341
18	0	24938	873	210763
19		47568		420422
20	242	116186	3145	1162192

N. Van Cleemput Structure generation

Timings and results

<i>n</i>	<i>Cq</i>	<i>Sq</i>	<i>Mq</i>	<i>SMq</i>
10	0.0s	0.0s	0.0s	0.1s
11	0.0s	0.2s	0.0s	0.3s
12	0.0s	0.6s	0.0s	1.3s
13	0.0s	2.4s	0.0s	5.2s
14	0.0s	9.5s	0.0s	22.0s
15	0.0s	39.5s	0.0s	94.8s
16	0.0s	168.7s	0.3s	420.5s
17	0.0s	743.4s	0.0s	1903.5s
18	0.0s	3341.9s	3.8s	8850.1s
19	0.0s	15407.8s	0.0s	41812.1s
20	2.2s	72708.7s	54.0s	201745.4s

N. Van Cleemput Structure generation

Timings and results

<i>n</i>	<i>Sq</i>	<i>Mq</i>	<i>SMq</i>
16	33.8/s		95.2/s
17	13.7/s		39.6/s
18	7.5/s	229.7/s	23.8/s
19	3.1/s		10.1/s
20	1.6/s	58.2/s	5.8/s

N. Van Cleemput Structure generation

Timings and results

<i>n</i>	rate
15	34 915.0/s
16	26 690.0/s
17	34 245.9/s
18	26 345.4/s
19	30 030.1/s
20	24 939.7/s
21	27 901.5/s
22	24 211.2/s
23	25 896.3/s
24	22 863.0/s
25	24 116.9/s
26	21 932.9/s
27	22 641.9/s
28	20 952.4/s
29	21 461.8/s
30	20 078.5/s

N. Van Cleemput Structure generation

Generating Delaney-Dress graphs

Since the quotients are the units, we already have some colour information available.

Assigning the remaining colours can be done using the homomorphism principle.

N. Van Cleemput Structure generation

Generating Delaney-Dress graphs

<i>n</i>	Delaney-Dress graphs	time	rate
12	9 480	0.1s	94 800.00/s
13	17 205	0.1s	172 050.00/s
14	61 594	0.3s	205 313.33/s
15	123 953	0.4s	309 882.50/s
16	433 030	1.6s	270 643.75/s
17	931 729	2.5s	372 691.60/s
18	3 196 841	9.1s	351 301.21/s
19	7 258 011	16.3s	445 276.75/s
20	24 630 262	55.0s	447 822.95/s
21	58 309 071	105.9s	550 605.01/s
22	196 266 434	≈ 5m	568 064.93/s
23	481 330 615	≈ 12m	666 478.28/s
24	1 610 942 856	≈ 38m	691 629.25/s
25	4 071 117 829	≈ 1h	785 187.34/s
26	13 569 014 653	≈ 4h	826 265.50/s
27	35 202 390 477	≈ 10h	919 758.85/s
28	116 994 675 348	≈ 33h	960 576.60/s
29	310 624 700 725	≈ 3 days	1 049 801.45/s
30	1 030 455 432 427	≈ 11 days	1 084 892.06/s

N. Van Cleemput Structure generation