Combinatorial structures and algorithms: phase transition, enumeration and sampling

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Central questions

What does a random object γ in a combinatorial class $\mathcal{C}$ look like?

- how big is the largest component in γ? (phase transition)
- what is the chromatic number?

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How to efficiently sample a random object γ in $\mathcal{C}$?

E.g. a random planar graph

Outline

I. Phase transition

- Introduction to phase transition
- Erdős–Rényi random graph
  - Phase transition
  - Limit theorems for the giant component
  - Critical phase
- Random graphs with given degree sequence

II. Enumeration and random sampling

- Recursive decomposition
- Singularity analysis, Boltzmann sampler, probabilistic analysis
- Planar structures, minors and genus

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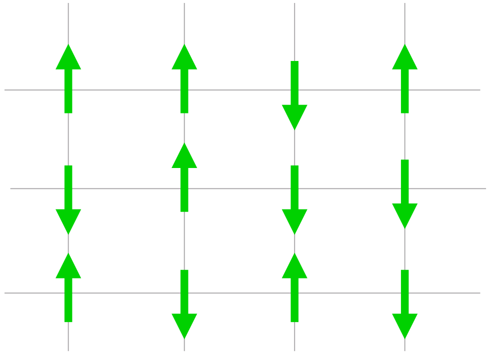
- PHASE TRANSITION IN THERMODYNAMICS

Phase transition

- PHASE TRANSITION IN STATISTICAL PHYSICS

Ising model

Given temperature T, (up or down) spins live on a lattice which interact with nearest neighbours



- Ordered phase at low temperatures
- Disordered phase at high temperatures

Phase transition

- PHASE TRANSITION IN COMPUTER SCIENCE

Random k-SAT problem

To determine whether or not a random k-CNF (conjunctive normal formula) $\mathcal{F}_k(n,m)$ with n variables and m clauses is satisfiable

E.g. a 3-CNF instance with 7 variables and 4 clauses

$$(x_1 \vee \overline{x_2} \vee x_5) \wedge (x_2 \vee x_3 \vee \overline{x_4}) \wedge (x_3 \vee \overline{x_4} \vee \overline{x_5}) \wedge (x_1 \vee x_5 \vee \overline{x_7})$$

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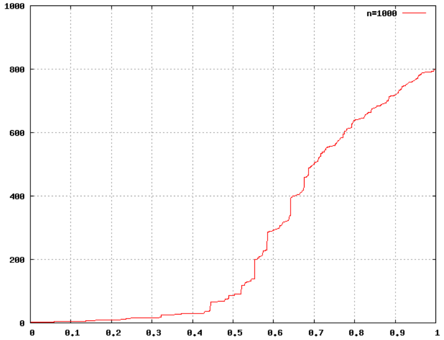
- Phase transition from satisfiability to unsatisfiability of $\mathcal{F}_k(n,m)$ around $\frac{m}{n} \sim \frac{2^k}{\ln 2}$
- Computational time required to find a satisfying truth assignment or determine it to be unsatisfiable increases drastically around $\frac{m}{n} \sim \frac{2^k}{k}$

Phase transition

- PHASE TRANSITION IN RANDOM GRAPH

It describes a dramatic change in the number of vertices in the largest component in a random graph by addition of a small number of edges around the critical value [ERDŐS–RÉNYI 60; BOLLOBÁS; ŁUCZAK; PERES; SPENCER, · · ·]



Phase transition

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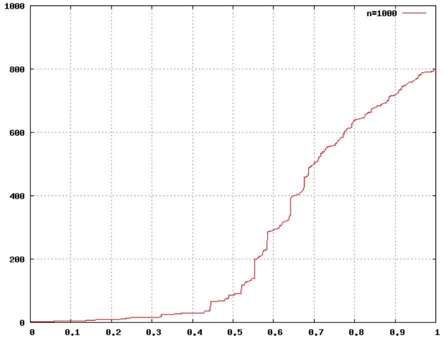
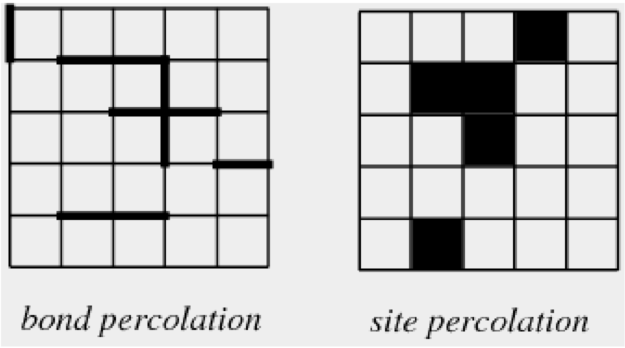


Cf. percolation theory.


bond percolation

site percolation

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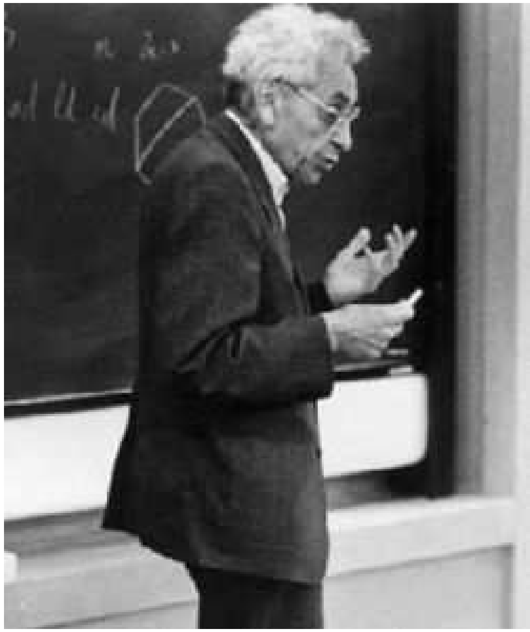
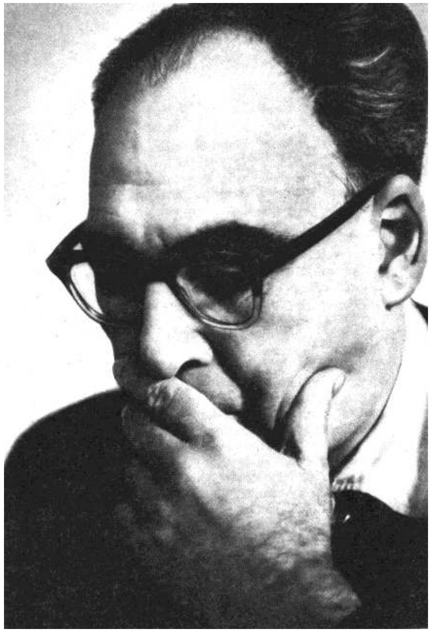
Binomial random graph

[ERDŐS–RÉNYI 60]

The binomial random graph $G(n,p)$



Paul Erdős (1913-1996)



Alfréd Rényi (1921-1970)

Binomial random graph

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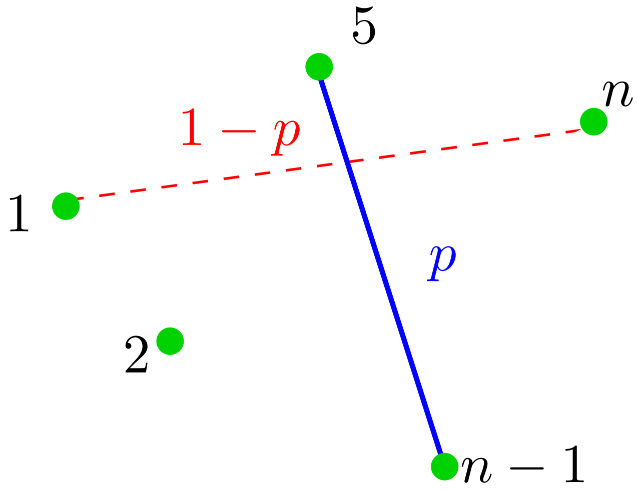

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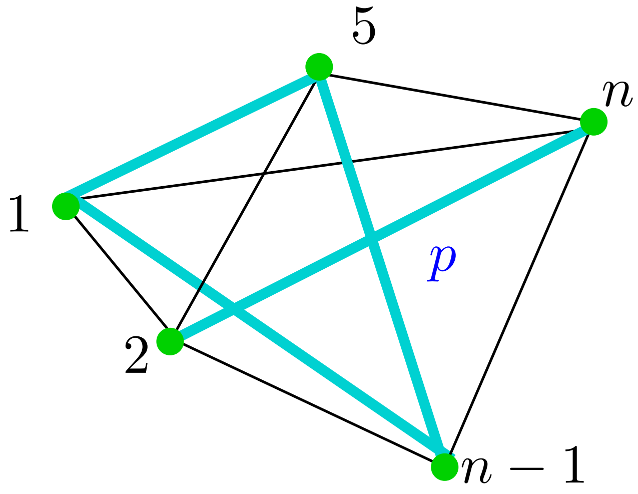

Expected degree

Suppose the edge probability $p = \frac{c}{n-1}$ for a constant $c > 0$.

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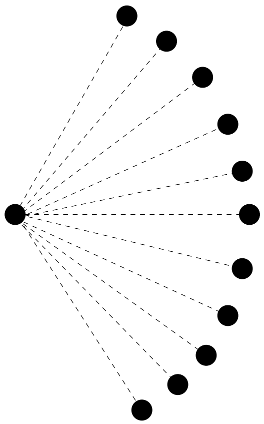

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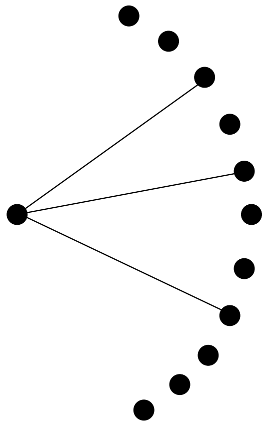
- The degree of a random vertex in $G(n, p)$ is a binomial random variable: $X \sim \mathrm{Bi}(n-1, p)$, i.e.

$$\mathbb{P}(X = i) = \binom{n-1}{i} p^i (1-p)^{n-1-i}$$



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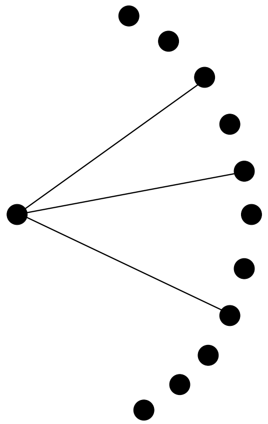

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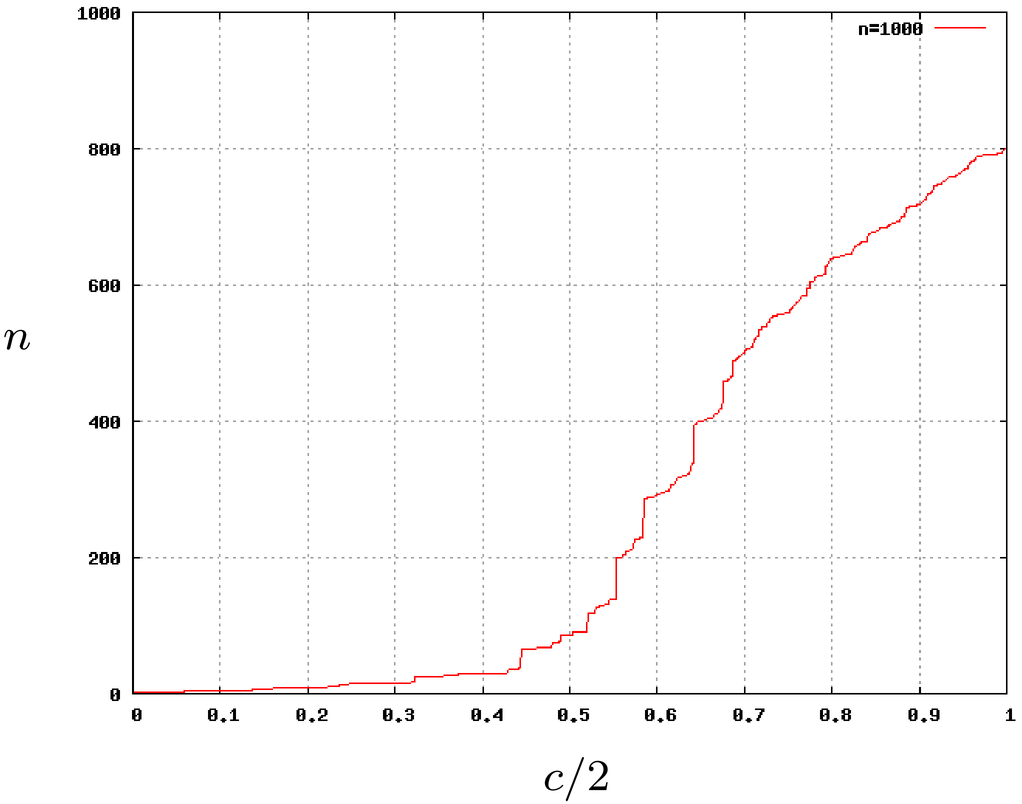

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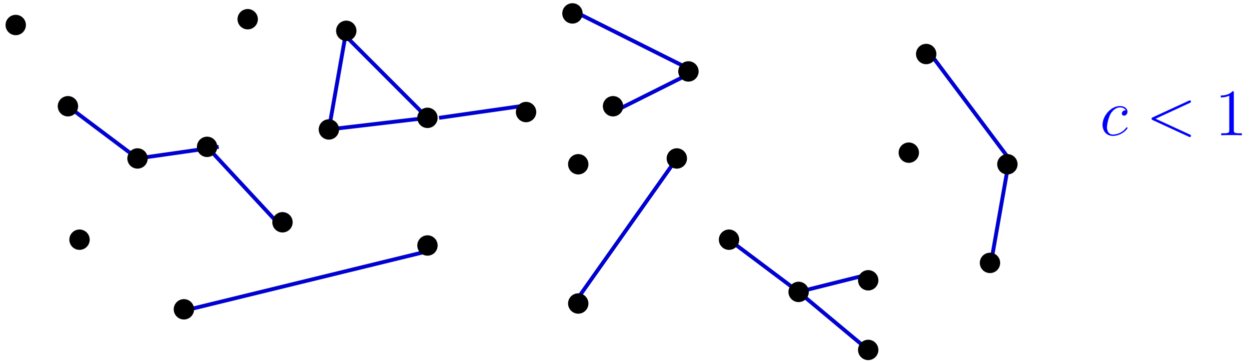

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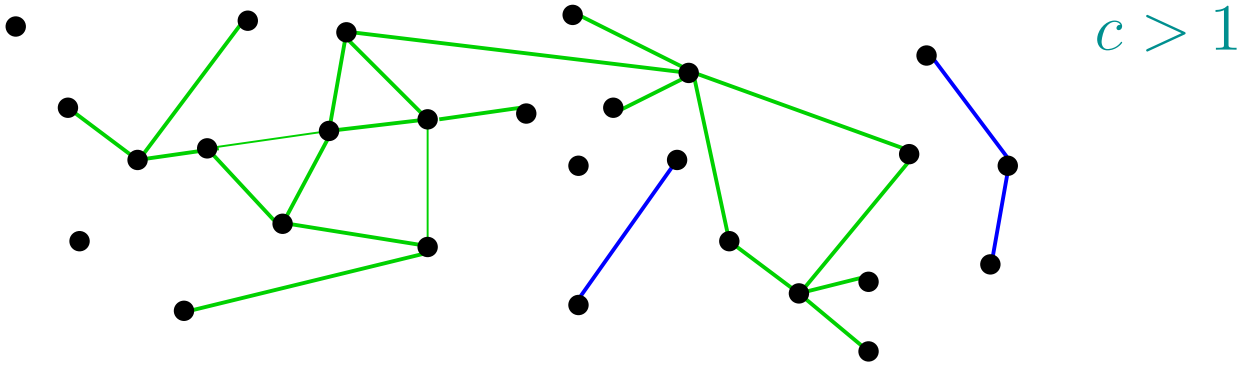
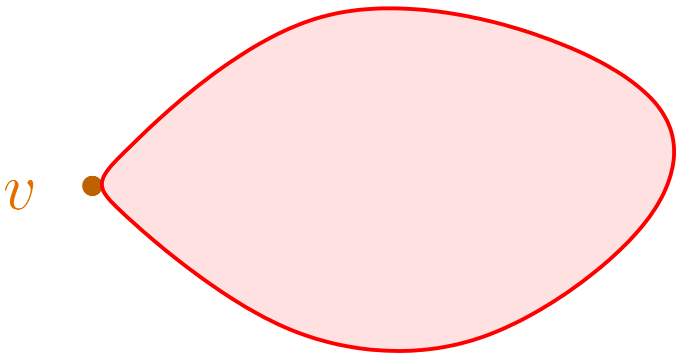
- When $c < 1$, with probability tending to 1 as $n \to \infty$ (whp) all the components have $O(\log n)$ vertices.
- When $c > 1$, whp there is a unique largest component of order $\Theta(n)$, while every other component has $O(\log n)$ vertices.



Exposing a component

[BREATH-FIRST-SEARCH: KARP 90]



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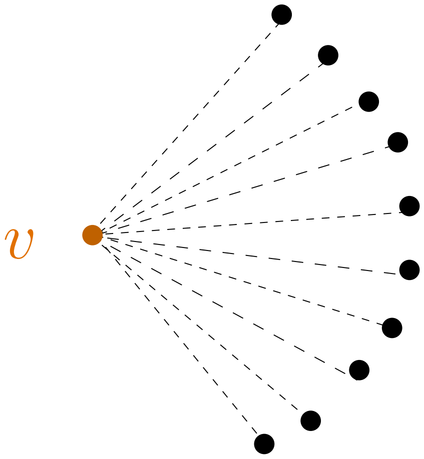

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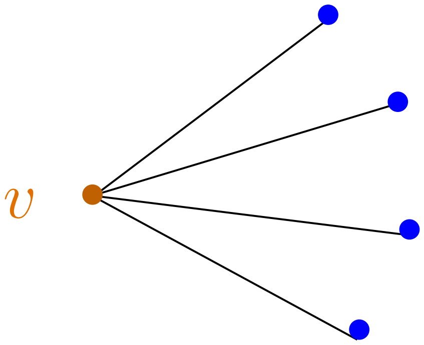

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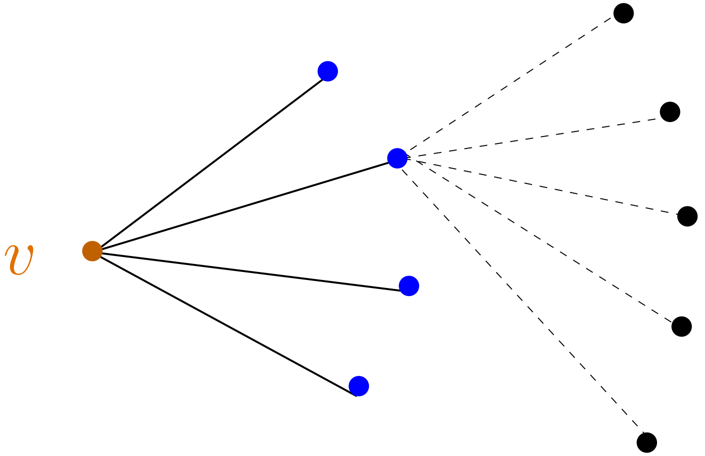

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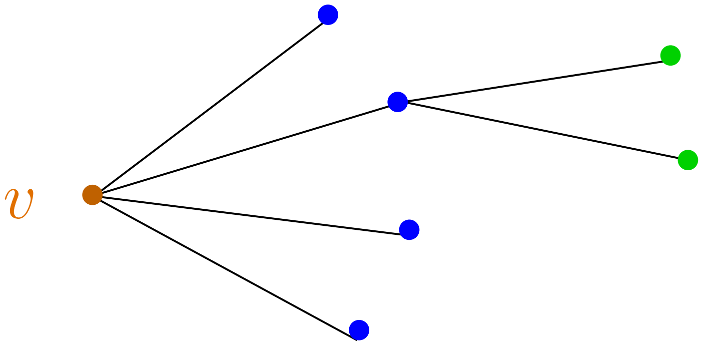

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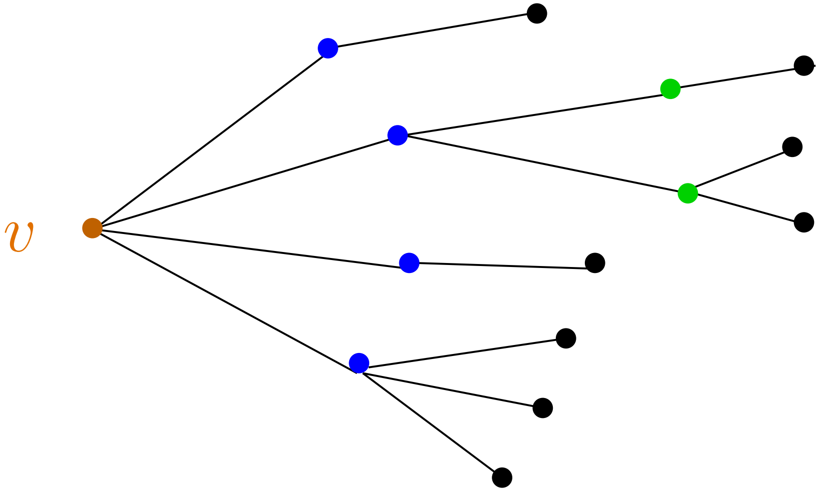

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- First we expose the neighbours („children”) of v
- Then we expose the neighbours of each neighbour of v
- We continue this procedure, until there are no more vertices contained in $C(v)$.

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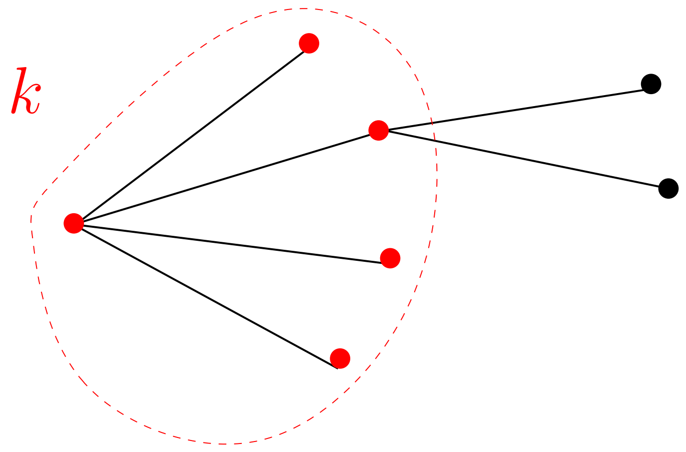

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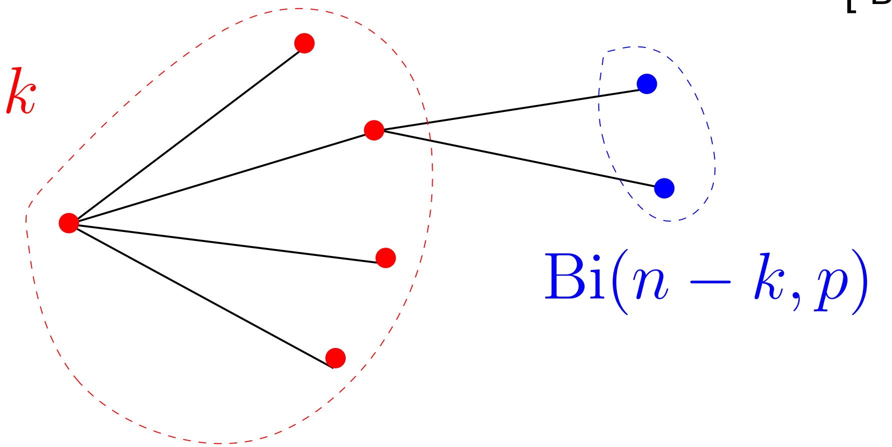

When $k \ll n$ vertices are exposed,

- the number of new neighbours (“children”) of a vertex: $\mathrm{Bi}(n-k,p)$
- the expected number of children: $(n-k)p = (n-k)\frac{c}{n-1} \sim c$.

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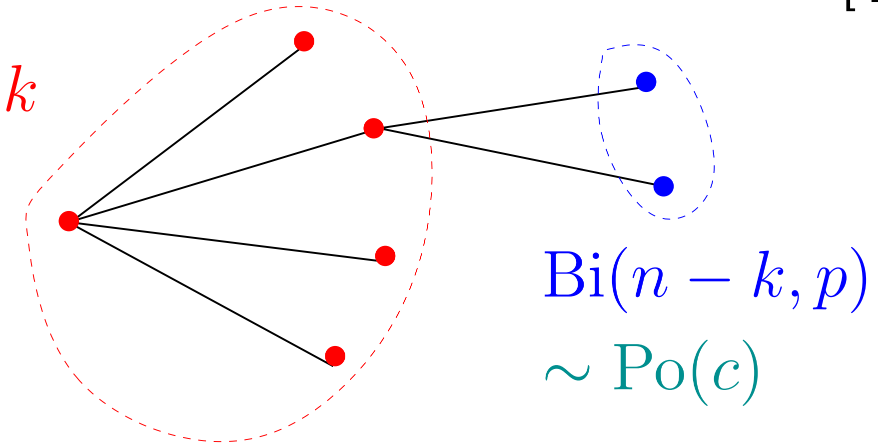

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$$\begin{aligned}\lim_{n\to\infty} \mathbb{P}(\mathrm{Bi}(n-k,p)=i) \quad &= \lim_{n\to\infty} \binom{n-k}{i} p^i (1-p)^{n-k-i} \\ &= \frac{c^i}{i!}e^{-c} = \mathbb{P}(\mathrm{Po}(c)=i)\end{aligned}$$

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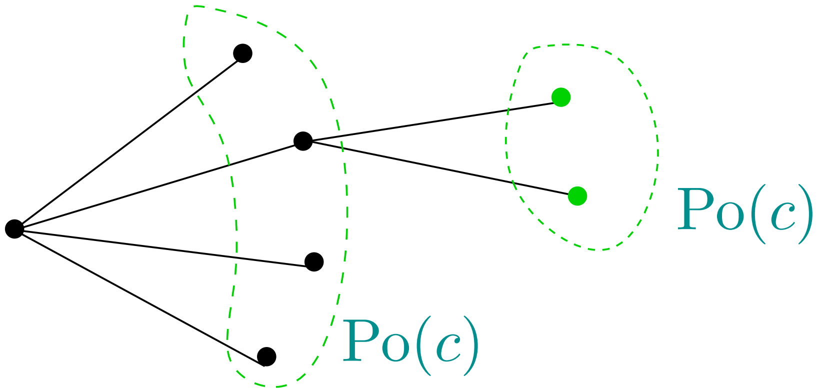

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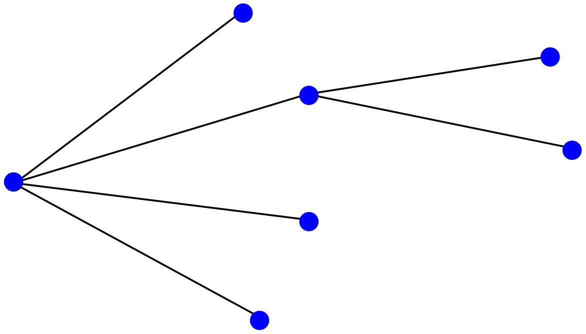
- If $c < 1$, the process dies out with probability 1.



It corresponds to a „small" component in $G(n,p)$

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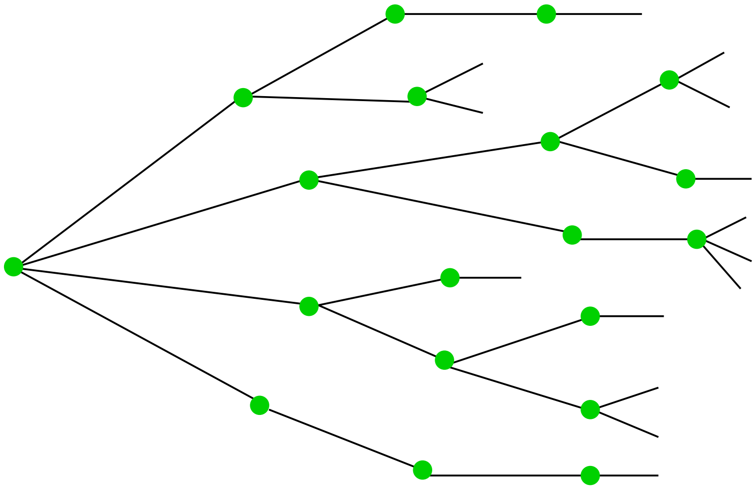

It corresponds to the „giant” component of order $\Theta(n)$ in $G(n,p)$

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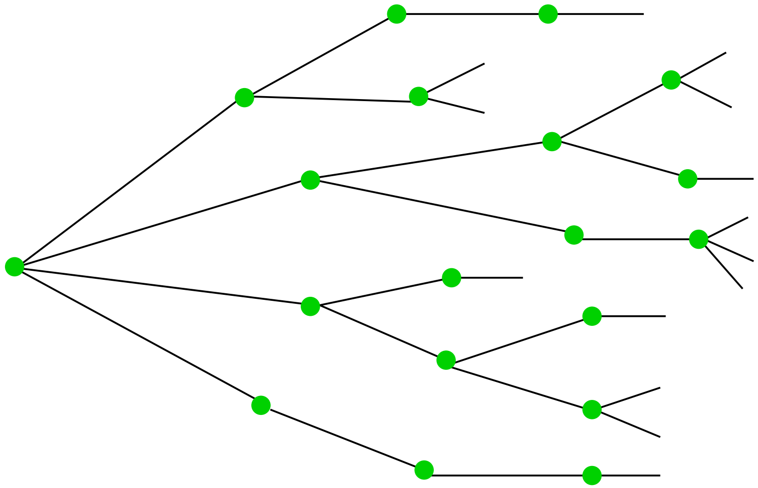
Survival probability ρ:

$1 - \rho = e^{-c\rho}$



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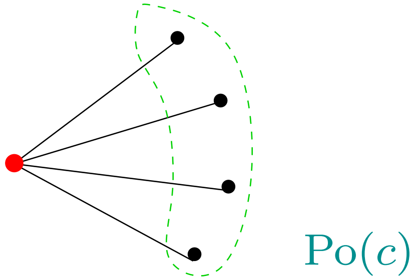
satisfies $q(z) = z \sum_k \mathbb{P}\left[\mathrm{Po}(c) = k\right] q(z)^k = z \sum_k e^{-c} \frac{c^k}{k!} q(z)^k = ze^{c(q(z)-1)}$.



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The extinction probability $1 - \rho := \sum_{i<\infty} \mathbb{P}\left[T = i\right] = q(1)$ satisfies

$$1 - \rho = q(1) = e^{c(q(1)-1)} = e^{c(1-\rho-1)} = e^{-c\rho}.$$

Giant component

Let $\mathcal{N}_p$ be the order of the giant component after the phase transition.

Then $\mathbb{E}(\mathcal{N}_p) = \rho n$ where $1 - \rho = e^{-c\rho}$, $\rho \neq 0$.

Giant component

Let $\mathcal{N}_p$ be the order of the giant component after the phase transition. Then $\mathbb{E}(\mathcal{N}_p) = \rho n$ and $\mathcal{N}_p = \rho n + o(n)$ whp where $1 - \rho = e^{-c\rho}$, $\rho \neq 0$.

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[PITTEL 90; BARREZ–BOUCHERON–DE LA VEGA 00]

The variance $\mathcal{N}_p$ satisfies $\sigma^2 := \mathrm{Var}(\mathcal{N}_p) = \frac{\rho - \rho^2}{(1-c(1-\rho))^2} n$.

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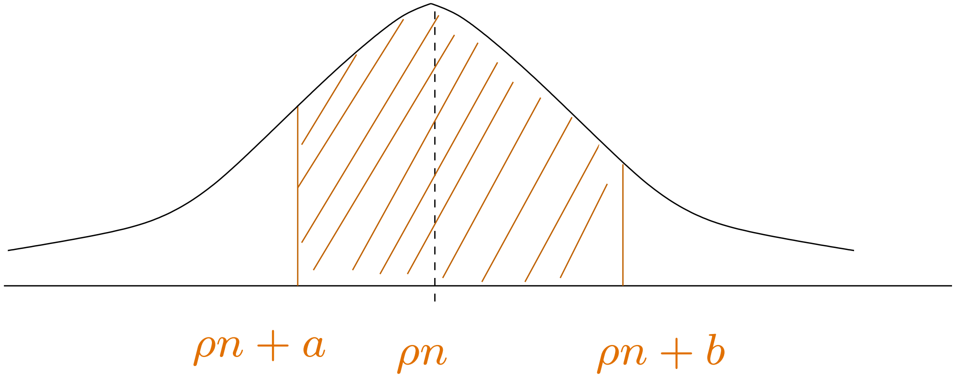
For any fixed numbers $a < b$

$$\mathbb{P}\left[\rho n + a \leq \mathcal{N}_p \leq \rho n + b\right] \sim \frac{1}{\sigma\sqrt{2\pi}} \int_a^b \exp\left[-\frac{x^2}{2\sigma^2}\right] dx.$$



Gaussian distribution

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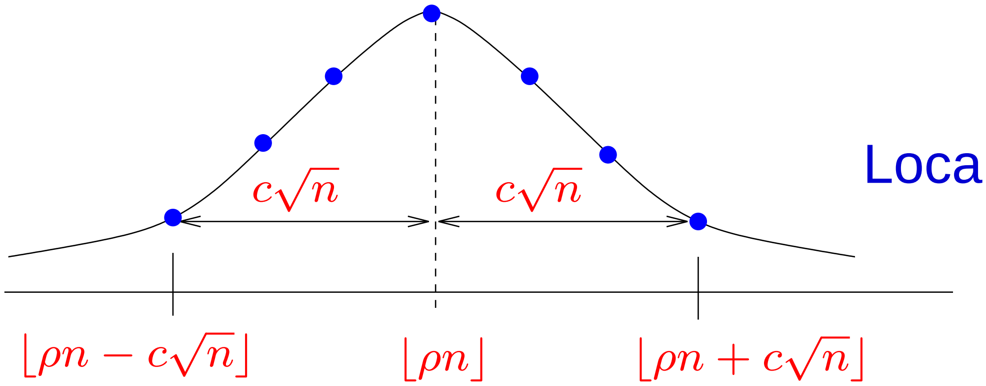

Locally?? Gaussian distribution

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Then $\mathbb{E}(\mathcal{N}_p) = \rho n$ and $\mathcal{N}_p = \rho n + o(n)$ whp where $1 - \rho = e^{-c\rho}$, $\rho \neq 0$.

Central Limit Theorem

[PITTEL 90; BARREZ–BOUCHERON–DE LA VEGA 00]

The variance $\mathcal{N}_p$ satisfies $\sigma^2 := \mathrm{Var}(\mathcal{N}_p) = \frac{\rho-\rho^2}{(1-c(1-\rho))^2} n$.

For any fixed numbers $a < b$

$$\mathbb{P}\left[\rho n + a \leq \mathcal{N}_p \leq \rho n + b\right] \sim \frac{1}{\sigma\sqrt{2\pi}} \int_a^b \exp\left[-\frac{x^2}{2\sigma^2}\right] dx.$$

Local Limit Theorem

[BEHRISCH–COJA-OGHLAN–K. 07+]

For any integer k with $k = \rho n + x$ and $x = O(\sqrt{n}\,) = O(\sigma)$,

$$\mathbb{P}\left[\mathcal{N}_p = k\right] \sim \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{x^2}{2\sigma^2}\right].$$

Joint distribution

- Let $\mathcal{M}_p$ denote $\#$ edges in the giant component in $G(n,p)$.

$$\mathbb{P}\left[\mathcal{N}_p = k \wedge \mathcal{M}_p = l\right] \sim \frac{1}{2\pi\sigma\sigma_{\mathcal{M}}\sqrt{1-\frac{\sigma_{\mathcal{N}\mathcal{M}}^2}{\sigma^2\sigma_{\mathcal{M}}^2}}} \exp\left[-\frac{\frac{x^2}{\sigma^2}-\frac{2\sigma_{\mathcal{N}\mathcal{M}}xy}{\sigma^2\sigma_{\mathcal{M}}^2}+\frac{y^2}{\sigma_{\mathcal{M}}^2}}{2\left(1-\frac{\sigma_{\mathcal{N}\mathcal{M}}^2}{\sigma^2\sigma_{\mathcal{M}}^2}\right)}\right]$$

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$$C(k,l) \sim \mathbb{P}\left[\mathcal{N}_p = k \wedge \mathcal{M}_p = l\right] \binom{n}{k}^{-1} p^{-l}(1-p)^{-\binom{n}{2}+\binom{n-k}{2}+l}$$

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Cf. asymptotic formula for $C(k,l)$ via

– enumerative method [BENDER–CANFIELD–MCKAY 90]

– saddle-point method [FLAJOLET–SALVY–SCHAEFFER 04]

The critical phase

What about the order of the largest component of $G(n,p)$ with $p = \frac{c_n}{n-1}$ when the expected degree $c_n \to 1$, in the so-called critical phase?

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[BOLLOBÁS 84]

Let $c_n = 1 + \lambda_n n^{-1/3} \log n$ where $\lambda_n n^{-1/3} \log n \to 0$ as $n \to \infty$.

- If $\lambda_n \to -\infty$, whp all components have $\ll n^{2/3}$ vertices.
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Scaling window of Mean-Field width of $n^{-1/3}$ (Percolation Theory)

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- If $\lambda_n \to \lambda$, whp the largest component has $\Theta(n^{2/3})$ vertices.
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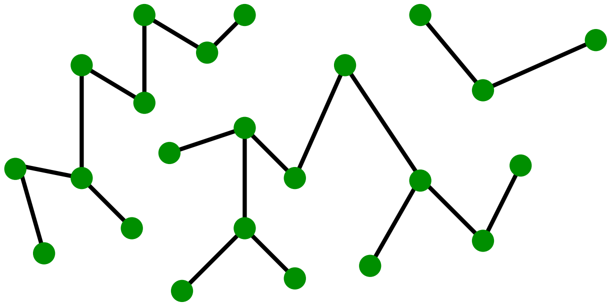

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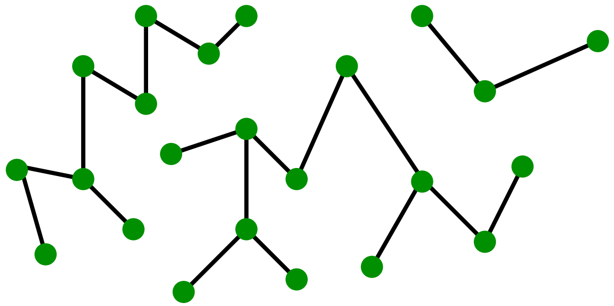
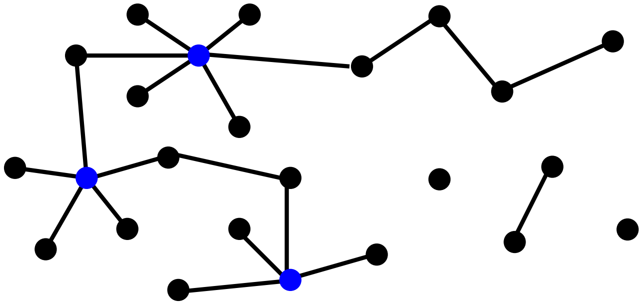


- In some complex systems/networks, e.g. www, epidemic networks, some vertices are of high degree, while most vertices are of low degree: non-homogeneous



Random graph models

Random graph processes

- To model and analyse dynamic nature of complex systems/networks arising from the real world
- Random „internet” graph [BOLLOBÁS–RIORDAN; COOPER–FRIEZE 03]
- Degree constraints [WORMALD; K.–SEIERSTAD 07; COJA-OGHLAN–K. 08+]

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Random graphs with given degree sequence

[Molloy–Reed 95, 98; Janson–M. Luczack 07+; K.–Seierstad 08]

Asymptotic degree sequence

[Molloy–Reed 95, 98]

Let $G_n(d_0(n), d_1(n), \ldots)$ be a uniform random graph on n vertices, $d_i(n)$ of which are of degree i.

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The asymptotic degree sequence $\mathcal{D} = \{d_0(n), d_1(n), \ldots\}$ satisfies:

- $\sum_{i \geq 0} d_i(n) = n$ and $d_i(n) = 0$ for $i \geq n$
- $\delta_i(n) = \frac{d_i(n)}{n} \to \delta_i^*$ as $n \to \infty$
- "well behaves" and $d_i(n) = 0$ whenever $i > n^{\frac{1}{4} - \varepsilon}$ for some $\varepsilon > 0$

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The phase transition in $G_n(\mathcal{D})$ occurs when

$$Q(\mathcal{D}) := \sum_i (i-2) i \delta_i(n) = 0.$$

(We will come back to this later)

Phase transition

[Molloy–Reed 95, 98]

If $Q(\mathcal{D}) < 0$, whp all components have $O(\log n)$ vertices.

If $Q(\mathcal{D}) > 0$, whp there is a unique component of order $\Theta(n)$, while all other components have $O(\log n)$ vertices.

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Given a degree sequence $\mathcal{D}_n = \{a_1, \ldots, a_n\}$ of $V = \{v_1, \ldots, v_n\}$ s.t.

$$a_i = \deg(v_i) \quad \text{for} \quad 1 \le i \le n,$$

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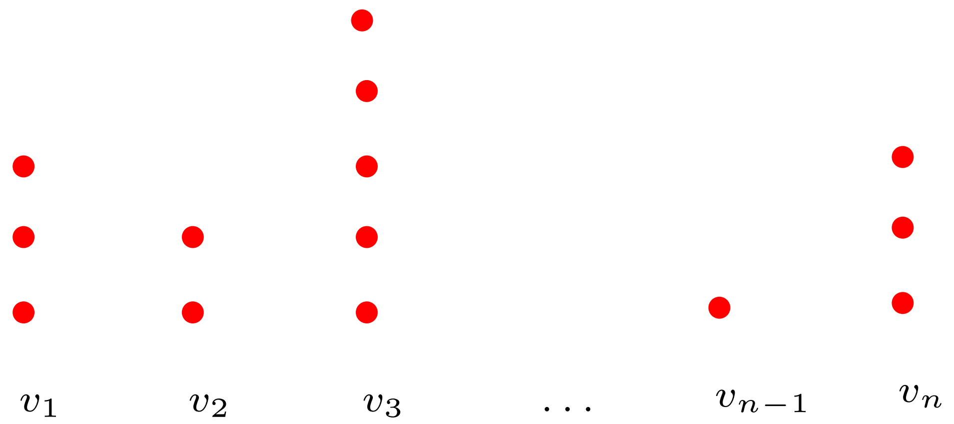

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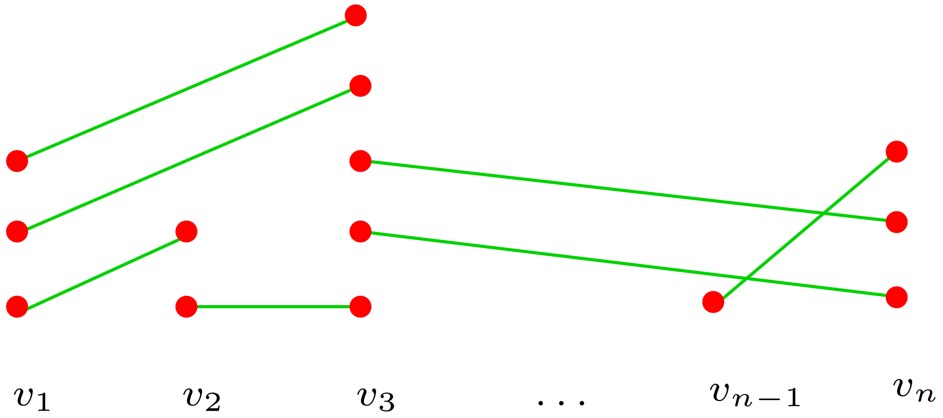

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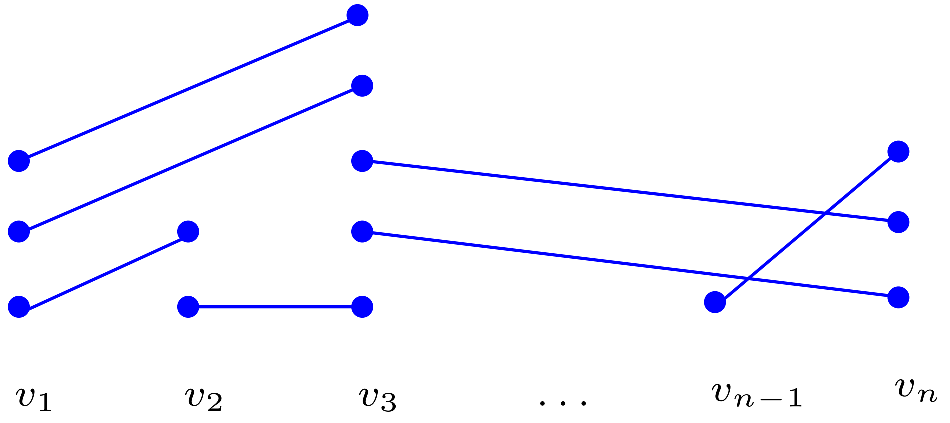
Then a random configuration $\mathcal{C}_n = L_n + M_n$.



Random configuration

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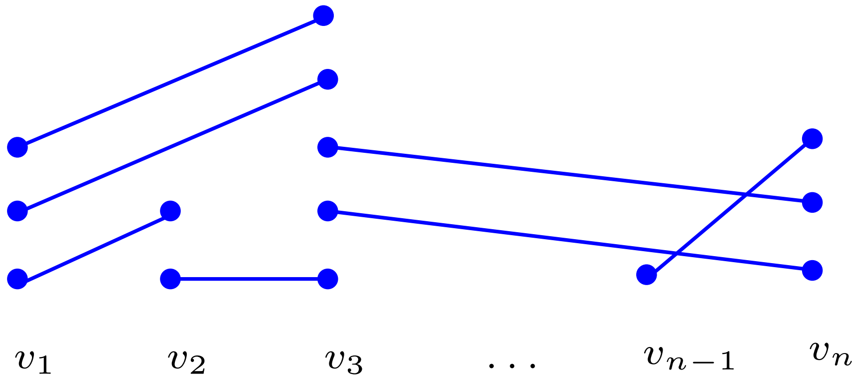
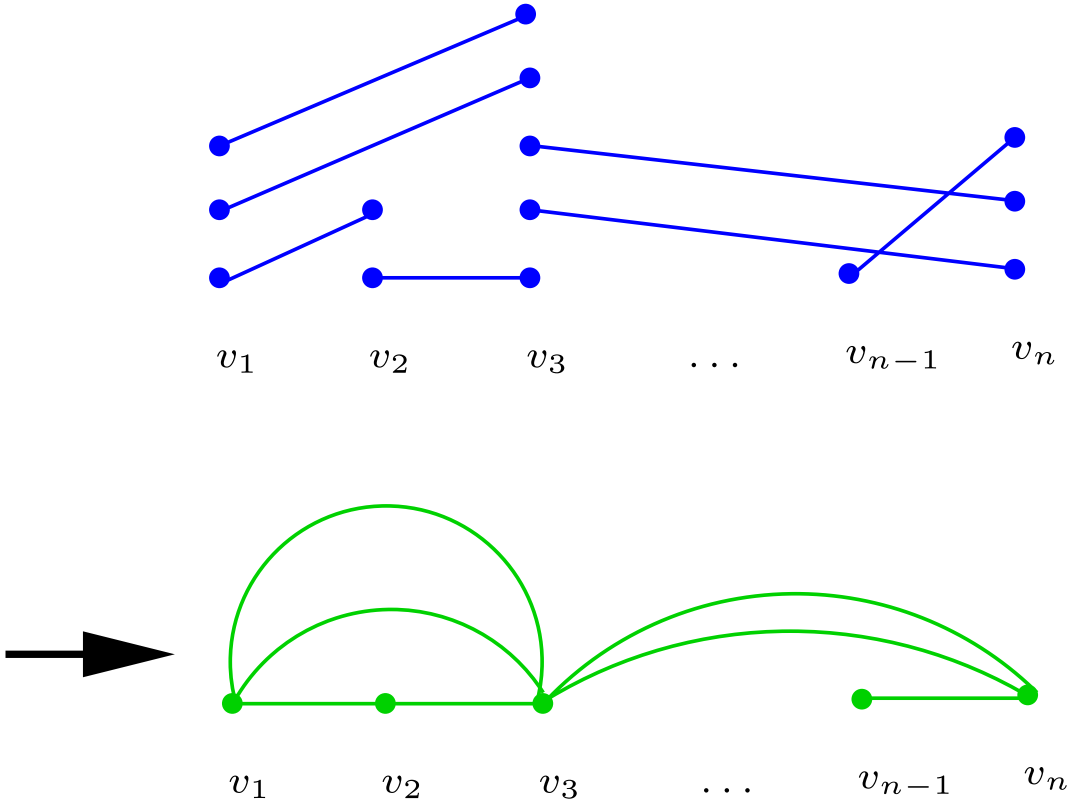


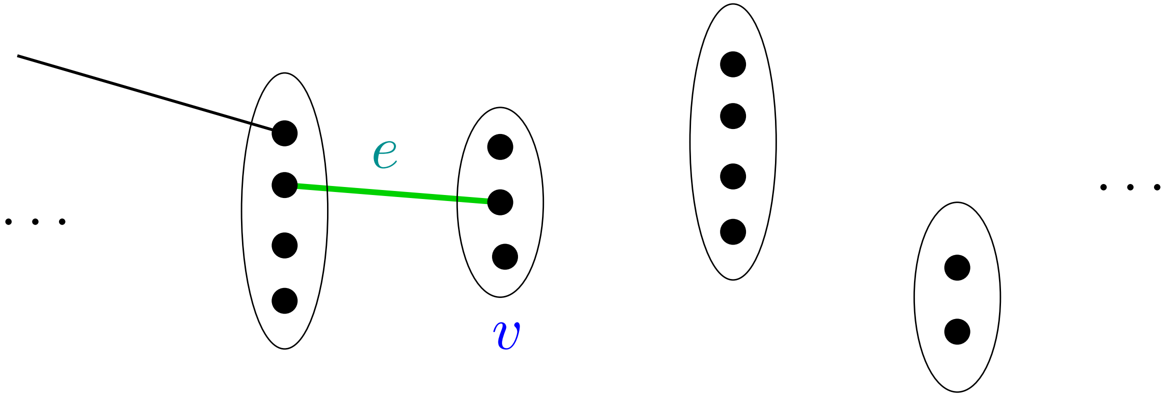
Random configuration

Given a configuration $\mathcal{C}_n$, let G_n^* be the multigraph obtained by

- identifying all a_i copies of v_i for every $i = 1, \ldots, n$, and
- letting the pairs of the perfect matching in $\mathcal{C}_n$ become edges.



Branching process



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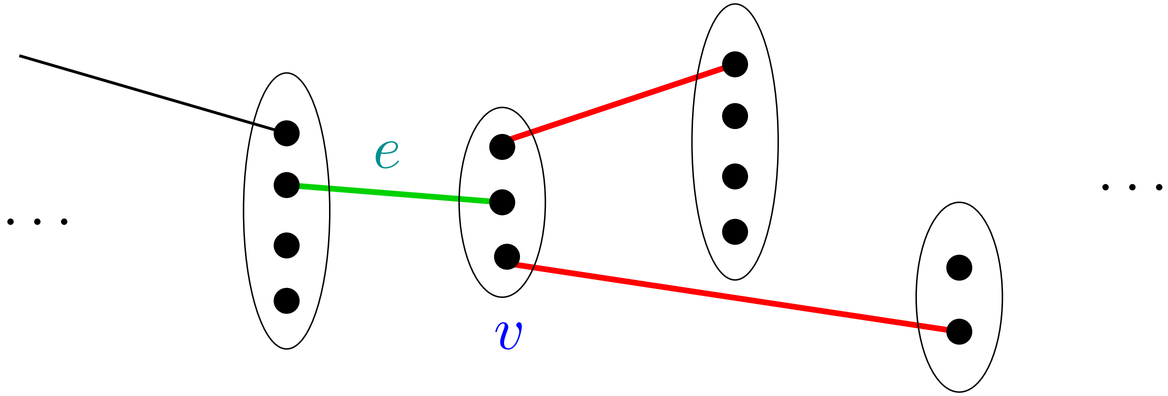

Let X be the number of children the edge e

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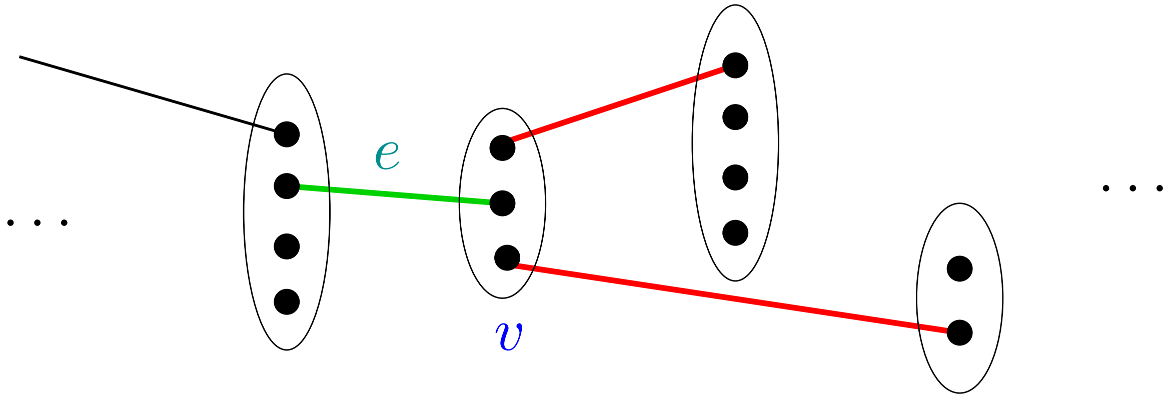

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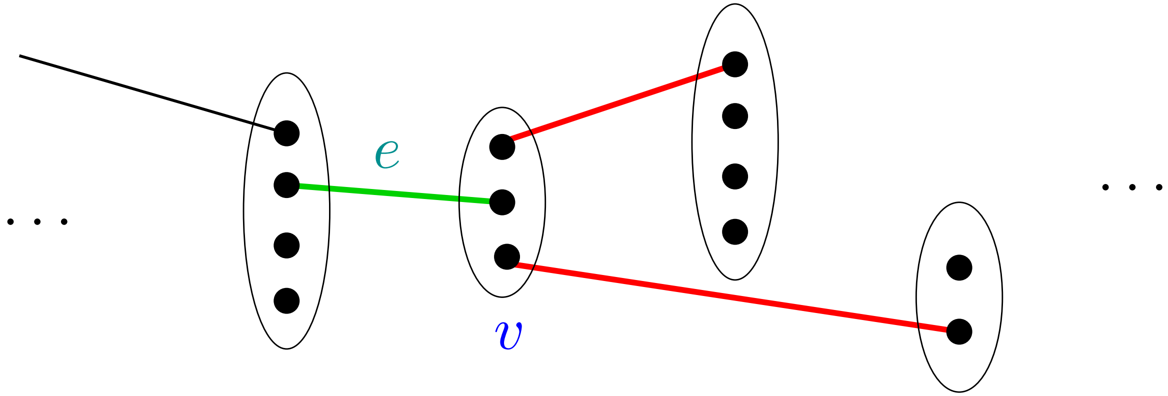

Let X be the number of children of the vertex v to which the edge e belongs. Its distribution is given by

$$\mathbb{P}[X = i - 1] = \frac{i\delta_i(n)}{\sum_i i\delta_i(n)}, \qquad \delta_i(n) = \frac{d_i(n)}{n} = \frac{|\{k : \deg(v_k) = i\}|}{n}.$$

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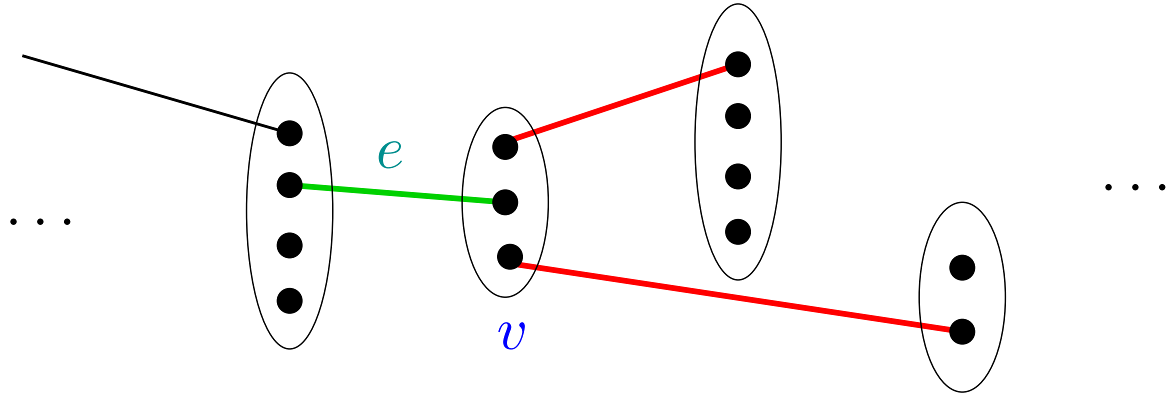

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$= \mathbb{P}[v$ is one of the d_i vertices of degree $i]$

$= \mathbb{P}[e$ is matched to one of the i clones of a vertex of degree $i]$

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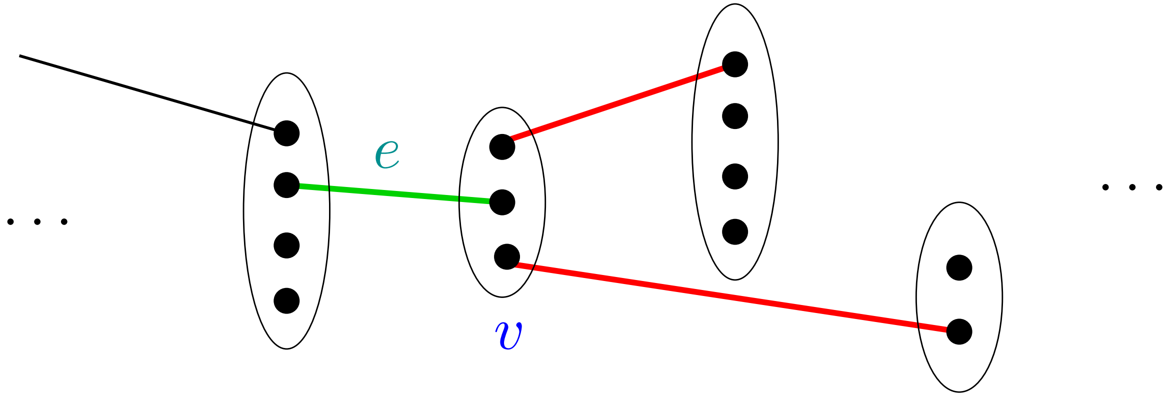

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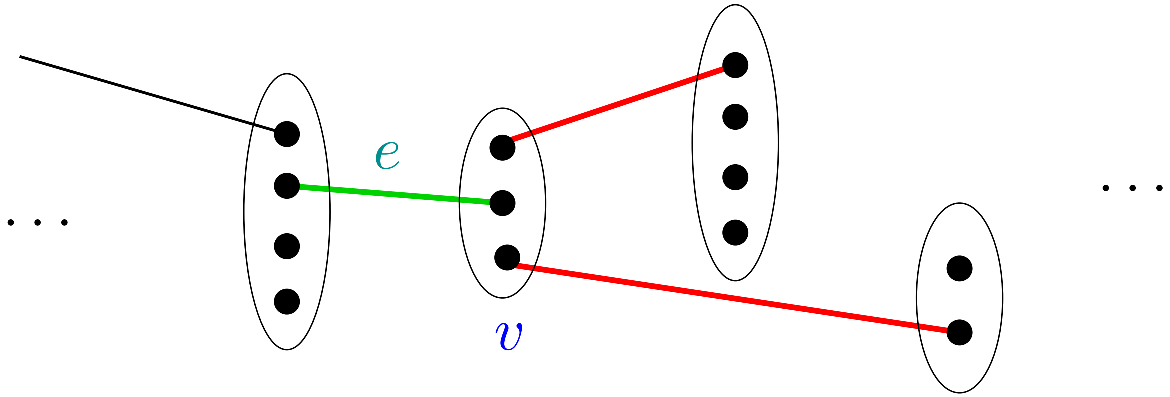

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$$\mathbb{E}[X] = \sum_i (i-1)\,\mathbb{P}[X = i-1] = \sum_i (i-1)\frac{i\delta_i(n)}{\sum_i i\delta_i(n)}.$$

The critical point of the branching process is when $\mathbb{E}[X] = 1$, that is,

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Graphs that can be embedded in the plane without crossing edges

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[Denise–Vasconcellos–Welsh 96]

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Markov chain (addition-deletion)

- upper bound on $\#$ planar graphs [Denise–Vasconcellos–Welsh 96]
- typical properties [McDiarmid–Steger–Welsh 05]

Planar graphs

Graphs that can be embedded in the plane without crossing edges

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$\exists$ alternative methods?

An alternative method?

“A nonstandard method of counting trees: Put a cat into each tree, walk your dog, and count how often he barks.” [*Proofs from THE BOOK*, M. AIGNER AND G. ZIEGLER]

Recursive decomposition

[Nijenhuis–Wilf 79; Flajolet–Zimmerman–Van Cutsem 94; Flajolet–Sedgewick 08+]

Recursive decomposition

[Nijenhuis–Wilf 79; Flajolet–Zimmerman–Van Cutsem 94; Flajolet–Sedgewick 08+]

Decomposition

Recursive Counting Formulas

Recursive decomposition

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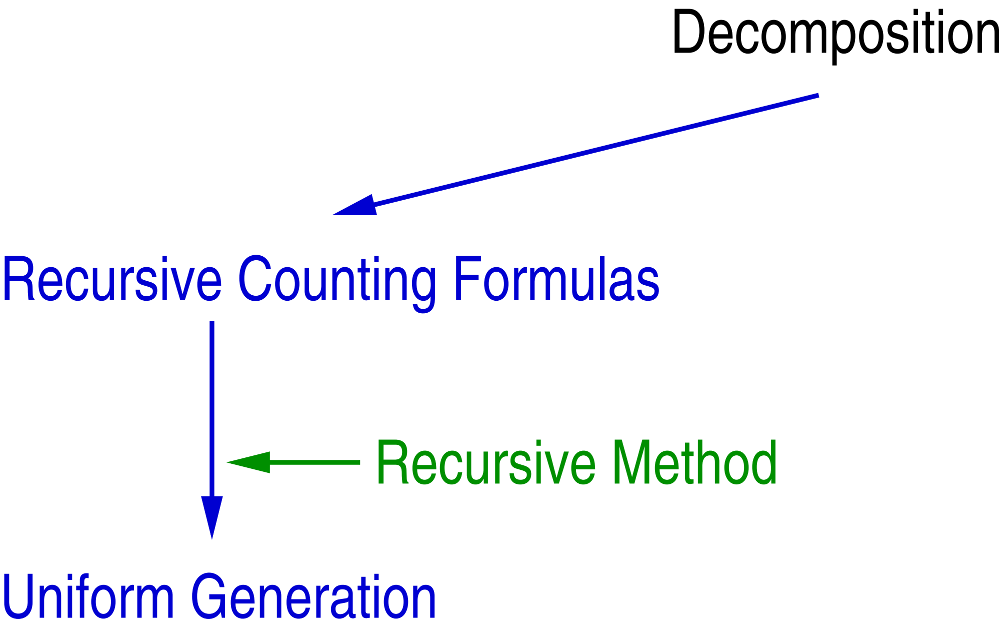

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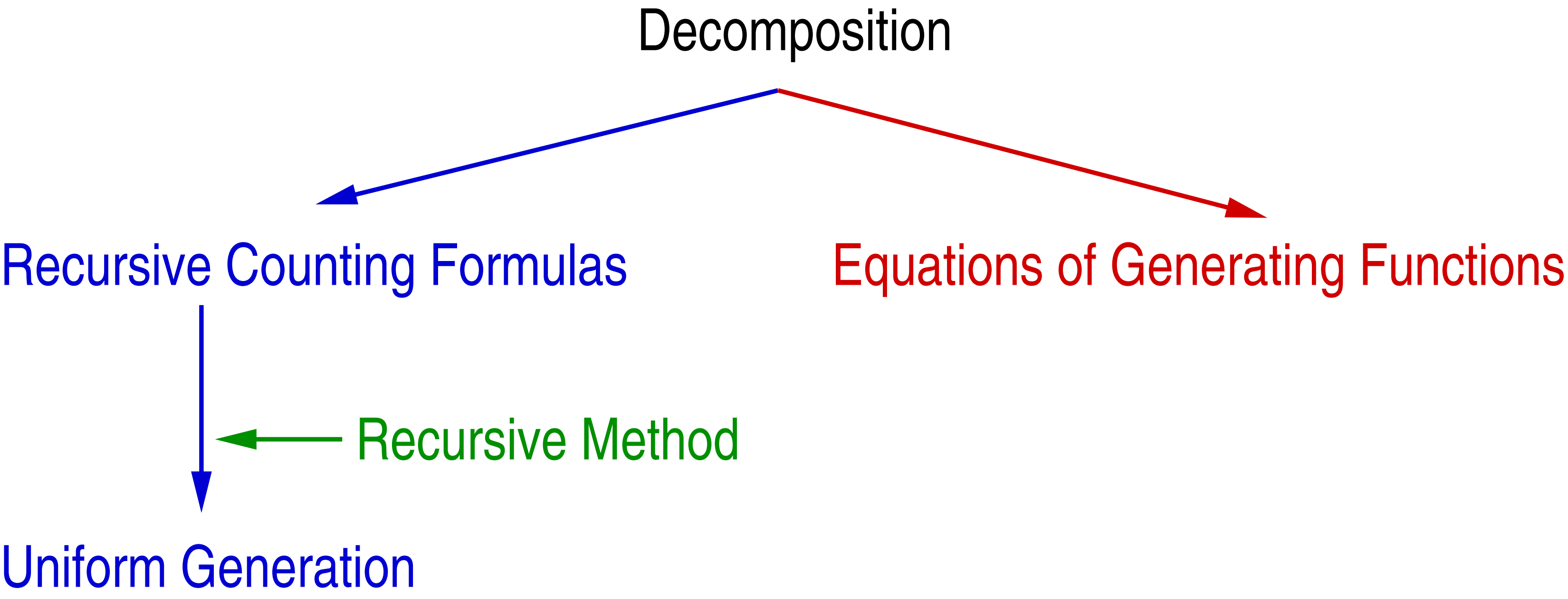

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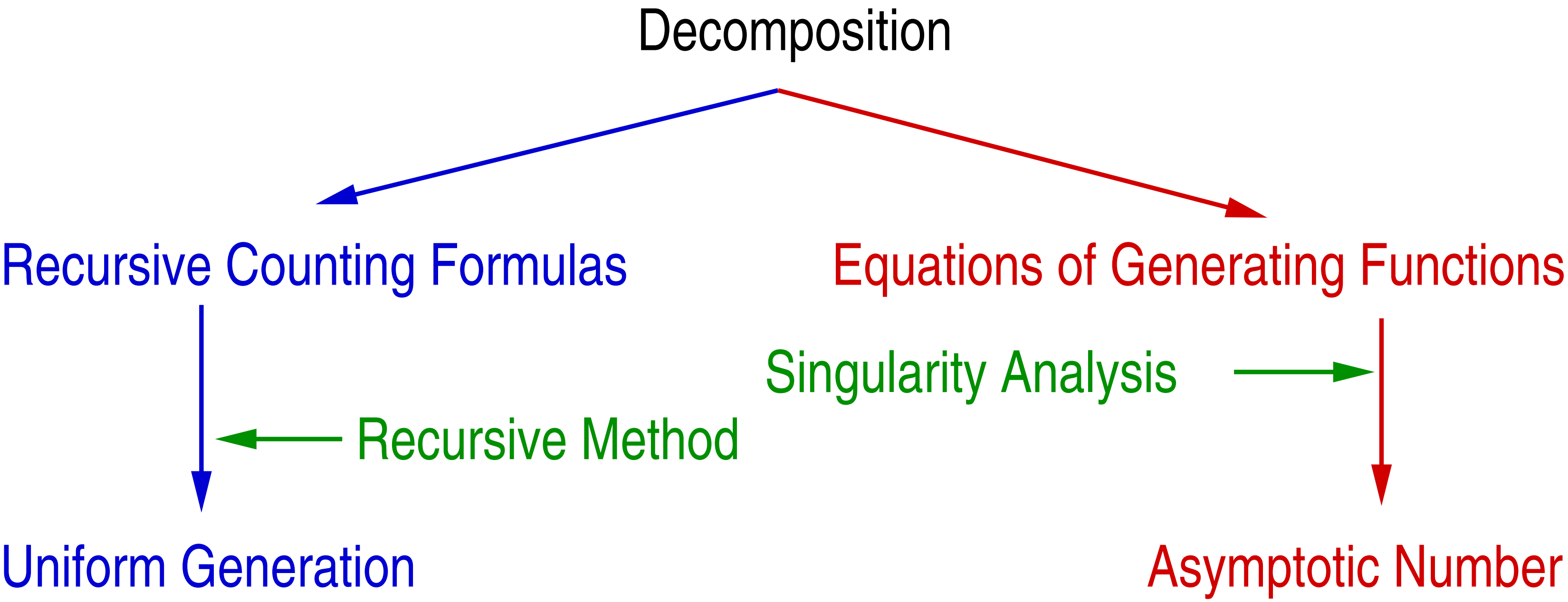

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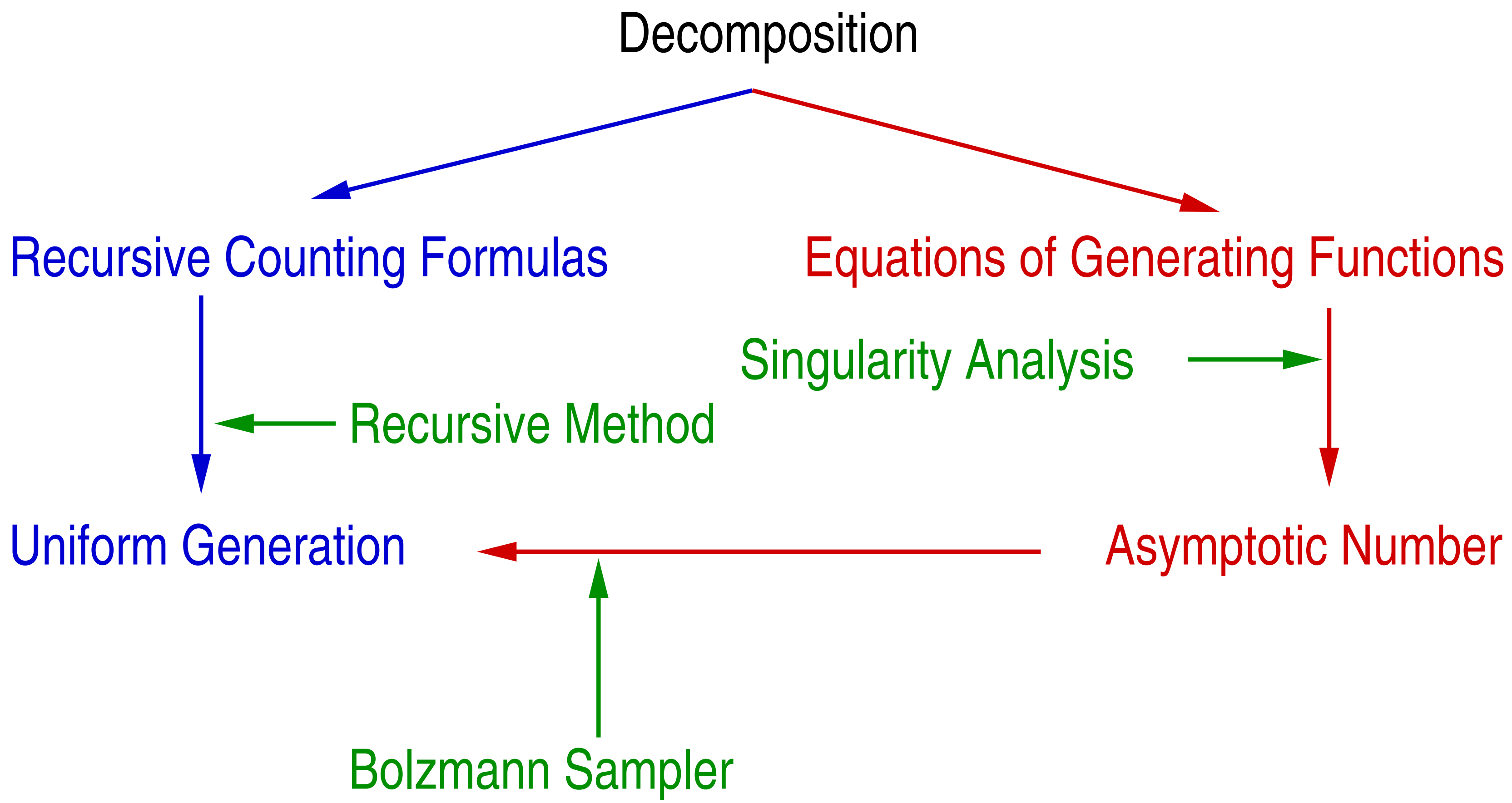

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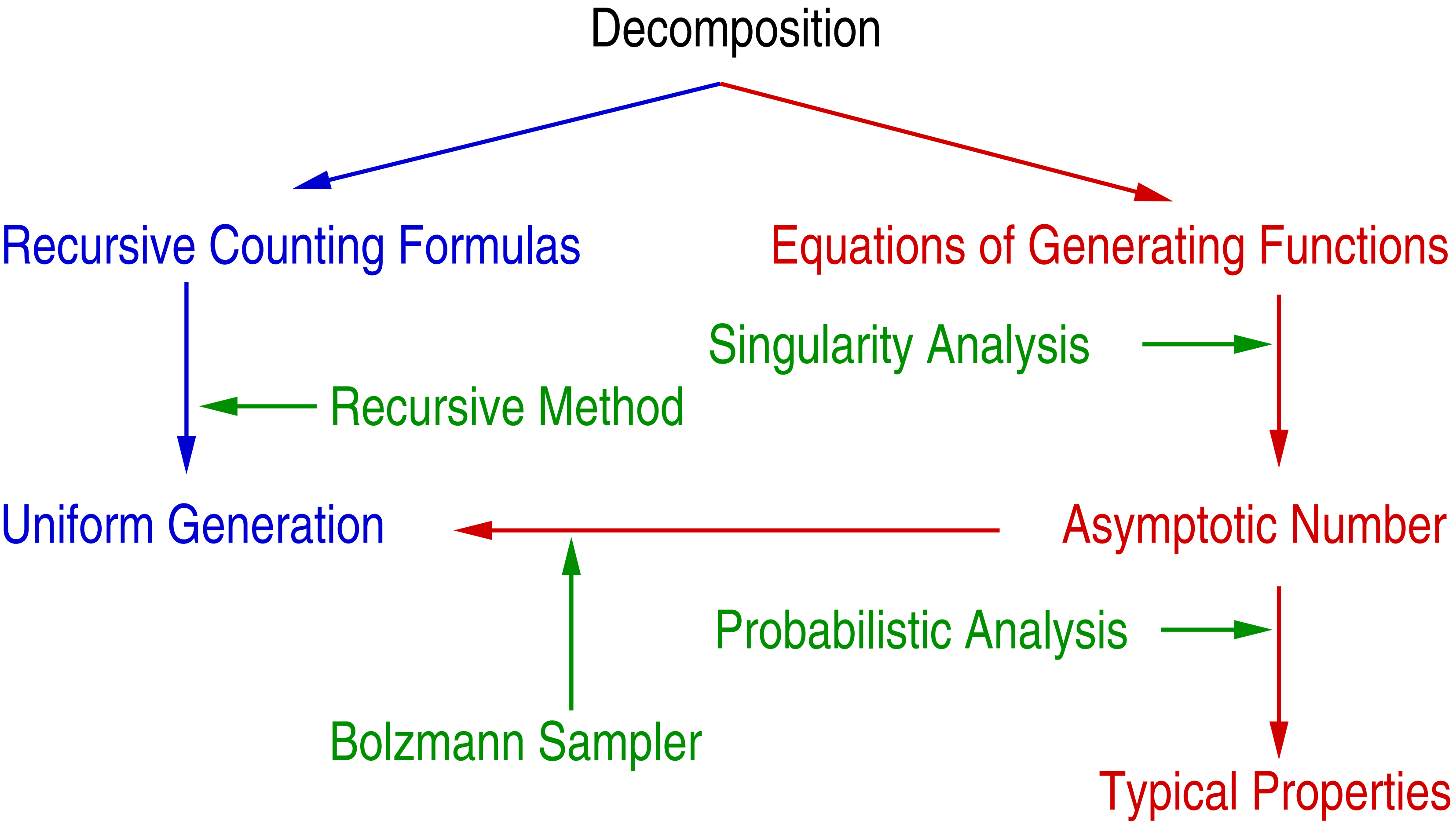

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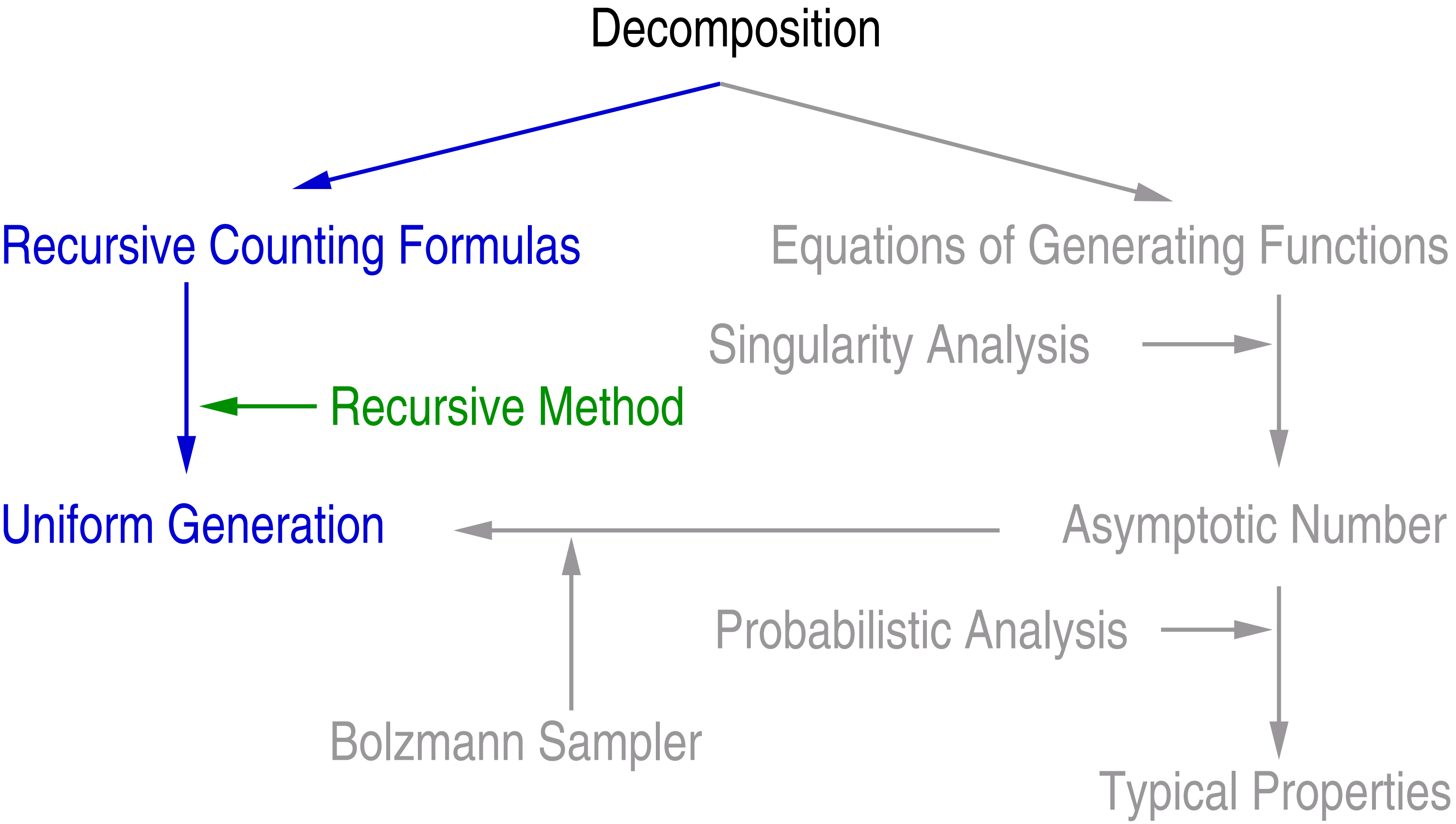

Labeled trees

For illustration of recursive decomposition method let us consider the set of labeled trees.

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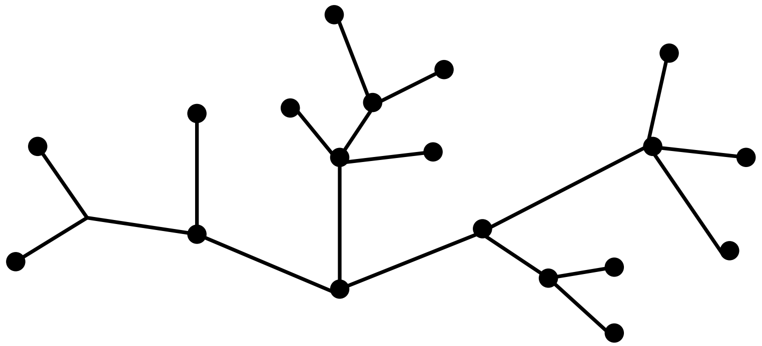

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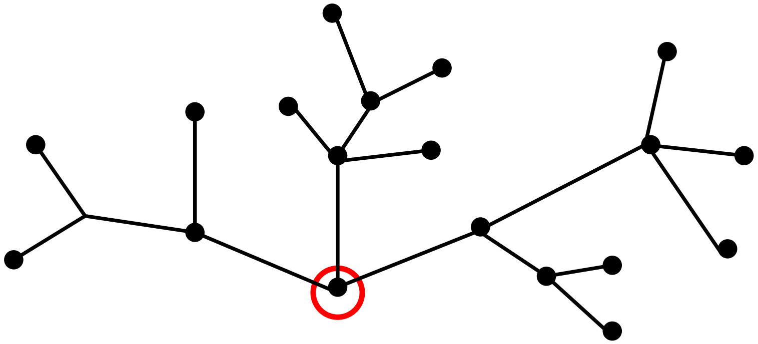

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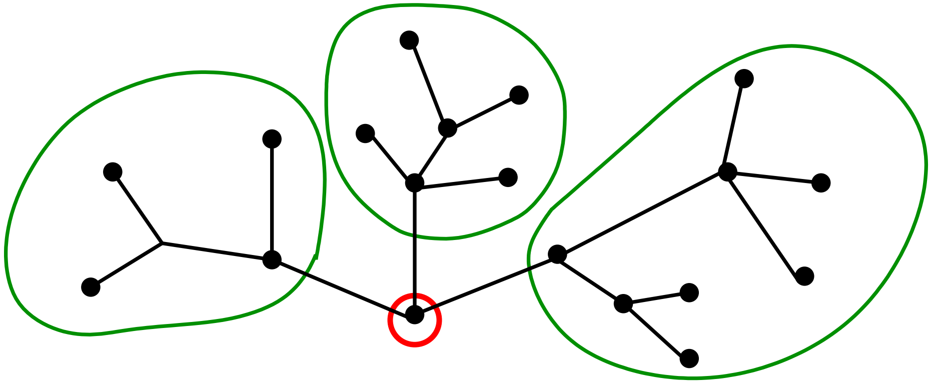

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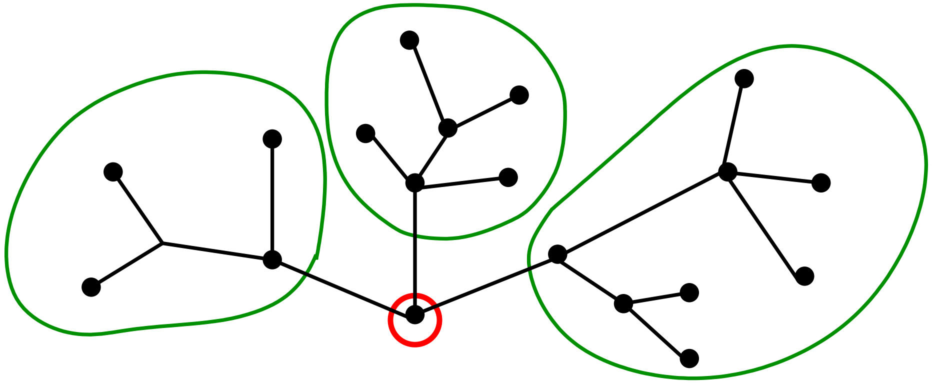

Let $t(n)$ be the number of rooted trees on $[n]$.

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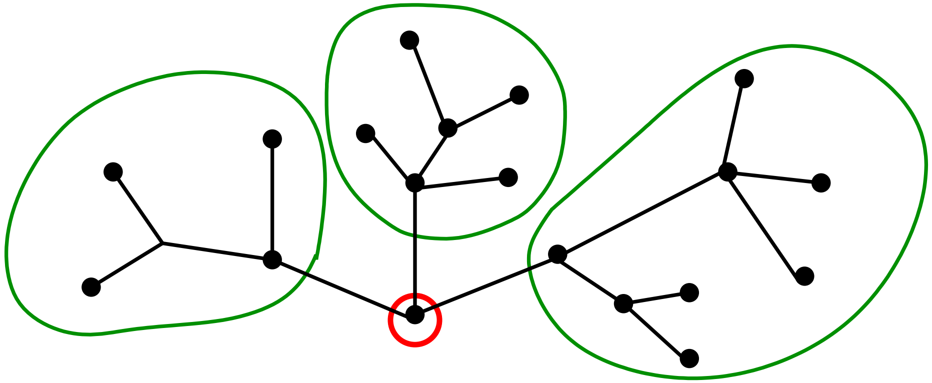

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$$\frac{t(n)}{n}$$

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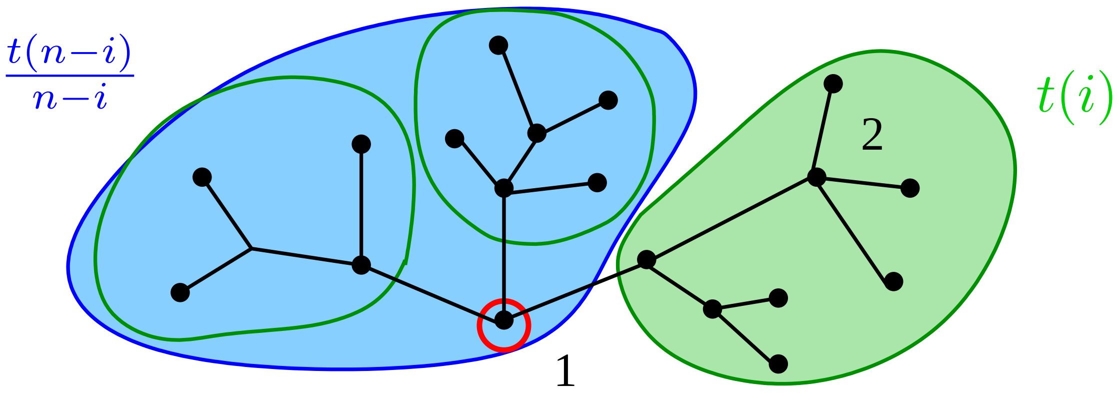
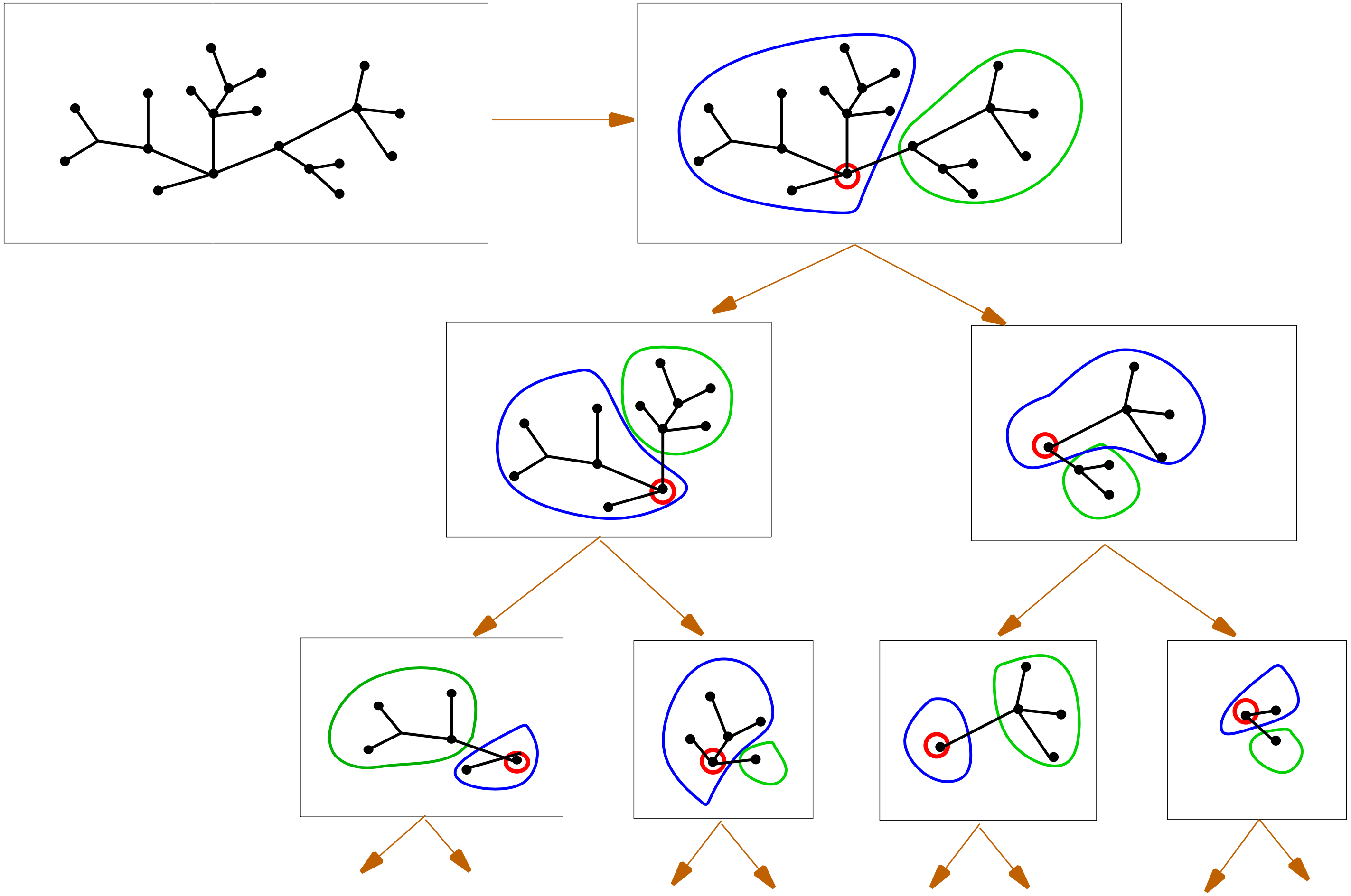


Let $t(n)$ be the number of rooted trees on $[n]$.

$$\frac{t(n)}{n} = \sum_i \binom{n-2}{i-1} t(i) \frac{t(n-i)}{n-i}$$

Recursive method

[Nijenhuis–Wilf 79; Flajolet–Zimmerman–Van Cutsem 94]



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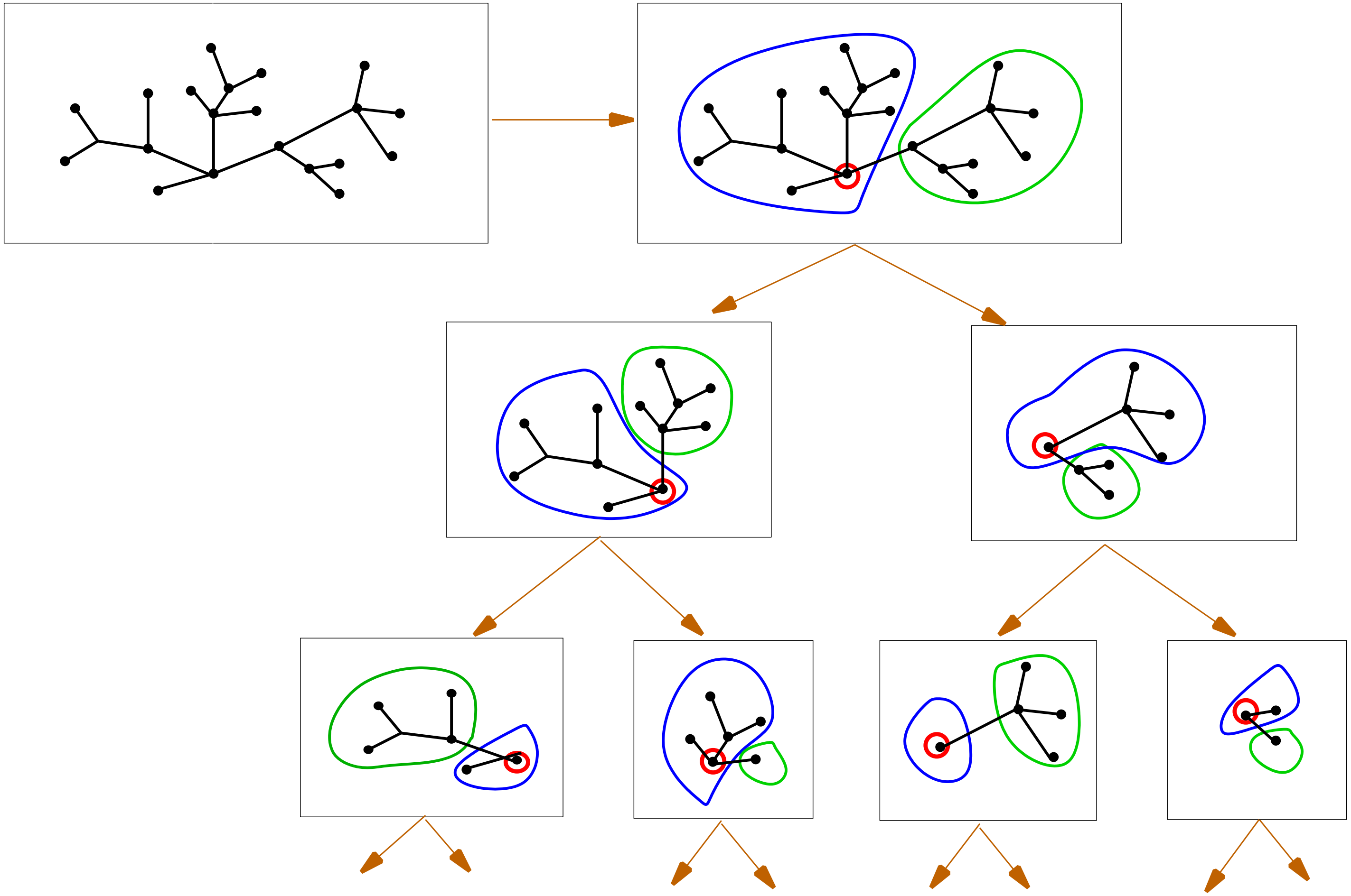
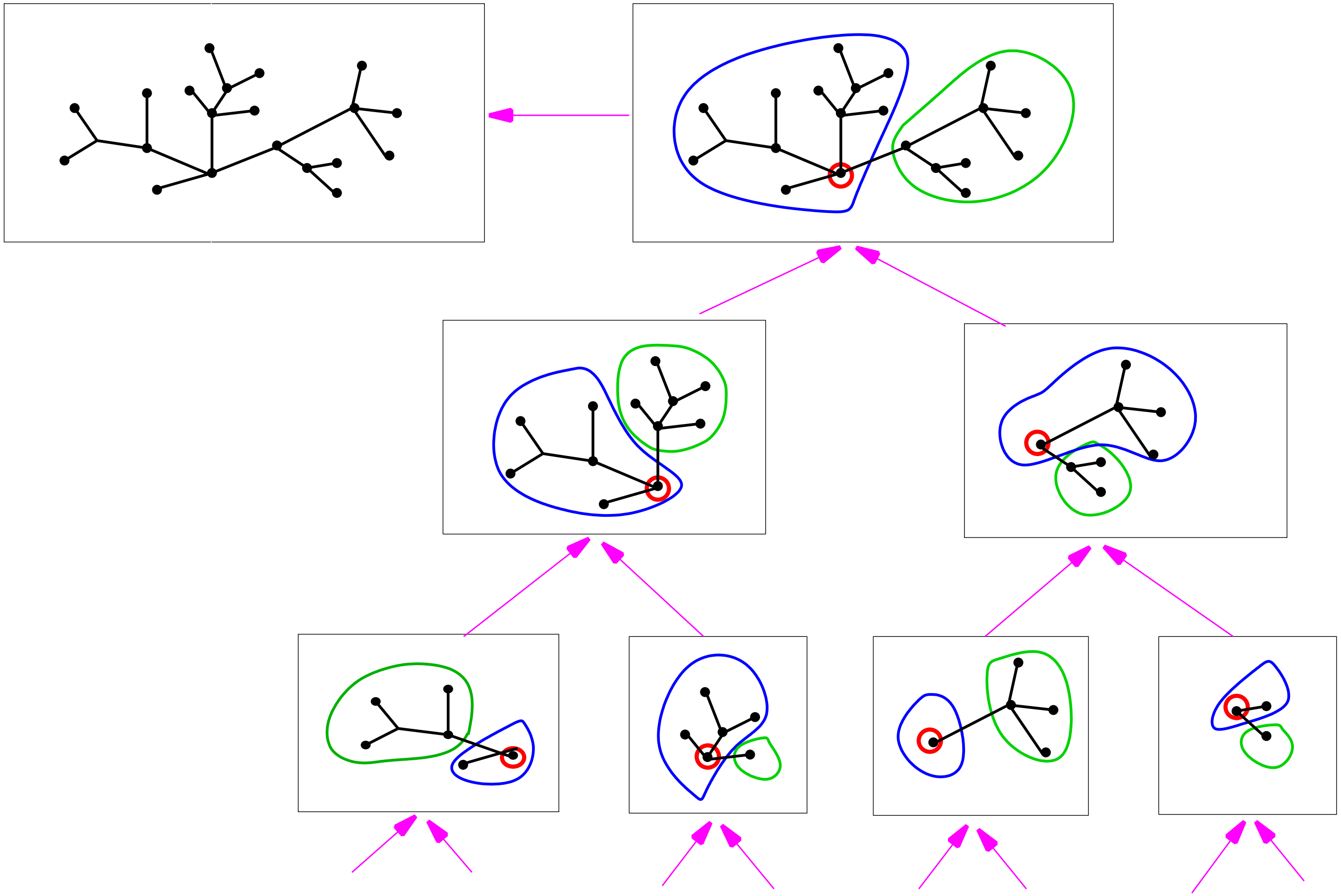


This yields a polynomial time algorithm to compute the exact number of trees.

Uniform Sampling

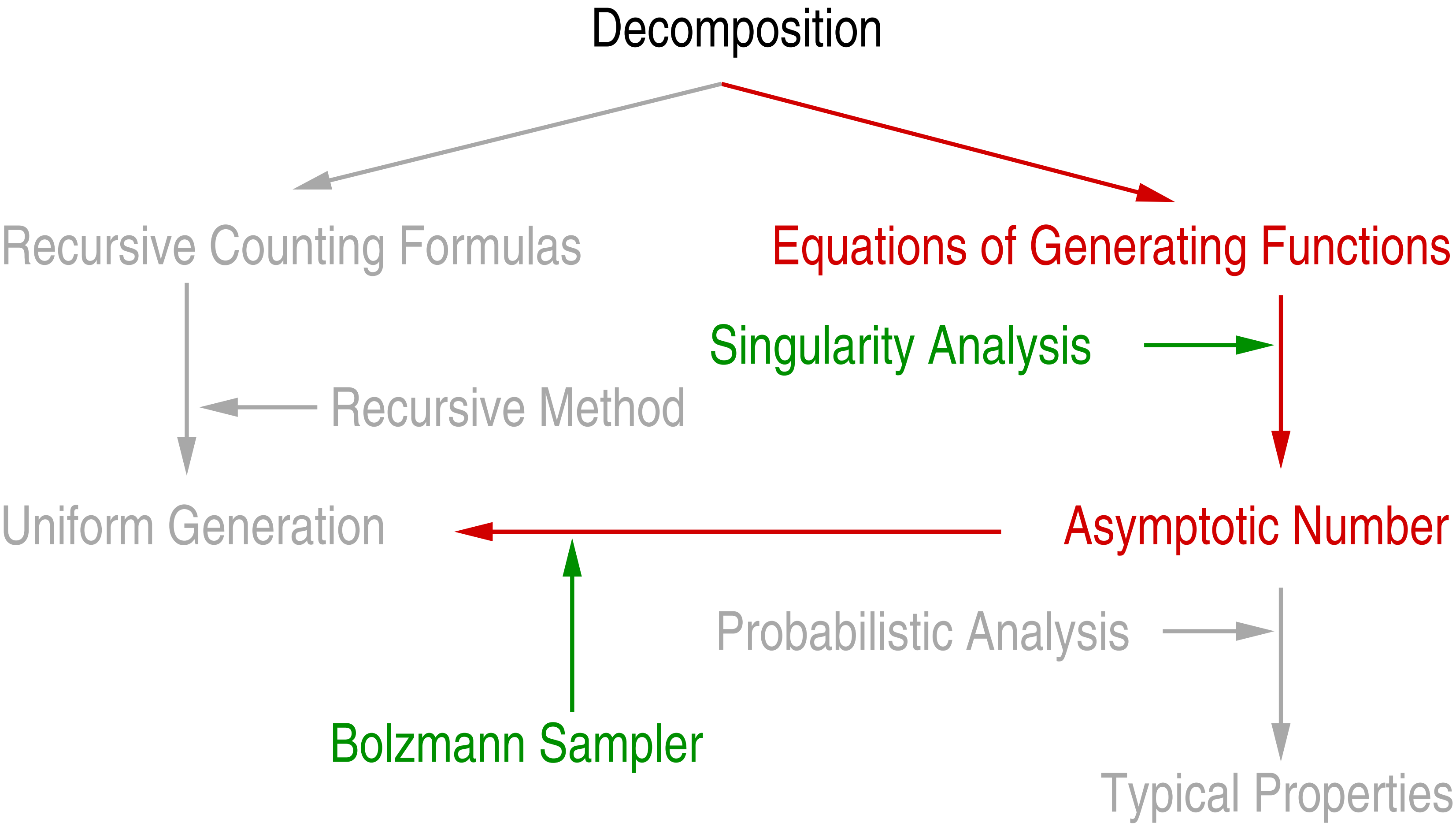
[NIJENHUIS–WILF 79; FLAJOLET–ZIMMERMAN–VAN CUTSEM 94]



Uniform sampling procedure as a reverse procedure of the decomposition.

Recursive decomposition

[Nijenhuis–Wilf 79; Flajolet–Zimmerman–Van Cutsem 94; Flajolet–Sedgewick 08+]



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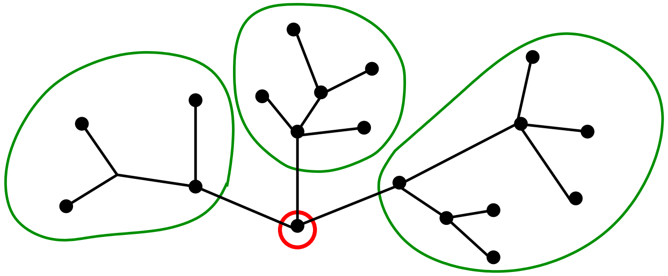
Singularity analysis

[FLAJOLET–SEDGEWICK 08+]

Let $\mathcal{T}$ denote the set of all rooted labeled trees and $T(z) = \sum_n \frac{t(n)}{n!} z^n$ be the corresponding generating function:

$$\mathcal{T} = \mathcal{Z} \times \mathrm{SET}(\mathcal{T})$$

$$T(z) = z\left(1 + T(z) + \frac{T(z)^2}{2!} + \frac{T(z)^3}{3!} + \cdots\right) = ze^{T(z)}.$$



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Its dominant singularity is e^{-1} and singular type $T(z) \sim 1 - \sqrt{2}(1 - ez)^{1/2}$:

$$t(n) \sim \frac{1}{\sqrt{2\pi}} n^{-3/2} e^n n!$$

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(Stirling's formula)

(Cayley's formula)

Boltzmann sampler

[DUCHON–FLAJOLET–LOUCHARD–SCHAEFFER 04]

Let $\mathcal{A}$ denote a combinatorial class, e.g. the set of rooted trees, and $A(z) = \sum_n \frac{a(n)}{n!} z^n$ be the corresponding generating function.

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Boltzmann sampler $\Gamma A(z)$ draws each object $\gamma \in \mathcal{A}$ according to

$$\mathbb{P}_z(\text{output } \ \gamma \in \mathcal{A}) = \frac{z^{|\gamma|}/|\gamma|!}{A(z)}.$$

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$$\mathcal{A} = \mathrm{SET}(\mathcal{B}) \quad \text{vs} \quad A(z) = e^{B(z)} = \sum_k \frac{B(z)^k}{k!},$$

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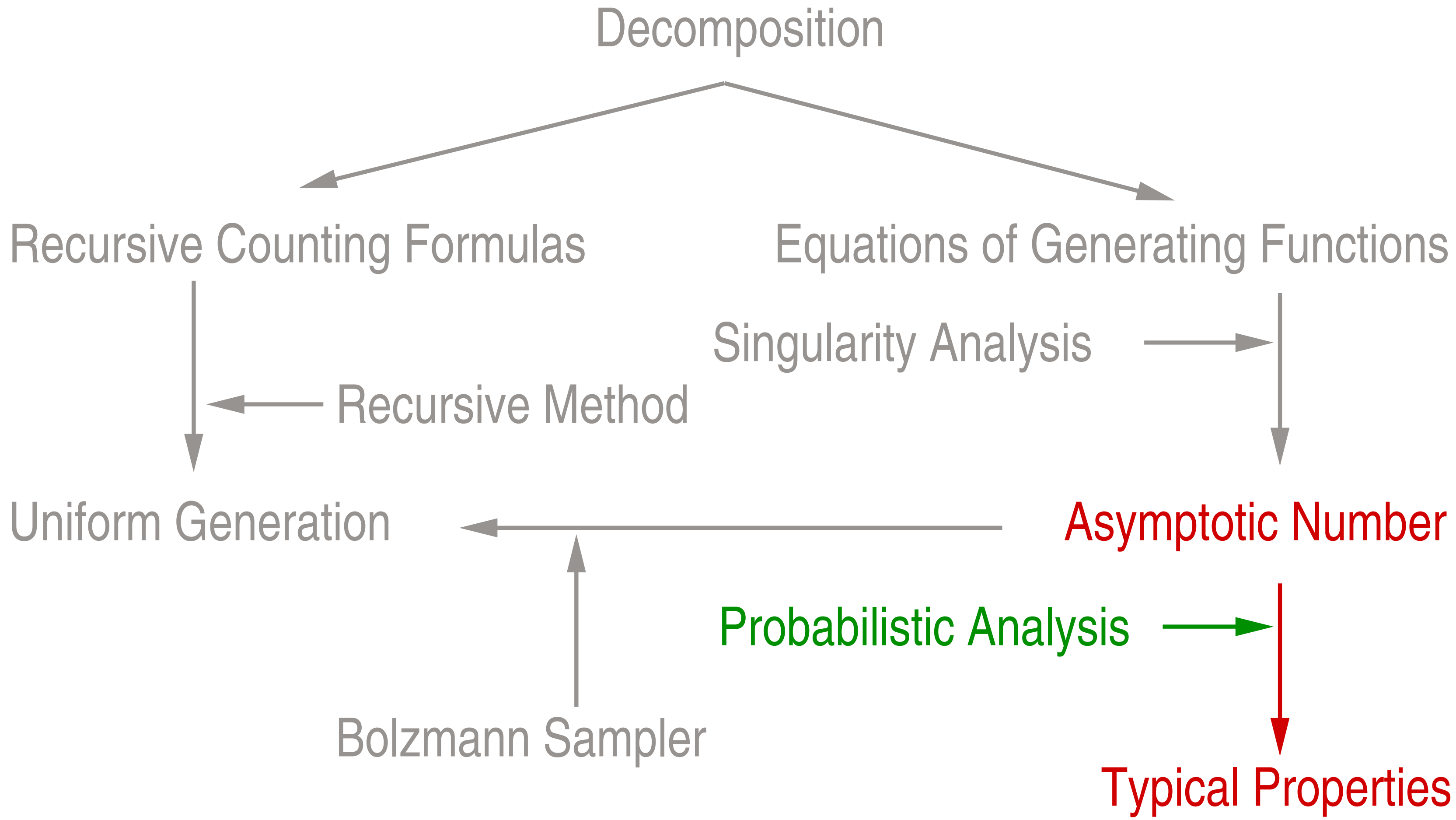
Boltzmann sampler $\Gamma A(z)$ draws each object $\gamma \in \mathcal{A}$ by

- **generating** a random number k according to $\mathbb{P}[X = k] = e^{-B(z)} \frac{B(z)^k}{k!}$
- **calling** $\Gamma B(z)$ independently k times and let $\gamma = \{\Gamma B(z), \ldots, \Gamma B(z)\}$

Recursive decomposition

[Nijenhuis–Wilf 79; Flajolet–Zimmerman–Van Cutsem 94; Flajolet–Sedgewick 08+]



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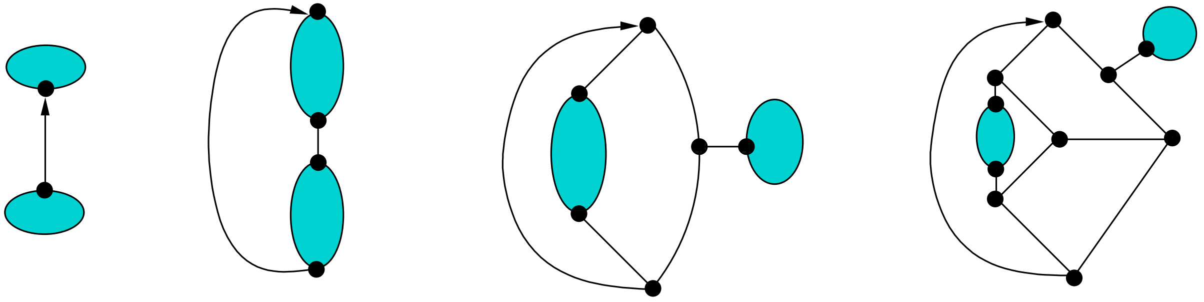
Typical Properties

Labeled cubic planar graphs

[Bodirsky–K.–Löffler–McDiarmid 07]



The number of cubic planar graphs on n vertices is asymptotically

$$\sim \alpha n^{-7/2} \rho^{-n} n!\,, \qquad \text{where } \rho^{-1} \doteq 3.1325$$

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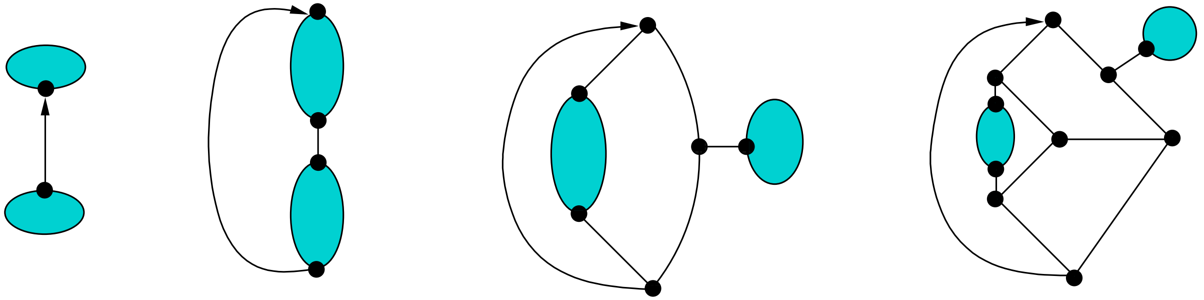

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What is the chromatic number of a random cubic planar graph G that is chosen uniformly at random among labeled cubic planar graphs on $[n]$?

Chromatic number

Let G be a cubic planar graph.

- $\chi(G) \leq 4$ [Four colour theorem]
- If G is connected and is neither a complete graph nor an odd cycle, $\chi(G) \leq \Delta(G) = 3$ [Brooks' theorem]

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- If G contains a component isomorphic to K_4, $\chi(G) = 4$.
- If G contains no isolated K_4, but at least one triangle, $\chi(G) = 3$.

Random cubic planar graphs

[Bodirsky–K.–Löffler–McDiarmid 07]

Let $G_n^{(k)}$ be a random k vertex-connected cubic planar graph on n vertices.

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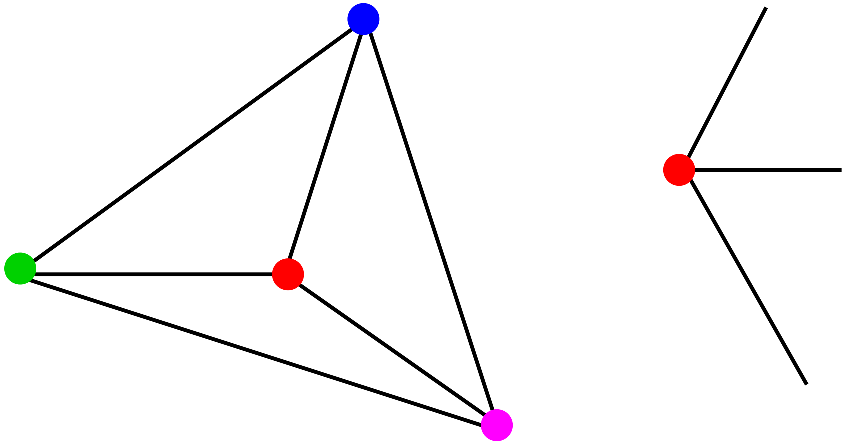
SUBGRAPH CONTAINMENTS

Let X_n be $\#$ isolated K_4's in $G_n^{(0)}$

$$\lim_{n\to\infty} \Pr(X_n > 0) = 1 - e^{-\frac{\rho^4}{4!}}$$



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Let $G_n^{(k)}$ be a random k vertex-connected cubic planar graph on n vertices.

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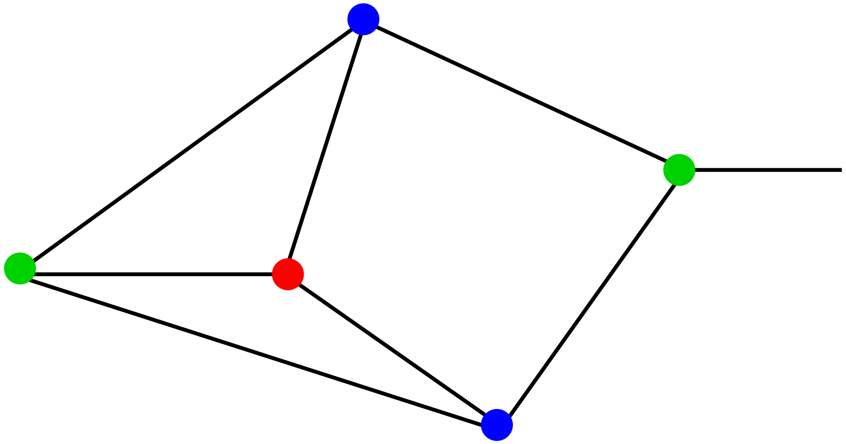
Let X_n be $\#$ isolated K_4's in $G_n^{(0)}$ and Y_n $\#$ triangles in $G_n^{(k)}$, $k > 0$. Then

$$\lim_{n\to\infty} \Pr(X_n > 0) = 1 - e^{-\frac{\rho^4}{4!}}, \qquad \lim_{n\to\infty} \Pr(Y_n > 0) = 1.$$



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CHROMATIC NUMBER

$$\lim_{n\to\infty} \Pr(\chi(G_n^{(0)}) = 4) = \lim_{n\to\infty} \Pr(X_n > 0) = 1 - e^{-\frac{\rho^4}{4!}}$$

$$\lim_{n\to\infty} \Pr(\chi(G_n^{(0)}) = 3) = \lim_{n\to\infty} \Pr(X_n = 0, Y_n > 0) = e^{-\frac{\rho^4}{4!}} \doteq 0.9995\,.$$

For $k = 1, 2, 3,$ $\quad \lim_{n\to\infty} \Pr(\chi(G_n^{(k)}) = 3) = \lim_{n\to\infty} \Pr(Y_n > 0) = 1\,.$

Outline

I. Phase transition

- Introduction to phase transition
- Erdős–Rényi random graph
  - Phase transition
  - Limit theorems for the giant component
  - Critical phase
- Random graphs with given degree sequence

II. Enumeration and random sampling

- Recursive decomposition
- Singularity analysis, Boltzmann sampler, probabilistic analysis
- Planar structures, minors and genus

Labeled planar structures

[GIMÉNEZ–NOY; BODIRSKY–GRÖPL–K.; MCDIARMID–STEGER–WELSH; OSTHUS–PRÖMEL–TARAZ; $\cdots$]

The number of planar structures on n vertices is asymp. $\sim \ \alpha\, n^{-\beta}\, \gamma^n n!$.

Classes	β	γ			
Forests	$5/2$	2.71			
Outerplanar graphs	$5/2$	7.32			
Planar graphs	$7/2^\dagger$	$27.2^\dagger$			
Cubic planar graphs	$7/2$	3.13			

† GIMÉNEZ–NOY 05 ;

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Let G_n be a random planar structure on n vertices. Then as $n \to \infty$,

- G_n is connected with probability tending to a constant p_{con}, and
- $\chi(G_n)$ is three with probability tending to a constant p_χ.

Classes	β	γ	p_{con}	p_χ	
Forests	$5/2$	2.71	$1/\sqrt{e}$	0	
Outerplanar graphs	$5/2$	7.32	0.861	1	
Planar graphs	$7/2^\dagger$	$27.2^\dagger$	$0.963^\dagger$	$?$	
Cubic planar graphs	$7/2$	3.13	≥ 0.998	0.999	

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Labeled planar structures

[Giménez–Noy; Bodirsky–Gröpl–K.; McDiarmid–Steger–Welsh; Osthus–Prömel–Taraz; · · ·]

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Running time of uniform sampler: $\tilde{O}(n^k)$ recursive method ($O(n^k)$ best)

Classes	β	γ	$p_{\rm con}$	p_χ	k
Forests	$5/2$	2.71	$1/\sqrt{e}$	0	3 $(1\ )$
Outerplanar graphs	$5/2$	7.32	0.861	1	4
Planar graphs	$7/2^\dagger$	$27.2^\dagger$	$0.963^\dagger$	$?$	7 $(2^\ddagger)$
Cubic planar graphs	$7/2$	3.13	≥ 0.998	0.999	6

$\dagger$ Giménez–Noy 05 ; $\ddagger$ Fusy 05

Unlabeled planar structures

Difficulty with unlabeled planar structures is symmetry:

Unlabeled planar structures

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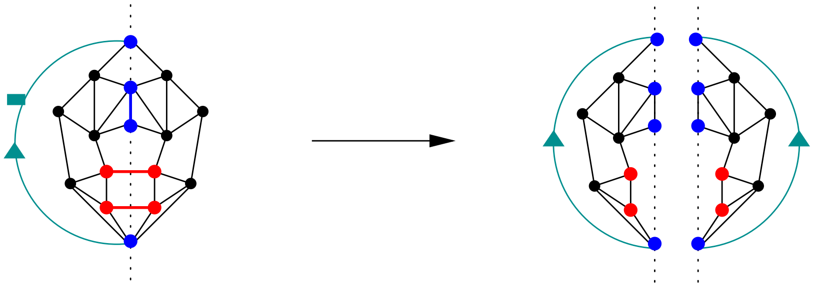
- Recursive method: decomposition along symmetry



Unlabeled planar structures

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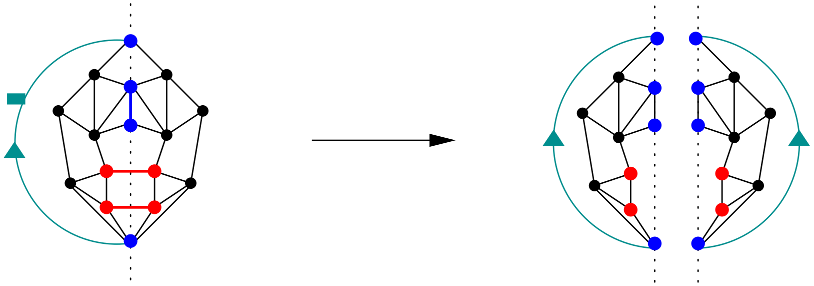

Classes	Asymptotic number	Uniform sampling
Outerplanar graphs		[BODIRSKY–K. 06]
2-con. planar graphs		[BODIRSKY–GRÖPL–K. 05]

Unlabeled planar structures

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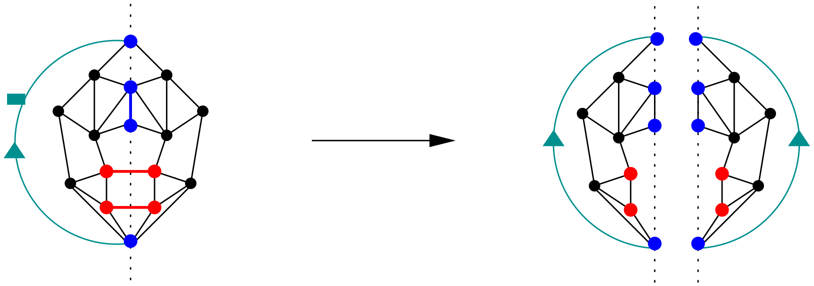

- Pólya theory: symmetry vs orbits of automorphism group of a graph

Classes	Asymptotic number	Uniform sampling
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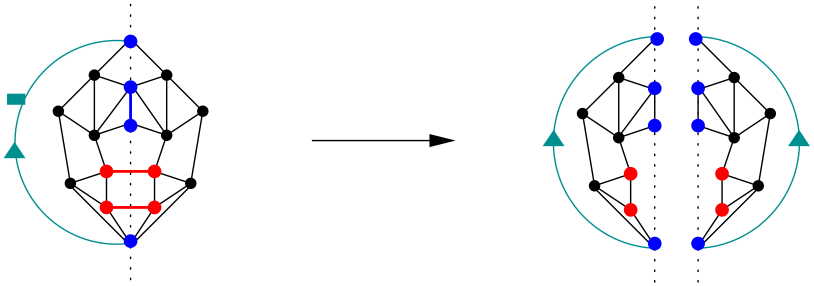
2-con. planar graphs		[Bodirsky–Gröpl–K. 05]

Unlabeled planar structures

Difficulty with unlabeled planar structures is symmetry:

- Recursive method: decomposition along symmetry



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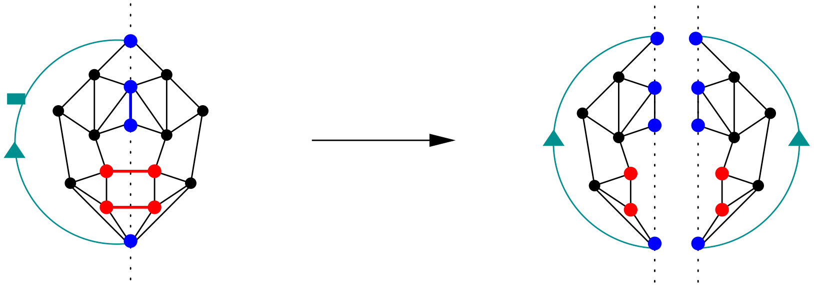

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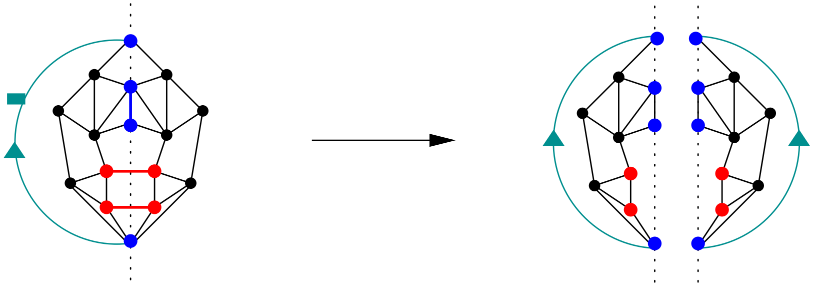

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  ⟶ Analytic expression for the series counting labeled planar graphs

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  - empirical/theoretical properties of a large system
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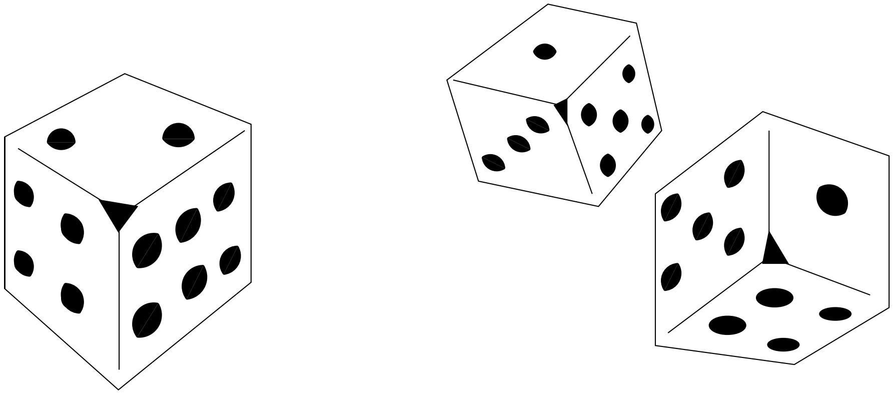

Thank you very much!