Projekti – OR 2024/2025
pri predmetu Finančni praktikum

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1 Osnovno o projektu

Osnove:

- Pričakovana obremenitev posameznega študenta za projekt je 60 ur.
- Vsak projekt izdela skupina. Skupina ima lahko dva ali tri študente. Skupine so naključne in jih določi učitelj.
- Študenti v isti skupini lahko dobijo različne ocene.
- Vsaka skupina dobi smernico. Pri določanju točne vsebine imate nekaj **fleksibilnosti**.
- Projekt mora vsebovati programiranje in **eksperimente**. Lahko si izberete programsko okolje, v katerem boste delali. Lahko najdete podatke na internetu, lahko jih pa tudi generirate sami.
- Na koncu projekta bo zagovor.
- Asistent J. Vidali in prof. R. Škrekovski sva na voljo na konzultacije, pomoč itd.

Za programiranje in poročila predlagamo, da uporabljate **GitHub**, ni pa nujno. Priporočamo tudi, da za programiranje uporabljate okolje **Sage** (SageMath) – gre za okolje, osnovano na programskem jeziku Python, z dodano podporo za matematiko (posebej bo prišla v upoštev podpora za grafe in celoštevilsko linearno programiranje).

Na koncu bomo imeli sestanek oziroma zagovor projekta s predavateljem in asistentom, kjer bo določena ocena projekta. Za zagovor, ki bo trajal do pol ure, lahko pripravite kratko predstavitev (max 20 min). Na zagovoru pričakujemo tudi argumentacijo smiselnosti vašega dela (zakaj se ste tako lotili) ter seveda razumevanje kode programa in eksperimentov.

Naloge:

- Razumevanje problema.
- Izbira natančnega problema (ali svojo varianto problema) iz reference.
- Izdelava kratkega (do 2 strani) opisa problema in načrta za nadaljnje delo.
- Programiranje rešitev ali rešitve izbranega problema.

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- Generiranje naključnih ali iskanje realnih podatkov za problem.
- Eksperimentiranje z napisanim programom in generiranimi podatki.
- Poročilo.
- Predaste, kar ste naprogramirali, s kratkimi navodili za uporabo (lahko tudi kot komentar v kodi). Koda programa mora biti lepo komentirana.
- Zagovor, kjer predstavite izdelek. Pomembno je, da razumete in lahko zagovarjate, kaj ste delali in uporabljali (tudi kodo programa).

Poročilo:

- Približno 5 strani (fleksibilno).
- Vsebuje jasen opis problema.
- Vsebuje glavne ideje programa ali psevdokodo.
- Vsebuje jasen opis generiranja ali izbiranja podatkov.
- Prikaže grafe, tabele ali drugačen opis eksperimentov (npr. kako se poveča čas izvajanja z velikostjo problema).

2 Koledar

Letos bomo imeli dva termina za projekt. Vsak študent izbere, v katerem terminu bo delal projekt. Termina ne smete spremeniti. *Rok za izbiro termina je 23. oktober 2024*, izbira pa bo potekala preko spletne učilnice.

Z **zvezdico** so označene težje naloge. Če bi se kdo rad lotil težje naloge, naj prosim obvesti asistenta **pred rokom za izbiro termina** (povejte, kdo bo v skupini in katere naloge bi se radi lotili). Ostali boste naključno razdeljeni v skupine, tem pa bo naključno dodeljena ena izmed nalog brez zvezdice.

Prvi termin:

- Dodelitev skupin in tem: 25. oktober 2024.
- Rok za kratek opis: 15. november 2024.
- Rok za poročilo in program: 13. december 2024.
- Zagovori: 16.–20. december 2024. Datumi bodo določeni kasneje.

Drugi termin:

- Dodelitev skupin in tem: 6. december 2024.
- Rok za kratek opis: 27. december 2024.
- Rok za poročilo in program: 31. januar 2025.
- Zagovori: 3.–7. februar 2025. Datumi bodo določeni kasneje.

3 Projekti

3.1 Metric Dimension

We say that a vertex s *resolves* a pair of vertices x, y in a graph G if $d(s,x) \neq d(s,y)$. A set of vertices S is a *resolving* set of G if every pair of vertices x, y of G is resolved by some vertex s from S. The *(vertex) metric dimension* of a connected graph G, denoted by $\dim(G)$, is defined as the size of a smallest set $S \subseteq V(G)$ which distinguishes all pairs of vertices in G.

We can similarly define the *edge metric dimension* of a connected graph G, denoted by $\mathrm{edim}(G)$, as the size of a smallest set $S \subseteq V(G)$ which distinguishes all pairs of edges, i.e., for each pair of edges e, f of G, there exists a vertex $s \in S$ such that $d(s,e) \neq d(s,f)$. Here, for an edge $e = uv$, we have $d(s,e) = \min\{d(s,u), d(s,v)\}$.

Another invariant which has been studied is the *mixed metric dimension*, where we resolve both edges and vertices in a graph, meaning that we want to distinguish every pair of vertices, every pair of edges, and every vertex from every edge. Denoted by $\mathrm{mdim}(G)$, it is the size of a smallest set $S \subseteq V(G)$ which distinguishes all pairs of vertices and edges.

This part involves various new and old metric dimensions. See the online survey [5] that gives an introduction and the state of the art of the topic.

Group 1: Identities with Vertex-, Edge-, and Mixed-metric Dimensions (2 students, part 1)

ILP models for these three metric dimension are known. Implement them in Sage in order to search for graphs for which

$$\dim(G) = \mathrm{edim}(G) = \mathrm{mdim}(G)$$

and also find graphs for which

$$\mathrm{mdim}(G) = \dim(G) + \mathrm{edim}(G).$$

For small graphs, apply a systematic search; for larger ones, apply some stochastic search. Do these graphs have any common structure? If so, maybe you can narrow your search to similar graphs in order to reduce the graph space and find even more such graphs. Also repeat your search for trees. Report your results.

Group 2: Fault-Tolerant Metric Dimension (2 students, part 1)

As defined above, in a graph G, a set S is *resolving* if for every pair $x, y \in V(G)$ there exists $s \in S$ such that $d(x,s) \neq d(y,s)$. A resolving set S for a graph G is *fault-tolerant* if $S \backslash \{v\}$ is also resolving for each $v \in S$. The *fault-tolerant metric dimension* of G is the cardinality of a smallest fault-tolerant resolving set S, and it is denoted by $\mathrm{ftdim}(G)$. Implement an ILP for computing the fault-tolerant metric dimension according to [8] and answer the following questions.

- Find graphs G with $\dim(G) = 2$ and $\mathrm{ftdim}(G) = 5, 6, 7$ or more.

For small graphs, apply a systematic search; for larger ones, apply a simulated annealing search. Report your results.

Group 3: Doubly-Resolving Metric Dimension (2 students, part 1)

A set $S \subseteq V(G)$ is a *doubly-resolving* set if for every pair of vertices $x, y \in V(G)$ there exists a pair of vertices $u, v \in S$ such that $d(x,u) - d(x,v) \neq d(y,u) - d(y,v)$. The *doubly resolving metric dimension* of a graph G is the cardinality of a smallest doubly-resolving set and it is denoted by $\mathrm{dbdim}(G)$. Implement an ILP for computing the doubly-resolving metric dimension according to [4] and answer the following questions.

- It is known that every doubly-resolving set is also a resolving set, hence $\text{dbdim}(G) \leq \dim(G)$. Find graphs (resp. trees) for which equality holds.
- Determine the doubly-resolving metric dimension of trees – possibly it could be a formula.
- Find graphs for which the doubly-resolving metric dimension differs from the mixed metric dimension.

For small graphs, apply a systematic search; for larger ones, apply a random search. Report your results.

Group 4: Metric dimension of directed graphs (2 students)

In a directed graph, if there is a directed path from a vertex u to a vertex v, then we take for the distance from u to v to be the length of a shortest such path. If such a path exists, we say that v is reachable from u. If there is no directed path from u to v, the we usually have $d(u,v) = \infty$ and consider that v is not reachable from u. If a directed graph is strongly connected then every vertex is reachable from every other vertex.

We say that a vertex s *resolves* a pair of vertices x and y if both x and y are reachable from s but on distinct distances, i.e., $d(s,x) \neq d(s,y)$. A set of vertices S resolves G if every pair of vertices of G is *resolved* by some vertex form S. The smallest size of such a set S is the *metric dimension* of the directed graph G.

Write an ILP model to determine the metric dimension of directed graphs. Then, consider clockwise directed circulant graphs $C(n,d)$. Note that they are strongly connected. For many small values of n and d, determine the metric dimension of $C(n,d)$, and then try to guess/obtain a general formula for the metric dimension of $C(n,d)$. Report your results.

3.1.1 Weak metric dimension

Let $S \subseteq V(G)$ and $a,b \in V(G) \cup E(G)$. We define $\Delta_S(a,b)$ as the sum of distance differences from a and b to each vertex of S, i.e., $\Delta_S(a,b) = \sum_{s\in S} |d(s,a) - d(s,a)|$. We abbreviate $\Delta_{V(G)}(a,b) = \Delta(a,b)$.

The *weak (vertex) k-metric dimension* $\text{wdim}_k(G)$ of a graph G is defined as the cardinality of a smallest set of vertices S such that for every pair of vertices $x,y \in V(G)$, we have $\Delta_S(x,y) \geq k$. Similarly, the *weak edge k-metric dimension* $\text{wedim}_k(G)$ of a graph G is defined as the cardinality of a smallest set of vertices S such that for every pair of edges $e,f \in E(G)$, we have $\Delta_S(e,f) \geq k$. Finally, the *weak mixed k-metric dimension* $\text{wmdim}_k(G)$ of a graph G is defined as the cardinality of a smallest set of vertices S such that for every pair of vertices or edges $a,b \in V(G) \cup E(G)$, we have $\Delta_S(a,b) \geq k$. The maximum values of k for which the weak k-metric dimension, the weak edge k-metric dimension and the weak mixed k-metric dimension are defined are denoted by $\kappa(G)$, $\kappa'(G)$, and κ"(G), respectively.

Group 5: Weak Mixed k-Metric Dimension (2 students, part 2)

Following the paper [6], implement an ILP model for this invariant, and then write separate small programs in Sage to answer each of following questions by exhaustive search.

1. Determine κ"(G) and $\text{wmdim}_k(G)$ for cycles, complete graphs, bipartite complete graphs, hypercubes and Cartesian products of cycles, and try to guess the possible formulas based on the computations.

2. Try to determine the graphs G for which $\mathrm{wmdim}_k(G)$ is small, say 1, 2, 3. Also, determine graphs for which $\mathrm{wmdim}_k(G)$ is large, say n or $n-1$ or $n-2$, where n is the order of G.

For small graphs, apply a systematic search; for larger ones, apply some stochastic search. Report your results.

3.1.2 Adjacency metric dimension

In the case of adjacency metric dimension, a pair of vertices x and y of a graph G is resolved by a set of vertices S if S contains a vertex v that is adjacent to precisely one of x and y. We look for a smallest set S that resolves every pair of vertices in G and denote its size by $\dim_A(G)$. See Section 5 from the survey [5] for more details.

Note that the problem of finding the adjacency metric dimension of a graph G can be formulated as an integer linear programming problem in the following way. For $u, v \in V(G)$, we define the integer

$$n_{u,v} = \begin{cases} 1 & \text{if } uv \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

The ILP is now stated as follows.

$$\begin{aligned} & \min \sum_{v \in V(G)} x_v \\ \text{s.t.} \quad & \sum_{u \in V(G)} \left| n_{u,v} - n_{u,w} \right| \cdot x_u + x_v + x_w \geq 1 \qquad \text{for every } v, w \in V(G), \\ & x_v \in \{0,1\} \qquad \text{for every } v \in V(G). \end{aligned}$$

We then have $x_v = 1$ if and only if $v \in S$.

Group 6: Adjacency metric dimension – A (2 students, part 1)

Implement the ILP model for the adjacency metric dimension as described above. Next, answer the following questions.

1. Determine which graphs G satisfy $\dim_A(G) = 1, 2$, or 3.

2. Determine which graphs G satisfy $\dim_A(G) = n, n-1, n-2$, where n is order of G.

3. For trees G of order n, determine the lower and upper bounds of $\dim_A(G)$ in terms of the order n. We expect the lower bound will be around $n/2$ and the upper bound should be $n-2$. Also, describe the trees that achieve these bounds.

Group 7: Adjacency metric dimension – B (2 students, part 2)

Use the ILP implementations from the previous group for $\dim(G)$ and $\dim_A(G)$ in order to answer the following questions.

1. Find the graphs for which $\dim(G) = \dim_A(G)$.

2. Study this metric on cartesian, strong and direct products; in particular on grid graphs and toroidal grid graphs.

3. Since $\dim(G) \leq \dim_A(G)$, try to find if there exists a constant c such that $\dim_A(G) \leq c \dim(G)$.

3.1.3 Partition dimension

The *distance* of a vertex v to a given set P of vertices in a graph G is defined as $d(v,P) = \min\{d(v,x) \mid x \in P\}$. Here, we partition the vertices of a given graph into disjoint sets $P_1, P_2, \ldots, P_k$, and for each vertex v of G, we have the *distance vector* $r(v) = (d(v,P_1), d(v,P_2), \ldots, d(v,P_k))$ to the sets of the partition. We want every pair of distinct vertices u and v to have different distance vectors, i.e., $r(u) \neq r(v)$ – if this is the case, we say that we *distinguish* u and v. The *partition dimension* of a graph G is the smallest number k for which there exists a partition $P_1, P_2, \ldots, P_k$ which distinguishes every pair of vertices in G. We write $\mathrm{pdim}(G) = k$. See [5] for details.

We want to test the following conjecture that is proposed in [5]:

Conjecture 1. *If T is a spanning tree of a unicyclic graph G, then* $\mathrm{pdim}(G) \leq \mathrm{pdim}(T) + 1$.

The work will be split into three groups – the first one, A, will deal with small graphs, and the second one, B, with larger graphs. We then want to apply the tools and experience from A and B to some other graphs, considered by group C.

Group 8: Partition dimension – A (2 students, part 1)

Write a program and check the above conjecture systematically for small unicyclic graphs as far as it goes. In order to do so, implement the ILP model for the partition dimension as proposed by J. Vidali.

Let n and D be the order and the diameter of the graph G, respectively, and let k be the maximal number of disjoint sets considered. The ILP is now stated as follows.

$$
\begin{aligned}
& \min t \\
\text{s.t.} \quad & \sum_{i=1}^{k} x_{u,i,0} = 1 && \text{for every } u \in V(G), \\
& i \cdot x_{u,i,0} \leq t && \text{for every } u \in V(G),\ 1 \leq i \leq k, \\
& \sum_{j=0}^{D} x_{u,i,j} \leq 1 && \text{for every } u \in V(G),\ 1 \leq i \leq k, \\
& n \cdot \sum_{j=0}^{D} x_{u,i,j} \geq \sum_{v \in V(G)} x_{v,i,0} && \text{for every } u \in V(G),\ 1 \leq i \leq k, \\
& x_{u,i,0} + x_{v,i,j} \leq 1 && \text{for every } u, v \in V(G),\ 1 \leq i \leq k,\ d(u,v) < j \leq D, \\
& \sum_{\substack{v \in V(G) \\ d(u,v) = j}} x_{v,i,0} \geq x_{u,i,j} && \text{for every } u \in V(G),\ 1 \leq i \leq k,\ 1 \leq j \leq D, \\
& D + \sum_{j=0}^{D} j \cdot (x_{u,i,j} - x_{v,i,j}) \geq (D+1) y_{u,v,i} && \text{for every } u, v \in V(G),\ 1 \leq i \leq k, \\
& \sum_{i=1}^{k} (y_{u,v,i} + y_{v,u,i}) \geq 1 && \text{for every } u, v \in V(G), \\
& x_{u,i,j} \in \{0,1\} && \text{for every } u \in V(G),\ 1 \leq i \leq k,\ 0 \leq j \leq D, \\
& y_{u,v,i} \in \{0,1\} && \text{for every } u, v \in V(G),\ 1 \leq i \leq k.
\end{aligned}
$$

We then have $x_{u,i,j} = 1$ if and only if $d(u,P_i) = j$ – in particular, we have $x_{u,i,0} = 1$ if and only if $u \in P_i$. Note that the ILP will be infeasible if we choose $k < \mathrm{pdim}(G)$. However, choosing k too large may give a problem that is too complex. It is thus advised to start with a small k (say, 3) and then increase it until a solution is obtained.

Use geng to generate unicyclic graphs of a given order. Report your results.

Group 9: Partition dimension – B (2 students, part 1)

Write programs that check for larger graphs, considering where the previous group ended. Use some metaheuristic, say Simulated annealing, for the larger graphs. One possibility is that each time you start with the partition $\{v_1\}, \{v_2\}, \{v_3\}, \ldots, \{v_n\}$, i.e., each vertex in its own set, and you try to join two sets into one. Later, when the sets are larger, you can try to reduce some set by moving its vertices into other sets. As there is no guarantee that you will find the right value of $\mathrm{pdim}(G)$, repeat your evaluation a few times. Report your results.

Group 10: Partition dimension – C (2 students, part 2)

Apply the tools from the groups A and B to evaluate the partition dimension of the following families of graphs.

1. Cartesian products of graphs, in particular $C_n \square C_m$.
2. Circulant graphs $C(n, \{d_1, d_2, \ldots, d_k\})$
3. Hypercubes Q_n.

In order to deal with larger graphs, we can run multiple jobs in parallel on a server by dealing with some subcases. For example, to consider each subset of some vertices v_1, v_2, v_3 being members of the resolving set that we are looking for, one can run 8 jobs simultaneously. Report your results.

3.2 Packing colorings

In a packing coloring, we want to color vertices of a graph by colors $1, 2, 3, \ldots$ so that each pair of vertices of color i is at distance $\geq i + 1$. The smallest number of colors need to color a given graph in such a way is the *packing coloring number* of that graph, $\chi_\rho(G)$. See [1, 7].

Group 11: Packing coloring of subcubic planar graphs (2 students)

We want to find a planar subcubic graph with the packing coloring number as large as possible.

First, implement an ILP model to determine the packing coloring number for a given graph. Next, write a procedure which generates a planar subcubic graph from an existing one. For example, we may randomly select a face f in such a graph G, insert a new vertex v into f, subdivide some of the edges of f, and connect v to some randomly chosen vertices of degree ≤ 2 on the face f. At the end, v should have degree ≤ 3. In addition you can also randomly remove some vertex or edge or randomly rewire some edge while taking care that the graph G is still planar and subcubic.

Finally, having done these two things done, apply as many as possible tests to obtain such a graph with the packing coloring number as large as possible. What is the maximum number you get, how do graphs that achieve the maximum look like? Report your results.

Group 12: Packing coloring of subdivisions of subcubic graphs (2 students)

The subdivision $S(G)$ of a graph G is the graph obtained from G by putting a vertex on every edge of G. Thus, these new vertices are of degree 2.

We want to test the following conjecture: *for every subcubic graph G, $\chi_\rho(G) \leq 5$ holds*, with the possibility of finding a counterexample, i.e., a graph with packing coloring number at least 6, (but perhaps this will not be easy, if possible at all).

First, implement an ILP model to determine the packing coloring number for a given graph. Then, do the following.

(a) Test the conjecture systematically for all small subcubic graphs G, say the order of G to be up to 15 or even more.

(b) Next, apply a stochastic search for larger graphs.

(c) Examine the structure of graphs with the largest value of $\chi_\rho(G)$ obtained in (a) and (b). Perhaps this value will be 5. Implement a new stochastic search amongst similar graphs.

Report your results.

Group 13: Shift Graphs (2 students)

Let n be a positive integer with $n > 2$. The *shift graph* $G_{n,2}$ is defined as follows.

- The vertices of $G_{n,2}$ correspond to the 2-intervals $[a_1, a_2]$ such that $1 \leq a_1 < a_2 \leq n$.
- Two vertices $[a_1, a_2]$ and $[b_1, b_2]$ are adjacent if and only if $a_2 = b_1$.

Here, are all these numbers are integers. The graph $G_{n,2}$ is called the *shift graph* for the parameter n. The following theorem is known.

Theorem 2. *If H is an induced subgraph of $G_{n,2}$ and H does not contain the complete bipartite graph $K_{a,b}$ (with $a + b \leq n - 2$) as a subgraph, then*

$$\chi(H) \leq a + b.$$

Keep the following in mind:

- Various subgraphs H of $G_{n,2}$ can be obtained by systematically or randomly removing vertices from $G_{n,2}$.
- To ensure that H does not contain $K_{a,b}$ as a subgraph, it is sufficient to consider the following:
  - if H has at least a vertices corresponding to intervals of the form $[*, i]$ for some i, then it has strictly fewer than b vertices corresponding to intervals of the form $[i, *]$ for the same i; and symmetrically,
  - if H has at least b vertices corresponding to intervals of the form $[*, i]$ for some i, then it has strictly fewer than a vertices corresponding to intervals of the form $[i, *]$ for the same i.

Your task is using a computer search to find as many subgraphs H and values of a, b, and n such that equality holds in the above theorem, i.e., $\chi(H) = a + b$. For small values of n, use a systematic search; for larger values, apply a stochastic approach.

3.3 Odd colorings

Group 14: Strong odd colorings of graphs (2 students)

An *odd coloring* of a graph is a proper coloring where, in the neighborhood of each vertex, some color appears an odd number of times. Recently, a stronger form of this concept has been introduced. We define it as follows.

A *strong odd coloring* of a simple graph G is a proper coloring of the vertices of G such that for every vertex v and every color c, either c is used an odd number of times in the open neighborhood $N_G(v)$, or no neighbor of v is colored by c. The *strong odd chromatic number* of a graph G is the smallest number of colors needed to color the graph in this way, and it is denoted by $\chi_{\text{so}}(G)$.

This project involves the following tasks.

1. Write a procedure that determines $\chi_{\text{so}}(G)$ for a given graph G.
2. Determine when a unicyclic graph has a strong odd chromatic number equal to 1, 2, 3, or 4. It is known that the strong odd chromatic number of a unicyclic graph is bounded by 4, as established in the referenced paper.
3. Generate outerplanar graphs and investigate whether any have a strong odd chromatic number greater than 7.

For additional details on this kind of colorings and above mentioned classes of graphs, consult the paper Strong Odd Coloring of Graphs.

3.4 Graph indices

Group 15: Pingdingshan number (2 students)

For a connected graph G, we define the Pingdingshan number, denoted by $\mathrm{PDS}(G)$, as the number of paths in the graph, including trivial paths of length 0. Here, we define a path of G of length ℓ as a sequence of vertices $(v_0, v_1, \ldots, v_\ell)$ of G without repetitions (i.e., $v_i \neq v_j$ for all $0 \le i < j \le \ell$) such that every pair of consecutive vertices is connected by an edge of G (i.e., $v_{i-1}v_i$ is an edge of G for all $1 \le i \le n$). Implement a function $\mathrm{PDS}(G)$ that (efficiently) calculates the Pingdingshan number for a given graph G.

Next, for each of the following classes of connected graphs: all graphs, bipartite graphs, triangle-free graphs, and cubic graphs on n vertices, we aim to identify which graph on n vertices have the biggest possible value of the Pingdingshan number. In order to do so, follow the following instructions.

1. For small values of n, say up to 12, perform an exhaustive search through graphs in the class on n vertices.
2. Based on the results from the previous task, make a conjecture about the optimal graphs.
3. For larger values of n, test your hypothesis stochastically.

3.4.1 Sigma irregularities

Irregularity measures quantify to what degree a certain graph is irregular. Thus, they give the value 0 for regular graphs, and a larger value means the graph should be more irregular. Amongst many such measures are also the following two.

The *sigma irregularity* index $\sigma(G)$ is defined as

$$\sigma(G) = \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2.$$

Similarly, the following variant of σ-irregularity, called the *sigma total irregularity*, has been introduced:

$$\sigma_t(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) - d_G(v))^2 .$$

Thus, the sum in the first measure runs through all edges, and in the second it runs through all pairs of vertices.

Group 16: Sigma total irregularity of triangle-free graphs (2 students)

We aim to identify the triangle-free graphs of order n that have the maximum possible sigma total irregularity. To achieve this, follow these steps:

1. First, for small values of n, find the optimal graphs through a systematic search.
2. Second, attempt to generalize your findings for larger n, and test them thoroughly.
3. Formulate a precise conjecture about what the optimal graph(s) will be, and test your conjecture by making small alterations to your candidate(s) – that is, you should always obtain a graph with a smaller sigma total irregularity. Here, you may use some metaheuristic approach.

3.5 Extremizing Antiregular Graphs

The total σ-irregularity is given by

$$\sigma_t(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) - d_G(v))^2 ,$$

where $d_G(z)$ indicates the degree of a vertex z within the graph G. Our aim is to generalize the σ_t irregularity index so that its minimum is still attained by regular graphs, but its maximum is attained by antiregular graphs, i.e., graphs with only one repetition in their degree sequence (in other words, all pairs of vertices except one have different degrees). Specifically, we define the index $\sigma_t^{f(n)}(G)$ as

$$\sigma_t^{f(n)}(G) = \sum_{\{u,v\} \subseteq V(G)} |d_G(u) - d_G(v)|^{f(n)},$$

where $n = |V(G)|$ and $f(n)$ is a function defined for $n \geq 4$. See the paper [3] for more details.

Group 17: Extremizing Antiregular Graphs by Modifying Total σ-Irregularity (2 students)

Below are three problems for which we seek solutions.

Problem 3. *Let $f(n) = \frac{1}{n}$. Is the maximum value of $\sigma_t^{f(n)}(G)$ achieved when G is an antiregular graph?*

Problem 4. *Let $f(n) = c$, where c is a real number in the interval $(0,1)$. Is the maximum value of $\sigma_t^{f(n)}(G)$ achieved when G is an antiregular graph?*

Problem 5. *Let $f(n)$ be a positive function such that $\lim_{n\to\infty} f(n) = 0$. Identify trees that attain the maximum value of $\sigma_t^{f(n)}$.*

Your task is to verify whether the answer to each of these questions is positive or negative through computer testing. Additionally, you should attempt to identify the trees that are extremal. To do this, follow these instructions.

1. For small graphs, apply a systematic search; for larger graphs, apply a stochastic search.
2. Test various values of $c \in (0,1)$, including values close to 0 and values close to 1.

Group 18: Chemical graphs (2 students)

A graph is considered chemical if its vertices have degrees at most 4. If a chemical graph has a_i vertices of degree i, $1 \le i \le 4$, then its degree sequence is denoted by $(1^{a_1}, 2^{a_2}, 3^{a_3}, 4^{a_4})$.

It is evident that the minimum value of $\sigma_t^{f(n)}$ is attained by regular graphs, exemplified by structures like a cycle C_n or graphs with degree sequences such as $(1^0, 2^0, 3^0, 4^n)$. Henceforth, our focus lies on chemical graphs exhibiting the maximum value of $\sigma_t^{f(n)}$.

Theorem 6. *Let $n \ge 7$, $f(n) \le \log_3\left(\frac{3n^2}{3n^2-8}\right)$, and let $(1^{a_1}, 2^{a_2}, 3^{a_3}, 4^{a_4})$ be a degree sequence of a chemical graph G with the maximum value of $\sigma_t^{f(n)}(G)$. Then,*

1. *If $n = 4k-1$, then $a_1 = a_3 = a_4 = k$ and $a_2 = k-1$;*
2. *If $n = 4k$, then $a_1 = a_2 = a_3 = a_4 = k$;*
3. *If $n = 4k+1$, then $a_1 = a_2 = a_3 = k$ and $a_4 = k+1$;*
4. *If $n = 4k+2$, then either $a_1 = a_3 = k$ and $a_2 = a_4 = k+1$, or $a_1 = a_3 = k+1$ and $a_2 = a_4 = k$.*

Since for chemical graphs the difference between degrees of vertices is bounded, we conjecture the following.

Conjecture 7. *The same graphs as in Theorem 6 have maximum value for $\sigma_t^{f(n)}$ if $f(n) = \frac{1}{n}$.*

Conjecture 8. *The same graphs as in Theorem 6 have maximum value for $\sigma_t^{f(n)}$ if $f(n) = c$ is a constant in the interval $(0, 1)$.*

Your task is to determine whether the answer of each of the two questions is positive or negative by testing/experimenting. In order to do so, follow the instructions.

1. For small graphs, apply a systematic search; for larger ones, apply some stochastic search.
2. Take many different values for $c \in (0, 1)$. Let some of them be very close to 0, and some very close to 1.

3.6 Domination number

A subset D of the vertices of the graph is called a *dominating set* of the graph if every vertex v of the graph is in D or adjacent to a vertex of D. The *domination number* of a graph, denoted by $\gamma(G)$, is the size of a smallest dominating set of the graph.

A subset D of the vertices of the graph is called a *total dominating set* of the graph if every vertex v of the graph is adjacent to a vertex of D. The *total domination number* of a graph, denoted by $\gamma_t(G)$, is the size of a smallest total dominating set of the graph.

An interested reader can find more about domination in graphs in the book [2].

Group 19: SDCTD domination (2 or 3 students)

A *simultaneously dominating and complement total dominating set* (SDCTD set for short) of G is defined as a set D which is at a same time a dominating set of G and a total dominating set of $\overline{G}$. The minimum cardinality of a SDCTD set of G is denoted by $\bar{\gamma}(G)$ and is called the *SDCTD* number of G. This variety of graph domination was proposed recently by Sergio Bermudo – a Spanish mathematician from Seville.

The ILP model for determining a smallest SDCTD set D of G is given by

$$
\begin{aligned}
\min \sum_{v \in V(G)} x_v & \\
\text{s.t.} \quad \sum_{w \in N_G(v)} x_w + x_v \geq 1 & \qquad \text{for every } v \in V(G) \\
\sum_{w \in N_{\overline{G}}(v)} x_w \geq 1 & \qquad \text{for every } v \in V(G), \\
x_v \in \{0,1\} & \text{ for every } v \in V(G),
\end{aligned}
$$

and then $D = \{v \in V(G) : x_v = 1\}$.

Implement the above ILP and try to find some interesting relations or properties of $\bar{\gamma}$. Here are few possibilities for illustration.

1. Which graphs of order n attain minimum and which attain maximum values of this domination number?
2. How does this invariant behave with regard to the Cartesian product and other graph products? Can you generate a Vizing-type conjecture?
3. How does $\bar{\gamma}(G)$ behave when the minimum/maximum degree of G is bounded?
4. Calculate $\bar{\gamma}(G)$ for graphs G of diameter 2.
5. Can you bound $\bar{\gamma}(G) + \bar{\gamma}(\bar{G})$ in terms of n?

For small graphs, apply a systematic search; for larger ones, apply a stochastic search.

Group 20: Graphs of type (SB) and domination on their cartesian products (2 students, part 1)

A graph H is of type (SB) if it has diameter 2 and it has two adjacent vertices h_1, h_2 such that

- h_1, h_2 do not have a common neighbour; and
- H has a vertex h^* that is not adjacent to h_1 and not adjacent to h_2, i.e., $h^* \nsim h_1$ and $h^* \nsim h_2$.

We may then partition the vertex set of H as $V(H) = \{h_1, h_2\} \cup A_1 \cup A_2 \cup A^*$, where A_1 is the set of vertices adjacent to h_1, A_2 is the set of vertices adjacent to h_2, and A^* is the set of vertices not adjacent to h_1 or h_2.

Now, consider the following tasks, report your results and provide the graphs for the group C:

(s1) First, write a procedure that can test if a given graph is of type (SB). Then, find all graphs up to $n \leq 10$ vertices that are of this type. How many are there for each small n?

(s2) Next, we want to construct graphs of type (SB) of higher order n randomly.

(s3) We also want to obtain a new graph of type (SB) from a given graph of type (SB) by a small random modification. For example, once you have obtained a graph G as it is described in (s1) or (s2), randomly add/remove a few vertices and/or edges in $A_1 \cup A_2 \cup A^*$ and then start introducing new edges in $A_1 \cup A_2 \cup A^*$ until you obtain a graph of type (SB).

(s4) Use (s1)–(s3) to verify what values the domination number of cartesian product of two graphs of type (SB) can take.

Note 1. One possible way for (s2) is the following: take a pair of adjacent vertices h_1 and h_2, and then fix the sets A_1, A_2, A^* as described above. Now start inserting edges into the set $A_1 \cup A_2 \cup A^*$ until you get a diameter 2 graph.

Note 2. One possibility for (s3) is to randomly add/remove a few vertices and/or edges in $A_1 \cup A_2 \cup A^*$ and afterwards again start introducing edges in $A_1 \cup A_2 \cup A^*$ until you obtain a graph of type (SB).

3.6.1 Domination on modular product graphs

The *modular product* $G \diamond H$ of graphs G and H is a graph with vertex set $V(G) \times V(H)$ that is the union of the cartesian product, the direct product, and the direct product of the complements of G and H:

$$G \diamond H = G \square H \cup G \times H \cup \bar{G} \times \bar{H}.$$

More precisely, two vertices (g, h) and (g', h') of $G \diamond H$ are adjacent if

1. $g = g'$ and $hh' \in E(H)$ or $gg' \in E(G)$ and $h = h'$; or
2. $gg' \in E(G)$ and $hh' \in E(H)$; or
3. (for $g \neq g'$ and $h \neq h'$) $gg' \notin E(G)$ and $hh' \notin E(H)$.

The edges from 1. are the cartesian product edges, the edges from 2. belong to the direct product of G and H, and the edges from 3. are those of the direct product of the complements.

Group 21: Domination on modular product graphs – A (2 students, part 1)

First, implement a function returning the modular product $\diamond$ of given graphs. Then, apply a systematic search for small graphs and use some meta-heuristic (say, simulated annealing) for larger graphs in order to find a graph that solves the following problem.

Problem 9. *Find graphs G that satisfy $\gamma(G \diamond G) \geq \gamma(G) + 2$.*

It is known that if such a graph exists, its diameter must be 2. One can implement a stohastic construction of such graphs in the following way.

1. First, randomly choose a non-complete connected graph G on n vertices.
2. If the diameter of G is larger than 2, then randomly choose two vertices at maximal distance, say u and v. Randomly insert a new edge connecting non-consecutive vertices in a shortest path $P = p_0 p_1 p_2 p_3 \cdots p_k$ connecting $u = p_0$ and $v = p_k$ in order to shorten the distance between u and v. Repeat this step until the diameter decreases to 2.
3. Calculate the domination number of G (which now has diameter 2), hoping it is large.
4. Next, modify the graph a little, say, by randomly removing a few edges, and go to step 2.

Group 22: Domination on modular product graphs – B (1 student, part 2)

Provided by the data and code from groups 20 and 21, test the following claim.

Claim 1. *For a graph G of diameter ≥ 3 and a graph H of type (SB), $\gamma(G \diamond H) \leq 4$ holds.*

Moreover, find as many pairs G, H as possible for which the bound 4 is achieved. Report your results.

3.7 Edge coloring

To obtain an edge coloring of a graph G of maximum degree Δ, we assign colors (actually numbers $1, 2, \ldots$) to edges so that every pair of adjacent edges (i.e., sharing a common vertex) has different colors. For such a coloring, we need at least Δ colors.

Group 23: Rich-neighbor edge-colorings (2 students)*

In an edge coloring, an edge e is called *rich* if all edges adjacent to e have different colors. An edge coloring is called a *rich-neighbor edge coloring* if every edge is adjacent to some rich edge. The smallest number of colors for which there exists such a coloring is denoted by $\chi'_{\mathrm{rn}}(G)$. For example, $\chi'_{\mathrm{rn}}(K_4) = 6$.

We want to verify the following conjecture:

Conjecture 10. *For every graph G of maximum degree Δ, $\chi'_{\mathrm{rn}}(G) \leq 2\Delta - 1$ holds.*

Test the above conjecture for

- non-regular graphs;
- regular multigraphs;
- non-regular multigraphs.

In order to do so, use the code from
`https://github.com/anejrozman/Rich-neighbour-edge-coloring`
or implement it yourself. Try to test the conjecture on smaller graphs as systematically as possible. For larger graphs of maximum degree $\Delta \geq 4$, apply a random search. Report your results.

Group 24: $\mathbb{Z}_2^3$-connectivity (2 students)**

First, we define the $(\mathbb{Z}_2^3, +_2)$ *group*. It consists of the set of all eight binary 3-vectors

$$\mathbb{Z}_2^3 = \{(0,0,0), (0,0,1), (0,1,0), \ldots, (1,1,1)\}$$

with operation $+_2$, which sums two elements binary and componentwise, e.g., $(0,0,1) + (1,0,1) = (1,0,0)$.

Now we define the concept of $\mathbb{Z}_2^3$-*connectivity*. Let G be a graph. A function $\delta : V(G) \to \mathbb{Z}_2^3$ is *zero-sum* if $\sum_{v \in V(G)} \delta(v) = (0,0,0)$. We say that a graph G is $\mathbb{Z}_2^3$-*connected* if for every zero-sum function δ of G, there exists a function $f : E(G) \to \mathbb{Z}_2^3 \setminus (0,0,0)$ such that for every vertex v of G and its incident edges $e_1, e_2, \ldots$, $\delta(v) = f(e_1) + f(e_2) + \cdots$ holds.

Problem 11. *Find a bridgeless graph G that is not $\mathbb{Z}_2^3$-connected with the smallest possible number of 2-edge-cuts.*

Note that the Petersen graph with every edge subdivided is not $\mathbb{Z}_2^3$-connected and it has 15 2-edge-cuts. We also know that graphs with less than four 2-edge-cuts are $\mathbb{Z}_2^3$-connected. So the answer to above problem will be a graph with the number of 2-edge-cuts between 4 and 15. We want to know the right number of 2-edge-cuts or at least to reduce the gap between 4 and 15. Apply a systematic search and report your results.

3.8 Snarks

Every cubic graph has chromatic index 3 or 4 (by Vizing's theorem). A *snark* is a cubic bridgeless graph that has chromatic index 4. Very often it is assumed that snarks additionally must be 3-edge-connected and without triangles (and sometimes even without 4-cycles). Many examples of snarks can be found on the site House of Graphs.

Group 25: Introducing 4-cycles in snarks (2 students)

We want to test whether (and when) introducing 4-cycles in a snark preserves the chromatic index (i.e., the chromatic index remains 4). Introducing a 4-cycle can be done at least in two ways.

1. Take two edges ab and cd in G and subdivide them twice so that you obtain a path au_1u_2b from the edge ab and a path cv_1v_2d from the edge cd. Next, connect u_1 with v_1 and u_2 with v_2.
2. Let ab be an edge of G and a_1, a_2 be the other two neighbors of a, and let b_1, b_2 be the other two neighbors of b. Remove the vertices a and b, add new vertices a_1', a_2', b_1', b_2', add new edges $a_1a_1', a_2a_2', b_1b_1', b_2b_2'$, and connect a_1', a_2', b_1', b_2' into a 4-cycle in some random order.

Download some small snarks from House of Graphs and apply the above operations (iteratively and randomly) to study when the newly constructed graph preserves the chromatic index.

3.9 Fullerenes

Fullerenes are a unique class of carbon molecules composed entirely of carbon atoms arranged in a hollow, spherical, ellipsoidal, or cylindrical structure. In 1996, Sir Harold Kroto, Robert Curl, and Richard Smalley were awarded the Nobel Prize in Chemistry for their discovery of buckminsterfullerene (C_{60}), a new form of carbon with a unique spherical structure.

From a graph-theoretical perspective, a fullerene is a 3-regular, planar graph where each face is either a pentagon or a hexagon. This means the molecular structure of fullerenes can be modeled as a graph in which each carbon atom corresponds to a vertex, and each bond between atoms corresponds to an edge. The most famous fullerene, C_{60}, is modeled as a truncated icosahedron, a polyhedral graph with 12 pentagonal and 20 hexagonal faces. These graph-theoretical representations help in understanding fullerenes' structural stability and chemical reactivity, making them useful in various applications such as nanotechnology, drug delivery, energy storage, and molecular electronics.

Group 26: Diameter of icosahedral fullerenes (2 students)**

The construction of icosahedral fullerenes $F_{i,j}$ is based on a hexagonal lattice, where two integers i and j define the steps in two lattice directions. The fullerene is formed by arranging hexagons and introducing 12 pentagons to close the structure, giving it a spherical shape. The order of such a fullerene is given by $n = 20(i^2 + ij + j^2)$. The parameters i and j determine the fullerene's size and symmetry, and by varying them, a family of icosahedral fullerenes can be systematically generated. For a detailed explanation of this construction method, please refer to the paper Fullerene Graphs and Some Relevant Graph Invariants for more details.

Construct the icosahedral fullerene $F_{i,j}$ of type (i, j). Note that its order is given by $n = 20(i^2 + ij + j^2)$. After constructing the fullerene, compare the ratio of the graph's diameter to $\sqrt{n}$, specifically $\frac{\text{diam}(G)}{\sqrt{n}}$. Your task is to find the optimal ratio between i and j that minimizes this value. Additionally, explore the analogous problem of finding the ratio between i and j that maximizes this value.

Group 27: Distance vector of non-tubical nanotube fullerenes of type (5,0) (2 students)

This project investigates the structure of non-tubical nanotube fullerenes of type $(5,0)$, which consist of $n = 10k$ vertices, with the diameter given by $\frac{n}{5} - 1$. These graphs contain an arbitrarily long cylindrical part, comprised entirely of hexagons, and are closed on both ends by patches made up of 6 pentagons. This construction leads to a combination of flat, hexagonal regions and curved, pentagonal regions, influencing both the symmetry and distance distribution in the graph.

The vertices of these graphs are grouped into k distinct orbits, with each orbit containing 10 vertices. The main goal of the project is to compute the distance vector for a vertex from each orbit as precisely as possible. The distance vector of a vertex is defined so that its i-th coordinate represents the number of vertices located at distance exactly i from the selected vertex. Understanding the distribution of distances across the graph is essential for revealing the fullerene's geometric properties and structure.

For further details on the construction and properties of these nanotube fullerenes, please refer to the paper Wiener Dimension: Fundamental Properties and (5,0)-Nanotubical Fullerenes.

3.10 Various topics

Group 28: Laplacian integral graphs (2 students)

We say that a graph is *Laplacian integral* if all its Laplacian eigenvalues are integers. Find as many as possible unicyclic and bicyclic graphs for which the Laplacian eigenvalues are integers. Apply an exhaustive search for graphs of small order, and apply some stochastic search for larger orders. Try to find a pattern/method for constructing Laplacian integral graphs or at least give some structural property. Apply a systematic search and report your results.

You may find the following two links useful:

- `https://users.fmf.uni-lj.si/mohar/Papers/Spec.pdf`
- `https://web.mit.edu/~jadbabai/www/ESE680/Laplacian_Thesis.pdf`

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