DIRECTED ORDERED ACYCLIC GRAPHS

ENUMERATION, UNIFORM SAMPLING, AND LINKS WITH CLASSICAL LABELLED DAGS

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joint work with Alfredo Viola & Antoine Genitrini

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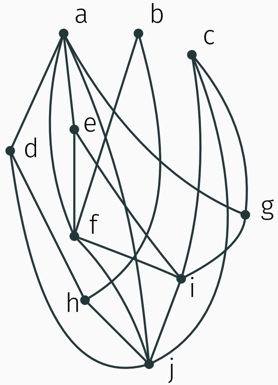
Séminaire CALIN

LIPN

Directed Acyclic Graphs

Directed Acyclic Graph (DAG)

- A finite set of vertices V e.g. $\{a, b, c, \ldots, j\}$;
- a set of directed edges $E \subseteq V \times V$;
- no cycles.



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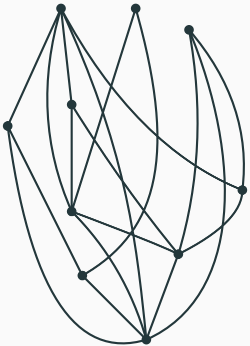

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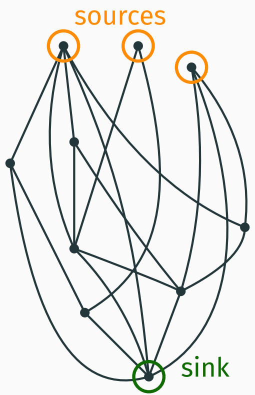

Why DAGs?

Omnipresent data structure:

- Encoding partial orders in scheduling problems;
- Git histories;
- Bayesian networks in probabilities;
- Genealogy trees (those are not trees!);
- Class inheritance in OOP...

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- Inclusion-exclusion

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Unlabelled DAGs:

- Counting by vertices and sources: [Rob77] ●

Problems:

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

Still missing

- Finer control over the number of edges?
- Unlabelled structures / other ways of breaking symmetries?

Outline of the presentation

Background

Directed ordered acyclic graphs

↳ *Definition and recursive decomposition*

Intermezzo: labelled DAGs

↳ *another way of counting*

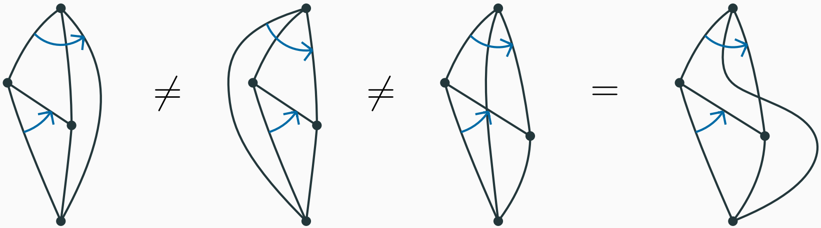
Asymptotic analysis

↳ *Matrix encoding*
↳ *Asymptotic result*
↳ *Faster sampler*

A new kind of DAG

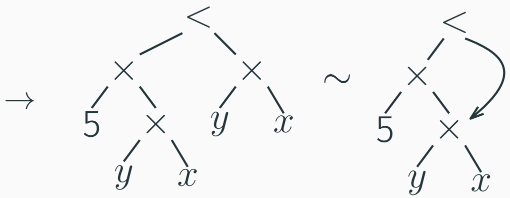
Directed Ordered Acyclic Graphs

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



Motivations

- Compacted trees [GGKW20; EFW21] are DOAGs



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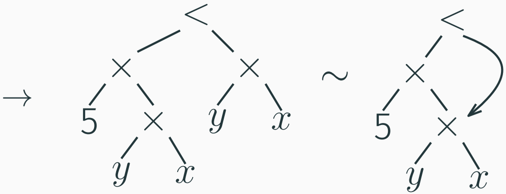

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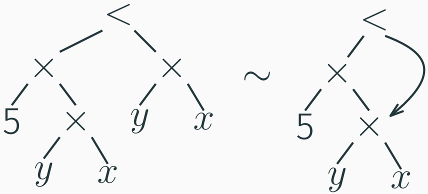
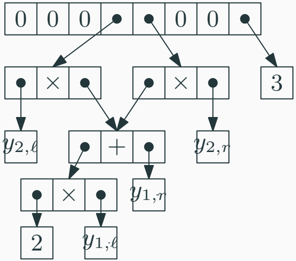


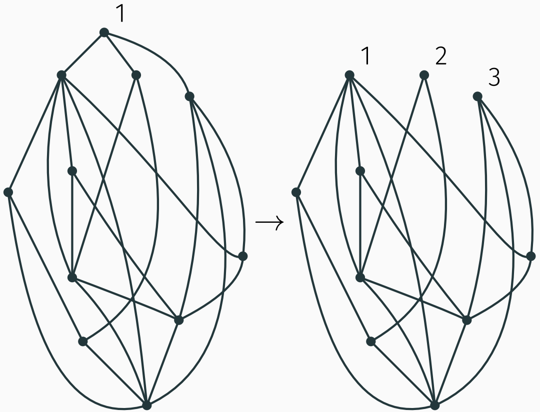
(also known as **hash-consing** in functional programming);

- Real-life implementations of DAGs have an **ordering**; $\rightarrow$



Recursive decomposition

Idea: remove the smallest source and see what is left.



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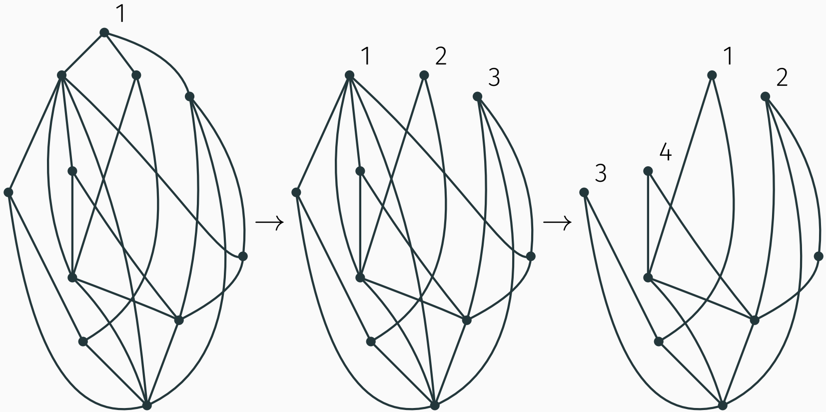

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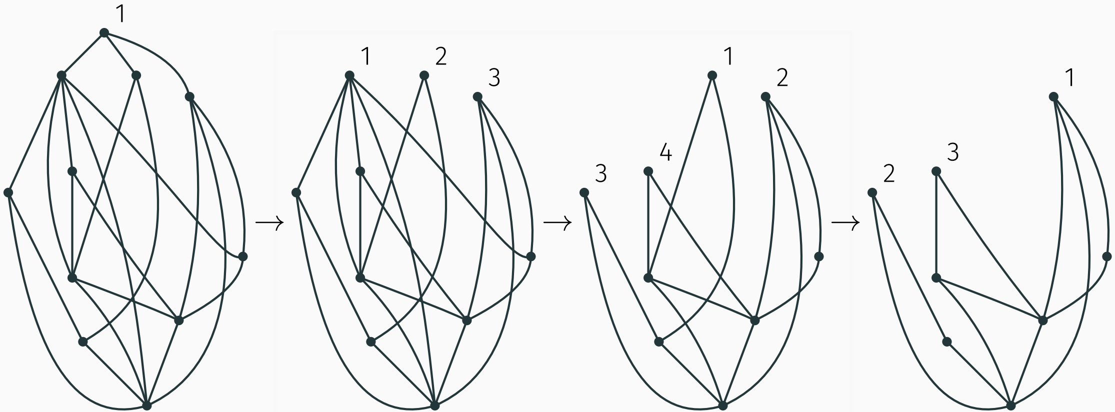

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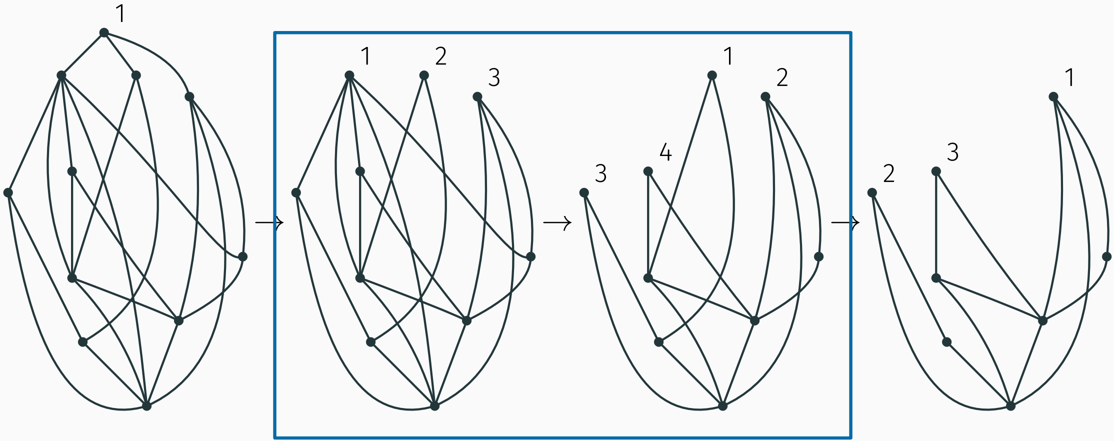

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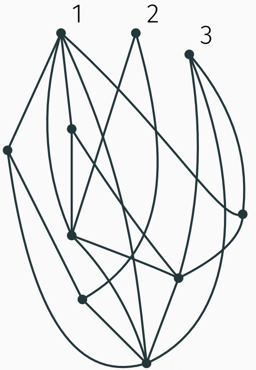

n vertices, m edges, k sources

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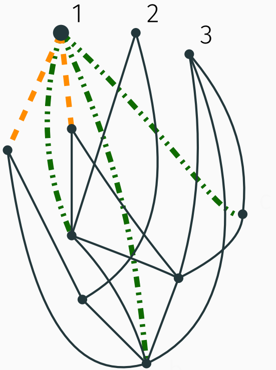

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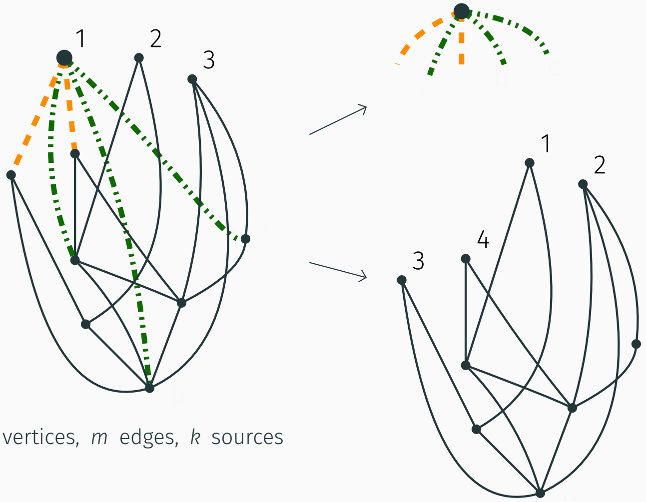

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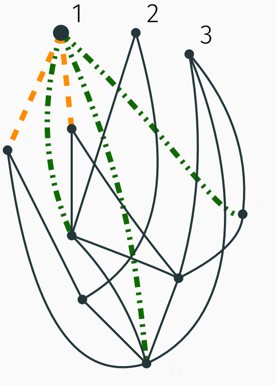

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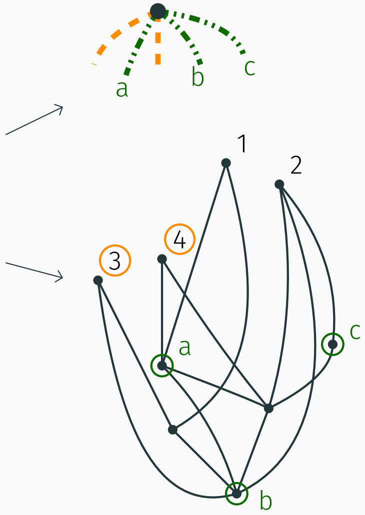

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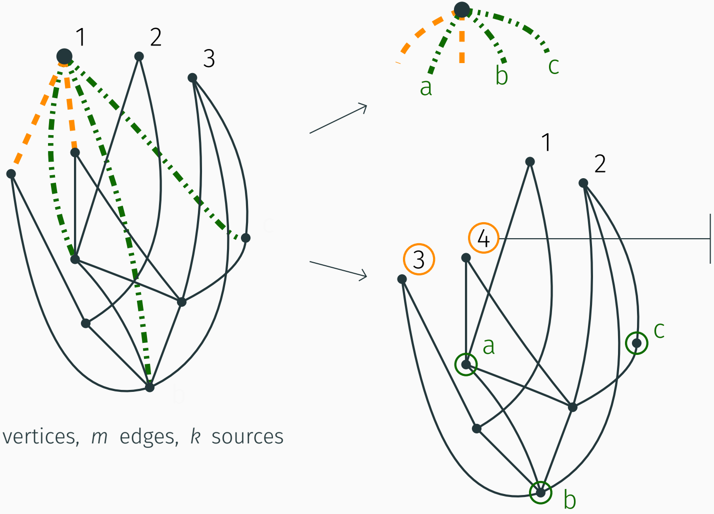

s edges to new sources

n vertices, m edges, k sources

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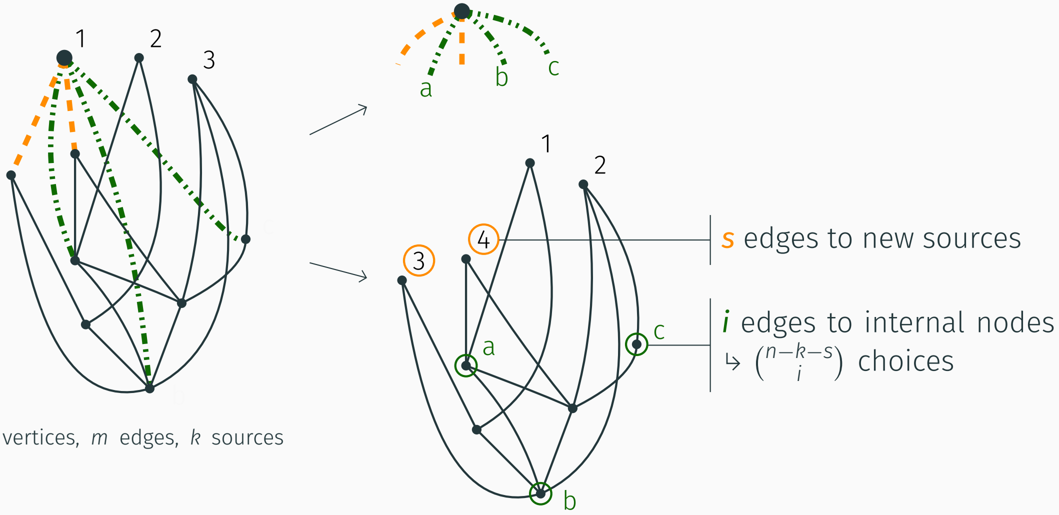

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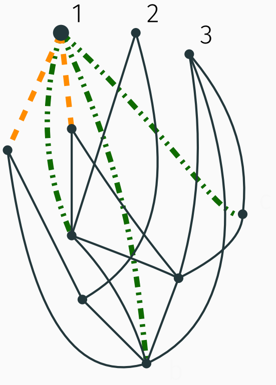

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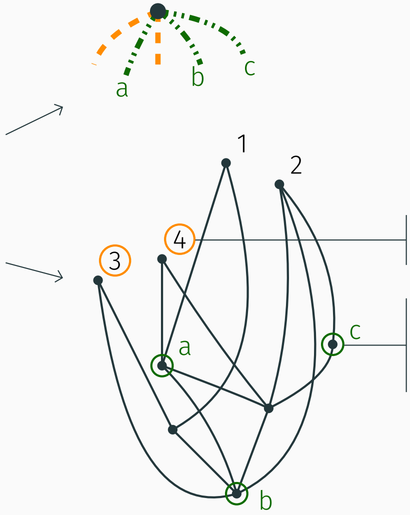
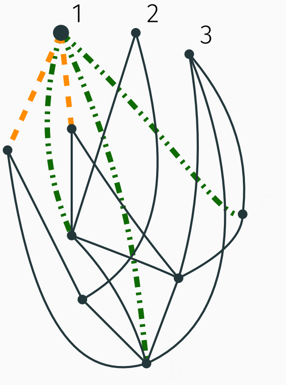


s edges to new sources

i edges to internal nodes
↳ $\binom{n-k-s}{i}$ choices

$(n-1)$ vertices, $(m-i-s)$ edges, $(k+s-1)$ sources

Recursive decomposition



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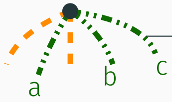
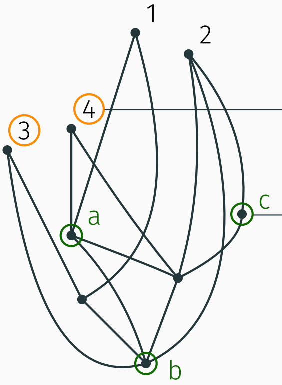


permute the edges
interleave with
↳ $i!\binom{i+s}{i}$ choices



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Recurrence formula

Counting formula

$$
\begin{aligned}
D_{n,m,k} &= \#\{\textit{DOAGs with } n \textit{ vertices, } m \textit{ edges and } k \textit{ sources}\} \\
&= \sum_{i+s>0} D_{n-1,m-i-s,k+s-1} \binom{n-k-s}{i} i! \binom{i+s}{i}
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Complexity: computing all $D_{n,m,k}$ for $n, k \leq N$ and $m \leq M$ costs:
→ $O(N^4 M)$ arithmetic operations;
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In practice: about 400 edges in a few minutes.

Random sampling = counting

Do the same, but backwards!

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Do the same, but backwards!

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

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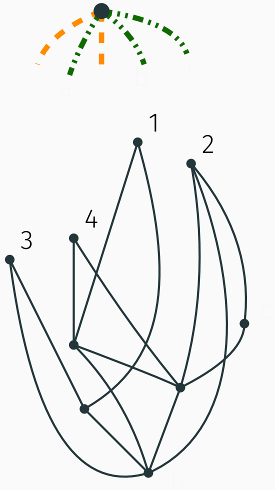

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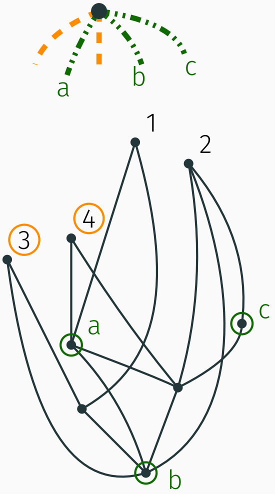

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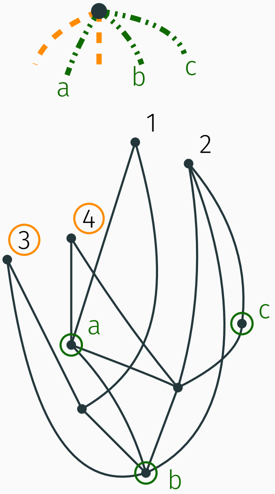

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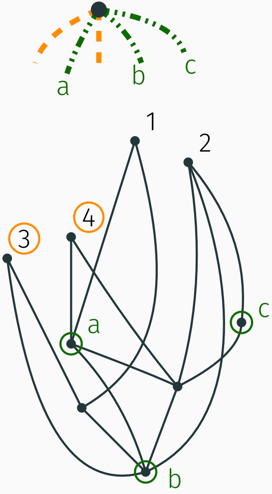

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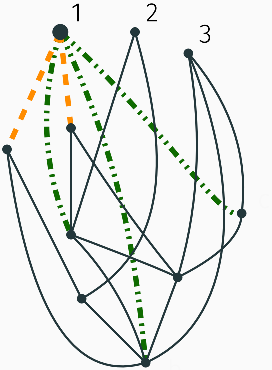

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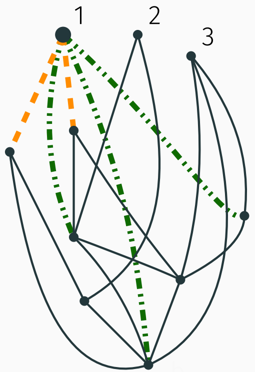

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↳ out-degree of v

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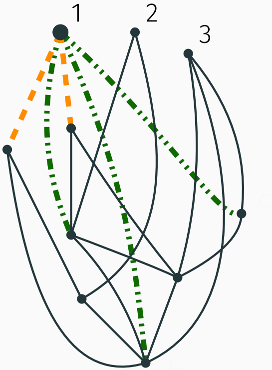

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In practice: about 400 edges in a few ms.

Conclusion

- New model
- New way of counting
- Control over the number of edges

Antoine Genitrini, Martin Pépin, and Alfredo Viola. “Unlabelled ordered DAGs and labelled DAGs: constructive enumeration and uniform random sampling”. In: *XI Latin and American Algorithms, Graphs and Optimization Symposium*. Eslevier. 2021

Outline of the presentation

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↳ *Definition and recursive decomposition*

Intermezzo: labelled DAGs

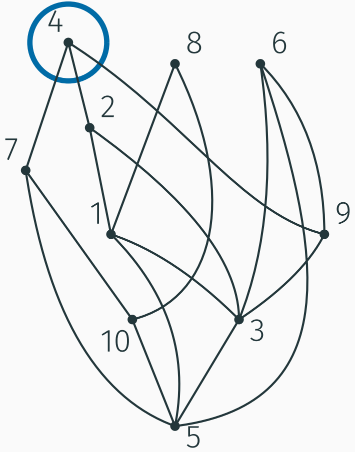
↳ *another way of counting*

Asymptotic analysis

↳ *Matrix encoding*
↳ *Asymptotic result*
↳ *Faster sampler*

What about labelled DAGs?

Idea: mark one source, and remove it.



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

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

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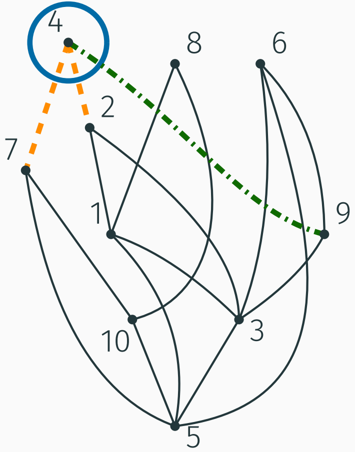

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Consequences on labelled DAGs

- Counting formula without inclusion-exclusion;
- Effective sampler with fixed number of edges and vertices.

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Problem: relative growth of n and m?

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- sparse case: $m \sim c \cdot n$?
- are there critical values for c?

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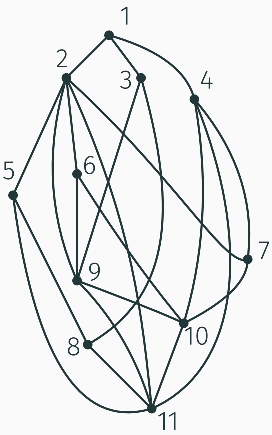
- sparse case: $m \sim c \cdot n$?
- are there critical values for c?

Simplification: Drop one parameter: only count by vertices.

$$D_n \stackrel{\text{def}}{=} \#\{\text{DOAG with } n \text{ vertices, one source.}\}$$

Matrix encoding



1	2	3	4	5	6	7	8	9	10	11	
											1
											2
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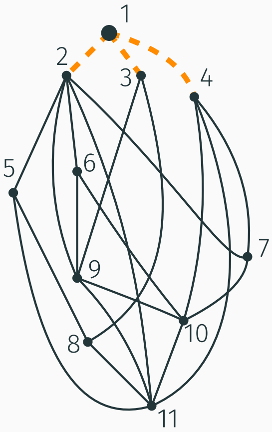

	1	2	3	4	5	6	7	8	9	10	11
1		**1**	**2**	**3**							
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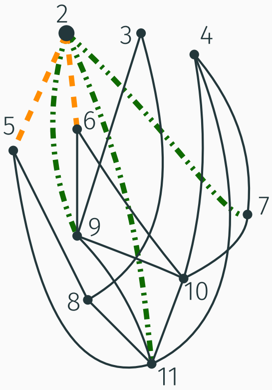

1	2	3	4	5	6	7	8	9	10	11	
	1	**2**	**3**								1
				1	**3**	**5**		**2**		**4**	2
											3
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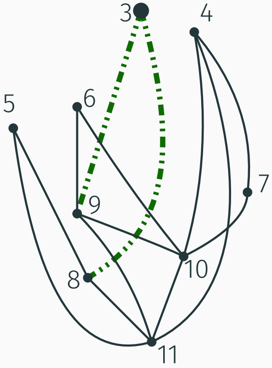

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2					**1**	**3**	**5**		**2**		**4**
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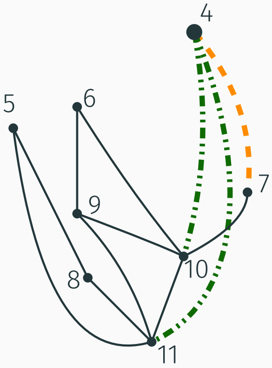
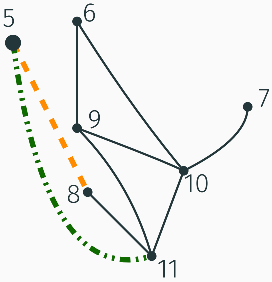
10											
11											

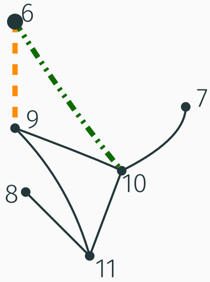


	1	2	3	4	5	6	7	8	9	10	11
1		**1**	**2**	**3**							
2					**1**	**3**	**5**		**2**		**4**
3								**2**	**1**		
4							**3**			**1**	**2**
5											
6											
7											
8											
9											
10											
11											

Matrix encoding

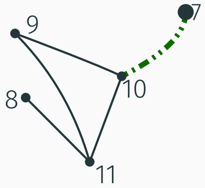


1	2	3	4	5	6	7	8	9	10	11	
	1	**2**	**3**								1
				1	**3**	**5**		**2**		**4**	2
							2	**1**			3
						3			**1**	**2**	4
							2			**1**	5
											6
											7
											8
											9
											10
											11



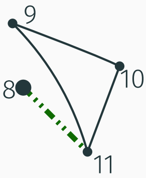
1	2	3	4	5	6	7	8	9	10	11	
	1	**2**	**3**								1
				1	**3**	**5**		**2**		**4**	2
							2	**1**			3
						3			**1**	**2**	4
							2			**1**	5
								1	**2**		6
											7
											8
											9
											10
											11

Matrix encoding



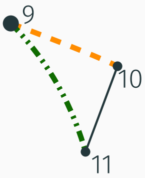
1	2	3	4	5	6	7	8	9	10	11	
	1	**2**	**3**								1
				1	**3**	**5**		**2**		**4**	2
							2	**1**			3
						3			**1**	**2**	4
							2			**1**	5
								1	**2**		6
									1		7
											8
											9
											10
											11

Matrix encoding



	1	2	3	4	5	6	7	8	9	10	11
1		**1**	**2**	**3**							
2					**1**	**3**	**5**		**2**		**4**
3								**2**	**1**		
4							**3**			**1**	**2**
5								**2**			**1**
6									**1**	**2**	
7										**1**	
8											**1**
9											
10											
11											

Matrix encoding



1	2	3	4	5	6	7	8	9	10	11	
	1	**2**	**3**								1
				1	**3**	**5**		**2**		**4**	2
							2	**1**			3
						3			**1**	**2**	4
							2			**1**	5
								1	**2**		6
									1		7
										1	8
									2	**1**	9
											10
											11

Matrix encoding

1	2	3	4	5	6	7	8	9	10	11	
	1	**2**	**3**								1
				1	**3**	**5**		**2**		**4**	2
							2	**1**			3
						3			**1**	**2**	4
							2			**1**	5
								1	**2**		6
									1		7
										1	8
									2	**1**	9
										1	10
											11

Matrix encoding

1	2	3	4	5	6	7	8	9	10	11	
	1	**2**	**3**								1
				1	**3**	**5**		**2**		**4**	2
							2	**1**			3
						3			**1**	**2**	4
							2			**1**	5
								1	**2**		6
									1		7
										1	8
									2	**1**	9
										1	10
											11

Matrix encoding

1. strict upper triangular matrix;

1	2	3	4	5	6	7	8	9	10	11	
	1	**2**	**3**								1
				1	**3**	**5**		**2**		**4**	2
							2	**1**			3
						3			**1**	**2**	4
							2			**1**	5
								1	**2**		6
									1		7
										1	8
									2	**1**	9
										1	10
											11

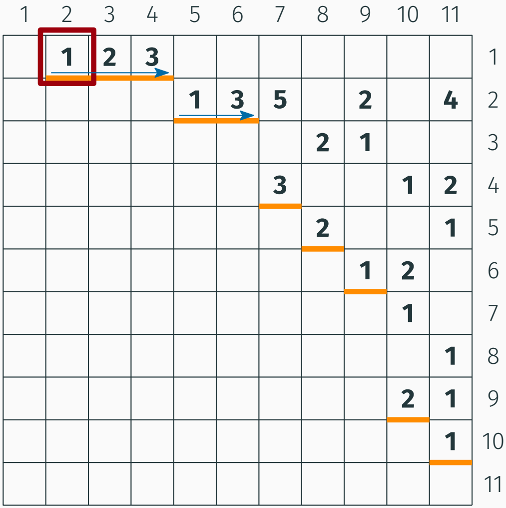
Matrix encoding

1. strict upper triangular matrix;
2. there is an element at $(1, 2)$;

	1	2	3	4	5	6	7	8	9	10	11
1		**1**	**2**	**3**							
2					**1**	**3**	**5**		**2**		**4**
3								**2**	**1**		
4							**3**			**1**	**2**
5								**2**			**1**
6									**1**	**2**	
7										**1**	
8											**1**
9										**2**	**1**
10											**1**
11											

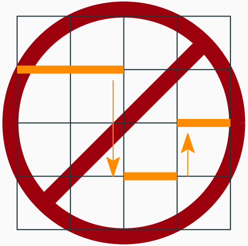
Matrix encoding

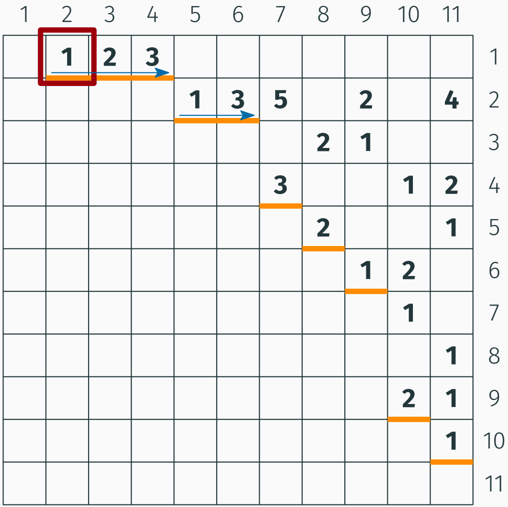
1. strict upper triangular matrix;
2. there is an element at $(1, 2)$;
3. increasing numbers above orange lines;



Matrix encoding

1. strict upper triangular matrix;
2. there is an element at $(1, 2)$;
3. increasing numbers above orange lines;
4. orange lines go down.





Asymptotic result

Number of mono-source DOAGs

$$D_n \underset{n\to\infty}{\sim} \frac{c}{\sqrt{n}} e^{n-1} \text{¡}n-1!$$

for $c \approx 0.30256$ *and where* $\text{¡}m! = \prod_{k=1}^{m} k!$.

Number of mono-source DOAGs

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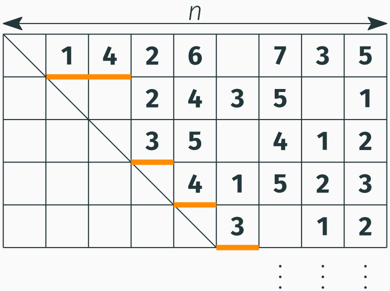
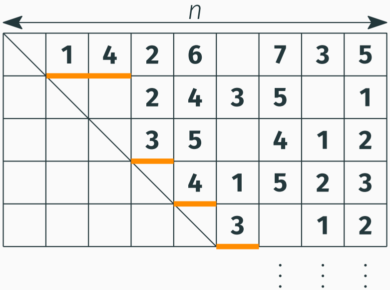


Asymptotic result

Number of mono-source DOAGs

$$D_n \underset{n\to\infty}{\sim} \frac{c}{\sqrt{n}}\, e^{n-1}\, ¡n-1!$$

for $c \approx 0.30256$ *and where* $¡m! = \prod_{k=1}^{m} k!$.



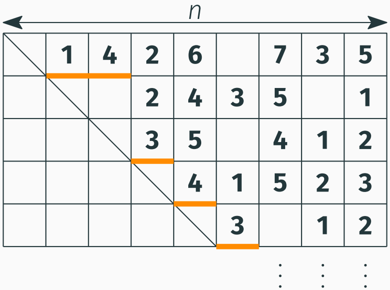
$\approx (n-1)!$ possible rows

Asymptotic result

Number of mono-source DOAGs

$$D_n \underset{n\to\infty}{\sim} \frac{c}{\sqrt{n}}\, e^{n-1}\ \text{¡}n-1!$$

for $c \approx 0.30256$ *and where* $\text{¡}m! = \prod_{k=1}^{m} k!$.



$\approx (n-1)!$ possible rows

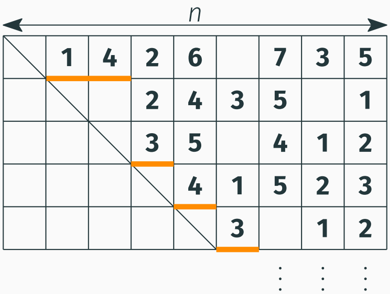
$\approx (n-2)!$ possible rows

Asymptotic result

Number of mono-source DOAGs

$$D_n \underset{n\to\infty}{\sim} \frac{c}{\sqrt{n}} e^{n-1} \text{¡}n-1!$$

for $c \approx 0.30256$ *and where* $\text{¡}m! = \prod_{k=1}^{m} k!$.



$\approx (n-1)!$ possible rows

$\approx (n-2)!$ possible rows

$\approx (n-3)!$ possible rows

$\approx (n-4)!$ possible rows

etc

$\Rightarrow \text{¡}n-1!$

Proof sketch (1/3)

The plan: 1. Upper bound 2. Lower bound 3. Bootstrapping

Proof sketch (1/3)

The plan: **1. Upper bound** 2. Lower bound 3. Bootstrapping

Proof sketch (1/3)

The plan: **1. Upper bound** 2. Lower bound 3. Bootstrapping

6	**1**		**5**		**2**	**4**		**3**	$=$	**6**	**1**	**5**	**2**	**4**	**3**	$\star$			

Proof sketch (1/3)

The plan: **1. Upper bound** 2. Lower bound 3. Bootstrapping

6	1		5		2	4		3

$=$

6	1	5	2	4	3

$\star$

$$\text{Variation} = \textsc{Seq}(\mathcal{Z}) \star \textsc{Set}(\mathcal{Z})$$

Proof sketch (1/3)

The plan: **1. Upper bound** 2. Lower bound 3. Bootstrapping

6	1		5		2	4		3	=	6	1	5	2	4	3	$\star$			

$$\text{Variation} = \textsc{Seq}(\mathcal{Z}) \star \textsc{Set}(\mathcal{Z})$$

$$V(z) = (1-z)^{-1}e^{z}$$

Proof sketch (1/3)

The plan: **1. Upper bound** 2. Lower bound 3. Bootstrapping

6	1		5		2	4		3

=

6	1	5	2	4	3

$\star$

$$\text{Variation} = \textsc{Seq}(\mathcal{Z}) \star \textsc{Set}(\mathcal{Z})$$

$$V(z) = (1-z)^{-1}e^{z}$$

$$v_n = e \cdot n! - o(1)$$

Proof sketch (1/3)

The plan: **1. Upper bound** 2. Lower bound 3. Bootstrapping

6	1		5		2	4		3

=

6	1	5	2	4	3

$\star$

$$\text{Variation} = \textsc{Seq}(\mathcal{Z}) \star \textsc{Set}(\mathcal{Z})$$

$$V(z) = (1-z)^{-1} e^{z}$$

$$v_n = e \cdot n! - o(1)$$

$\#\{\text{DOAG matrices}\} = \#\{\text{collections of rows}\} \leq \#\{\text{collections of variations}\}$

Proof sketch (1/3)

The plan: **1. Upper bound** 2. Lower bound 3. Bootstrapping

6	**1**		**5**		**2**	**4**		**3**	=	**6**	**1**	**5**	**2**	**4**	**3**	$\star$			

$$\text{Variation} = \textsc{Seq}(\mathcal{Z}) \star \textsc{Set}(\mathcal{Z})$$

$$V(z) = (1-z)^{-1} e^z$$

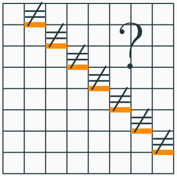
$$v_n = e \cdot n! - o(1)$$

$\#\{\text{DOAG matrices}\} = \#\{\text{collections of rows}\} \leq \#\{\text{collections of variations}\}$

$$D_n \leq \prod_{k=1}^{n-1} v_k \leq e^{n-1} \text{ ¡} n - 1!$$

Proof sketch (2/3)

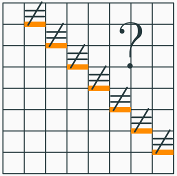
The plan: 1. Upper bound **2. Lower bound** 3. Bootstrapping

{DOAG matrices} $\supseteq$ 

(constraints are automatically satisfied)

Proof sketch (2/3)

The plan: 1. Upper bound **2. Lower bound** 3. Bootstrapping

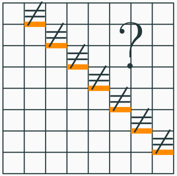
{DOAG matrices} $\supseteq$ 

(constraints are automatically satisfied)

$\#\, \boxed{\neq \mid ? \mid ? \mid ? \mid ? \mid ? \mid ? \mid ? \mid ?} = v_k - v_{k-1}$

Proof sketch (2/3)

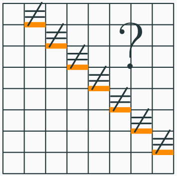
The plan: 1. Upper bound **2. Lower bound** 3. Bootstrapping

{DOAG matrices} $\supseteq$  (constraints are automatically satisfied)

$\#$  $= v_k - v_{k-1} = e \cdot k! \cdot \left(1 - \frac{1}{k} - o\left(\frac{1}{(k-1)!}\right)\right)$

Proof sketch (2/3)

The plan: 1. Upper bound **2. Lower bound** 3. Bootstrapping

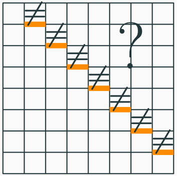
{DOAG matrices} $\supseteq$  (constraints are automatically satisfied)

$$\# \boxed{\neq \mid ? \mid ? \mid ? \mid ? \mid ? \mid ? \mid ? \mid ?} = v_k - v_{k-1} = e \cdot k! \cdot \left(1 - \frac{1}{k} - o\left(\frac{1}{(k-1)!}\right)\right)$$

$$D_n \geq e^{n-1} \text{ ¡}n - 1\text{!} \prod_{k=2}^{n-1} \left(\frac{k-1}{k} + o\left(\frac{1}{(k-1)!}\right)\right)$$

Proof sketch (2/3)

The plan: 1. Upper bound **2. Lower bound** 3. Bootstrapping

{DOAG matrices} $\supseteq$ 

(constraints are automatically satisfied)

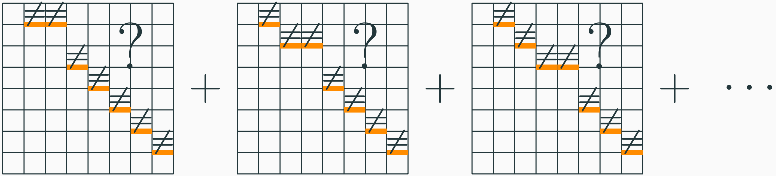
$$\#\,\boxed{\neq}\boxed{?}\boxed{?}\boxed{?}\boxed{?}\boxed{?}\boxed{?}\boxed{?}\boxed{?} = v_k - v_{k-1} = e \cdot k! \cdot \left(1 - \frac{1}{k} - o\left(\frac{1}{(k-1)!}\right)\right)$$

$$D_n \geq e^{n-1}\,\text{¡}n-1!\prod_{k=2}^{n-1}\left(\frac{k-1}{k} + o\left(\frac{1}{(k-1)!}\right)\right) \geq e^{n-1}\,\text{¡}n-1!\,\frac{A}{n} \quad \text{for some } A > 0$$

Proof sketch (2’/3)

The plan: 1. Upper bound **2’. Better lower bound** 3. Bootstrapping

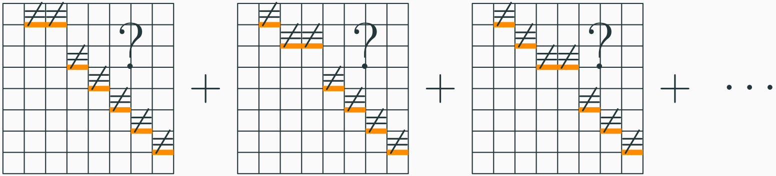
{DOAG matrices} $\supseteq$



Proof sketch (2'/3)

The plan: 1. Upper bound **2'. Better lower bound** 3. Bootstrapping

{DOAG matrices} ⊇

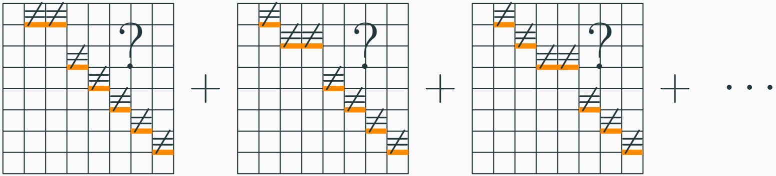


$$D_n \geq \frac{A' \cdot \ln(n)}{n} e^{n-1} \text{¡}n - 1!$$

Proof sketch (2’/3)

The plan: 1. Upper bound **2’. Better lower bound** 3. Bootstrapping

{DOAG matrices} $\supseteq$



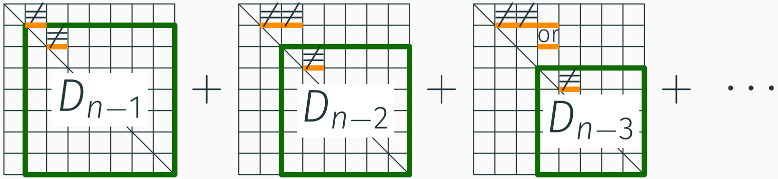
$$D_n \geq \frac{A' \cdot \ln(n)}{n}\, e^{n-1}\, \text{¡}n-1!$$

$$P_n = \frac{D_n}{e^{n-1}\, \text{¡}n-1!} \quad \Rightarrow \quad \frac{A' \cdot \ln(n)}{n} \leq P_n \leq 1$$

Proof sketch (3/3)

The plan: 1. Upper bound 2'. Better lower bound **3. Bootstrapping**

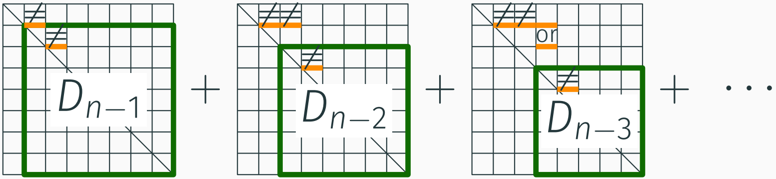
{DOAG matrices} =



Proof sketch (3/3)

The plan: 1. Upper bound 2'. Better lower bound **3. Bootstrapping**

$\{$DOAG matrices$\} =$

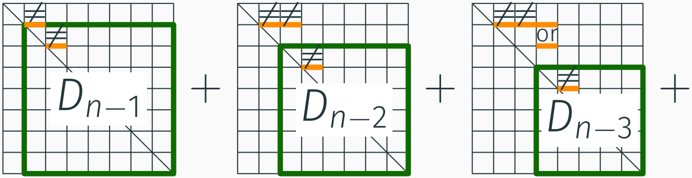


$$D_n = (v_{n-1} - v_{n-2})D_{n-1} + \frac{1}{2}(v_{n-1} - 2v_{n-2} + v_{n-3})v_{n-3}D_{n-2} + \cdots$$

Proof sketch (3/3)

The plan: 1. Upper bound 2'. Better lower bound **3. Bootstrapping**

$\{\text{DOAG matrices}\} =$



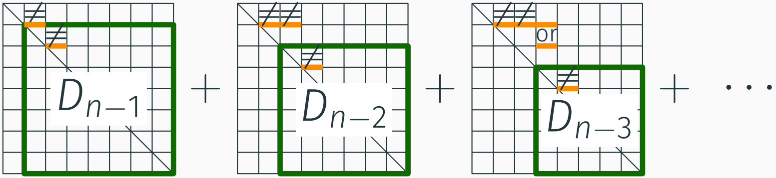
$+ \cdots$

$$D_n = (v_{n-1} - v_{n-2})D_{n-1} + \frac{1}{2}(v_{n-1} - 2v_{n-2} + v_{n-3})v_{n-3}D_{n-2} + \cdots$$

$$P_n = \left(1 - \frac{1}{n-1}\right) P_{n-1} + \frac{1}{2(n-2)} \left(1 - \frac{2}{n-1} + \frac{1}{(n-1)(n-2)}\right) P_{n-2} + \cdots$$

Proof sketch (3/3)

The plan: 1. Upper bound 2'. Better lower bound **3. Bootstrapping**

{DOAG matrices} = 

$$D_n = (v_{n-1} - v_{n-2}) D_{n-1} + \frac{1}{2}(v_{n-1} - 2v_{n-2} + v_{n-3}) v_{n-3} D_{n-2} + \cdots$$

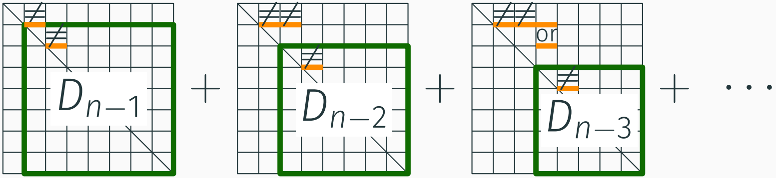
$$P_n = \left(1 - \frac{1}{n-1}\right) P_{n-1} + \frac{1}{2(n-2)} \left(1 - \frac{2}{n-1} + \frac{1}{(n-1)(n-2)}\right) P_{n-2} + \cdots$$

$$P_n \sim P_{n-1}$$

Proof sketch (3/3)

The plan: 1. Upper bound 2'. Better lower bound **3. Bootstrapping**

{DOAG matrices} =



$$D_n = (v_{n-1} - v_{n-2})D_{n-1} + \frac{1}{2}(v_{n-1} - 2v_{n-2} + v_{n-3})v_{n-3}D_{n-2} + \cdots$$

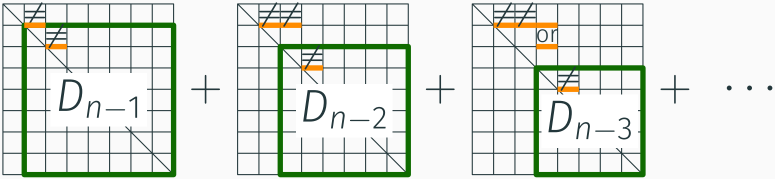
$$P_n = \left(1 - \frac{1}{n-1}\right)P_{n-1} + \frac{1}{2(n-2)}\left(1 - \frac{2}{n-1} + \frac{1}{(n-1)(n-2)}\right)P_{n-2} + \cdots$$

$$P_n \sim P_{n-1}$$

Proof sketch (3/3)

The plan: 1. Upper bound 2'. Better lower bound **3. Bootstrapping**

{DOAG matrices} =



$$D_n = (v_{n-1} - v_{n-2})D_{n-1} + \frac{1}{2}(v_{n-1} - 2v_{n-2} + v_{n-3})v_{n-3}D_{n-2} + \cdots$$

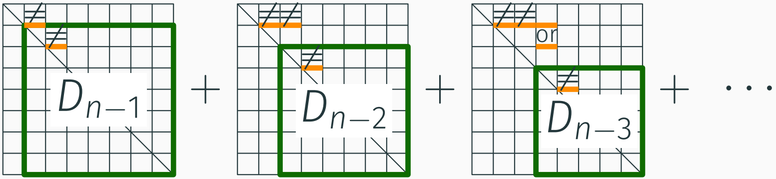
$$P_n = \left(1 - \frac{1}{n-1}\right) P_{n-1} + \frac{1}{2(n-2)} \left(1 - \frac{2}{n-1} + \frac{1}{(n-1)(n-2)}\right) P_{n-2} + \cdots$$

$$P_n = P_{n-1}\left(1 - \frac{1}{2n} + O\left(n^{-2}\right)\right)$$

Proof sketch (3/3)

The plan: 1. Upper bound 2'. Better lower bound **3. Bootstrapping**

{DOAG matrices} =



$$D_n = (v_{n-1} - v_{n-2}) D_{n-1} + \frac{1}{2}(v_{n-1} - 2v_{n-2} + v_{n-3}) v_{n-3} D_{n-2} + \cdots$$

$$P_n = \left(1 - \frac{1}{n-1}\right) P_{n-1} + \frac{1}{2(n-2)} \left(1 - \frac{2}{n-1} + \frac{1}{(n-1)(n-2)}\right) P_{n-2} + \cdots$$

$$P_n = P_{n-1}\left(1 - \frac{1}{2n} + O\left(n^{-2}\right)\right) \Rightarrow P_n \sim c \cdot n^{-\frac{1}{2}}$$

Random sampling again!

Corollary

$$\frac{D_n}{\#\{\textit{collections of variations of length } 1, 2, \ldots, n-1\}} \sim c \cdot n^{-\frac{1}{2}}$$

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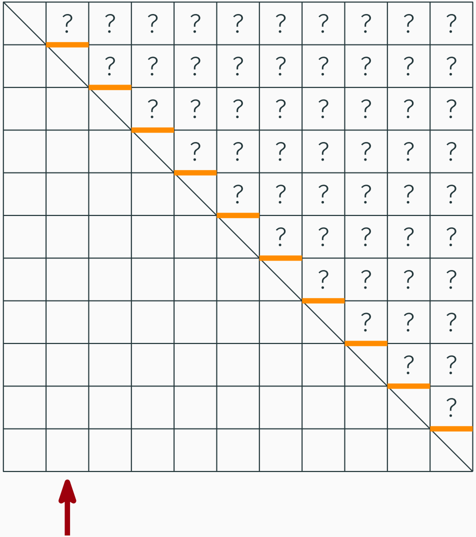
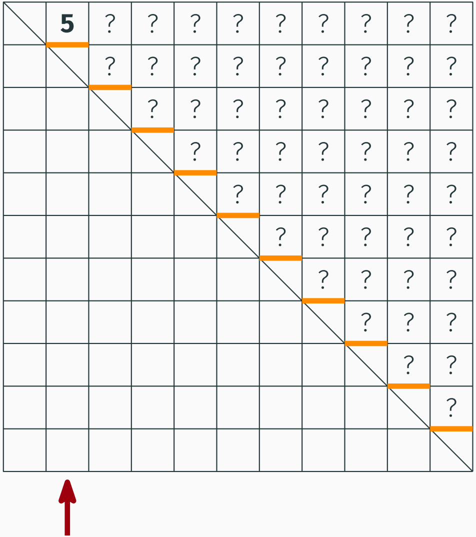
Better complexity:

$$\begin{aligned} &\mathsf{Cost}(\text{one full generation}) + \#\text{rejections} \times \mathsf{Cost}(\text{one failed generation}) \\ &= \frac{n^2}{2} \log_2(n) + O(\sqrt{n} \cdot \mathbf{Cost}(\text{one failed generation})) \end{aligned}$$

Early rejection



Early rejection



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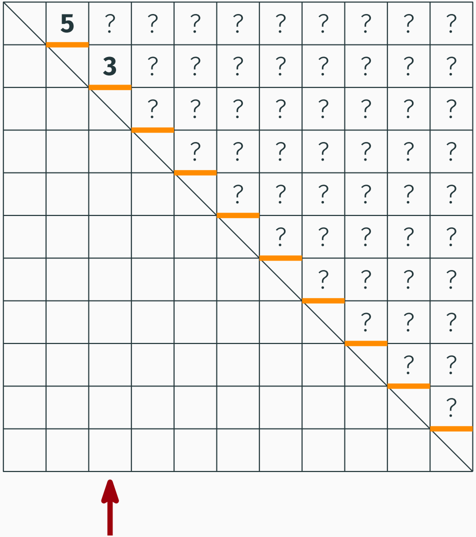

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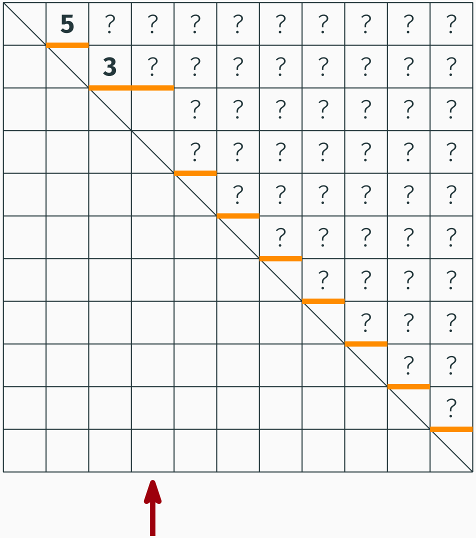

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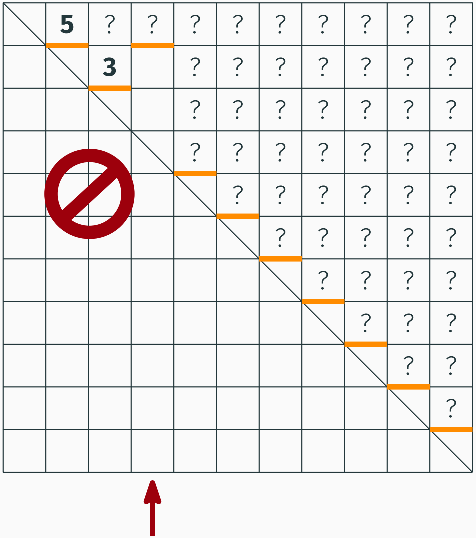

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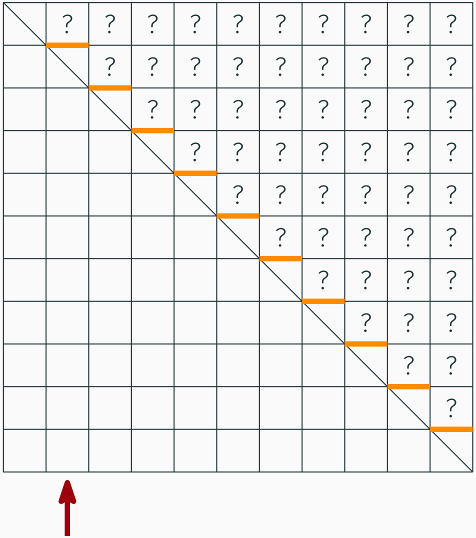

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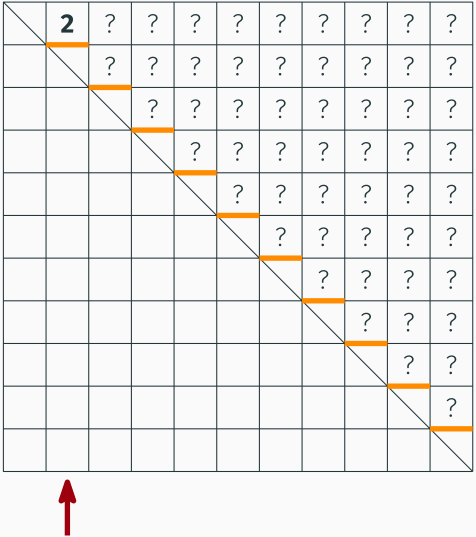

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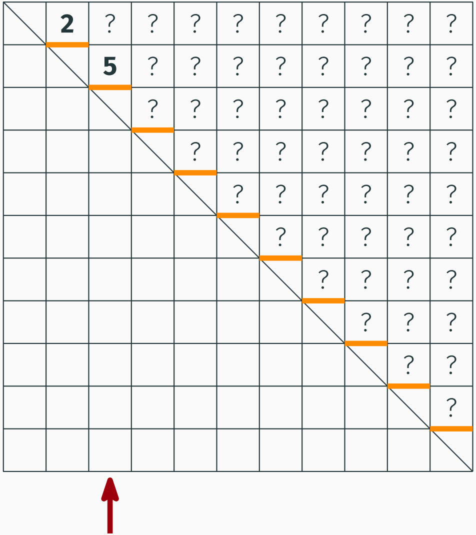

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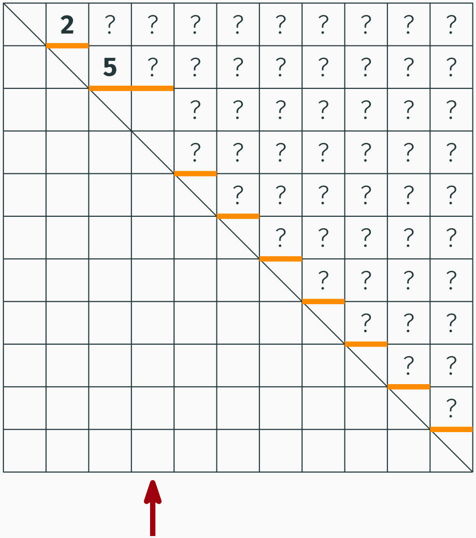

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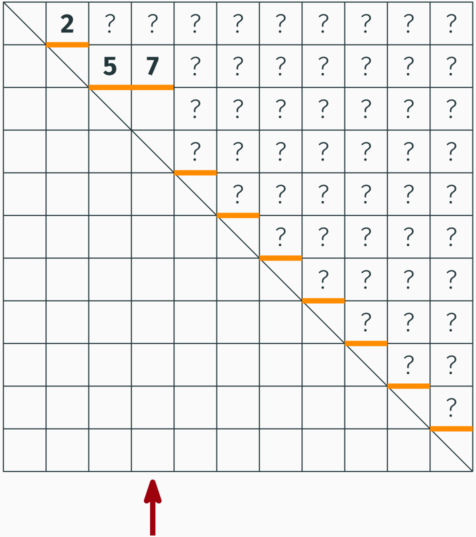

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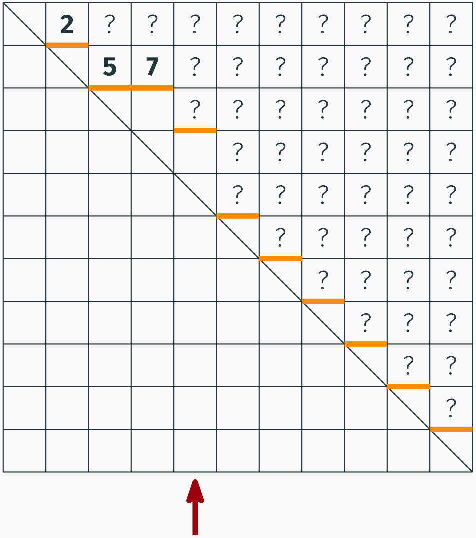

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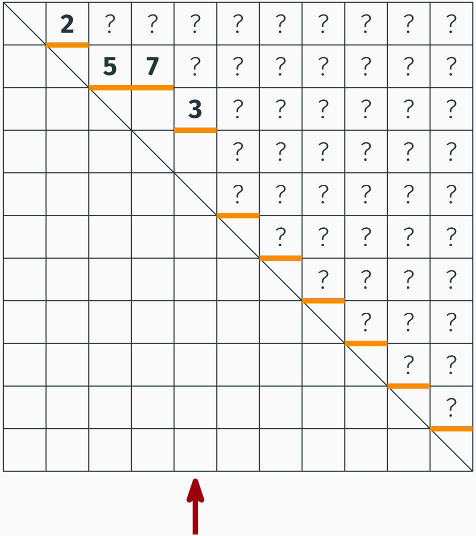

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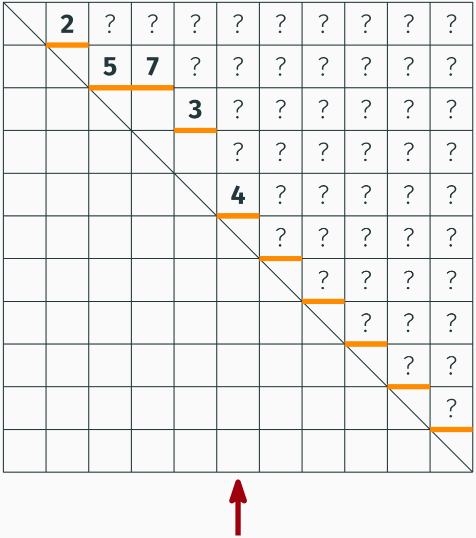

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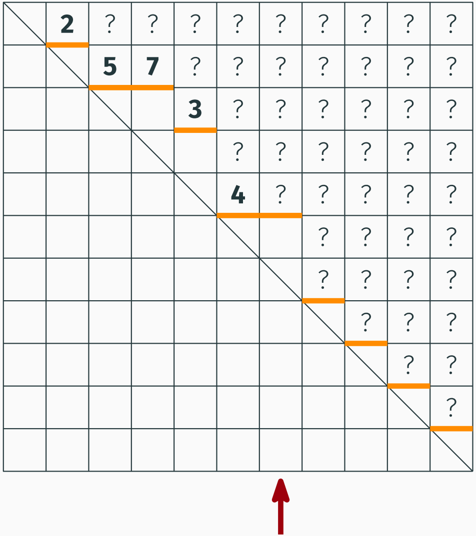

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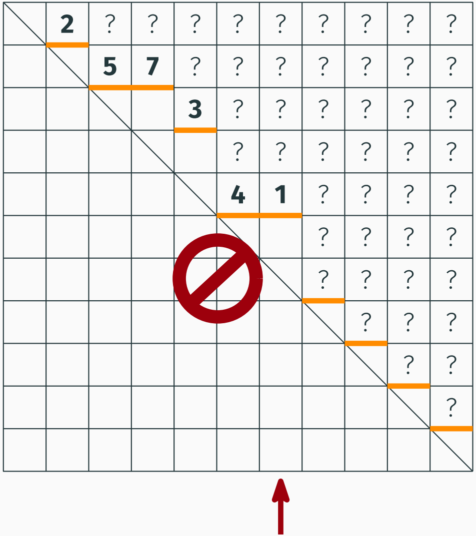

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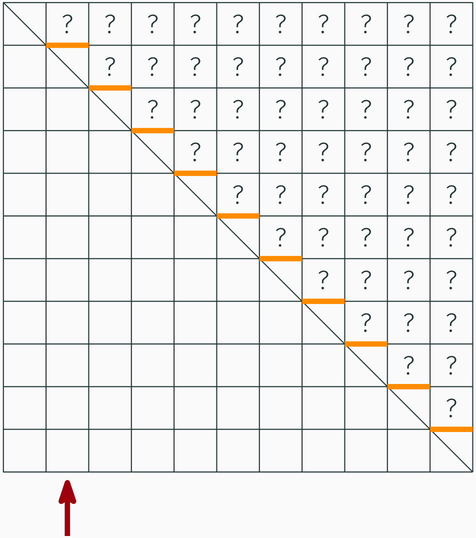

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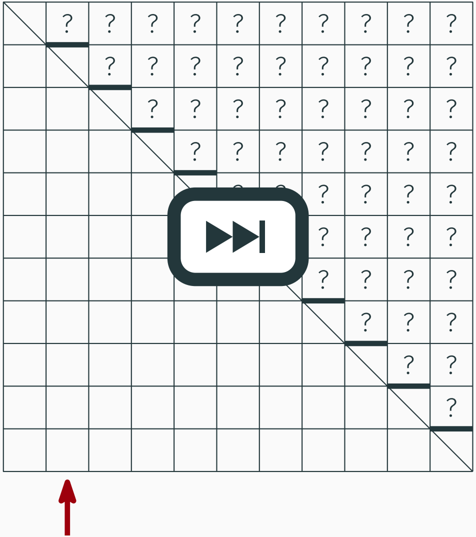

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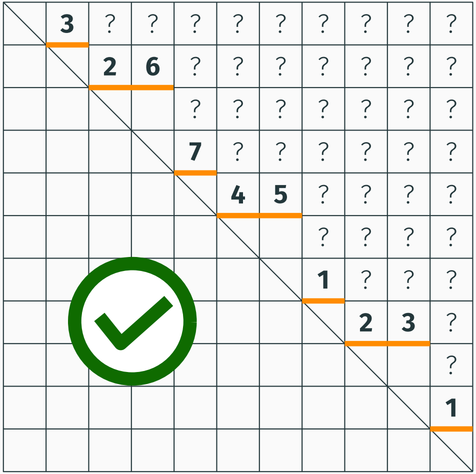

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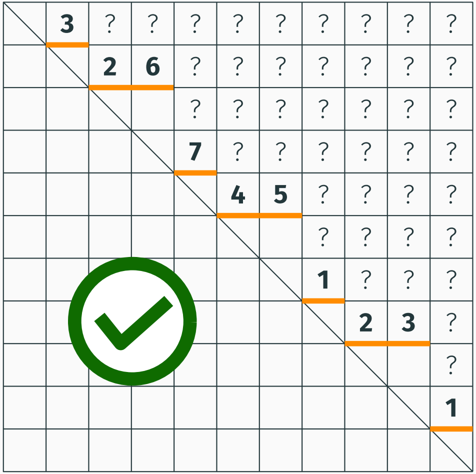

Complexity $= O(n \ln(n))$

Total complexity $= \dfrac{n^2}{2} \log_2(n) + O\left(\sqrt{n} \cdot n \ln(n)\right)$

Perspectives

- Law of the number of edges?

Perspectives

- Law of the number of edges?
- Multigraph equivalent: DOAMG
    - Identical to compacted plane trees
    - We have to count by edges
    - Simpler recurrence relation
    - No asymptotics (yet)
    - Collaborations with Alfredo Viola (Montevideo) and Michael Wallner (TU Wien)

- New model: DOAG
- New way of counting
- Control over the number of edges
- When forgetting edges:
  - (Fun?) asymptotic results
  - Optimal uniform sampler

https://github.com/Kerl13/randdag

https://wkerl.me

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