Constructive enumeration and uniform random sampling of DAGs

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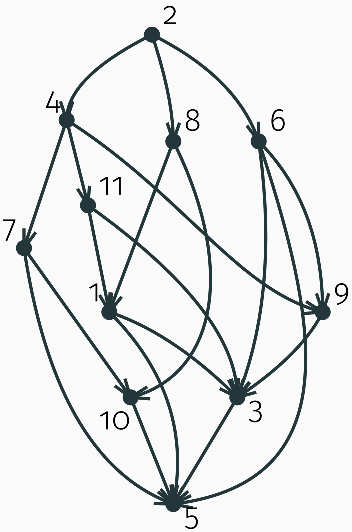
Outline

Directed Acyclic Graphs

- A finite set of vertices V e.g. $\{1, 2, \ldots, n\}$;
- a set of directed edges $E \subseteq V \times V$;
- no cycles: $v_1 \to v_2 \to \cdots \to v_n = v_1$.



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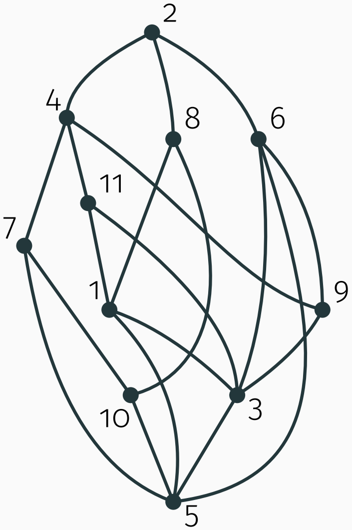

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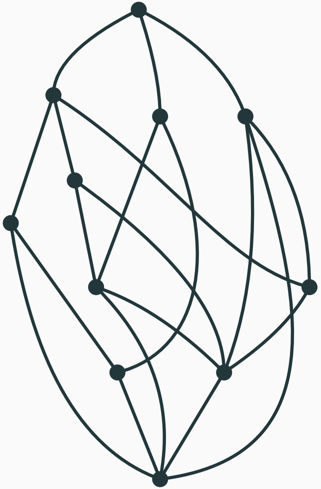

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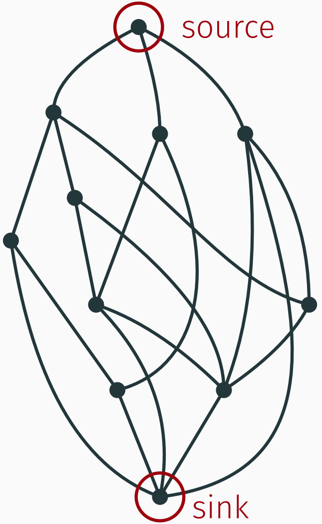

Goals and motivations

- Counting
  - Starting point for many quantitative studies...
  - ... And for random generation

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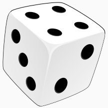
- Uniform random generation
  - Testing and simulations
  - Uniformity as a default generation strategy
  - Can be biased as needed



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Problems:

- Inclusion-exclusion
- No or little control over the number of edges

Still missing

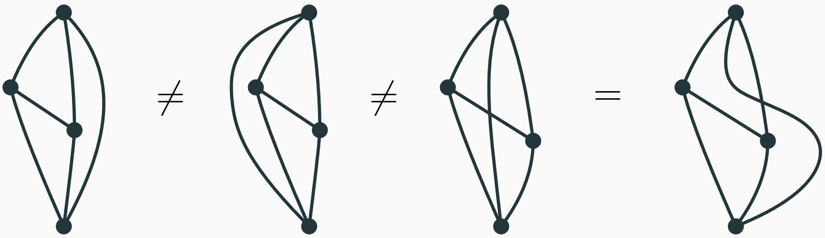
- Finer control over the number of edges?
- Sampling of unlabelled structures?

Outline

A new kind of DAG

Directed Ordered Acyclic Graphs (DOAGs)

DOAG = Unlabelled DAG
+ a total order on the **outgoing** edges of each vertex
+ only one sink and one source



Motivation

- Real-life implementations of DAGs have an **ordering**; →

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struct vertex {
  int           out_degree;
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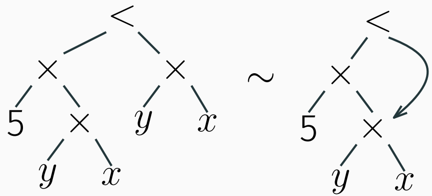

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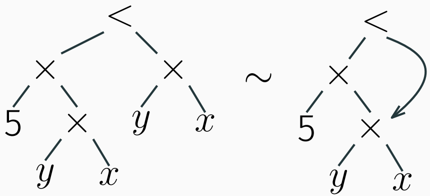
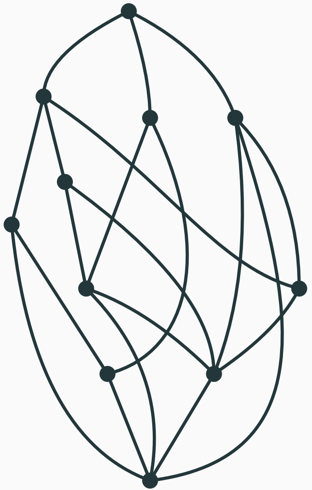


- Models **unlabelled** objects.

Recursive decomposition: multi-source DOAGs

Idea: remove the source and see what is left.



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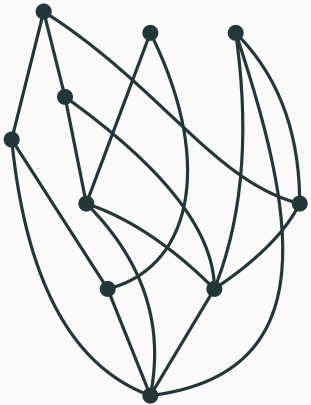

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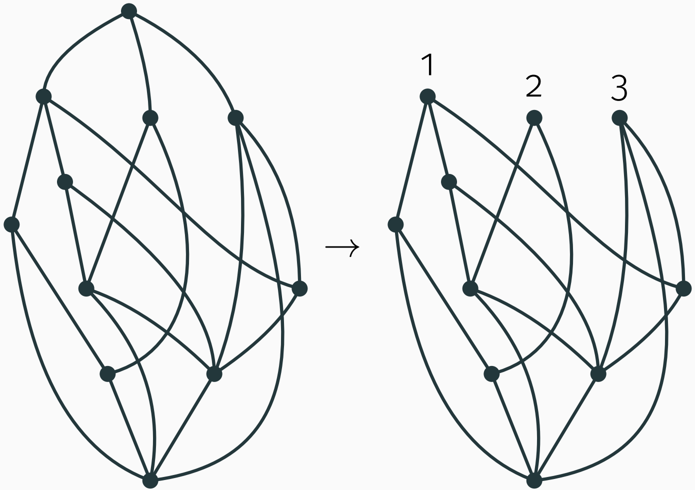

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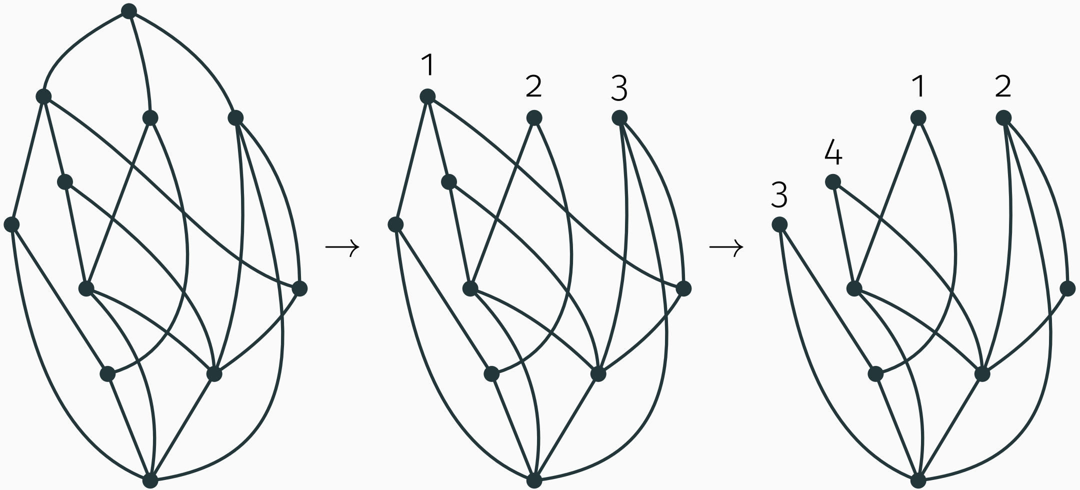

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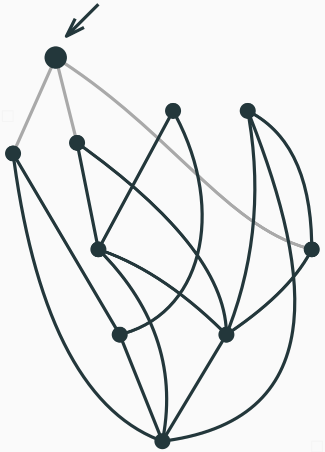

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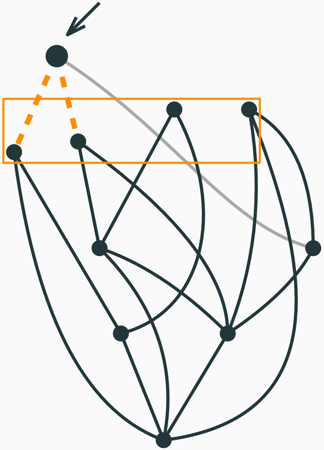

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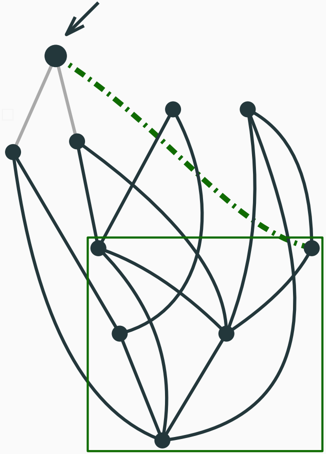

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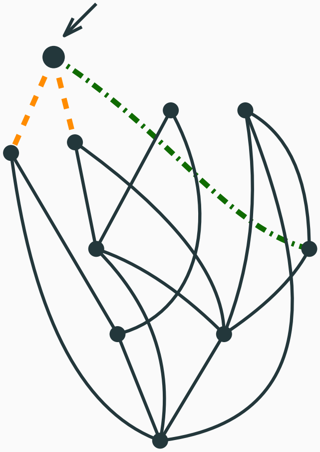

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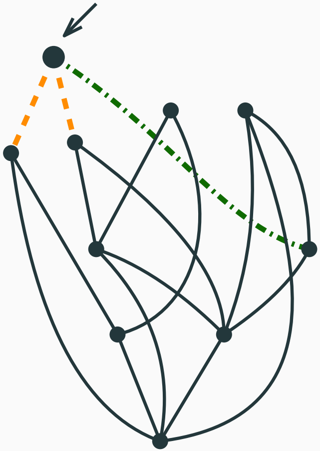

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$$D_{n,m,k} = \#\text{DOAGs with } n \text{ vertices, } m \text{ edges, } k \text{ sources}$$
$$= \sum_{s+q>0} D_{n-1,m-s-q,k-1+q} \binom{n-k-q}{s} \binom{s+q}{q} s!$$

Complexity of the counting

$$
\begin{aligned}
D_{1,m,k} &= \mathbb{1}_{\{m=0 \wedge k=1\}} & \\
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Computing $D_{n,m,k}$ for all $n, k \leq N$ and $m \leq M$ takes $O(N^4 M)$ arithmetic operations.

In practice we reach $M = 400$, $N = M + 1$.

Random sampling

Do the same, but backwards.

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1. Select (s, q) with probability $\frac{D_{n-1,m-s-q,k-1+q}\binom{n-k-q}{s}\binom{s+q}{q}s!}{D_{n,m,k}}$;

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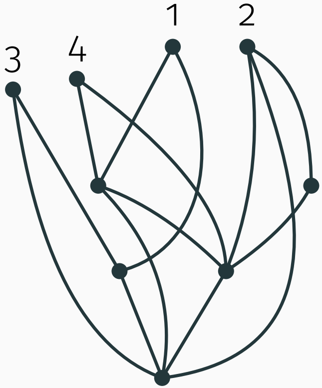

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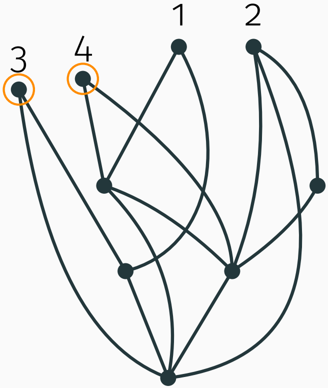

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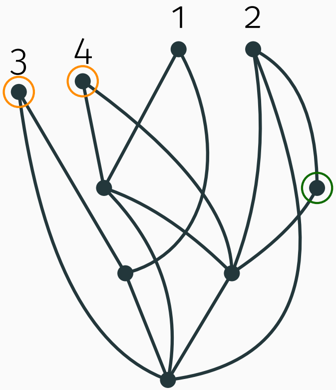

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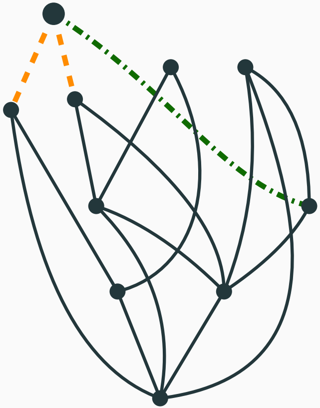

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5. Connect them to the new sources.

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4. (bonus) sum in the lexicographic order for $(s+q, s)$.

Complexity of the sampling algorithm

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In practice it takes a few milliseconds.

Outline

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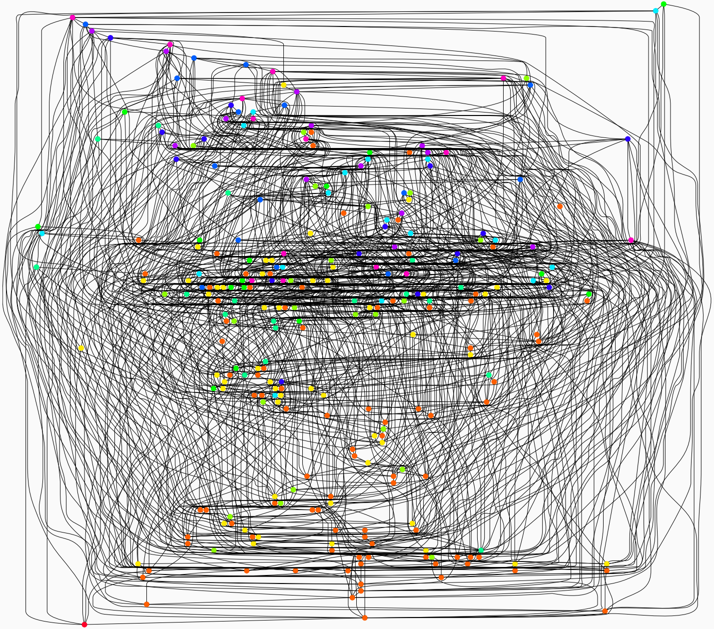
- Counting: $O(N^2 d^4)$ arithmetic operations.
- Sampling $O(Nd^2)$ arithmetic operations.
- In practice we reached $m = 1500$ with $d = 2$ and $m = 1000$ with $d = 10$.

Your next favourite wallpaper



Uniform DOAG with $m = 1000$ edges and with out-degree bounded by $d = 10$.

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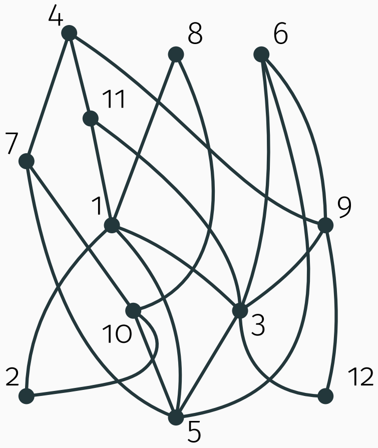

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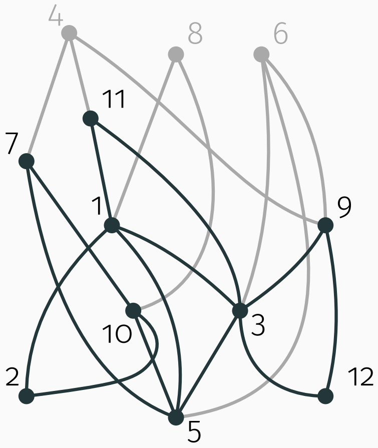

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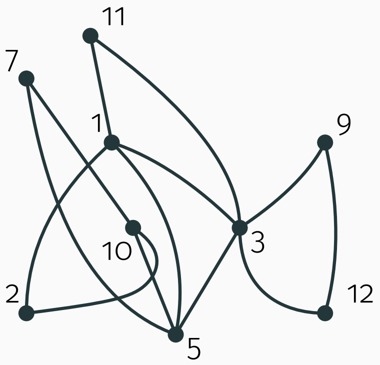

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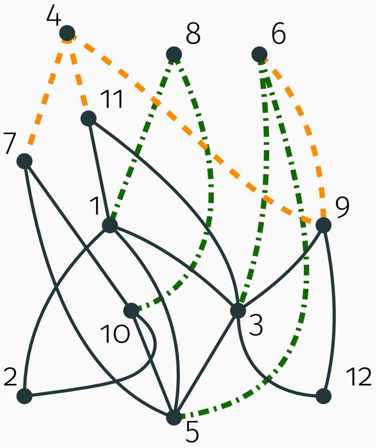

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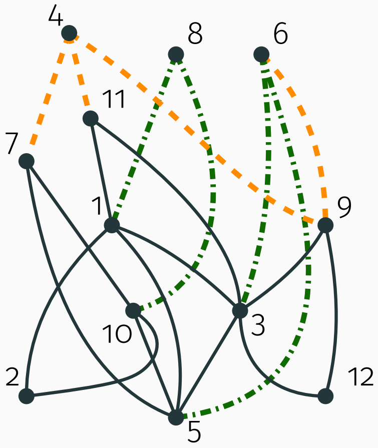

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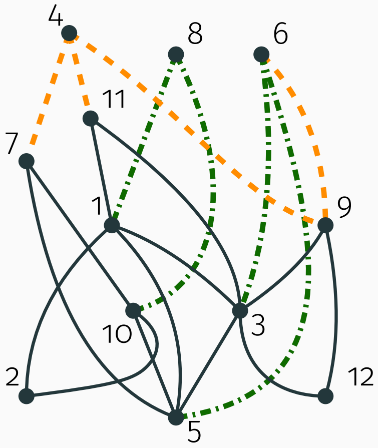

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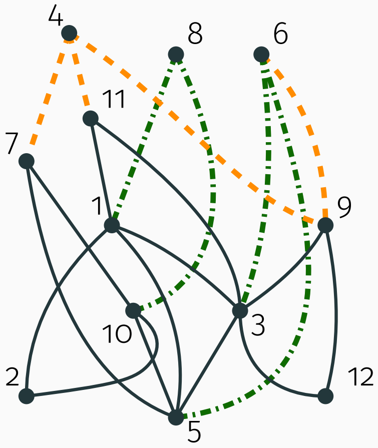

$A_{n,k}$ = #DAGs with n vertices, k sources

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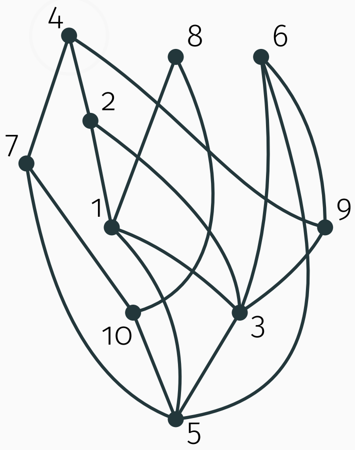
→ Use our approach!

Vertex-by-vertex decomposition of labelled DAGs

Idea: mark one source, and remove it.



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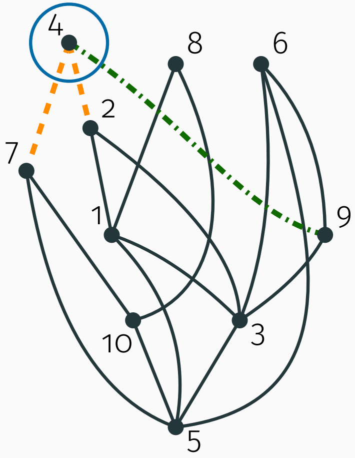

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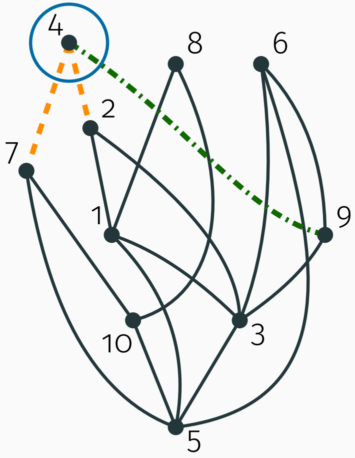

$A_{n,m,k}$ = #DAGs (one sink, k sources)

$$k \cdot A_{n,m,k} =$$

$$n \cdot \sum_{s+q>0} A_{n-1,m-s-q,k-1+q} \binom{k-1+q}{q} \binom{n-q-k}{s}$$

Outline

Conclusion

Initial questions:

- Finer control over the number of edges?
- Sampling of unlabelled structures?

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We presented:

- a new model of DAGs: DOAGs;
- a new way of counting.

Future work

- Can we get rid of the one-sink-one-source constraint while retaining weak connectivity?
- Is there a symbolic method operator hidden behind the vertex-by-vertex decomposition?
- Asymptotics?
- Can we get closer to sampling regular unlabelled DAGs?

Thank you for your attention!

I. M. Gessel.
Counting acyclic digraphs by sources and sinks.
Discrete Mathematics, 160(1):253 – 258, 1996.

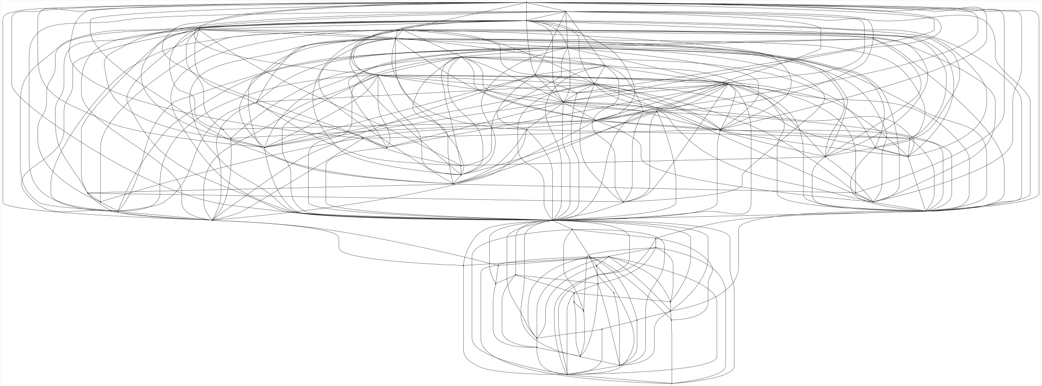
J. Kuipers and G. Moffa.
Uniform random generation of large acyclic digraphs.
Stat. and Computing, 25(2):227–242, 2015.

G. Melançon, I. Dutour, and M. Bousquet-Mélou.
Random generation of directed acyclic graphs.
Electron. Notes Discret. Math., 10:202–207, 2001.

R.W. Robinson.
Counting labeled acyclic digraphs.
New Directions in the Theory of Graphs, pages 239–273, 1973.

R. W. Robinson.
Counting unlabeled acyclic digraphs.
In *Combinatorial Mathematics V*, Lecture Notes in Mathematics, pages 28–43. Springer, 1977.

A biased DOAG



DOAG with 3 bottlenecks: every path from a source to a vertex must go through one of these 3 points.