

# Asymptotical Behaviour of Directed Graphs

Angel Garrido, Facultad de Ciencias de la UNED

## Abstract

Among the different graphs, Bayesian Networks are the most successful class of models to represent uncertain knowledge. But the representation of conditional independencies (CIs, in acronym) does not have uniqueness. The reason is that probabilistically equivalent models may have different representations. And this problem is overcome by the introduction of the concept of *Essential Graph*, as unique representant of each equivalence class. They represent *CI models* by *graphs*. Such mathematical and graphical tools containing both, directed or/and undirected edges; hence, producing respectively either *Directed Graphs (DGs)*, in particular acyclic elements, or *Directed Acyclic Graphs (DAGs)*, either *Undirected Graphs (UGs)*, or *Chain Graphs (CGs)*, in the mixed case.

So, DAG models are generally represented as Essential Graphs (EGs). Knowing the ratio of EGs to DAGs is a valuable tool, because through this information we may decide in which space to search. If the ratio is low, we may prefer to search the space of DAG models, rather than the space of DAGs directly, as it was usual until now. The most common approach to learning DAG models is that of performing a search into the space of either DAGs or DAG models (EGs). It is preferable, from a mathematical point of view, to obtain the more exact solution possible, studying its asymptotic behaviour. But also it is feasible to propose a Monte Carlo Chain Method (MCMC) to approach the ratio, avoiding the straightforward enumeration of EGs. And a many more elegant construct, if very difficult, through the Ihara Zeta function for counting graphs.

Here we will show some new results about the Graphs and its equivalence classes. And also the study of the enumerative asymptotic behaviour, according its different possible situations.

**Keywords:** Graph Theory, Combinatorics, Enumeration of graphs, Asymptotical Analysis.

**Mathematics Subject Classification:** 68R10, 68R05, 05C78, 78M35.

## 1. Introduction

An *Essential Graph (EG)* is a very useful graphical representation of any Markov equivalence classes.

In relation with the Essential Graph, each directed edge would have the same direction in all the graphs that belongs to its equivalence class. There is

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a bijective correspondence (one-to-one) among the set of Markov equivalence classes and the set of essential graphs, their representatives.

The labeled or unlabeled character of the graph means whether their nodes or edges are distinguishable or undistinguishable.

For this, we will say that it is *vertex-labeled*, *vertex-unlabeled*, *edge-labeled*, or *edge-unlabeled*.

The labeling will be considered as a mathematical function, referred to a value or name (label), assigned to its elements, either nodes, edges, or both, which makes them distinguishable.

Because many times it will be useful to associate with each edge a number, called its *weight*, acting as label.

In such way, we must to assign certain mastery of some link on another. Then, we call such mathematical constructs *edge-weighted*, or more simply, *weighted-graphs*, usually denoted by

$$w(a, b)$$

So, if we take the set of *n-essential graphs*, and denote its cardinal by  $a_n$ , applying the *IEP*, we may obtain

$$a_n = \sum_{s=1, \dots, p} (-1)^{s+1} \sum_{\substack{i_j \\ j \in \{1, \dots, s\}}} c(A_{i_1} \cap A_{i_2} \cap \dots \cap A_{i_s})$$

where

$$A_k = \{G \in E : k \text{ is a terminal node of } G\},$$

with

$$k = 1, 2, \dots, n \quad [*]$$

## 2. Searching for adequate bounds

Let  $a_n$  be the number of essential (labeled) DAGs.

And also let  $a_n$  be the number of (labeled) DAGs.

Then,  $a_n$  is given by the recurrence equation

$$a_n = \sum_{s=1}^n (-1)^{s+1} C_{n,s} \left( 2^{\binom{n-s}{2}} - n + s \right)^s a_{n-s}$$

with  $a_0 = 1$

Whereas (Robinson, 1973) obtain for the number of labeled n-DAGs,

$$a_n' = \sum_{s=1}^n (-1)^{s+1} C_{n,s} \left(2^{n-s}\right)^s a_{n-s}'$$

with  $a_0' = 1$

The basic idea is to count the number of  $n$ -DAGs considering each digraph as created by adding terminal nodes to a DAG with lesser number of nodes. After this addition, we obtain a new DAG. So, the new formula would be recursive, and it is a direct application of the *IEP*. From which, we can reach directly the equation.

We may rewrite the equation as

$$\sum_{s=0}^n (-1)^{n-s} C_{n,s} (2^s - s)^{n-s} a_s = 0$$

with  $n \geq 1$ .

Another case of application of *Inclusion-Exclusion Principle* is to find the cardinal of the set of essential DAGs,  $E$ , with a set of nodes  $\{1, 2, \dots, n\}$ .

For this, we will start from a family of sets as the aforementioned  $\{A_k\}_{k=1}^n$ .

Therefore, to know the cardinal of  $E$ , first we compute the intersection that appears in the last summatory, for  $j = 1, 2, \dots, n$ . With the total allowed connection numbers, from a given node being

$$2^{n-s} - n + s$$

So, the number of possible ways of adding directed edges from the essential graph until all the  $s$  terminal nodes will be

$$[2^{n-s} - n + s]^s$$

If we denote  $a_n$  the number of *essential*  $n$ -DAGs, this would be

$$a_n = \sum_{s=1}^n (-1)^{s+1} C_{n,s} \left(2^{n-s} - (n-s)\right)^s a_{n-s}$$

with  $a_0 = 1$

Robinson obtains a very similar expression. In such case, the purpose was to obtain a number of labeled  $n$ -DAGs. It would be

$$a_n' = \sum_{s=1}^n (-1)^{s+1} C_{n,s} \left(2^{n-s}\right)^s a_{n-s}'$$

with  $a_0' = 1$

If we denote  $e_n$  the number of *essential  $n$ -graphs*, also labeled, it holds

$$a_n \leq e_n \leq a_n'$$

I.e. both precedent values,  $a_n$  and  $a_n'$ , are the lower and upper bounds of  $e_n$ , for each selected order,  $n$ .

So, it holds

$$\frac{1}{13.6} \leq \frac{a_n}{a_n'}$$

And also

$$\frac{1}{13.6} a_n' \leq e_n \leq a_n'$$

where we obtain lower and upper bounds for the cardinal of essential graphs.

### 3. The Ihara zeta function

The *Riemann Zeta Function* may be definable on all the complex values,  $s$ , such that

$$Re(s) > 1$$

Being this definition possible by the series

$$\zeta(s) \equiv \sum_{n=1}^{\infty} \frac{1}{n^s}$$

And also may be representable by the *Euler's Product Formula*, by the convergent product over all the primes, denoted by  $p$ , in this way

$$\zeta(s) \equiv \prod_p \frac{1}{1 - p^{-s}}$$

It is an important special function that arises in definite integration, being intimately related with deep results surrounding the Prime Number Theorem.

The notation for the variable as  $s$ , instead of the usual complex  $z$ , is preserved until today in deference to Bernhard Riemann and its seminal paper of 1859.

Taking on the real line the subinterval  $(1, +\infty) \subset \mathbf{R}$ , the Riemann zeta function can be also defined by this improper integral,

$$\zeta(s) \equiv \frac{1}{\Gamma(s)} \int_0^{\infty} \frac{x^{s-1}}{e^x - 1} dx = \frac{1}{\Gamma(s)} \lim_{b \rightarrow \infty} \int_0^b \frac{x^{s-1}}{e^x - 1} dx$$

About the expression "zeta function", it must be certainly said in plural, because there are many versions, adapted to different situations and fields of applications.

For instance,

- Artin - Mazur zeta function of a Dynamical System,
- Dedekind zeta function of a number field,
- Epstein zeta function of a quadratic form,
- Ihara zeta function of a graph,
- Igusa zeta function,
- Wierstrass zeta function, connected with elliptic functions,

and many others.

For our purposes, we take advantage on the fact that the *Riemann Zeta Function* may be *generalizable to graphs*, according (Ihara, 1966).

This function was first defined in terms of discrete subgroups. J. P. Serre suggested can be reinterpreted graph-theoretically.

And it was (Sunada, 1985) who put this into practice.

In this version, it is denoted by  $\varsigma_G$ , and defined by

$$\varsigma_G(s) \equiv \left[ \prod_p \left( 1 - s^{L(p)} \right) \right]^{-1}$$

This product is taken over all prime walks,  $p$ , on the graph  $G$ , being  $L(p)$  the length of the *prime*  $p$ .

Also  $\varsigma_G$  is always the reciprocal of a polynomial

$$\varsigma_G(s) \equiv \frac{1}{\det(I - T s)}$$

where  $T$  is edge adjacency operator (Hashimoto, 1990).

Recall that the *adjacency operator*,  $A$ , is acting on the space of functions defined on the set of nodes of  $G = (V, E)$ . Being  $o(e)$  and  $t(e)$  the origin and terminus of  $e$ , respectively, it is defined by

$$(Af)(x) = \sum_{e \in E_x} f[t(e)]$$

where  $E_x \equiv \{e \in E : o(e) = x\}$

(Bass, 1992) also gave a determinant formula involving the adjacency operator.

For any *Graph*,  $G$ , the function  $\varsigma_G$  can be expressed in terms of  $\varsigma$ , depending of their distinct dimensional values, here denoted by  $n$ .

So,

If  $n = 1$ , then  $\varsigma_G(s) = 2\varsigma(s)$

If  $n = 2$ , then  $\varsigma_G(s) = 4\varsigma(s-1)$

If  $n = 3$ , then  $\varsigma_G(s) = 4\varsigma(s-2) + 2\varsigma(s)$

If  $n = \infty$ , then  $\varsigma_G(s) = \frac{8}{3}\varsigma(s-3) + \frac{16}{3}\varsigma(s-1)$

And in the limit, when  $n \rightarrow \infty$ , it holds

$$\varsigma_G(s) = \frac{2^n \varsigma(s-n+1)}{\Gamma(n)}$$

with  $s$  next to the transition point

$\varsigma_G(s)$  is a decreasing function of  $s$ , that is,

$$\varsigma_G(s_1) > \varsigma_G(s_2), \text{ if } s_1 < s_2$$

If the average degree of nodes, also called *mean coordination number of the graph*, is finite, then there exists exactly a value of  $s$ , denoted  $s_{\text{transition}}$ , where the Zeta Function changes from infinite to finite, or vice versa. It is also called *dimension of the Graph*, or the *Complex Network*.

#### 4. About its asymptotic behaviour

Analyzing the asymptotic behaviour of the ratio, i.e. studying the convergence of ratios among the number of classes, or essential graphs, and the number of graphs (exactly DAGs), we may develop

$$\begin{aligned} A(n) &\equiv \frac{a_n}{a_n} \Rightarrow \\ \Rightarrow \lim_{n \rightarrow \infty} A(n) &= \lim_{n \rightarrow \infty} \frac{\sum_{s=1}^n (-1)^{s+1} C_{n,s} (2^{n-s} - (n-s))^s a_{n-s}}{\sum_{s=1}^n (-1)^{s+1} C_{n,s} (2^{n-s})^s a_{n-s}} = \\ &= \frac{\lim_{n \rightarrow \infty} \left\{ \sum_{s=1}^n (-1)^{s+1} C_{n,s} (2^{n-s} - (n-s))^s a_{n-s} \right\}}{\lim_{n \rightarrow \infty} \left\{ \sum_{s=1}^n (-1)^{s+1} C_{n,s} (2^{n-s})^s a_{n-s} \right\}} = \\ &= \frac{\lim_{n \rightarrow \infty} \left\{ (-1)^{s+1} C_{n,s} (2^{n-s} - (n-s))^s a_{n-s} \right\}}{\lim_{n \rightarrow \infty} \left\{ (-1)^{s+1} C_{n,s} (2^{n-s})^s a_{n-s} \right\}} = \\ &= \frac{\lim_{n \rightarrow \infty} \left\{ C_{n,s} (2^{n-s} - (n-s))^s a_{n-s} \right\}}{\lim_{n \rightarrow \infty} \left\{ C_{n,s} (2^{n-s})^s a_{n-s} \right\}} = \\ &= \frac{\lim_{n \rightarrow \infty} \left\{ (2^{n-s} - (n-s))^s a_{n-s} \right\}}{\lim_{n \rightarrow \infty} \left\{ (2^{n-s})^s a_{n-s} \right\}} = \\ &= \frac{\lim_{n \rightarrow \infty} \left\{ (2^{n-s} - (n-s))^s \right\}}{\lim_{n \rightarrow \infty} \left\{ (2^{n-s})^s \right\}} \frac{\lim_{n \rightarrow \infty} \{a_{n-s}\}}{\lim_{n \rightarrow \infty} \{a_{n-s}\}} = \\ &= \lim_{n \rightarrow \infty} \left( \frac{(2^{n-s} - (n-s))^s}{(2^{n-s})^s} \right) \lim_{n \rightarrow \infty} \left( \frac{a_{n-s}}{a_{n-s}} \right) \end{aligned}$$

Or analogously we may consider

$$\begin{aligned}
\lim_{n \rightarrow \infty} A(n) &= \lim_{n \rightarrow \infty} \frac{\sum_{s=1}^n (-1)^{s+1} C_{n,s} \left(2^{n-s} - (n-s)\right)^s a_{n-s}}{\sum_{s=1}^n (-1)^{s+1} C_{n,s} \left(2^{n-s}\right)^s a_{n-s}'} = \\
&= \lim_{n \rightarrow \infty} \sum_{s=1}^n \frac{\left\{ (-1)^{s+1} C_{n,s} \left(2^{n-s} - (n-s)\right)^s a_{n-s} \right\}}{\left\{ (-1)^{s+1} C_{n,s} \left(2^{n-s}\right)^s a_{n-s}' \right\}} = \\
&= \sum_{s=1}^{\infty} \lim_{n \rightarrow \infty} \frac{\left\{ (-1)^{s+1} C_{n,s} \left(2^{n-s} - (n-s)\right)^s a_{n-s} \right\}}{\left\{ (-1)^{s+1} C_{n,s} \left(2^{n-s}\right)^s a_{n-s}' \right\}} = \\
&= \frac{\lim_{n \rightarrow \infty} \left\{ (-1)^{s+1} C_{n,s} \left(2^{n-s} - (n-s)\right)^s a_{n-s} \right\}}{\lim_{n \rightarrow \infty} \left\{ (-1)^{s+1} C_{n,s} \left(2^{n-s}\right)^s a_{n-s}' \right\}} = \\
&= \frac{\lim_{n \rightarrow \infty} \left\{ C_{n,s} \left(2^{n-s} - (n-s)\right)^s a_{n-s} \right\}}{\lim_{n \rightarrow \infty} \left\{ C_{n,s} \left(2^{n-s}\right)^s a_{n-s}' \right\}} = \\
&= \frac{\lim_{n \rightarrow \infty} \left\{ \left(2^{n-s} - (n-s)\right)^s a_{n-s} \right\}}{\lim_{n \rightarrow \infty} \left\{ \left(2^{n-s}\right)^s a_{n-s}' \right\}} = \\
&= \left[ \lim_{n \rightarrow \infty} \frac{\left(2^{n-s} - (n-s)\right)^s}{\left(2^{n-s}\right)^s} \right] \left[ \frac{\lim_{n \rightarrow \infty} \{a_{n-s}\}}{\lim_{n \rightarrow \infty} \{a_{n-s}'\}} \right] = \\
&= \lim_{n \rightarrow \infty} \left( \frac{2^{n-s} - (n-s)}{2^{n-s}} \right)^s \lim_{n \rightarrow \infty} \left( \frac{a_{n-s}}{a_{n-s}'} \right)
\end{aligned}$$

But we will dispose of previous and known results, as

$$fixed\ s, \frac{n-s}{2^{n-s}} \rightarrow 0^+ \Rightarrow 1 - \left( \frac{n-s}{2^{n-s}} \right) \rightarrow 1^-$$

Hence,

$$\begin{aligned}
&\lim_{n \rightarrow \infty} \left\{ \sum_{s=1}^n \left( \frac{2^{n-s} - (n-s)}{2^{n-s}} \right)^s A(n-s) \right\} = \\
&= \left\{ 1 - \lim_{n \rightarrow \infty} \sum_{s=1}^n \left( \frac{(n-s)}{2^{n-s}} \right)^s \right\} \{ \lim_{n \rightarrow \infty} A(n-s) \}
\end{aligned}$$

being

$$A(n-s) \equiv \frac{a_{n-s}}{a_{n-s}'}$$

and

$$1 - \varsigma_G(n-s) = \lim_{n \rightarrow \infty} \sum_{s=1}^n \left( \frac{2^{n-s} - (n-s)}{2^{n-s}} \right)^s$$

That is,

$$\varsigma_G(n-s) \equiv \lim_{n \rightarrow \infty} \sum_{s=1}^n \left( \frac{(n-s)}{2^{n-s}} \right)^s$$

So, returning to our initial step,

$$\begin{aligned} \lim_{n \rightarrow \infty} A(n) &= \lim_{n \rightarrow \infty} \left\{ \left[ 1 - \varsigma_G(n-s) \right] A(n-s) \right\} = \\ &= \left[ 1 - \lim_{n \rightarrow \infty} \varsigma_G(n-s) \right] [\lim_{n \rightarrow \infty} A(n-s)] \end{aligned}$$

Considering the subsequent collection of partial sums, depending on  $n$ ,

$$\sum_{s=1}^n \frac{n-s}{2^{n-s}}$$

it holds

$$\begin{aligned} \sum_{s=1}^n \left[ 1 - \frac{n-s}{2^{n-s}} \right] &= n - \sum_{s=1}^n \frac{n-s}{2^{n-s}} \Rightarrow \\ \Rightarrow \sum_{s=1}^n \left[ 1 - \frac{n-s}{2^{n-s}} \right]^s &\leq n - \sum_{s=1}^n \left( \frac{n-s}{2^{n-s}} \right)^s \end{aligned}$$

and its asymptotical behaviour, when  $n \rightarrow \infty$ , these may establish a correspondence with a modified version of the Zeta Function of Riemann,  $\chi_G$ . It is the so called *Ihara-Selberg of the  $n$ -graph  $G_n$* .

But operating here on the increasing value of  $n-s$ , i.e., with

$$\chi_G(n-s)$$

So, we obtain that denoting the ratio among terms of the series as

$$c = \lim_{n \rightarrow \infty} \frac{\left\{ \sum_{s=1}^n (-1)^{s+1} C_{n,s} \left( 2^{n-s} - (n-s) \right)^s a_{n-s} \right\}}{\left\{ \sum_{s=1}^n (-1)^{s+1} C_{n,s} \left( 2^{n-s} \right)^s a_{n-s} \right\}}$$

and taking into account which



$$\begin{aligned}
c &= \lim_{n \rightarrow \infty} \frac{\left\{ \sum_{s=1}^n \left| (-1)^{s+1} C_{n,s} \left( 2^{n-s} - (n-s) \right)^s \right| a_{n-s} \right\}}{\left\{ \sum_{s=1}^n \left| (-1)^{s+1} C_{n,s} \left( 2^{n-s} \right)^s \right| a_{n-s} \right\}} = \\
&= \lim_{n \rightarrow \infty} \frac{\left\{ \left| (-1)^{s+1} C_{n,s} \left( 2^{n-s} - (n-s) \right)^s \right| a_{n-s} \right\}}{\left\{ \left| (-1)^{s+1} C_{n,s} \left( 2^{n-s} \right)^s \right| a_{n-s} \right\}} = \\
&= \lim_{n \rightarrow \infty} \frac{\left\{ \left| C_{n,s} \left( 2^{n-s} - (n-s) \right)^s \right| a_{n-s} \right\}}{\left\{ \left| C_{n,s} \left( 2^{n-s} \right)^s \right| a_{n-s} \right\}} = \\
&= \left( \lim_{n \rightarrow \infty} \left\{ 1 - \varsigma_G(n-s) \right\} \right) \left( \lim_{n \rightarrow \infty} A(n-s) \right)
\end{aligned}$$

In our case, once fixed  $s$ , for every natural  $n$ ,

$$\begin{aligned}
&a_{n-s} \leq a_{n-s}' \Rightarrow \\
&\Rightarrow (-1)^{s+1} C_{n,s} \left( 2^{n-s} - (n-s) \right)^s a_{n-s} \leq (-1)^{s+1} C_{n,s} \left( 2^{n-s} \right)^s a_{n-s}'
\end{aligned}$$

This proves the convergence of the series, and as a consequence, the convergence of the ratio among both.

As

$$(n-s) \geq 0$$

then

$$2^{n-s} - (n-s) \leq 2^{n-s}$$

So, being  $n \in \mathbf{N}$ , it holds

$$C_{n,s} \in \mathbf{N}, \forall s: 1 \leq s \leq n$$

and therefore

$$\begin{aligned}
&\left[ 2^{n-s} - (n-s) \right]^s \leq \left( 2^{n-s} \right)^s \Rightarrow \\
&\Rightarrow C_{n,s} \left( 2^{n-s} - (n-s) \right)^s \leq C_{n,s} \left( 2^{n-s} \right)^s \Rightarrow \\
&\Rightarrow \sum_{i=1}^n (-1)^{s+1} C_{n,s} \left( 2^{n-s} - (n-s) \right)^s a_{n-s} \leq \sum_{s=1}^n (-1)^{s+1} C_{n,s} \left( 2^{n-s} \right)^s a_{n-s}'
\end{aligned}$$

Hence, from the convergence of the second series we induce the convergence of the first. And symmetrically, in case of divergence of the first, the divergence of the second.

Furthermore

$$a_{n-s} \leq a'_{n-s}, \forall n, \text{ once fixed } s \Rightarrow \\ \Rightarrow \exists \Phi_1 = \left[ 1 - \lim_{n \rightarrow \infty} \varsigma_G(n-s) \right] \left[ \lim_{n \rightarrow \infty} A(n-s) \right]$$

once fixed  $s$ , when  $n$  increases to  $\infty$ ,

$$\Phi_1 = \frac{1}{10 \varsigma(5/2)} = \frac{1}{5\varsigma_G(5/2)}$$

equivalence classes for each digraph, or equivalently,

$$\Phi_1^{-1} = 10 \varsigma(5/2) = 5/2 \varsigma_G(7/2)$$

digraphs for each equivalence class, or essential graph.

In the bidimensional case, it holds

$$\exists \Phi_2^* \equiv \lim_{n \rightarrow \infty} \left( \left\{ \varsigma_G(n) \right\} \left[ A^*(n-s) \right] \right) \Rightarrow \\ \Rightarrow \Phi_2^* = \frac{1}{10} \varsigma(3/2) = \frac{1}{40} \varsigma_G(5/2)$$

and so dually,

$$\exists \left( \Phi_2^* \right)^{-1} \equiv \lim_{n \rightarrow \infty} \left( \left\{ \varsigma_G(n) \right\} \left[ A^*(n-s) \right] \right)^{-1} \Rightarrow \\ \Rightarrow \left( \Phi_2^* \right)^{-1} = \frac{10}{\varsigma(3/2)} = \frac{4}{\varsigma_G(5/2)}$$

## 5. Conclusion

It will be so reached the limit situation, reflecting the degree of fitness to the proposed model.

Now we can support on a many more powerful analytical framework, so improving our theoretical basis, being coherent with the precedent results.

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