Enumeration of labelled graphs

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TYPESET 2005 APRIL 25 9:57 IN PDFIATEX ON A LINUX SYSTEM

BT Research at Martlesham, Suffolk



- Cambridge-Ipswich high-tech corridor
- 2000 technologists
- 15 companies
- UCL, Univ of Essex

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$$P(1) = 1$$

$$P(2) = 1-q$$

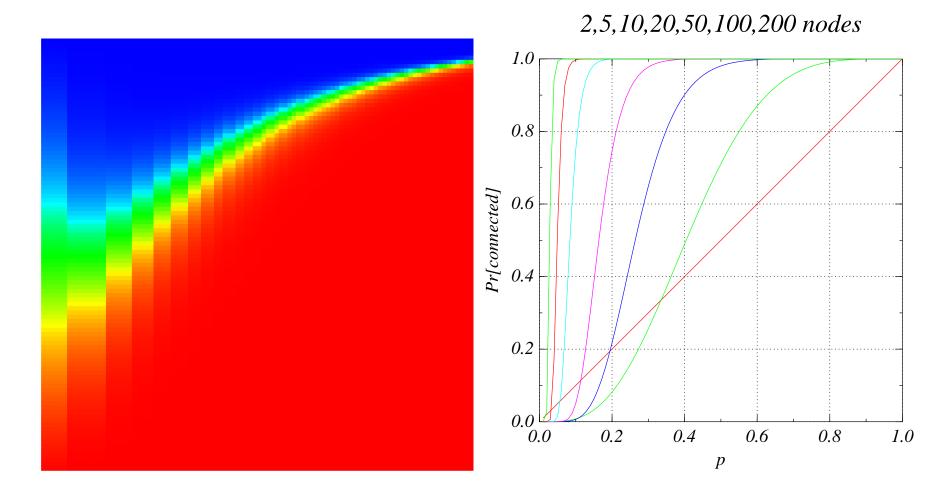
$$P(3) = (2q+1)(q-1)^{2}$$

$$P(4) = (6q^{3}+6q^{2}+3q+1)(1-q)^{3}$$

$$P(5) = (24q^{6}+36q^{5}+30q^{4}+20q^{3}+10q^{2}+4q+1)(q-1)^{4}$$

• as $n \to \infty$, we have $P(n) \to 1 - nq^{n-1}$.

Connectivity for the Bernoulli model



x-axis: $\log(n = \text{number of nodes}), n = 2, \dots, 100$

y-axis: p, 0 at top, 1 at bottom

blue=0 red=1

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- The claim: the number C(n,n+k) of labelled (étiquetés) connected graphs with n nodes and excess (edges-nodes) = $k\geqslant 2$ is

$$A_{k}(1)\sqrt{\pi} \left(\frac{n}{e}\right)^{n} \left(\frac{n}{2}\right)^{\frac{3k-1}{2}} \left[\frac{1}{\Gamma(3k/2)} + \frac{A'_{k}(1)/A_{k}(1) - k}{\Gamma((3k-1)/2)} \sqrt{\frac{2}{n}} + \mathcal{O}\left(\frac{1}{n}\right) \right]$$

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	k	1	2	3	4	5	6	7
•	$A_k(1)$	5/24	5/16	1105/1152	565/128	82825/3072	19675/96	1282031525/688128
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Airy in Playford:

www.ast.cam.ac.uk/~ipswich/History/Airys_Country_Retreat.htm

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• Also, on pages 4 and 24, I think S should have the expansion $1-(5/4)\alpha+(15/4)\alpha^2+\dots$

Asymptotic expansion of $C(n, n+k)/n^{n+\frac{3k-1}{2}}$

 $\xi \equiv \sqrt{2\pi}$ green: from [bcm90] red: from [fss04] (with removal of factor e)

k	type	$[n^0]$	$[n^{-1/2}]$	$[n^{-1}]$	$[n^{-3/2}]$
-1	tree	1	0	0	0
0	unicycle	$\xi rac{1}{4}$			
1	bicycle	$\frac{5}{24}$			
2	tricycle	$\xi \frac{5}{256} \ \xi \frac{5}{256}$	$-\frac{35}{144}$		
3	quadricycle	$\frac{221}{1512} \ \frac{221}{24192}$	$-\sqrt{\pi}\frac{35}{96}$		
4	pentacycle	$\xi \frac{113}{196608}$			

blue: conjectured by KMB from numerical experiments

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0	unicycle	$\xi rac{1}{4}$	$-\frac{7}{6}$	$\xi \frac{1}{48}$	$\frac{131}{270}$	$\xi rac{1}{1152}$	$-\frac{4}{2835}$?
1	bicycle	$\frac{5}{24}$	$-\xi \frac{7}{24}$	$\frac{25}{36}$	$-\xi \frac{7}{288}$	$-\frac{79}{3240}$?	
2	tricycle	$\xi rac{5}{256}$	$-\frac{35}{144}$	$\xi \frac{1559}{9216}$	$-\frac{55}{144}$		
3	quadricycle	$\frac{221}{24192}$	$-\xi \frac{35}{10706}$				

Counting

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$$|S| = \sum_{x \in S} 1$$

Exponential generating functions

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exponential generating function for all connected labelled graphs:

$$c(w,z) = \log(g(w,z))$$

$$= z + w\frac{z^2}{2} + (3w^2 + w^3)\frac{z^3}{6} + (16w^3 + 15w^4 + 6w^5 + w^6)\frac{z^4}{4!} + \dots$$

rooted labelled trees

$$T(z) = z \exp(T(z)) = \sum_{n=1}^{\infty} n^{n-1} \frac{z^n}{n!} = z + \frac{2}{2!} z^2 + \frac{9}{3!} z^3 + \cdots$$

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unrooted labelled trees

$$W_{-1}(z) = T(z) - T(z)^2 / 2 = z + \frac{1}{2!}z^2 + \frac{3}{3!}z^3 + \frac{16}{4!}z^4 + \dots$$

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unicyclic labelled graphs

$$W_0(z) = \frac{1}{2} \log \left[\frac{1}{1 - T(z)} \right] - \frac{1}{2} T(z) - \frac{1}{4} T(z)^2 = \frac{1}{3!} z^3 + \frac{15}{4!} z^4 + \frac{222}{5!} z^5 + \frac{3660}{6!} z^6 + .$$

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bicyclic labelled graphs

$$W_1(z) = \frac{T(z)^4 (6 - T(z))}{24 (1 - T(z))^3} = \frac{6}{4!} z^4 + \frac{205}{5!} z^5 + \frac{5700}{6!} z^6 + \dots$$

Theory 1

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• Ramanujan's Q-function is defined for $n=1,2,3,\ldots$:

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- $T(z) = z \exp(T(z))$

- to get the large-n asymptotics of Q, we first consider the related function $R(n) \equiv 1 + \frac{n}{n+1} + \frac{n^2}{(n+1)(n+2)} + \dots, \ n = 1, 2, 3, \dots$
 - \triangleright we have $Q(n)+R(n)=n!\,e^n/n^n$
 - \triangleright let D(n) = R(n) Q(n)

 - $D(n) \sim \sum_{k=1}^{\infty} c(k)[z^n] (T(z)-1)^k$, where $c(k) \equiv [\delta^k] \log(\delta^2/2/(1-(1+\delta)e^{-\delta}))$
 - ▶ this gives $D(n) \sim \frac{2}{3} + \frac{8}{135} n^{-1} \frac{16}{2835} n^{-2} \frac{32}{8505} n^{-3} + \frac{17984}{12629925} n^{-4} + \frac{668288}{492567075} n^{-5} + O(n^{-6})$
- now using $Q(n)=(n!\,e^n/n^n\!-\!D(n))/2$, we get
 - $\begin{array}{l} \triangleright \ \ Q(n) \ \ \sim \ \ \frac{1}{2} n^{1/2} \sqrt{2\pi} \frac{1}{3} + \frac{1}{24} \sqrt{2\pi} n^{-1/2} \frac{4}{135} \, n^{-1} + \frac{1}{576} \sqrt{2\pi} n^{-3/2} + \frac{8}{2835} \, n^{-2} \\ \ \frac{139}{103680} \sqrt{2\pi} n^{-5/2} + \frac{16}{8505} \, n^{-3} \frac{571}{4976640} \sqrt{2\pi} n^{-7/2} \frac{8992}{12629925} \, n^{-4} + \frac{163879}{418037760} \sqrt{2\pi} n^{-9/2} \\ \ \frac{334144}{492567075} \, n^{-5} + \frac{5246819}{150493593600} \sqrt{2\pi} n^{-11/2} + O\left(n^{-6}\right) \end{array}$

- Let W_k be the egf for connected labelled (k+1)-cyclic graphs
 - ▶ for unrooted trees $W_{-1}(z) = T(z) T^2(z)/2$, $[z^n]W_{-1}(z) = n^{n-2}$
 - ▶ for unicycles $W_0(z) = -(\log(1-T(z))+T(z)+T^2(2)/2)/2$
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- Knuth and Pittel's tree polynomials $t_n(y)$ $(y \neq 0)$ are defined by $(1-T(z))^{-y} = \sum_{n=0}^{\infty} t_n(y) \frac{z^n}{n!}$
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 - ▶ we can compute these for y > 0 from $t_n(1) = 1$; $t_n(2) = n^n(1+Q(n))$; $t_n(y+2) = n t_n(y)/y + t_n(y+1)$
- ullet thanks to this recurrence, the asymptotics for t_n follow from the known asymptotics of Q

Let $\xi = \sqrt{2\pi}$. All results agree with numerical estimates on this page.

- the number of connected unicycles is $C(n,n)=n![z^n]W_0(z)=\frac{1}{2}Q(n)n^{n-1}+3/2+t_n(-1)-t_n(-2)/4$
 - $\stackrel{C(n,n)}{\sim} \sim \frac{1}{4} \, \xi \, n^{-1/2} \frac{7}{6} \, n^{-1} + \frac{1}{48} \, \xi \, n^{-3/2} + \frac{131}{270} \, n^{-2} + \frac{1}{1152} \, \xi \, n^{-5/2} + \frac{4}{2835} \, n^{-3} \frac{139}{207360} \, \xi \, n^{-7/2} + \frac{8}{8505} \, n^{-4} \frac{571}{9953280} \, \xi \, \left(n^{-1} \right)^{9/2} \frac{4496}{12629925} \, n^{-5} + \frac{163879}{836075520} \, \xi \, n^{-11/2} + O \left(n^{-6} \right)$

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- the number of connected bicycles is $C(n,n+1)=n![z^n]W_1(z)=\frac{5}{24}t_n(3)-\frac{19}{24}t_n(2)+\frac{13}{12}t_n(1)-\frac{7}{12}t_n(0)+\frac{1}{24}t_n(-1)+\frac{1}{24}t_n(-2)$
 - $\stackrel{C(n,n+1)}{\stackrel{n^n}{=}} \sim \frac{5}{24} n \frac{7}{24} \xi n^{1/2} + \frac{25}{36} \frac{7}{288} \xi n^{-1/2} \frac{79}{3240} n^{-1} \frac{7}{6912} \xi n^{-3/2} \frac{413}{4860} n^{-2} + \frac{973}{1244160} \xi n^{-5/2} \frac{4}{3645} n^{-3} + \frac{3997}{59719680} \xi n^{-7/2} + \frac{2248}{5412825} n^{-4} \frac{163879}{716636160} \xi n^{-9/2} + \frac{83536}{211100175} n^{-5} \frac{5246819}{257989017600} \xi n^{-11/2} + O\left(n^{-6}\right)$

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$$\stackrel{C(n,n)}{\sim} \sim \frac{1}{4} \, \xi \, n^{-1/2} - \frac{7}{6} \, n^{-1} + \frac{1}{48} \, \xi \, n^{-3/2} + \frac{131}{270} \, n^{-2} + \frac{1}{1152} \, \xi \, n^{-5/2} + \frac{4}{2835} \, n^{-3} - \frac{139}{207360} \, \xi \, n^{-7/2} + \frac{8}{8505} \, n^{-4} - \frac{571}{9953280} \, \xi \, \left(n^{-1} \right)^{9/2} - \frac{4496}{12629925} \, n^{-5} + \frac{163879}{836075520} \, \xi \, n^{-11/2} + O \left(n^{-6} \right)$$

- the number of connected bicycles is $C(n,n+1)=n![z^n]W_1(z)=\frac{5}{24}t_n(3)-\frac{19}{24}t_n(2)+\frac{13}{12}t_n(1)-\frac{7}{12}t_n(0)+\frac{1}{24}t_n(-1)+\frac{1}{24}t_n(-2)$
 - $\stackrel{C(n,n+1)}{\stackrel{n^n}{=}} \sim \frac{5}{24} \, n \frac{7}{24} \, \xi \, n^{1/2} + \frac{25}{36} \frac{7}{288} \, \xi \, n^{-1/2} \frac{79}{3240} \, n^{-1} \frac{7}{6912} \, \xi \, n^{-3/2} \frac{413}{4860} \, n^{-2} + \frac{973}{1244160} \, \xi \, n^{-5/2} \frac{4}{3645} \, n^{-3} + \frac{3997}{59719680} \, \xi \, n^{-7/2} + \frac{2248}{5412825} \, n^{-4} \frac{163879}{716636160} \, \xi \, n^{-9/2} + \frac{83536}{211100175} \, n^{-5} \frac{5246819}{257989017600} \, \xi \, n^{-11/2} + O \left(n^{-6} \right)$
- similarly, for the number of connected tricycles we get

$$\stackrel{C(n,n+2)}{\stackrel{n}{n}} \sim \frac{5}{256} \, \xi \, n^{5/2} - \frac{35}{144} \, n^2 + \frac{1559}{9216} \, \xi \, n^{3/2} - \frac{55}{144} \, n + \frac{33055}{221184} \, \xi \, n^{1/2} - \frac{41971}{136080} + \frac{31357}{2654208} \, \xi \, n^{-1/2} + \frac{1129}{81648} \, n^{-1} + O \left(n^{-3/2} \right)$$

• we now have all the results needed to calculate the asymptotic probability P(n,n+k) that a randomly chosen graph with n nodes and n+k edges is connected (for $n\to\infty$ and small fixed k)

- we now have all the results needed to calculate the asymptotic probability P(n,n+k) that a randomly chosen graph with n nodes and n+k edges is connected (for $n\to\infty$ and small fixed k)
- the total number of graphs is $g(n,n+k)\equiv \binom{\binom{n}{2}}{n+k}$. This can be asymptotically expanded:

$$\begin{array}{c} > \frac{g(n,n-1)}{\sqrt{\frac{2}{\pi}}e^{n-2}\left(\frac{n}{2}\right)^{n}n^{-3/2}} \sim 1 + \frac{7}{4}n^{-1} + \frac{259}{96}n^{-2} + \frac{22393}{5760}n^{-3} + \frac{54359}{10240}n^{-4} + \frac{52279961}{7741440}n^{-5} + \\ \frac{777755299}{103219200}n^{-6} + O\left(n^{-7}\right) \end{array}$$

$$\frac{g(n,n+0)}{\sqrt{\frac{2}{\pi}}e^{n-2}\left(\frac{n}{2}\right)^{n}n^{-1/2}} \sim \frac{1}{2} - \frac{5}{8}n^{-1} - \frac{53}{192}n^{-2} - \frac{4067}{11520}n^{-3} - \frac{9817}{20480}n^{-4} - \frac{10813867}{15482880}n^{-5} - \frac{217565701}{206438400}n^{-6} - \frac{11591924473}{7431782400}n^{-7} + O\left(n^{-8}\right)$$

$$\begin{array}{l} \triangleright \ \frac{g(n,n+1)}{\sqrt{\frac{2}{\pi}}e^{n-2}\left(\frac{n}{2}\right)^{n}n^{3/2}} \sim \frac{1}{4} - \frac{21}{16}n^{-1} + \frac{811}{384}n^{-2} - \frac{43187}{23040}n^{-3} + \frac{159571}{73728}n^{-4} - \frac{55568731}{30965760}\,n^{-5} \\ + \frac{2867716177}{1238630400}n^{-6} - \frac{3215346127}{2123366400}n^{-7} + \frac{1317595356557}{475634073600}n^{-8} + O\left(n^{-9}\right) \end{array}$$

> ...

$$\triangleright g(n, n+k) \sim \sqrt{\frac{2}{\pi}} e^{n-2} \left(\frac{n}{2}\right)^n n^{k-1/2} \left(2^{-k-1} + O(n^{-1})\right)$$

$$\frac{P(n,n-1)}{2^n e^{2-n} n^{-1/2} \xi} \sim \frac{1}{2} - \frac{7}{8} n^{-1} + \frac{35}{192} n^{-2} + \frac{1127}{11520} n^{-3} + \frac{5189}{61440} n^{-4} + \frac{457915}{3096576} n^{-5} + \frac{570281371}{1857945600} n^{-6} + \frac{291736667}{495452160} n^{-7} + O\left(n^{-8}\right)$$

 \triangleright check: n = 10, exact=0.1128460393, asymptotic=0.1128460359

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•
$$\frac{P(n,n+0)}{2^n e^{2-n}\xi} \sim \frac{1}{4}\xi - \frac{7}{6}n^{-1/2} + \frac{1}{3}\xi n^{-1} - \frac{1051}{1080}n^{-3/2} + \frac{5}{9}\xi n^{-2} + O(n^{-3})$$

 \triangleright check: n = 10, exact=0.276, asymptotic=0.319

•
$$\frac{P(n,n-1)}{2^n e^{2-n} n^{-1/2} \xi} \sim \frac{1}{2} - \frac{7}{8} n^{-1} + \frac{35}{192} n^{-2} + \frac{1127}{11520} n^{-3} + \frac{5189}{61440} n^{-4} + \frac{457915}{3096576} n^{-5} + \frac{570281371}{1857945600} n^{-6} + \frac{291736667}{495452160} n^{-7} + O(n^{-8})$$

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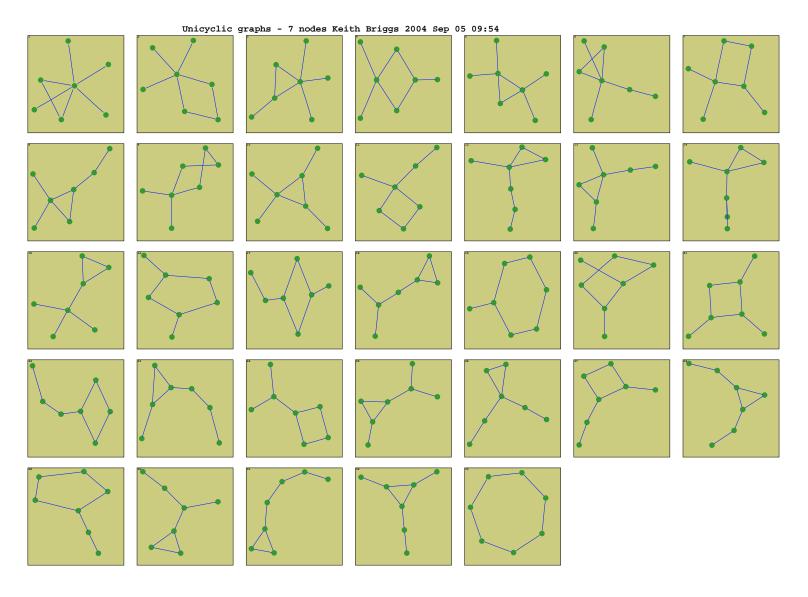
•
$$\frac{P(n,n+0)}{2^n e^{2-n}\xi} \sim \frac{1}{4}\xi - \frac{7}{6}n^{-1/2} + \frac{1}{3}\xi n^{-1} - \frac{1051}{1080}n^{-3/2} + \frac{5}{9}\xi n^{-2} + O(n^{-3})$$

 \triangleright check: n = 10, exact=0.276, asymptotic=0.319

$$\frac{P(n,n+1)}{2^n e^{2-n} n^{1/2} \xi} \sim \frac{5}{12} - \frac{7}{12} \xi n^{-1/2} + \frac{515}{144} n^{-1} - \frac{28}{9} \xi n^{-3/2} + \frac{788347}{51840} n^{-2} - \frac{308}{27} \xi n^{-5/2} + O\left(n^{-3}\right)$$

- \triangleright check: n = 10, exact=0.437, asymptotic=0.407
- \triangleright check: n = 20, exact=0.037108, asymptotic=0.037245
- \triangleright check: n = 100, exact=2.617608 $\times 10^{-12}$, asymptotic=2.617596 $\times 10^{-12}$

Example of unlabelled case - unicycles for n=7



The unlabelled case - unicycles

- Christian Bower's idea: A connected unicyclic graph is an undirected cycle of 3 or more rooted trees. Start with a single undirected cycle (or polygon) graph. It must have at least 3 nodes. Hanging from each node in the cycle is a tree (a tree is of course a connected acyclic graph). The node where the tree intersects the cycle is the root, thus it is (combinatorially) a rooted tree.
 - ▶ A000081 is undirected cycles of exactly 1 rooted tree
 - ▶ A001429 is undirected cycles of 3 or more rooted trees
 - ▶ A027852 is undirected cycles of exactly 2 rooted trees
 - ▶ A068051 is undirected cycles of 1 or more rooted trees
- this gives formulae which should be amenable to analysis, but let's first do some brute-force numerics to get a feel for the behaviour
- I calculated the counts up to $n=20000\,$ nodes, and tried to guess the form of the asymptotic expansion and then the values of the coefficients

Transforms

A027852 is undirected cycles of exactly 2 rooted trees

$$A_{27852}(x) = \frac{1}{2} (A_{81}(x)^2 + A_{81}(x^2))$$

A068051 is undirected cycles of 1 or more rooted trees

$$A_{68051}(x) = -\frac{1}{2} \sum_{k=1}^{\infty} \frac{\phi(k)}{k} \left(\log(1 - A_{81}(x^k)) \right) + \frac{2A_{81}(x) + A_{81}(x)^2 + A_{81}(x^2)}{4(1 - A_{81}(x^2))}$$

• A001429 is undirected cycles of 3 or more rooted trees

$$A_{1429}(x) = A_{68051}(x) - A_{27852}(x) - A_{81}(x)$$

Asymptotics of A81 (unlabelled rooted trees) [fin03]

- d = 2.9557652856519949747148175241231...
- $\bullet \frac{A81(n)}{d^n} n^{3/2} \sim$
- 0.4399240125710253040409033914 +
- $0.4416990184010399369262808877 n^{-1} +$
- $0.2216928059720368062220256792 n^{-2} +$
- $0.8676554908288089633384550125 n^{-3} +$
- $0.6252197622721944695355918318 n^{-4} +$
- $32.3253941706451396137450650501 n^{-5} + \dots$

Asymptotics for unlabelled unicycles

 \bullet I get that the number c(n,n) of connected unlabelled unicyclic graphs behaves like

$$\left(\frac{c(n,n)}{d^n} - \frac{1}{4^n}\right) n^{3/2} \sim -0.4466410059 + 0.44311055235n^{-1} + 0.91158865326n^{-2} + O(n^{-3})$$

 the coefficients are poorly determined (unlike in a similar analysis of the labelled case)

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