Invariant Graph Characteristics from the Zeta Function
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Abstract
We describe here the problem of enumerating graphs, in particular, Directed Acyclic Graphs (DAGs, in acronym), or Bayesian Networks (BNs). All them will be analyzed by the elegant and useful Ihara Zeta Function.

Keywords: Graph Theory, Combinatorics, Enumeration of graphs, Graph labeling, Asymptotic Analysis.

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

1. Introduction
The Ihara zeta function was firstly defined by Ihara studying discrete subgroups of the two-by-two special linear groups. Zeta functions of graphs were studied not only by Ihara [34] [35], but many other works on it, as may be Sunada, Hashimoto, Bartholdi, and Bass. So, Jean Pierre Serre [47] suggested can be reinterpreted graph-theoretically, in his book Trees. And it was Toshikazu Sunada, in 1985, who put this suggestion into practice.

Storm [54] defined the Ihara-Selberg zeta function for Hypergraphs.

The Ihara zeta function is denoted by \( \zeta_G \), and it will be defined by

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

or equivalently,

\[
\prod_p \left( 1 - \frac{L(p)}{s} \right) \equiv \frac{1}{\zeta_G(s)}
\]

Such formula is analogous to the Euler product for the Riemann zeta function.

In fact, we have an infinite product to work with.

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

Let $G$ be a graph, and

$$A \equiv (a_{ij})$$

its adjacency matrix, which as we known, will be a

$$(c \{V(G)\} \times c \{V(G)\}) - \text{matrix}$$

with entries

$$a_{ij} \equiv \begin{cases} \text{cardinal of undirected edges connecting } n_i \text{ to } n_j, \text{ being } i \neq j \\
\text{double of the cardinal of loops at the node } n_i, \text{ if } i = j \end{cases}$$

As our graphs have no loops neither multiple edges, such entries will be either zero or one, according to the adjacency or not adjacency of its respective pairs of nodes.

Suppose that we take now $D$, as the diagonal matrix such that its entry $d_i$ is the degree of the $i$-th node minus one, and let

$$r - 1 = c \{E(G)\} - c \{V(G)\}$$

Then, The Ihara zeta function will be expressed as

$$\zeta_G(s)^{-1} \equiv \left(1 - s^2\right)^{r-1} \det \left( I - As + Du^2 \right)$$

It is very interesting to look at the logarithmic derivative of the Ihara zeta function,

$$s \frac{d}{ds} \ln \left[ \zeta_G(s) \right]$$

We have

$$\ln \left[ \zeta_G(s) \right] = \ln \left[ \prod_p \left( 1 - s^{L(p)} \right)^{-1} \right] =$$

$$= \ln \left[ \prod_p \left( 1 - s^{L(p)} \right)^{-1} \right] = - \sum_p \ln \left( 1 - s^{L(p)} \right)$$

and taking the derivative,
\[
\frac{d}{ds} \left[ \zeta_G(s) \right] = \frac{d}{ds} \left[ - \sum_p \ln \left( 1 - s^{L(p)} \right) \right] = - \sum_p \frac{1}{1-s^{L(p)}} \frac{d}{ds} \left( 1 - s^{L(p)} \right) =
\]

\[
= - \sum_p \frac{1}{1-s^{L(p)}} \left[ -L(p) \right] L(p) = \sum_p \frac{L(p) s^{L(p)-1}}{1-s^{L(p)}}
\]

and now multiplying by \( s \),

\[
s \frac{d}{ds} \left[ \zeta_G(s) \right] = s \sum_p \frac{L(p) s^{L(p)-1}}{1-s^{L(p)}} = \sum_p \frac{L(p) s^{L(p)}}{1-s^{L(p)}}
\]

But such expression may be improved by the geometric series identity,

\[
\sum_{n \in \mathbb{N}^*} s^n = \frac{1}{1-s}
\]

giving

\[
s \frac{d}{ds} \left[ \zeta_G(s) \right] = \sum_p L(p) s^{L(p)-1} \left[ 1 + s^{L(p)} + s^{2L(p)} + s^{3L(p)} + \ldots \right] =
\]

\[
= \sum_p L(p) \left[ s^{L(p)} + s^{2L(p)} + s^{3L(p)} + s^{4L(p)} + \ldots \right]
\]

If we denote

\[
N_k = \sum_{p: \ L(p)\mid k} L(p)
\]

it holds

\[
s \frac{d}{ds} \left[ \zeta_G(s) \right] = \sum_{k \in \mathbb{N}} N_k s^k
\]

Where the coefficient \( N_k \), being associated with the term \( s^k \), will report us the number of prime paths with a number of nodes which divides \( k \).

We may translate the results from closed geodesics to cycles, considering the elements of a group, or instead, working on graphs.

We say that a cycle is primitive, if it is not the \( r \)-multiple of some other cycles, being \( r \geq 2 \).

A closed geodesic which is not the power of another is called a prime geodesic.

It is possible to establish an equivalence relation on the set of prime paths in the graph. According such relation, two closed paths are equivalent, if they are the same path with a different starting point.

Mathematically expressed, let \( E \) and \( F \) two cycles,
\[ E = (e_i)_{i=1}^n \]

\[ F = (f_i)_{i=1}^n \]

Both will be equivalent, if there is a fixed \( k \in \mathbb{Z}/n\mathbb{Z} \), such that

\[ e_i = f_{i+k} \quad \forall i \in \mathbb{Z}/n\mathbb{Z} \]

This says that all indices are considered module \( n \ (mod \ n) \). So, we are reducing to the first cycle. And we are imposing the aforementioned equivalence relation via cyclic permutation.

Therefore, two prime geodesics are said to be equivalent, if one is obtained from another by a cyclic permutation of edges.

An equivalence class of prime geodesics is called a prime geodesic class, or simply a prime, \( \varphi \). Given a path, \( \gamma \), we denote by \( L(\gamma) \) its length. The length of a prime, \( \varphi \), is the length of any of its representatives. A prime cycle is the equivalence class of primitive cycles which have no backtracking or tails.

Given a graph, \( G \), with a symmetric digraph, \( D_G \), we may associate to each of its edges \( (e) \) an invariant, \( s_e \), and so, define the function

\[ g(C) \equiv \prod_{e \text{ edge in } C} s_e \]

for a prime cycle. Such function \( g \) inform about the edges involved in a particular prime cycle, and also about how many times they are used.

The edge zeta function of \( G \) is a function of \( s_e \in \mathbb{C} \), given by

\[ \varepsilon_G(s) \equiv \prod_{\text{prime cycles}} [1 - g(C)]^{-1} \]

And specializing each \( s_e \) to \( s \), we obtain the Ihara function of \( G \), by

\[ \zeta_G(s) \equiv \prod_{\text{prime cycles}} [1 - s^{L(C)}]^{-1} \]

being denoted as \( L(C) \) the length of a representative of the prime cycle, \( [C] \).

For a finite graph where every node has at least degree two, the zeta function give us the cardinal of edges in the graph.

And what happens in the case of degree one? When the edges are incident to a degree one node, they are ignored by the zeta function. It is because in this situation, only admits two possibilities, either have a backtracking or a tail.

If we consider as \( I \) the identity matrix, it holds
\[ \zeta_G(s) = (1 - s)^\chi(G) \det \left[ I - sA + s^2(D - I) \right] \]

where \( \chi(G) \) will be the Euler characteristics, or Euler number (a notable topological invariant), of the graph \( G \).

Recall that this number is reachable by

\[ \chi(G) = c[V(G)] - c[E(G)] \]

The Ihara zeta function, \( \zeta_G \), will be always representable as the reciprocal of a polynomial

\[ \zeta_G(s) \equiv \frac{1}{\det(I - Ts)} \]

that is,

\[ \zeta_G(s)^{-1} \equiv \det(I - Ts) = \det(I - sT) \]

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

Therefore, the edge zeta function is the reciprocal of a multivariate polynomial in, at most, \( 2c(E(G)) \) variables.

An important fact indeed, because it implies the possibility of to be computed in polynomial time.

Observe that the maximum degree of the reciprocal of the Zeta function is the double of the number of edges in the graph, its size, i.e. \( 2c(E(G)) \).

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

\[ (Af)(x) = \sum_{e \in E_x} f[t(e)], \text{ where } E_x \equiv \{ e \in E : o(e) = x \} \]

We may define the directed edge matrix, \( T \), of a graph, \( G \). For this, firstly we need a labeling of the directed edges (in the associated digraph).

Then, such matrix, \( T \), has as its \((i,j)\)-entry,

\[ t_{ij} = \begin{cases} 
1, & \text{if } t(e_i) = o(e_j), \text{ and } e_i \neq e_j \\
0, & \text{otherwise}
\end{cases} \]

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

Recall that the set of eigenvalues of a matrix, \( A \), is called its Spectrum, usually denoted either by \( \text{Spec}(A) \), or \( \lambda(A) \).
\[ \lambda(A) \equiv \{ \lambda_i \}_{i=1}^n \]

being \( \lambda_i \) its eigenvalues, for every index \( i \in I \).

Then, we have as determinant of \( A \),

\[ \det (A) = \prod_{i=1}^{n} \lambda_i = \begin{pmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & \lambda_n \end{pmatrix} \]

And the set of graph eigenvalues of the adjacency matrix is known as the Spectrum of the Graph.

If we have a graph, \( G \), with \( n_i \) – fold degenerate eigenvalues, \( \lambda_i \), the usual expression for its spectrum will be

\[ \text{Spec}(G) = \prod_{i=1}^{m} (\lambda_i)^{n_i} \]

Sometimes it will be denoted by

\[ \begin{pmatrix} \lambda_1 & \lambda_2 & \ldots & \lambda_m \\ n_1 & n_2 & \ldots & n_m \end{pmatrix} \]

Let \( G \) and \( H \) be two graphs. They are called cospectral, if its adjacency matrices have the same spectra.

An important result of the theory of Ihara zeta function, characterizing this question on \( k \)-regular graphs, is the following

\textit{Theorem (Mellein)}.

Suppose \( G \) and \( H \) are both \( k \)-regular graphs.

Then, \( G \) and \( H \) are cospectral if and only if

\[ \zeta_G(s) = \zeta_H(s), \ \forall s \]

So, whenever a \( k \)-regular graph is uniquely determined by its spectrum, it is possible to conclude that its Ihara zeta function is also uniquely determined.

For any Graph, \( G \), the function \( \zeta_G \) can be expressed in terms of the Riemann zeta function, \( \zeta \), for different dimension values, \( n \).

So,

If \( n = 1 \), then \( \zeta_G(s) = 2 \zeta(s) \).

If \( n = 2 \), then \( \zeta_G(s) = 4 \zeta(s - 1) \).

If \( n = 3 \), then \( \zeta_G(s) = 4 \zeta(s - 2) + 2 \zeta(s) \).

If \( n = \infty \), then \( \zeta_G(s) = \frac{8}{3} \zeta(s - 3) + \frac{16}{3} \zeta(s - 1) \).

Recall that \( \zeta_G(s) \) is a decreasing function of \( s \).

That is,
\[\zeta_G(s_1) > \zeta_G(s_2) \text{, if } s_1 < s_2\]

And in the limit, if \(n \rightarrow \infty\), when \(s\) is next to the transition point, it holds

\[\zeta_G(s) = \frac{2^n \cdot c(s - n + 1)}{\Gamma(n)}\]

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.

### 2. Enumerating Graphs

About the foundations of Graph Theory, there exists many adequate surveys, as [9] [10] [27].

For Graphical Enumeration, it may be convenient to see for instance [6] [11] [14] [21] [28], among others.

A very elegant construct, if certainly difficult, may be through the Ihara Zeta function.

It is also possible to use Generating Functions to count labeled DAGs. For this mathematical construct, it is necessary to make intervene the Inclusion-Exclusion Principle (IEP).

So, if we take the set of \(n\)-essential graphs, and denote its cardinal by \(a_n\), applying the aforementioned IEP, we may obtain

\[a_n = \sum_{s=1, \ldots, p} (-1)^{s+1} \sum_{i_j \in \{1, \ldots, s\}} C_{n,s} c(A_{i_1} \cap A_{i_2} \cap \ldots \cap A_{i_s})\]

where

\[A_k = \{G \in E : k \text{ is a terminal node of } G\}, \text{ with } k = 1, 2, \ldots, n \quad[^*]\]

Let \(a_n\) and \(a_n'\) be the number of essential labeled \(n\) – DAGs, and the number of labeled \(n\) – DAGs, respectively. Then, \(a_n\) is given by the recurrence equation

\[a_n = \sum_{s=1}^{n} (-1)^{s+1} C_{n,s} \left(2^{n-s} - n + s\right)^{s} a_{n-s}, \text{ with } a_0 = 1\]

Whereas

\[a_n' = \sum_{s=1}^{n} (-1)^{s+1} C_{n,s} \left(2^{n-s}\right)^{s} a_{n-s} ', \text{ with } a_0' = 1\]
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

\[ \sum_{s = 0}^{n} (-1)^{n-s} s^{n-s} n \binom{n}{s} 2^{s-s} a_s = 0, \text{ with } n \geq 1 \]

Another case of application of IEP is to find the cardinal of the set of essential DAGs, \( E \), with a set of labeled nodes, with labelings that belongs to \( \{1, 2, \ldots, n\} \). For this, we start with a family of sets, as the aforementioned \( \{A_k\}_{k=1}^n \). See the precedent formula \([*]\), where \( A_k \) represents the subclass of graphs concluding at the node labeled by \( k \).

Therefore, to know the cardinal of \( E \), first we compute the intersection that appears in the last summatory, for \( j = 1, 2, \ldots, n \), being these

\[ \sum_{j \in \{1, \ldots, s\}} c \left( A_1 \cap A_{i_2} \cap \ldots \cap A_s \right) \]

related with the aforementioned principle (IEP).

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

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

3. Asymptotical behaviour

Analyzing the asymptotic behaviour of its ratios, i.e. studying the convergence of the quotient of cardinals, among the number of essential graphs, and the number of DAGs (acronym of Directed Acyclic Graphs), we may develop this so

\[
A(n) \equiv \frac{a_n}{a_n} \implies \\
\lim_{n \to \infty} A(n) = \lim_{n \to \infty} \frac{\sum_{s=1}^{n} (-1)^{s+1} s^{n-s} n \binom{n}{s} \left(2^{s-n} - (n-s)\right) a_{n-s}}{\sum_{s=1}^{n} (-1)^{s+1} s^{n-s} n \binom{n}{s} \left(2^{s-n} - (n-s)\right) a_{n-s}}
\]

being
\[ A(n - s) \equiv \frac{a_{n-s}}{a_{n-s}} \]

and

\[ \zeta_G(n - s) \equiv \lim_{n \to \infty} \sum_{s=1}^{n} \left( \frac{(n - s)^{\frac{s}{2}}}{n^{s}} \right) \]

and turning to our initial step,

\[ \lim_{n \to \infty} A(n) = \left[ 1 - \lim_{n \to \infty} \zeta_G(n - s) \right] \left[ \lim_{n \to \infty} A(n - s) \right] \]

we can consider the series

\[ \sum_{s=1}^{n} \frac{n - s}{2^{n-s}} \Rightarrow \sum_{s=1}^{n} \left[ 1 - \frac{n - s}{2^{n-s}} \right] = n - \sum_{s=1}^{n} \frac{n - s}{2^{n-s}} \]

and its asymptotical behaviour, when \( n \to \infty \). These may establish an analytical correspondence with a version of the Riemann zeta function, the so called *Ihara zeta function of the \( n \)-graph, \( G_n \).

But operating here on the increasing value of \( n - s \), i.e. with \( \zeta_G(n - s) \). Nevertheless, this proof would be very complex. Instead, we may apply here an interesting result, which permits to finalize our demonstration.

So, we obtain the ratio among terms of the series (by applying the precedent Lemma),

\[
\lim_{n \to \infty} \left\{ \sum_{s=1}^{n} \frac{(-1)^{s+1}}{C_{n,s}} \left[ \frac{2^{n-s}}{(n-s)^{\frac{s}{2}}} \right] a_{n-s} \right\} = \lim_{n \to \infty} \left\{ \sum_{s=1}^{n} \frac{(-1)^{s+1}}{C_{n,s}} \left[ \frac{2^{n-s}}{(n-s)^{\frac{s}{2}}} \right] a_{n-s} \right\} = \lim_{n \to \infty} \left\{ \frac{(-1)^{s+1}}{C_{n,s}} \left[ \frac{2^{n-s}}{(n-s)^{\frac{s}{2}}} \right] a_{n-s} \right\} = \lim_{n \to \infty} \left\{ \frac{2^{n-s}}{(n-s)^{\frac{s}{2}}} \right\} a_{n-s} = \left[ \lim_{n \to \infty} \left( \frac{2^{n-s}}{(n-s)^{\frac{s}{2}}} \right) \right] \left[ \lim_{n \to \infty} \frac{a_{n-s}}{a_{n-s}} \right] = \left[ \lim_{n \to \infty} \left\{ 1 - \zeta_G(n - s) \right\} \right] \left[ \lim_{n \to \infty} A(n - s) \right] \]

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4. Applying the Ihara zeta function

We establish from now these auxiliary and useful notation

\[ f(n - s) = 1 - \frac{n - s}{2^{n-s}} \Rightarrow f(n) = 1 - \frac{n}{2^n} \]

that is,

\[ 1 - f(n - s) = \frac{n - s}{2^{n-s}} \Rightarrow 1 - f(n) = \frac{n}{2^n} \]

But as we known

\[ \lim_{n \to \infty} \frac{n - s}{2^{n-s}} = \lim_{n \to \infty} \frac{n}{2^n} = 0 \]

and by this procedure,

\[ [1 - \{f(n - s)\}]^s = 1 - \left(\frac{n - s}{2^n}\right)^s \]

Hence

\[ \lim_{n \to \infty} [1 - \{f(n - s)\}]^s = \lim_{n \to \infty} \left\{1 - \left(\frac{n - s}{2^n}\right)^s\right\} = 1 \]

and

\[ \lim_{n \to \infty} \sum_{i=1}^{n} \left(\frac{n - s}{2^n}\right)^s = n - \lim_{n \to \infty} \sum_{i=1}^{n} \left(\frac{n - s}{2^n}\right)^s = \]

\[ = n - \lim_{n \to \infty} \sum_{i=1}^{n} [1 - f(n - s)]^s = n - [n - \zeta(n) (n - s)] = \zeta(n - s) \]

These last terms must regulate the asymptotical behaviour, by its limit values.

And respect to its reciprocal function

\[ \zeta^{-1}(n - s) = \lim_{n \to \infty} \left[\sum_{i=1}^{n} \left(1 - \frac{n - s}{2^n}\right)^{-s}\right] \]

whith this may appears \( \Phi^{-1}_i \) from \( \Phi_i \), as they are described in the subsequent step.

Note that we can take

\[ f(n - s) = \frac{2^n - (n - s)}{2^n}, \text{ for each } n \in \mathbb{N}, \text{ once fixed } s \]
So, by

\[ \zeta_G (n - s) = \lim_{n \to \infty} \sum_{i=1}^{n} [f(n - s)]' \]

it holds

\[ \exists \Phi_A = \left[ n - \lim_{n \to \infty} \sum_{i=1}^{n} [f(n - s)]' \right] [\lim_{n \to \infty} A(n - s)] = \]

\[ = \left[ n - \lim_{n \to \infty} \zeta_G (n - s) \right] [\lim_{n \to \infty} A(n - s)] , \]

fixed s, when n increases to \( \infty \) \( \Rightarrow \)

\[ \Rightarrow \Phi_A = \frac{1}{10 \sqrt{5/2}} = \frac{1}{\zeta_G (5/2)} \simeq 0.07 \]

DAGs for each equivalence class, or equivalently,

\[ \Phi_A^{-1} = 10 \zeta (5/2) \]

hence, passing from Riemann to Ihara zeta function,

\[ \Phi_A^{-1} = 5/2 \zeta_G (7/2) \simeq 13.6 \]

This will be the number of equivalence classes for each DAG.

So far, we have supposed \textit{dimension one}.

Because in case of \textit{dimension two}, where the new functions are denoted \( \Phi_B \) and \( \Phi_B^{-1} \), respectively, it holds

\[ \Phi_B = \frac{1}{10 \zeta (5/2)} = \frac{1}{5/2 \zeta_G (7/2/2)} , \text{ and } \Phi_B^{-1} = 4 \zeta (7/2 - 1) = 4 \zeta (5/2) \]

And translating this from Riemann to Ihara Zeta Function, we obtain

\[ \Phi_B^{-1} = 5/2 \zeta_G (7/2) \]

Note that the “labeled” or “unlabeled” character of the considered graphs is relevant, because they are very distinct situations, giving so different ratios.

It is obvious that the enumeration of unlabeled essential graphs results more complex than in the labeled case. Also, its symmetries can be used.

Recall that permutating between the positions of two symmetric nodes is an operation that when acting on graphs, leaves the shape unaffected.

For the case of unlabeled graphs (Sunada, 1985), denoted here by the letter "c", we have
\[ c_n \equiv \text{cardinal of the set of unlabeled n-DAGs} \]

and

\[ c_n^* \equiv \text{cardinal of the set of unlabeled essential n-DAGs} \]

And so, we can find (applying our previous Lemma) that

\[ c_{n-s} \leq c_{n-s}^*, \forall n, \text{ once fixed } s \Rightarrow \]

\[ \exists \Phi_c = \lim_{n \to \infty} (s_G(n) [C(n-s)]) , \]

fixed \( s \), and when \( n \to \infty \),

with \( C(n-s) \equiv \lim_{n \to \infty} \sum_{s=1}^{n} \frac{c_{n-s}}{c_{n-s}^*} \Rightarrow \]

\[ \Phi_c \equiv \{ \lim_{n \to \infty} s_G(n) \} \{ \lim_{n \to \infty} C(n-s) \} = \frac{1}{10} \zeta(3/2) = \frac{1}{20} \zeta_G(3/2) \simeq 0.26 \]

essential graphs for each unlabeled DAG, in the case of dimension one.

And symmetrically,

\[ \exists (\Phi_c)^* \equiv \{ \lim_{n \to \infty} [s_G(n)] \}^{-1} \{ \lim_{n \to \infty} [C(n-s)] \}^{-1} = \frac{10}{\zeta(3/2)} = \frac{20}{\zeta_G(3/2)} \simeq 3.73 \]

unlabeled DAGs for each essential graph, which coincides with our precedent analytical results.

In case of dimension two, it holds

\[ \exists \Phi_c^* \equiv \lim_{n \to \infty} \left( \left\{ s_G(n) \right\} \left[ C^*(n-s) \right] \right) = \frac{1}{10} \zeta(3/2) = \frac{1}{30} \zeta_G(5/2) \simeq 0.26 \]

and dually,

\[ \exists \left( \Phi_c^* \right)^{-1} \equiv \lim_{n \to \infty} \left( \left\{ s_G(n) \right\} \left[ C^*(n-s) \right] \right)^{-1} = \frac{10}{\zeta(3/2)} = \frac{4}{\zeta_G(5/2)} \simeq 3.73 \]

5. Conclusion

And it is so in the limit situation, reflecting the degree of fitness of the proposed model, based in analytical framework, to the precedent computational results, as the shown by [1], or [20].

References


Translated with commentaries by R. C. Read, in *Combinatorial enumeration of groups, graphs...* Springer.


