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Curriculum networks

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There are many different approaches to curriculum content sequencing that are mostly based on teacher’s experience and developed within certain government or institution guidelines. The aim of this paper is to propose measures that can evaluate the quality of content sequencing. Our measures are based on the representation of curriculum content as simple directed connected graphs, where educational units correspond to vertices and edges connect educational units with its prerequisites. Educational unit can correspond to a certain topic, lesson, section or course. We also analyze these measures and determine graphs that correspond to the most complex and the least complex curriculums.

In many cases, the consensus on curriculum content sequencing must be obtained and hence disputes among experienced teachers might be resolved by using here proposed objective measures. Moreover, these measures might be a cornerstone for the development of software for curriculum content sequencing which might be a valuable assistance for independent lifelong learning. Also, in Croatia, Complete Curriculum Reform is currently in progress, so we think that this topic is one of very important and current topics.
We will survey the existing results and show the recent progress we made on studying $M$-Lipschitz mappings of graphs (simple, finite and connected). A $M$-Lipschitz mapping of graph $G = (V, E)$ with root $v_0 \in V$ is a mapping of $V$ to $\mathbb{Z}$ such that $f(v_0) = 0$ and for every edge $(u, v) \in E$ holds that $|f(u) - f(v)| \leq M$.

First, we will turn our attention to the special case of $M = 1$, continuing in work of Loebl et al. [2]. One can view 1-Lipschitz mapping as a homomorphism from some graph to an infinite path with a loop added to each vertex. This definition generalizes the concept of random walk on a path into the graph-indexed random walk and its slightly different version was originally motivated by a problem in statistical physics [1].

We will be interested in a range and an average range. A range of 1-Lipschitz mapping $f$ of rooted graph $G$ is the size of the set $\{x | x = f(v) \text{ for some } v \in V\}$. An average range of rooted graph $G$ is an arithmetic average of ranges of all 1-Lipschitz mappings of $G$. We will show an explicit formulas for an average range of some classes of graphs including paths, cycles, complete graphs, dragon graphs and lollipops.

Furthermore, we will tackle $M$-Lipschitz mappings in an algorithmic way and we will introduce two new problems and show our results on them. $M$-MAXRANGE asks for the maximum possible range among all the $M$-Lipschitz mappings of the given graph $G$. The problem of partial $M$-Lipschitz mapping extension – $M$-LIPEXT – gets on an input the graph $G$ and some subset $H$ of the vertices of $G$ together with the function $f_H : H \rightarrow \mathbb{Z}$. Our task is to determine if there is an $M$-Lipschitz mapping $f$ of $G$ such that $f_H \subseteq f$.

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On the magic of labyrinth patterns

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An $n \times n$ pattern is obtained by starting with the unit square, dividing it into $n \times n$ congruent smaller subsquares and coloring some of them in black (which means that they will be cut out), and the rest in white.

Sierpiński carpets are (self-similar) fractals in the plane that originate from the well-known Sierpiński carpet. They are constructed in the following way: start with the unit square, divide it into $n \times n$ congruent smaller subsquares and cut out $m$ of them, corresponding to a given $n \times n$ pattern (called the generator of the Sierpiński carpet). Repeat this construction step with all the remaining subsquares ad infinitum. The resulting object is a fractal of Hausdorff and box-counting dimension $\log(n^2 - m)/\log(n)$, called a Sierpiński carpet.

By using special patterns, which we called “labyrinth patterns”, and which we described with the help of the graph associated to a pattern, we created and studied a special class of carpets, called labyrinth fractals. Labyrinth fractals are self-similar, and mixed labyrinth fractals are not self-similar.

During this talk we will show how, by choosing the labyrinth patterns in an appropriate way, one can obtain... almost everything.

The results stem from joint work with Bertran Steinsky and Gunther Leobacher.
Cusp catastrophe in lattice based models of phase transitions

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Catastrophe theory studies the critical points of smooth functions, by which we can gain insight into the behavior of systems of interest. We let $F(x, u)$ denote the function called universal unfolding, where the function $f(x)$ represents the state of the system and the parameter $u$ describes dependency of the system on external forces. The cusp catastrophe is universal unfolding of the function $f(x) = x^4$.

It has been shown that this catastrophe is manifested in many systems [3]. Here we are going to focus on systems in which the phase transition occurs. A known example is Van der Waals equation of state of the ideal gas from which we can easily come to the cusp catastrophe surface (the set of critical points of all partial functions $F_u(x)$ of $F$). Even more remarkable occurrence of the cusp catastrophe appears in the lattice based models of ferromagnetism, in particular in the Ising model. In spite of simplicity of the model in which a block of iron is regarded as a collection of atoms whose positions are fixed in a crystalline lattice, and each atom has a magnetic spin being either upward or downward, the equation of state is also described by no other than cusp catastrophe surface.

References


Maximal matchings and packings

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A matching $M$ in a graph $G$ is a collection of edges of $G$ such that no two edges from $M$ have a vertex in common. The number of edges of $M$ is called the size of the matching. Small matchings are not interesting – they are easy to find and enumerate. Hence, we are mostly interested in matchings that are as large as possible. There are two ways to quantify the idea of “large” matchings, one of them based on their cardinality, the other based on the set inclusion.

A matching $M$ is maximum if there is no matching in $G$ with more edges than $M$. The cardinality of any maximum matching in $G$ is called the matching number of $G$. A matching $M$ in $G$ is maximal if it cannot be extended to a larger matching in $G$, i.e., if no other matching in $G$ contains it as a proper subset. Obviously, every maximum matching is also maximal, but the opposite is generally not true. The cardinality of any smallest maximal matching in $G$ is the saturation number of $G$.

A closely related concept of packing is a generalization of matching. An $H$-packing of $G$ is a collection of vertex-disjoint subgraphs of $G$ such that each component is isomorphic to $H$. Hence, a matching of $G$ is a $P_2$-packing in $G$, where $P_2$ denotes a path on 2 vertices. Again, we are interested only in large packings. If a packing is a spanning subgraph, we say that the packing is perfect; if no other $H$-packing has more components, the packing is maximum; finally, if an $H$-packing cannot be extended to a valid $H$-packing, we say that it is a maximal $H$-packing. The $H$-packing number and $H$-saturation number are defined in the same way as for matchings.

Maximal matchings and packings can serve as models of several physical and technical problems such as the block-allocation of a sequential resource or adsorption of dimers and/or polymers on a structured substrate or a molecule. When that process is random, it is clear that the substrate can become saturated by a number of units much smaller than the theoretical maximum. The respective saturation numbers provide an information on the worst possible case of clogging; they measure how inefficient the adsorption or the allocation process can be. However, in order to assess its efficiency, we also need to know how likely it is that
a given number of units will saturate the substrate. Hence, we must study the enumerative aspects of the problem.

In this talk we present several results about the enumerative aspects of maximal matchings and maximal $P_m$-packings in paths and cycles.
Lego-like spheres and tori, enumeration and drawing

Mathieu Dutour Sikirić
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We consider maps on the sphere or torus for which every vertex has degree $k$ and faces are of size $a$ or $b$. We suppose that faces are arranged in clusters with each cluster containing one $a$-gon or one $b$-gon. We suppose that all such clusters are isomorphic. We report the obtained results for spheres and tori. We also give details on the computer enumeration method used to get those maps. Then we expose in detail the program that we wrote to make the drawings of those maps in a practical way.
An enumeration of non-directed diagonally convex polyominoes

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Already 20 years ago, column-convex polyominoes and directed diagonally convex polyominoes were well explored models. By contrast, nothing was known about general (i.e., non-directed) diagonally convex polyominoes. So in her habilitation thesis, published in 1996, Mireille Bousquet-Mélou wrote: “En comparant aux tableaux précédents les nombreux travaux effectués, on est d’abord frappé par le fait que la convexité diagonale n’a été que peu étudiée”. In the meantime, the things have not changed. Combinatorialists somehow got used to this gap in their knowledge.

But the gap will be filled (at least partly) in this lecture. Namely, we have enumerated nondirected diagonally convex polyominoes by perimeter. The perimeter generating function is very complicated and satisfies an algebraic equation of degree eight. The Taylor series expansion of that generating function is

\[ x^4 + 2x^6 + 7x^8 + 28x^{10} + 122x^{12} + 556x^{14} + 2618x^{16} + 12634x^{18} + 62128x^{20} + 310212x^{22} + 1568495x^{24} + 8014742x^{26} + 41323641x^{28} + 214719610x^{30} + \ldots \]
On the Graovac-Ghorbani index of bipartite graphs

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The atom-bond connectivity (ABC) index is a well-known degree-based molecular structure descriptor with a variety of chemical applications. In 2010 Graovac and Ghorbani introduced a distance-based analog of this index, the Graovac-Ghorbani (GG) index, which yielded promising results when compared to analogous descriptors. In this talk, we investigate the structure of graphs that maximize and minimize the GG index. Specifically, it is shown that amongst all bipartite graphs, the minimum GG index is attained by a complete bipartite graph, while the maximum GG index is attained by a path or a cycle-like graph; the structure of the resulting graph depends on the number of vertices. Along the way, we also derive an asymptotic estimate of the GG index of paths. In order to obtain our results, we introduce a normalized version of the GG index and call it the normalized Graovac-Ghorbani (NGG) index. Finally, we discuss some related open questions as a potential extension of this work.
Some improvements to the fault-tolerant group Steiner tree problem

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We are given an undirected graph $G = (V, E)$ with edge costs $c : E \to \mathbb{R}^+$, a collection of $k$ subsets $G_1, G_2, \ldots, G_k$ that are called groups and some vertex $r$. Our goal is to compute a subgraph $H$ of minimum cost $c(H) = \sum_{e \in E(H)} c(e)$ such that, for each $i \in [k]$ there exist at least two paths between vertices in $G_i$ and $r$. This problem is known as a fault-tolerant group Steiner tree problem (FGST) which generalizes a very important combinatorial optimization problems such as Steiner tree and set cover problem. This talk presents some improvements over results of Khandekar et al. (2012) to the specific version of FGST where each group $G_i$ contains at most $\gamma = O(1)$ vertices.
Counting the number of closed walks in a graph

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Let $G$ be a graph without loops and multiple edges, and with the vertex set $V = \{1, 2, \ldots, n\}$. A walk of length $k$ in $G$ is any sequence of (not necessarily distinct) vertices $v_1, v_2, \ldots, v_k, v_{k+1} \in \{1, 2, \ldots, n\}$ such that for each $i = 1, 2, \ldots, k$ there is an edge between the vertices $v_i$ and $v_{i+1}$. A walk starting and terminating at vertex $v \in \{1, 2, \ldots, n\}$ is called a closed walk at $v$. A closed walk in a graph is called a spanning closed walk if it passes through all vertices of the graph. A graphlet in a graph is a small connected induced rooted subgraph of the graph.

In this talk, a formula for counting the number of closed walks of certain length at a particular vertex of a graph will be presented. The formula is based on the number of spanning closed walks in the graphlets of particular types. The number of spanning closed walks in a rooted graph is counted by using the inclusion-exclusion principle.

This investigation is related to the network alignment problem. The presented spectral formula is applied to defining the measure of similarity between vertices of considered networks (i.e. graphs with large number of vertices).

The talk is based on the results exposed in the papers:

- Jovanović I.M., Closed walks and graphlets, accepted for publication in Utilitas Mathematica, UM 13-338. (ISSN 0315-3681, M23), and

On the torsion group of elliptic curves induced by Diophantine triples over quadratic fields

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If \(a, b, c\) are elements of some commutative ring and \(ab + 1\), \(ac + 1\) and \(bc + 1\) are squares in a ring, than \(\{a, b, c\}\) is called a Diophantine triple.

The problem of extendibility of Diophantine triples in \(Q\) is closely connected with the properties of elliptic curves induced by them.

The possible torsion groups of elliptic curves induced by Diophantine triples over quadratic fields, which do not appear over \(Q\), are \(\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/10\mathbb{Z}\), \(\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}\) and \(\mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}\).

We showed that all these torsion groups indeed appear over some quadratic field. Moreover, we proved that there are infinitely many Diophantine triples over quadratic fields which induce elliptic curves with these torsion groups.

Joint work with A. Dujella and I. Soldo.
Incidence coloring of graphs

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An incidence in a graph $G$ is a pair $(v, e)$ where $v$ is a vertex of $G$ and $e$ is an edge of $G$ incident to $v$. Two incidences $(v, e)$ and $(u, f)$ are adjacent if at least one of the following holds: (1) $v = u$, (2) $e = f$, or (3) $vu \in \{e, f\}$. An incidence coloring of $G$ is a coloring of its incidences assigning distinct colors to adjacent incidences. The originators, Brualdi and Quinn Massey (R. A. Brualdi, J. J. Quinn Massey, Incidence and strong edge colorings of graphs, Discrete Math. 122(1–3) (1993), 51–58), conjectured that every graph $G$ admits an incidence coloring with at most $\Delta(G) + 2$ colors. The conjecture is false in general (B. Guiduli, On incidence coloring and star arboricity of graphs, Discrete Math. 163(1–3) (1997), 275–278), but there are many classes of graphs for which it holds. We will present main results from the field and introduce some of our recent ones. Namely, we will focus on incidence coloring of Cartesian products of graphs (P. Gregor, B. Lužar, and R. Sotáč, On incidence coloring conjecture in Cartesian products of graphs, Discrete Appl. Math. 213 (2016), 93–100) and subquartic graphs (P. Gregor, B. Lužar, and R. Sotáč, Note on incidence chromatic number of subquartic graphs, J. Combin. Optim. (2016), published online).
Similarity graphs and growth curve clustering

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The problem of growth curve clustering is analyzed and its connection with the spectral methods is described. It is shown that a nearly optimal curve partition can be obtained from the eigen decomposition of a specific matrix associated with a certain type of graph which contains information on similarities between curves. Results are illustrated on the set of synthetically generated set of curves and on one real world example.
On the total positivity via Aissen-Schoenberg-Whitney theorem

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Total positivity (TP) is a powerful concept that arises in various branches of mathematics. A matrix $M = [m_{i,j}]_{i,j \geq 0}$ is totally positive if all its minors are non-negative real numbers. A remarkable spectral property of an $n \times n$ totally positive matrix $M$ is that $M$ has $n$ distinct positive eigenvalues. Any totally positive matrix can be realized as a matrix of generalized complete homogeneous symmetric functions evaluated at non-negative real numbers. Total positivity of some types of triangular matrices, including Catalan triangles by Aigner and by Shapiro can be proved using the Aissen-Schoenberg-Whitney Theorem. On the base of these ideas, we demonstrate TP of some combinatorial matrices. In addition, we present a class of totally positive matrices, defined by means of hyper-sequences that are recently introduced by Dil and Mezö.

References


Computable intermediate value theorem (generalization)

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Let \( f: [a, b] \rightarrow \mathbb{R} \) be a continuous function. The intermediate value theorem states that if \( u \) is any number in the interval \( (f(a), f(b)) \), then there exists a number \( c \in (a, b) \) such that \( f(c) = u \). As a consequence of this theorem we get a result, which states that if \( f: [0, 1] \rightarrow \mathbb{R} \) is a continuous function such that \( f(0) < 0 \) and \( f(1) > 0 \), then it has a root in the segment \([0, 1]\).

Let us now take a computable function \( f: [0, 1] \rightarrow \mathbb{R} \) such that \( f(0) < 0 \) and \( f(1) > 0 \). Then there exists a computable number \( x \in [0, 1] \) such that \( f(x) = 0 \). This is a computable version of the intermediate value theorem. In this paper we observe a generalization of this theorem.

Suppose that \( K \) is a connected subset of \( \mathbb{R}^2 \) which intersects both components of \( \mathbb{R}^2 \setminus S \). Then \( K \) certainly intersects \( S \). The question is does the following implication hold:

\[
K \text{ computable } \implies K \text{ intersects } S \text{ in a computable point}.
\] (1)

Suppose \((X, d, \alpha)\) is a computable metric space. Let \( U \) and \( V \) be disjoint and computably enumerable open sets in this space and let \( S = X \setminus (U \cup V) \). Suppose \( K \subseteq X \) is a chainable continuum which intersects \( U \) and \( V \). We prove that (1) holds under assumption that \( K \cap S \) is totally disconnected. From this result it follows that if \( A \) is a computable arc which intersects \( U \) and \( V \), then \( A \) intersects \( S \) in a computable point.

Key words: computable metric space, chainable continuum, computable compact set, computably enumerable open set, computable point

MSC 2010: 03D78
References


Absolute real root separation

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While the separation (the minimal nonzero distance) between roots of a polynomial is a classical topic, its absolute counterpart (the minimal nonzero distance between their absolute values) does not seem to have been studied much. We present the general context and give tight bounds for the case of real roots.

Joint work with Yann Bugeaud, Andrej Dujella, and Bruno Salvy.
Global forcing number for maximal matchings

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A matching in a graph \( G \) is any set of edges \( M \) such that every vertex in \( G \) is incident to at most one edge from \( M \). We say that matching \( M \) is maximal if there is no matching \( M' \) such that \( M \) is contained in \( M' \). A global forcing set for maximal matchings of a graph \( G \) is every set of edges \( S \) such that intersections of any two maximal matchings and \( S \) are different. The cardinality of the smallest global forcing set is called the global forcing number for maximal matchings in \( G \). We establish extremal values of global forcing number for maximal matchings on trees, on general graphs and on the class of graphs with given cyclomatic number. Also, we characterize graphs for which extremal values are obtained.
Finding largest small polygons via symbolic computations

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A small polygon is a convex polygon (in a plane) of unit diameter. The problem of determining the largest area of small \( n \)-gons was already studied by Reinhardt in 1922. He showed that for \( n \) odd the regular \( n \)-gon is optimal. For even \( n \) this is not the case. For \( n = 6 \) the largest area \( F_6 \), a plane hexagon of unit area can have, satisfies a 10th degree irreducible equation with integer coefficients. This is the famous Graham’s largest little hexagon (1975). R.L. Graham (with S.C. Johnson) needed factoring a 40-degree polynomial with up to 25-digit coefficients. Graham introduced the diameter graphs by joining the vertices at maximal distance. For \( n=6 \) (resp. 8) there are 10 (resp. 31) possible diameter graphs. The case \( n = 8 \) was attacked by C. Audet, P. Hanson, F. Messine via global optimization (10 variables and 20 constraints) which produced (an approximate) famous Hansen’s little octagon.

In this talk we report on reduction for \( F_6 \) of the auxiliary polynomial to degree 14 (instead of 40) by rational substitutions (a “missed opportunity” in Graham and Johnson’s approach). Also for the first time, under axial symmetry conjecture, we obtained explicit equations for \( F_8 \) (resp. \( F_{10} \)) of degree 42 (resp. 152) via intriguing symbolic iterated discriminants computations (sometimes involving 2800 digit numbers).
Using Group Steiner Problem to model a government formation

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In democratic societies, after the elections, the goal of government formateur is to form a leading political majority in the parliament which aims to achieve a certain level of stability and expertness. In this talk, we present a Government Formation Problem (GFP) as an optimization problem which can be modelled by formulating several Group Steiner Problems on the corresponding social graph $G=(V,E)$ induced by political candidates (members) $V$. The edges $E$ describe a cooperability between members $V$ and the level of cooperability, namely, a cooperability distance, is assigned for every edge in $E$. Also, we are given set of candidates for (prime) minister and official positions in governmental departments (ministries). The goal is to find a prime minister and at least one minister for each ministry, such that all ministers are connected to prime minister while the total cooperability distance is minimized. Moreover, we add to our model a minister dispersity, i.e. a value of the optimal solution cost of the following problem: for a given ministry and a given minister candidate find a subset of officials such that for each ministry department there is at least one official who is eligible for that department and all officials are connected to the minister candidate, while the total cooperability distance is minimized. Using this two-stage approach, our covering and connectivity constraints are used to ensure the expertness and cooperability of a ministry/government and the minimum total cost of the final solution ensures the stability of the government. We show the NP-hardness of the problem and present an integer linear programming based algorithm to obtain a solution.

Keywords: Government Formation Problem, social graph, Team Formation Problem, integer linear programming
Balaban index is defined as \( J(G) = \frac{m}{m-n+2} \sum \frac{1}{\sqrt{w(u)w(v)}} \), where the sum is taken over all edges of a connected graph \( G \), \( n \) and \( m \) are the cardinalities of the vertex and the edge set of \( G \), respectively, and \( w(u) \) (resp. \( w(v) \)) denotes the sum of distances from \( u \) (resp. \( v \)) to all the other vertices of \( G \). In the talk, we present an upper bound for the Balaban index of \( r \)-regular graphs on \( n \) vertices, and also improved bound for fullerene graphs. Next we consider graphs of order \( n \) with minimum Balaban index. In the talk we will present also some other results and problems about this index and its sum variation.
Resonance graphs of carbon nanotubes and fullerenes

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University of Maribor, Slovenia

Carbon nanotubes are chemical compounds made of carbon which possess a cylindrical structure. Open-ended single-walled carbon nanotubes are called tubulenes. A fullerene is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. The resonance graph of a benzenoid system, tubulene or fullerene reflects the interference among its Kekulé structures.

In the talk some basic properties of resonance graphs will be considered and the differences according to the specific family of graphs will be presented.

Joint work with Petra Žigert Pleteršek, Tomislav Došlić and Dong Ye.
A structure theorem for some families of sets of non-negative integers

Salvatore Tringali
University of Graz, Austria

Let $H$ be a commutative (multiplicative) monoid with the property that every non-unit element can be written as a finite product of atoms.

For every $k \in \mathbb{N}^+$, let $U_k(H)$ denote the set of all $l \in \mathbb{N}^+$ for which there are atoms $u_1, \ldots, u_k, v_1, \ldots, v_l \in H$ such that $u_1 \cdots u_k = v_1 \cdots v_l$.

A fundamental result in factorization theory, commonly referred to as the Structure Theorem for Unions of Sets of Lengths, states that, for all sufficiently large $k$, the sets $U_k(H)$ are almost arithmetic progressions with the same difference and bound.

In this talk, I will present a generalization of the above result, which requires nothing beyond basic knowledge in additive combinatorics. In particular, the new approach allows to show for the first time that the Structure Theorem is still true for some classes of possibly non-cancellative monoids, including semigroups of modules and semigroups of (not necessarily invertible) ideals of Noetherian domains.
Some properties of hyperfibonacci sequences

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Hyperfibonacci sequences are defined starting with Fibonacci sequence as the first hyperfibonacci sequence \( \left( F_n^{(0)} \right)_{n \geq 0} = (f_n)_{n \geq 0} \). Each of the following hyperfibonacci sequences \( \left( F_n^{(r+1)} \right) \) is the sequence of all partial sums of the previous hyperfibonacci sequence \( \left( F_n^{(r)} \right) \), i.e., \( F_n^{(r+1)} = \sum_{0}^{n} F_n^{(r)} \). Some formulas similar to those valid for Fibonacci numbers are presented, e.g., \( F_n^{(r+1)} = F_n^{(r)} + F_n^{(r)} + \binom{n+r}{r-1} \) (a generalization of \( f_{n+2} = f_{n+1} + f_n \)), a formula \( F_n^{(r)} = \sum_{0}^{\left\lfloor \frac{n-1}{2} \right\rfloor} \binom{n-r-k-1}{r+k} \) (a generalization of \( f_n = \sum_{k=0}^{\left\lfloor \frac{n-1}{2} \right\rfloor} \binom{n-k-1}{k} \)).

References


On Candido’s identity

DARKO VELJAN
University of Zagreb, Croatia

The Candido identity published first in 1951, says that the square of the sum of three consecutive Fibonacci numbers is equal twice the sum of their fourth powers. We first provide an elegant one-sentence proof. Then we relate it to a much broader context including examples in combinatorics, geometry and number theory. The talk is based on author’s paper to appear in Mathematical Intelligencer.
Modelling efficient same-source multiple broadcasting

VIDA VUKAŠINOVIĆ
Jožef Stefan Institute, Slovenia

In this work we study same-source multiple broadcasting under communication model with restrictions that: a) different messages cannot arrive in the same vertex at a unit time step (1-in port model), b) every received message can be sent to neighbors only in the next step (no-buffer model), and c) at every step, a message is sent only to vertices which have not received it yet (non-repeating model). We use the concept of level-disjoint partitions to study how many messages and in what time can be simultaneously broadcasted under the communication model from a given source vertex in a given graph. We provide a necessary condition in terms of girth and eccentricity of the root for existence of $k$ same-rooted level-disjoint partitions of optimal height and we provide a structural characterization of graphs that admit simultaneous broadcasting of two messages from a given vertex.

Joint work with Petr Gregor and Riste Škrekovski.
Measuring vertex importance (centrality) in a graph has been extensively studied and it is one of the central topics in the complex network theory. In chemistry, the importance of atoms in molecule is completely opposite and it seems that peripheral atoms are much more significant. Here, inspired by complex network theory counterparts, peripherality indices will be proposed and their usefulness in QSAR studies will be demonstrated by showing that descriptors based on the concept of peripherality can be used in study of biological activity of phenethylamines. It will be shown that the biological activity can be well predicted by a simple linear one-parameter model using newly defined descriptors.
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