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Contents

Abstract

Two systems are modeled in this thesis. First, we consider a multi-component stochastic monotone binary system, or SMBS for short. The reliability of an SMBS is the probability of correct operation. A statistical approximation of the system reliability is provided for these systems, inspired in Monte Carlo Methods. Then, we are focused on the diameter constrained reliability model (DCR), which was originally developed for delay sensitive applications over the Internet infrastructure. The computational complexity of the DCR is analyzed. Networks with an efficient (i.e., polynomial time) DCR computation are offered, termed Weak graphs.
Second, we model the effect of a dynamic epidemic propagation. Our first approach is to develop a SIR-based simulation, where unrealistic assumptions for SIR model (infinite, homogeneous, fully-mixed population) are discarded.

Finally, we formalize a stochastic process that counts infected individuals, and further investigate node-immunization strategies, subject to a budget constraint. A combinatorial optimization problem is here introduced, called Graph Fragmentation Problem. There, the impact of a highly virulent epidemic propagation is analyzed, and we mathematically prove that Greedy heuristic is suboptimal.

Keywords— Stochastic Binary System, Recursive Variance Reduction Method, Diameter Constrained Reliability, Graph Theory, Complexity Theory, GRASP, SIR Model, Monte Carlo Methods, Epidemic Model

List of publications issued from this thesis work

This thesis was written following a Swedish PhD style. The chapters of this thesis are based on the following published papers:

1. "Diameter-Constrained Reliability: Complexity, Factorization and Exact computation in Weak Graphs", Eduardo Canale, Juan Piccini, Franco Robledo, and Pablo Romero. In Proceedings of the 8th Latin America Networking Conference (LANC 2014), Article No. 12, Pages 1-7, Montevideo, Uruguay.

2. "Recursive Variance Reduction Method in Stochastic Monotone Binary Systems", Eduardo Canale, Héctor Cancela, Juan Piccini, Franco Robledo, Pablo Romero, Gerardo Rubino, and Pablo Sartor. In the Proceedings of the 7th International Workshop on Reliable Networks Design and Modeling (RNDM 2015), pages 135-141, Munich, Germany.

3. "Node-Immunization Strategies in a Stochastic Epidemic Model", Juan Piccini, Franco Robledo, and Pablo Romero. Proceedings of the International Workshop in Machine learning, Optimization and big Data (MOD 2015), Taormina, Italy. Published in the Volume 9432 of the series Lecture Notes in Computer Science, pages 222-232.

4. "A counter-intuitive result on SIR-based Node-immunisation Heuristics", Juan Piccini, Franco Robledo, and Pablo Romero. Submitted to the International Journal of Metaheuristics.

5. "Graph Fragmentation Problem", Juan Piccini, Franco Robledo, and Pablo Romero. In Proceedings of the 5th International Conference on Operations Research and Enterprise Systems (ICORES 2016), Rome, Italy.

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Chapter 1

Introduction

1.1 Systems

In this thesis we work with systems. A *System* is a set of interacting or interdependent components that entail a complex/intricate whole. The importance of systems in today's world is evident. Just consider Power Distribution Networks, Transportation Networks in general, Internet, among others.

Leaving aside questions of efficiency, a system can be in two basic states: operating or not operating (up/down, working/not working, one/zero, on/off, etc.), where the meaning of the term "operating" depends on the context. The correct operation of a system (e.g., a car, a plane, a network, etc.) depends on the correct operation and interactions of their components.

Usually, it is hard to know deterministically when a certain component will fail. Thus, a natural way to model the system's functioning is probabilistically. Sometimes, under certain hypothesis the probability of system failure can be computed explicitly from the probability of failure of its components. This occurs for instance when components fail at random and the failure of one component does not affect the operation of the others. For each state or configuration, the system works or not. This measure is timeless (in a sense that time is not an explicit variable). It depends only of the states of system components, hence the term "*static system*".

Therefore, if we know the configurations for which the system works and their probabilities or weights, we can calculate the probability that the system works, whether explicitly or approximately. In dependent systems, the failure of one component affects the others, which in turn affects system performance. A natural way to model cascade failures is by means of *dynamic systems*. The spatial structure of the system is the ground on which failures evolve.

The object in reliability analysis is to assign a number to each system. As a consequence, reliability analysis falls within the scope of *Metrology*. Thus, reliability is a measure associated to *static systems*. But in most of real-life situations, time plays an relevant role. System configurations change over time and an adequate measure is the system *Resilience*. Resilience is the ability (of a system) to cope with change. In computer networking this implies the ability to provide and maintain an acceptable level of service in the face of faults and challenges to normal operation. Threats and challenges for services can range from simple misconfiguration over large scale natural disasters to targeted attacks.

In order to represent a system, usually a point of departure is to draw a diagram, where nodes represent components that perform a particular task or change in any way as a certain input or influence. The links in turn can represent physical connections, stimuli, influences, interactions, inputs, or other relation.

In this thesis, on/off systems are represented by graphs. Components can be either nodes or links. Already at this stage components under failure are labeled or removed from the system. Therefore it is not surprising the strong correlation between the correct operation of a system and certain properties (such as connectivity) of the underlying graph used to represent it.

1.2 Terminology

The following terminology will be adopted in this thesis. It has been almost entirely taken from PhD thesis of Dr. Claudio Risso.

1. **Graph**
   A *graph* is an ordered pair $G = (V,E)$ comprising a finite set V of *vertices* (or *nodes*) together with a set E of *edges* (or *lines*), which are pairs of vertices of V. When E is a multiset of pairs of vertices (not necessarily distinct), such a graph is called *multigraph* or *pseudograph*, otherwise is called *simple*. Simple also requires graphs with no *loops* (edges connected at both ends to the same vertex). When pairs of nodes in E are unsorted pairs, the graph is referred to as *undirected*. To avoid ambiguity, if the type of the graph is not specified the graph is assumed to be undirected and simple.

2. **Adjacent vertices**
   Given a graph G and two vertices, if these vertices are connected by an edge they are called *adjacent*, whereas the edge is called *incident* to the vertices.

3. **Neighborhood**
   Let $G = (V,E)$ be a graph. Given any node $v \in V$, the *neighborhood* of v or $N(v)$, is the set of nodes adjacent to v.

4. **Degree**
   Let $G = (V,E)$ be a graph. Given any node $v \in V$ we denote as $d_G(v)$ to the number of nodes adjacent to it (i.e. $|N(v)|$). This number is called *degree of* v.

5. **Path**
   Let G be a graph. Given two vertices u and v, a *path* from u to v consists of a sequence of distinct vertices starting at u and ending at v, such that each two consecutive vertices in the sequence are adjacent to each other.

6. **Connected vertices**
   Let G be an undirected graph. Two vertices u and v of G are called *connected* if G contains a path from u to v. Otherwise, they are called disconnected.

7. **Connected Graph**
   A graph G is said to be *connected* if every pair of vertices in the graph is connected.

8. **Articulation Point**
   Let G be a graph, an *articulation point* or *cut-vertex* is any vertex whose removal disconnects the graph.

9. **k-node Connectivity**
   Let $G = (V,E)$ be an arbitrary undirected graph. If $G' = (V \setminus Y, E)$ is connected for all $Y \subseteq V$ where $|Y| < k$, then G is *k-vertex-connected* (or simply *k-connected*).

10. **Node Connectivity**
    Let k be the greatest integer for which G is k-node-connected. We call $k(G)$ to such number, which is referred to as *node connectivity* of G.

11. **k-edge Connectivity**
    Let $G = (V, E)$ be an arbitrary undirected graph. If $G' = (V, E \backslash X)$ is connected for all $X \subseteq E$ where $|X| < k$, then G is *k-edge-connected*.

12. **Edge-Connectivity**
    Let m be the greatest integer for which G is m-edge-connected. We call $\lambda(G)$ to such number, which is referred to as *edge connectivity* of G.

13. **Contraction**
    Let $e = xy$ be an edge of the graph G. By G/e we denote the graph obtained from G by *contracting* the edge e into a new vertex v_e, which becomes adjacent to all the former neighbors of x and y. When this transformation relaxes the premiss regarding the existence of an edge between nodes is called an *identification*.

14. **Resilience**
    Resilience is the ability (of a system) to cope with change. That is, the ability to continue operating in contexts where faults are dynamic.

15. **Stochastic Binary System**
    A *Stochastic Binary System* (SBS) represents a system S that fails randomly as a function of the random failure of its components. The states of any two components are statistically independent. The state of element i in the element's set T at some instant of interest is done by the outcome of a binary random variable X_i, where $p_i = P(X_i = 1)$ and $p = (p_1, \ldots, p_{|T|})$. The *state* of the system is done by the random vector $X = (X_1, \ldots, X_{|T|})$. The *structure* of the system is represented by a function $\phi : \{0,1\}^{|T|} \to \{0,1\}$ such that $\phi(X) = 1$ if the system works under state X, and $\phi(X) = 0$ otherwise. The triad (S, p, ϕ) is called *Stochastic Binary System*.

16. **Stochastic Monotone Binary System**
    If $x, y \in \{0,1\}^{|T|}$, we consider the relation $x \leq y$ whenever $x_i \leq y_i$ for all $i = 1, \ldots, |T|$, and $x < y$ if $x \leq y$ and $x_j < y_j$ for some $j = 1, \ldots, |T|$. According to this, the structure is *monotone* if $\phi(x) \leq \phi(y)$ whenever $x \leq y$. An SBS with monotone structure is called *Sthochastic Monotone Binary System* or SMBS.

17. **Source-Terminal Reliability**
    Let $G = (V, E)$ be a simple graph, s and t terminal nodes. The source-terminal reliability is the probability to find a path that connects the terminal nodes s and t.

18. **All-Terminal Reliability**
    Let G be a graph with perfect nodes. The all-terminal reliability is the probability that the resulting subgraph is connected, where nodes are perfect but links fail independently and probabilistically.

19. **Diameter Constrained Reliability**
    Let G be a graph with perfect nodes, $K \subseteq V$ a set of distinguished nodes, and d a positive integer. The diameter constrained reliability is the probability that for every pair of nodes in $K \times K$ there exists in G at least one path having all its links operational and length not greater than d.

20. **Stochastic Process**
    A *stochastic process* X is a collection $\{X_t : t \in \mathcal{T}\}$ where each X_t is an $\mathcal{F}$-valued random variable. Usually $\mathcal{F} = \mathbf{R}$ or $\mathcal{F} = \mathbf{Z}$. The parameter t represents time. We use $\mathcal{T} = \mathbf{Z}$ and $\mathcal{F} = \mathbf{Z}$.

21. **Decision Problem**
Is a problem π that takes as input some string σ over an alphabet Σ, and outputs "yes" or "no".

22. **Instance**
Given a decision problem π, we call an *instance* of it to a concrete set of parameters that can be used to univocally feed an algorithm in order to find an answer (Yes or No). Any decision problem π has an associated domain-set of instances D_π, where the problem makes sense. Let $Y_\pi \subseteq D_\pi$ be that subset of instances for which the answer is *Yes*.

In the field of Computational Complexity and Analysis of Algorithms the following are basic questions: when is an algorithm efficient? and when is a problem easy to be solved? The classical definition for the efficiency of an algorithm relies upon time-complexity and is: "the amount of time taken by an algorithm to run, as a function of the length of the string representing the input". As measuring translates into comparing, at this point we introduce some useful concept to compare algorithms. The following definition allow us to compare the complexity of two algorithms.

23. **Order of Complexity**
Let $f(x)$ and $g(x)$ be two real functions defined on some input string set, whose outputs (positive reals) respectively represent the time expended by two algorithms -running upon the some computer- to find a solution to an instance associated with each input string. We say that g is of *higher complexity order* than f (denoted as $f(x) = O(g(x))$, if and only if, there is a positive constant M such that for all sufficiently large strings x, $f(x)$ is at most M multiplied by $g(x)$. That is, exists x_0 and M such that: $f(x) \leq Mg(x)$, for all $|x| > x_0$.

This definition focuses on the tendency of the algorithm as the input increases in size, so, coefficients and lower order terms are usually excluded. For example, if the time required by an algorithm on all inputs of size n is at most $5n^3 + 3n$, the *asymptotic time complexity* is $O(n^3)$.

24. **Efficient Algorithm**
An algorithm is referred to as *efficient* or *tractable*, if and only if, its *asymptotic time complexity* is a monomial. In other words, for any input instance x of size n, the algorithm can find a solution in *polynomial time*. Formally, there is a $p \in \mathbb{N}$ such that the time required to the algorithm to find a solution ($f(x)$) is of *lower complexity order* than n^p (i.e. $f(x) = O(n^p)$).

Let us suppose that computing power (in terms of computations per second) increases by a factor of 1000 at decade, and we have to choose between four different algorithms to find solutions for a critical application, which demands an answer within a day. As a baseline, performance for these algorithms was computed on 2010 and the best all of them could do, was finding solutions within a day for instances of size 100. Besides, it is known that complexity orders for these algorithms are: n^2, n^{10}, 10^n and $n!$ respectively. The table 1.1 shows the expected size for instances that each algorithm can solve within a day, along decades, as computer performance evolves. We must observe that the first algorithm is the most promising one in terms of scalability. Although worse

in performance, the second algorithm shares a characteristic with the first one, decade after decade the size of the achievable instance increases by a common factor: $\sqrt{1000} \approxeq 31.62$ in the first case, $\sqrt[10]{1000} \approxeq 1.995$ in the second.

year	$O(n^2)$	$O(n^{10})$	$O(10^n)$	$O(n!)$
2010	100	100	100	100
2020	3,162	200	103	102
2030	100,000	398	106	104
2040	3,162,278	794	109	105
2050	100,000,000	1,585	112	106

Table 1.1: Affordable size of instances for algorithms of different complexity orders

Unlike polynomial time algorithms, third and fourth are respectively of exponential and over-exponential complexity. When this happens the size of instances behaves as immutable to evolution of computer's performance. This is the practical consequence of intractability, that is, we cannot rely on hardware efficiency improvements to find solutions for big instances. A polynomial time algorithm is usually a reasonable option. Problem is that there are many problems for which a polynomial time algorithm has never been found. Computational complexity theory as a branch of the "theory of computation" in "theoretical computer science and mathematics" is an abstract area. Outstanding contributors to this area were: Alan Turing, Stephen Cook and Richard Karp. A detailed analysis on it is out of the scope of this document, nevertheless we give here a descriptive/extendable set of concepts for *decision problems*, i.e., problems where the output limits to two values: Yes or No.

25. **The Class of $\mathcal{P}$-problems**
We say a decision problem π is of class $\mathcal{P}$, if and only if, there is an algorithm capable of finding answers (solutions) in polynomial time as a function of the instance size.

26. **The Class of $\mathcal{NP}$-problems**
We say a decision problem π is of class $\mathcal{NP}$, if and only if, there is an algorithm capable of checking a solutions (given by an external oracle) in polynomial time as a function of the instance size.

It is pretty clear that whether a problem can be *solved* in polynomial time it also can be *checked* in polynomial time, so $\mathcal{P} \subseteq \mathcal{NP}$. Although the opposite inclusion looks unlikely, until today no one has ever found a formal proof of it. In fact, the conjecture $\mathcal{P} \neq \mathcal{NP}$ is probably the most important open problem in computer science and we are not intending to search for an answer here. Instead, we take the usual approach to establish the intrinsic complexity of our problems, that is, we compare them to other well known complex problems.

27. **Polynomical Reduction**

Given any two decision problems π and π', and being D_π and $D_{\pi'}$ their respective sets of instances, we call *polynomial reduction* of π' to π ($\pi' \preccurlyeq \pi$) to any function $f : D_{\pi'} \to D_\pi$ of polynomial complexity, such that for all $d \in D_{\pi'}$, it fulfills that $d \in Y_{\pi'}$ if and only if $f(d) \in Y_\pi$.

The existence of a polynomial reduction from π' to π ($\pi' \preccurlyeq \pi$) means that if anyone develops an efficient algorithm to find solutions to any instance of π, through the reduction process it can be used as the kernel to construct an efficient algorithm to find solutions to any instance of π'.

28. **The Class of $\mathcal{NP}$-Hard problems**
Given a problem π we say that it is $\mathcal{NP}$-Hard if and only if for all $\pi' \in \mathcal{NP}$ it holds $\pi' \preccurlyeq \pi$.

29. **The Class of $\mathcal{NP}$-Complete problems**
Let π a $\mathcal{NP}$-Hard problem. If in addition $\pi \in \mathcal{NP}$, we say that π is $\mathcal{NP}$-Complete or $\mathcal{NP}$-C.

30. **The Class of $\sharp$P-Complete problems**
The class $\sharp\mathcal{P}$ is the set of the counting problems associated with the decision problems in the set $\mathcal{NP}$.

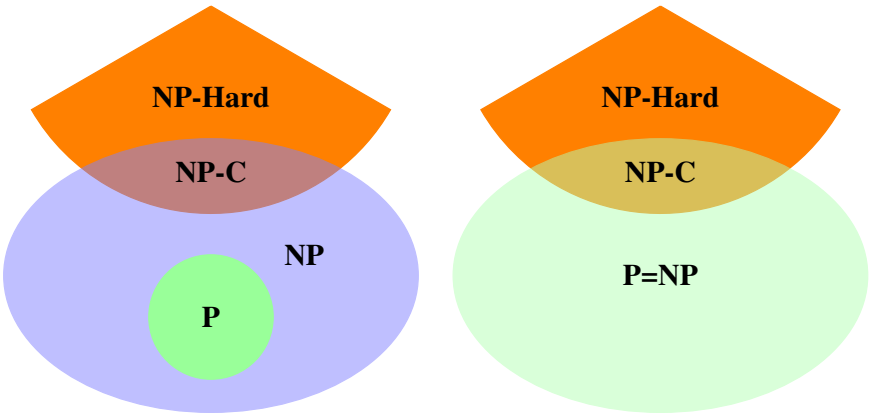

Figure 1.1: Inclusion relationship amid complexity types

The inclusion relationship admit different complexity types of problems is represented in figure 1.1. The representation on the left corresponds to the case where $\mathcal{P} \neq \mathcal{NP}$, the right one to $\mathcal{P} = \mathcal{NP}$. On 1971 Stephen Cook proved (Cook's theorem) that the boolean Satisfiability (SAT) problem is $\mathcal{NP}$-Complete, that is: the SAT is as hard as any other problem of $\mathcal{NP}$. An yet on 1972 Richard Karp started the construction of a list of polynomial reductions of SAT to other $\mathcal{NP}$ problems, thereby showing that all of them are $\mathcal{NP}$-Complete (Karp's 21 $\mathcal{NP}$-Complete problems). The standard procedure to prove that a problem $\pi \in \mathcal{NP}$ is $\mathcal{NP} - Complete$, consists in finding a well known $\mathcal{NP}$-Complete problem (π') and a polynomial reductions from π' to π (i.e. proving that $\pi' \preccurlyeq \pi$). Hence, the transitivity of "$\preccurlyeq$" guarantees that: $SAT \preccurlyeq \pi$. Complementarily and since SAT is the hardest $\mathcal{NP}$ problem (Cook's theorem), both complexities are equivalent and π is $\mathcal{NP}$-Complete too. It is worth pointing out that the previous procedure

guarantees π is $\mathcal{NP}-Hard$, even if we cannot prove $\pi \in \mathcal{NP}$.

31. **Optimization Problem**
Given a domain X for a set of n variables (e.g. $X = \mathbb{R}^n$, $X = \mathbb{N}^n$ or $X = \{0,1\}^n$), an objective function $f : X \to \mathbb{R}$ and a set of m constraints to be fulfilled $g : X \to \mathbb{R}^m$, an *Optimization Problem* consists in finding $\bar{x} \in X$, such that $f(\bar{x})$ is the minimum (or maximum) value of f while $g(\bar{x}) \leq 0$.

32. **Combinatorial Optimization Problem**
We call an Optimization Problem as a *Combinatorial Optimization Problem* (COP) when all variables are of integer type.

For example, the surface in figure 1.2 represents a hypothetical instance for a two variables problem of a generic (P) optimization problem. The goal is finding the points marked with blue dots in the figure.

On 1984 Narendra Karmarkar proved that when $X = \mathbb{R}^n$, g is a linear function and f is also linear (or even quadratic), the problem (P) can be solved in polynomial time. So Linear Programming (LP) problems are computationally easy to solve (i.e. they are in $\mathcal{P}$ class).

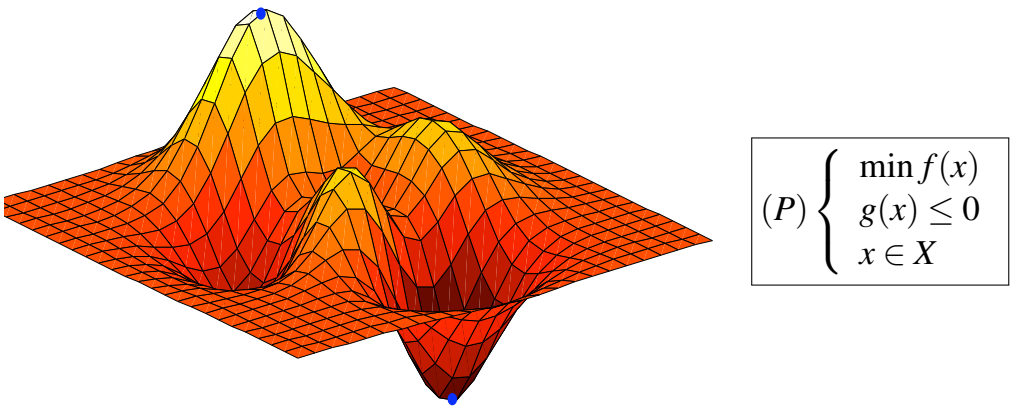

Figure 1.2: A generic optimization problem representation

However, when $X \subseteq \mathbb{Z}^n$ the problem (P) is hard in general, even when f and g are linear.

33. **GRASP**
Greedy Randomized Adaptive Search Procedure (GRASP) is a multi-start or iterative process, where feasible solutions are produced in a first phase, and neighbor solutions are explored in a second phase. The best overall solution is returned as the result. The first implementation is due to Tomas Feo and Mauricio Resende, were the authors address a hard set covering problem arising for Steiner triple systems

1.3 Structure of the Thesis

This thesis follows the Swedish style, and is organized in three parts. These parts have been ordered according to the logic of studying the reliability first, then resilience and finally the graph fragmentation problem. Chapter 2 includes elementary contributions on the diameter constrained reliability model, while Chapter 3 studies stochastic monotone binary systems. Chapters 4 and 5 deal with the second part, while Chapter 6 focuses in the third part.

1. In Part I we study how to measure the probability of correct operation of a static system, known as *System Reliability*. Chapter 2 focuses on the SBS, while Chapter 3 does in SMBS.

2. In Part II we study how to improve the *Resilience* of a dynamic system when failures propagate as an epidemic. This issue is addressed in the Chapters 4 and 5.

3. In Part III a combinatorial optimization problem is introduced. It is inspired in epidemic modeling, and finds applications in firefighting and electric networks.

   The goal is to protect (i.e., delete) specific nodes in a ground graph in order to minimize the expected number of deads, where an atacker picks a node uniformly at random and attacks its whole connected component. This problem is treated in Chapter 6.

Each chapter includes a corresponding peer-reviewed article. They are all accepted and published (the article from Chapter 5 is to appear).

Preliminary results about resilience are published in the Proceedings of the International Workshop in Machine learning, Optimization and big Data (MOD 2015), and presented in Chapter 4, while a more in-depth analysis is included in Chapter 5. There, we provide evidence of major shortcomings of a Greedy immunization heuristic to cope with an epidemic propagation.

In Chapter 6 we explore and go deeper into the ideas outlined above, now as a Graph Fragmentation Problem or GFP. We prove mathematically certain desired properties of candidate solutions.

Using these properties we define a *Greedy* notion for the GFP. We develop a more sophisticated GRASP heuristic enriched with a Path-Relinking post-optimization phase. Both heuristics are compared on the lights of certain graphs inspired by real-world systems.

1.4 Main Contributions

1.4.1 Reliability

Framework

In Chapter 2, the object under study is the exact evaluation of the Diameter Constrained Reliability (DCR). There, the hardness of an exact computation is established in an all-terminal scenario when the diameter is equal to two. Additionally, a new family of graphs is presented, which accepts an exact and efficient DCR evaluation.

The reliability of more abstract systems is studied in Chapter 3. There, we consider Stochastic Binary Systems. Recursive Variance Reduction (RVR) method shows to be suitable for network reliability analysis. Here, we show that RVR method preserves all their properties already known in network reliability, provided the SBS is monotone. Also a new method called F-Monte Carlo (FMC) is introduced.

Contributions

Chapter 2: Diameter-Constrained Reliability: Complexity, Factorization and Exact computation in Weak Graphs

- We prove that the DCR evaluation belongs to the $\mathcal{NP} - Hard$ class in an all-terminal scenario when the diameter is $d = 2$.
- A new family of graphs that accepts a polynomial-time DCR evaluation is introduced, called *Weak Graphs*. As a corollary, closed formulas are provided for the DCR evaluation of specific sub-families (i.e., trees, cycles, Monma graphs, graphs with free co-rank and planar graphs with a number of faces independent of the order).

Chapter 3: Recursive Variance Recursion Method in Stochastic Monotone Binary Systems

- We prove here that the reliability computation of an arbitrary SMBS belongs to the class of $\mathcal{NP}$-Hard problems.
- Two Monte Carlo approaches are introduced for the SMBS: RVR and FMC.
- We show that RVR method preserves all their properties already known in network reliability, provided the SBS is monotone.
- Methods are tested over different SMBS and compared with Crude Monte Carlo (CMC) method for three different definitions of “system works”.

1.4.2 Resilience under epidemic propagation of failures

Framework

In Chapters 4 and 5, the network is exposed to an epidemic failure process. A singleton is initially infected, and failures (i.e., the infection) is propagated through neighboring nodes. This dynamic system is first empirically studied (Chapter 4) and then formalized as a stochastic process and combinatorial problem (Chapter 5).

In this dynamic system a singleton node is initially infected. Then, it propagates the infection through neighboring susceptible nodes, following a probabilistic infection rule. Some nodes are chosen for node-immunization; they are not susceptible nodes (indeed, they fall in a third category, as in a traditional SIR model). The number of infected individuals represents the stochastic process under study, and the goal is to minimize the peak of infected nodes through time.

A Greedy immunization heuristic is presented, where nodes with the highest degree are immunized. We show both mathematically and empirically that Greedy heuristic is suboptimal. Furthermore, a Random heuristic outperforms Greedy in special scenarios. It is worth to observe that the class of infected individuals can be considered as failure elements in a network. With this analogy in mind, an epidemic process can adequately model cascade failures.

Contributions

Chapter 4: Node-Immunization Strategies in a Stochastic Epidemic Model

- A combinatorial optimization problem is formally presented. The goal is to minimize the infection subject to a budget constraint, choosing a node-immunization strategy.
- A performance analysis is carried out. There, Greedy is compared with a Random immunization heuristic.
- We empirically show that Greedy heuristic is not always the best choice.

Chapter 5: A counter-intuitive result on SIR-based Node-immunisation Heuristics

- We provide sufficient conditions for optimality.
- As a Corollary, we mathematically prove that Greedy is sub-optimal.
- The effect of the underlying network topology is empirically analyzed.

1.4.3 Graph Fragmentation Problem

Framework

In several real-world applications a malfunctioning of a single element is propagated through neighboring interconnected elements. In Chapter 6, we propose a combinatorial problem that models how to cope with an accident, choosing nodes for protection. We invite and challenge the operations research community to model and understand firefighting and related real-world problems.

Contributions

Chapter 6: Graph Fragmentation Problem

- The Graph Fragmentation Problem (GFP) is introduced. We are given a ground graph G and a budget constraint B. The goal is to protect (remove) B nodes from a graph G, in such a way that a random attack to an arbitrary node v affects the lowest expected number of nodes (where the whole connected component from v is affected).
- Elementary properties of the GFP were studied. Specifically, we prove that graph fragmentation and balancing are good strategies. Together, they define a Greedy notion for the problem.
- We mathematically prove that Greedy achieves an improvement in each additional protected node.
- A more sophisticated GRASP suitably customized heuristic enriched with a Path Relinking post-optimization scheme has been developed.
- The effectiveness of our more sophisticated heuristic has been tested on real-life telecommunication networks.

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Part I

Reliability in Static Systems

Chapter 2

Diameter-Constrained Reliability: Complexity, Factorization and Exact computation in Weak Graphs

In classical reliability analysis, the all-terminal reliability is the connectedness probability of a random graph. There, nodes are perfect but links fail with independent probabilities.

We consider a positive integer d and distinguished node-set K, called terminals. The diameter constrained reliability (DCR) is the probability that every pair of terminals are connected by paths composed by d links, or less. Since the DCR evaluation subsumes the classical reliability analysis, it belongs to the class of $\mathcal{NP}$-Hard problems as well.

Elementary properties of the DCR are studied in this paper. First, the intractability of the DCR evaluation is established even if $d = 2$ in an all-terminal scenario. Additionally, a special family of graphs is introduced, which accept a polynomial time evaluation.

Diameter-Constrained Reliability: Complexity, Factorization and Exact computation in Weak Graphs

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ABSTRACT

In this paper we address a problem from the field of network reliability, called diameter-constrained reliability. Specifically, we are given a simple graph $G = (V, E)$ with $|V| = n$ nodes and $|E| = m$ links, a subset $K \subseteq V$ of *terminals*, a vector $p = (p_1, \ldots, p_m) \in [0, 1]^m$ and a positive integer d, called *diameter*. We assume nodes are perfect but links fail stochastically and independently, with probabilities $q_i = 1 - p_i$. The *diameter-constrained reliability* (DCR for short), is the probability that the terminals of the resulting subgraph remain connected by paths composed by d links, or less. This number is denoted by $R^d_{K,G}(p)$.

The general DCR computation is inside the class of $\mathcal{NP}$-Hard problems, since is subsumes the complexity that a random graph is connected. In this paper the computational complexity of DCR-subproblems is discussed in terms of the number of terminal nodes $k = |K|$ and diameter d. A factorization formula for exact DCR computation is provided, that runs in exponential time in the worst case. Finally, a revision of graph-classes that accept DCR computation in polynomial time is then included. In this class we have graphs with bounded co-rank, graphs with bounded genus, planar graphs, and, in particular, Monma graphs, which are relevant in robust network design. We extend this class adding arborescence graphs. A discussion of trends for future work is offered in the conclusions.

Categories and Subject Descriptors

C.4 [**Performance of Systems**]: Reliability, availability, and serviceability; D.2.8 [**Mathematical Software**]: Reliability and Robustness—*computational complexity, performance measures*

General Terms

Network Reliability

Keywords

Computational Complexity, Network Reliability, Diameter-Constrained Reliability

1. INTRODUCTION

The definition of DCR has been introduced in 2001 by Héctor Cancela and Louis Petingi, inspired in delay-sensitive applications over the Internet infrastructure [10]. Nevertheless, its applications over other fields of knowledge enriches the motivation of this problem in the research community [12].

We wish to communicate special nodes in a network, called *terminals*, by d hops or less, in a scenario where nodes are perfect but links fail stochastically and independently. The all-terminal case with $d = n - 1$ is precisely the probability that a random graph is connected, or *classical reliability problem* (CLR for short). Arnon Rosenthal proved that the CLR is inside the class of $\mathcal{NP}$-Hard problems [24]. As a corollary, the general DCR is $\mathcal{NP}$-Hard as well, hence intractable unless $\mathcal{P} = \mathcal{NP}$.

The focus of this paper is the computational complexity of DCR subproblems in terms of the number of terminals k and diameter d, and the efficient computation of the DCR for distinguished graph topologies.

In Section 4, a formal definition of DCR is provided as a particular instance of a coherent stochastic binary system. The computational complexity of the DCR is discussed in terms of the diameter and number of terminals in Section 3. The contributions of this paper are two-fold. First, we close the complexity analysis of the DCR problem in terms of k and d. Indeed, we prove in this section that the DCR is in the computational class of $\mathcal{NP}$-Hard problems in the all-terminal scenario ($k = n$) with a given diameter $d \geq 2$. The computational complexity for other possible pairs for k and d is already available from prior literature from this area.

Then, we provide an exact DCR computation by means of a factor-

ization technique inspired in [20], in Section 4. Finally, we extend the class of known graphs that permit an efficient (i.e. polynomial time) computation for the DCR in Section 5. A particular but relevant family of these graphs are Monma graphs, which plays a key role in the design of robust network design [19, 23, 8]. Concluding remarks and open problems are summarized in Section 6.

2. TERMINOLOGY

We are given a system with m components. These components are either "up" or "down", and the binary state is captured by a binary word $x = (x_1, \ldots, x_m) \in \{0,1\}^m$. Additionally, we have a structure function $\phi : \{0,1\}^m \to \{0,1\}$ such that $\phi(x) = 1$ if the system works under state x, and $\phi(x) = 0$ otherwise. When the components work independently and stochastically with certain probabilities of operation $p = (p_1, \ldots, p_m)$, the pair (ϕ, p) defines a *stochastic binary system*, or SBS for short, following the terminology from [1]. An SBS is *coherent* whenever $x \leq y$ implies that $\phi(x) \leq \phi(y)$, where the partial order set $(\leq, \{0,1\}^m)$ is bit-wise (i.e. $x \leq y$ if and only if $x_i \leq y_i$ for all $i \in \{1, \ldots, m\}$). If $\{X_i\}_{i=1,\ldots,m}$ is a set of independent binary random variables with $P(X_i = 1) = p_i$ and $X = (X_1, \ldots, X_m)$, then $r = E(\phi(X)) = P(\phi(X) = 1)$ is the *reliability* of the SBS.

Now, consider a simple graph $G = (V, E)$, a subset $K \subseteq V$ and a positive integer d. A subgraph $G_x = (V, E_x) \subseteq G$ is *d-K-connected* if $d_x(u, v) \leq d, \forall \{u, v\} \subseteq K$, where $d_x(u, v)$ is the distance between nodes u and v in the graph G_x. Let us choose an arbitrary order of the edge-set $E = \{e_1, \ldots, e_m\}$, $e_i \leq e_{i+1}$. For each subgraph $G_x = (V, E_x)$ with $E_x \subseteq E$, we identify a binary word $x \in \{0,1\}^m$, where $x_i = 1$ if and only if $e_i \in E_x$; this is clearly a bijection. Therefore, we define the structure $\phi : \{0,1\}^m \to \{0,1\}$ such that $\phi(x) = 1$ if G_x is d-K-connected, and $\phi(x) = 0$ otherwise. If we assume nodes are perfect but links fail stochastically and independently ruled by the vector $p = (p_1, \ldots, p_m)$, the pair (ϕ, p) is a coherent SBS. Its reliability, denoted by $R^d_{K,G}(p)$, is called *diameter constrained reliability*, or DCR for short. A particular case is $R^{n-1}_{K,G}(p)$, called *classical reliability*, or CLR for short.

In a coherent SBS, a *pathset* is a state x such that $\phi(x) = 1$. A *minpath* is a state x such that $\phi(x) = 1$ but $\phi(y) = 0$ for all $y < x$ (i.e. a minimal pathset). A *cutset* is a state x such that $\phi(x) = 0$, while a *mincut* is a state x such that $\phi(x) = 0$ but $\phi(y) = 1$ if $y > x$ (i.e. a minimal cutset). We will denote $\mathcal{O}^K_d(G)$ to the set of all d-K-connected subgraphs of a ground graph G.

We recall a bit of terminology coming from graph theory, which will be used throughout this treatment. A graph $G = (V, E)$ is *bipartite* if there exists a bipartition $V = V_1 \cup V_2$ such that $E \subseteq \{\{x, y\} : x \in V_1, y \in V_2\}$. A *vertex cover* in a graph $G = (V, E)$ is a subset $V' \subseteq V$ such that V' meets all links in E.

Given two graphs G_1 and G_2 with the same vertex set V, $f : V \to V$ is a *K-isomorphism* from G_1 to G_2 if it is an isomorphism that fixes the set K. In that case G_1 and G_2 are *K-isomorphic*. Given a simple graph $G = (V, E)$ and $e = \{x, y\} \in E$, an *elementary division* of e is a couple of edges $e_1 = \{x, z\}$ and $e_2 = \{z, y\}$ that replace e in G, where $z \notin V$. Two graphs G_1 and G_2 are *homeomorphic* if there exists a graph G such that G_1 and G_2 can be obtained from G by means of a sequence of elementary divisions. If $P = \{V_1, \ldots, V_c\}$ is a partition of V, the *quotient graph* is $G' = (P, E')$, where $\{V_i, V_j\} \in E'$ if and only if $i \neq j$ and there exists an edge from a vertex of V_i to a vertex of V_j in E. We say v_j is *reachable* from v_i either when $v_i = v_j$ or there is a path from v_i to v_j. In a simple graph G, reachability is an equivalence relation, and c, the number of classes in the quotient graph, is the number of *connected components*. Given a simple graph $G = (V, E)$ with $n = |V|$ vertices and $m = |E|$ edges, its *rank* is $r(G) = n - c$, while its *co-rank* is $c(G) = m - n + c$. A *connected graph* verifies $c = 1$; then $r(G) = n - 1$ and $c(G) = m - n + 1$. In topological graph theory, the *genus of a graph* G is the least natural g such that G can be drawn without crossing itself in a surface with genus g. A *planar graph* verifies $g = 0$.

3. COMPUTATIONAL COMPLEXITY

The class $\mathcal{NP}$ is the set of problems polynomially solvable by a non-deterministic Turing machine [15]. A problem is $\mathcal{NP}$-Hard if it is at least as hard as every problem in the set $\mathcal{NP}$ (formally, if every problem in $\mathcal{NP}$ has a polynomial reduction to the former). It is widely believed that $\mathcal{NP}$-Hard problems are intractable (i.e. there is no polynomial-time algorithm to solve them). An $\mathcal{NP}$-Hard problem is $\mathcal{NP}$-Complete if it is inside the class $\mathcal{NP}$. Stephen Cook proved that the joint satisfiability of an input set of clauses in disjunctive form is an $\mathcal{NP}$-Complete decision problem; in fact, the first known problem of this class [13]. In this way, he provided a systematic procedure to prove that a certain problem is $\mathcal{NP}$-Complete. Specifically, it suffices to prove that the problem is inside the class $\mathcal{NP}$, and that it is at least as hard as an $\mathcal{NP}$-Complete problem. Richard Karp followed this hint, and presented the first 21 combinatorial problems inside this class [16]. Leslie Valiant defines the class $\#\mathcal{P}$ of counting problems, such that testing whether an element should be counted or not can be accomplished in polynomial time [26]. A problem is $\#\mathcal{P}$-Complete if it is in the set $\#\mathcal{P}$ and it is at least as hard as any problem of that class.

Recognition and counting minimum cardinality mincuts/minpaths are at least as hard as computing the reliability of a coherent SBS [1]. Arnon Rosenthal proved the CLR is $\mathcal{NP}$-Hard [24], showing that the minimum cardinality mincut recognition is precisely Steiner-Tree problem, included in Richard Karp's list. The CLR for both two-terminal and all-terminal cases are still $\mathcal{NP}$-Hard, as Michael Ball and J. Scott Provan proved by reduction to counting minimum cardinality $s - t$ cuts [22]. As a consequence, the general DCR is $\mathcal{NP}$-Hard as well. Later effort has been focused to particular cases of the DCR, in terms of the number of terminals $k = |K|$ and diameter d.

When $d = 1$ all terminals must have a direct link,

$$R^1_{K,G} = \prod_{\{u,v\} \subseteq K} p(uv),$$

where $p(uv)$ denotes the probability of operation of link $\{u, v\} \in E$, and $p(uv) = 0$ if $\{u, v\} \notin E$. The problem is still simple when $k = d = 2$. In fact,

$$R^2_{\{u,v\},G} = 1 - (1 - p(uv)) \prod_{w \in V - \{u,v\}} (1 - p(uw)p(wv)).$$

Héctor Cancela and Louis Petingi rigorously proved that the DCR is $\mathcal{NP}$-Hard when $d \geq 3$ and $k \geq 2$ is a fixed input parameter [11], in strong contrast with the case $d = k = 2$.

The literature offers two proofs that the DCR has a polynomial-time algorithm when $d = 2$ and k is a fixed input parameter [25, 6]. Pablo Sartor et. al. present a recursive proof [25], while Eduardo Canale et. al. present an explicit expression for $R^2_{K,G}$ that is computed in a polynomial time of elementary operations [7].

Here, we will prove that the DCR is inside the class of $\mathcal{NP}$-Hard problems in the all-terminal case with diameter $d \geq 2$. The main source of inspiration for the first result is the article authored by [11], where they proved that the DCR is $\mathcal{NP}$-Hard when $d \geq 3$ and $k \geq 2$ is a fixed input parameter. There, the authors prove first that the result holds for $k = 2$, and they further generalize the result for fixed $k \geq 2$. For our purpose it will suffice to revisit the first part. Before, we state a technical result:

LEMMA 1. *Counting the number of vertex covers of a bipartite graph is #$\mathcal{P}$-Complete [2].*

PROPOSITION 1. *The DCR is $\mathcal{NP}$-Hard when $k = 2$ and $d \geq 3$ [11].*

PROOF. Let $d' = d - 3 \geq 0$ and $P = (V(P), E(P))$ a simple path with node set $V(P) = \{s, s_1, \ldots, s_{d'}\}$ and edge set $E(P) = \{\{s, s_1\}, \{s_1, s_2\}, \ldots, \{s_{d'-1}, s_{d'}\}\}$. For each bipartite graph $G = (V, E)$ with $V = A \cup B$ and $E \subseteq A \times B$ we build the following auxiliary network:

$$G' = (A \cup B \cup V(P) \cup \{t\}, E \cup E(P) \cup I\}, \qquad (1)$$

where $I = \{\{s_{d'}, a\}, a \in A\} \cup \{\{b, t\}, b \in B\}$, and all links of G' are perfect but links in I, which fail independently with identical probabilities $p = 1/2$. Consider the terminal set $K = \{s, t\}$. The auxiliary graph G' is illustrated in Fig. 1. The reduction from the bipartite graph to the two-terminal instance is polynomial.

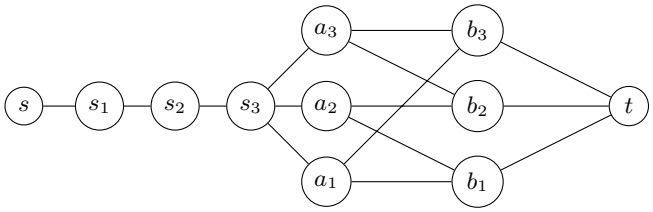

Figure 1: Example of auxiliary graph G'' with terminal set $\{s, t\}$ and $d = 6$, for the bipartite instance C_6.

A vertex cover $A' \cup B' \subseteq A \cup B$ induces a cutset $I' = \{\{s_{d'}, a\}, a \in A'\} \cup \{\{b, t\}, b \in B'\}$ (i.e. if all links in I' fail, the nodes $\{s, t\}$ are not connected). Reciprocally, that cutset determines a vertex cover. Therefore, the number of cutsets $|\mathcal{C}|$ is precisely the number of vertex covers of the bipartite graph $|\mathcal{B}|$. When $p = 1/2$, all cutsets are equally likely, and the source-terminal reliability evaluation at $p = 1/2$ is:

$$R^d_{\{s,t\},G'}(1/2) = 1 - \frac{|\mathcal{C}|}{2^{|A|+|B|}}$$

Finally, using the fact that $|\mathcal{B}| = |\mathcal{C}|$ and by substitution:

$$|\mathcal{B}| = 2^{|A|+|B|}(1 - R^d_{\{s,t\},G'}(1/2)).$$

Thus, the DCR for the two-terminal case is at least as hard as counting vertex covers of bipartite graphs. ♠ □

The result for $d \geq 3$ is a corollary of Proposition 1.

THEOREM 1. *The DCR is $\mathcal{NP}$-Hard when $k = n$ and $d \geq 3$.*

PROOF. Consider the auxiliary graph $G' = (V', E')$ from Fig. 1. Extend G' furthermore, and consider $G'' = (V'', E'')$, where $V'' = V'$ and $E'' = E' \cup \{\{a, a'\}, a \neq a', a, a' \in A\} \cup \{\{b, b'\}, b \neq b', b, b' \in B\}$. In words, just add links in order to connect all nodes from A, and all nodes from B. We keep the same probabilities of operation that in G', and the new links are perfect.

Consider now the all-terminal case $K = V''$ for G'', and given diameter $d \geq 3$. The key is to observe that the cutsets in the all-terminal scenario for G'' are precisely the $s - t$ cutsets in G', and they have the same probability.

Indeed, each pair of terminals from the set A are directly connected by perfect links; the same holds in B. The distance between s and $s_{d'}$ is $d' = d - 3 < d$, so these nodes (and all the intermediate ones) respect the diameter constraint. Finally, if there were an $s - t$ path (i.e. a path from s to t), the diameter of G'' would be exactly d. Therefore, $R^d_{\{s,t\},G'} = R^d_{V'',G''}$, and again:

$$\begin{aligned} |\mathcal{B}| &= 2^{|A|+|B|}(1 - R^d_{\{s,t\},G'}(1/2)) \\ &= 2^{|A|+|B|}(1 - R^d_{V'',G''}(1/2)). \end{aligned}$$

Thus, the DCR for the all-terminal case is at least as hard as counting vertex covers of bipartite graphs. ♠ □

THEOREM 2. *The DCR is $\mathcal{NP}$-Hard when $k = n$ and $d = 2$.*

PROOF. Given a graph $G = (V, E)$, consider $G' = (V \cup \{a, b\}, E \cup \{\{x, a\}, \{x, b\}, \forall x \in V\})$. By its definition, G' has diameter $d = 2$. All links are perfect, except the ones incident to a, with $p(ax) = 1/2$. Consider the DCR for G'. We will show that the number of minimum cardinality pathsets in G' is precisely the number of vertex covers in G'. Since counting minimum cardinality pathsets is at least as hard as computing the reliability of a coherent SBS [1], the result will follow.

A minimum cardinality pathset in G' contains all perfect links, and $\{a, x_1\}, \ldots, \{a, x_r\}$ for certain nodes $x_i \in V$. Since H is a minimum cardinality pathset, the graph $G_H = (V, H)$ has diameter 2, but the diameter is increased under any link deletion. Let $N_a = \{x : \{a, x\} \in H\}$ the set of neighbor vertices for the terminal node a. The key is to observe that *vertex a reaches every node in two steps if and only if N_a is a vertex cover*.

Indeed, suppose a reaches every node in two steps. Then, for any $x \in V \setminus N_a$ there exists a path xya, so $y \in N_a$ and thus N_a is a vertex cover. Conversely, if N_a covers V, let $x \in V$. Then, either $x \in N_a$ and x is adjacent with a, or $x \in V \setminus N_a$ and there exists $y \in N_a \cap N_x$, so xya is a path of two hops between x and a.

The minimality of N_a as a cover follows from the minimality of H as a pathset. □

The whole picture of DCR complexity is provided in Fig. 2, which closes the complexity analysis for different independent pairs (k, d).

4. FACTORIZATION IN DCR

Let us consider a network $G = (V, E)$ with perfect nodes and identical probabilities of operation $p_e = p \, \forall e \in E$. Denote $n =$

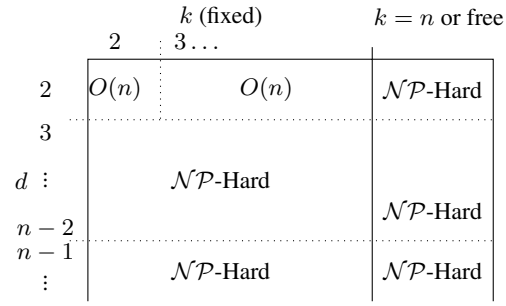

Figure 2: DCR Complexity in terms of the diameter d and number of terminals $k = |K|$

$|V|$ and $m = |E|$ the respective number of nodes and links in the network. Totaling exhaustive and mutually disjoint events, Michael Ball and Scott Provan observed that [2]

$$R_{V,G}(p) = \sum_{i=0}^{n} F_i p^{m-i}(1-p)^i, \tag{2}$$

being F_i the number of connected subgraphs $H = (V, E')$ for G such that $|E'| = m - i$. Therefore, the problem can be reduced to counting subgraphs. In particular, if c denotes the minimum cardinality cutset (mincut) then F_{m-c} is the number of those cutsets.

The classical reliability problem, CLR, is $\mathcal{NP}$-Hard (see Section 3 for a discussion of computational complexity). Since DCR is an extension of CLR, it is $\mathcal{NP}$-Hard as well. Once these classical problems are known to be computationally hard, the research community delved into the development of exact exponential algorithms, close approximations and polynomially solvable subclasses of the CLR.

The literature is vast, and we are forced to choose inspirational and most cited works. Remarkably, Moskowitz [21] proposed series parallel reductions and deletion of irrelevant edges, as well as the deletion-contraction principle (or Factoring Theorem): let $e = \{x, y\} \in E$ be an arbitrary edge, $G - e = (V, E - e)$ represents edge-deletion, $G * e$ is an edge contraction (the nodes $\{x, y\}$ are both identified with x, and the graph $G * e$ has possibly multiple edges), and K' is the new terminal-set after the identification of nodes x and y. Then:

$$R_{K,G} = (1 - p_e)R_{K,G-e} + p_e R_{K',G*e}. \tag{3}$$

A notorious computational method for rough estimations of $R_{K,G}$ is Crude Monte Carlo (CMC) and its enhancements [14]. The key idea is to pick N independent random graphs $G_1, \ldots, G_N$ that respect the correct probability law for the links, and set a binary random variable X_i to 1 if the desired condition is met or $X_i = 0$ otherwise. By Kolmogorov's strong law, the average random variable $\overline{X_N}$ converges almost surely to $P(X = 1)$, precisely the target probability (K-connectedness in the CLR, for instance). This estimation is unbiased, and its error can be reduced linearly with the sample size N. Unbiased estimations for $R_{K,G}$ are usually compared with respect to efficiency, which considers both expected square error (i.e., variance) and computational effort. Héctor Cancela and Mohammed El Khadiri developed a Recursive Variance Reduction (RVR) estimation for $R_{K,G}$, with clearly winning efficiency with respect to CMC [9]. Other valuable approximation methods are cross-entropy [18], antithetic variables and uniform bounds [5]. Here we just touched on the surface of CLR. The curious reader can find a recent survey in [4].

The DCR additionally requires the terminals to be connected by path composed not more that d hops. The new parameter d is called the *diameter*, and the target probability is denoted by $R^d_{K,G}$, following the terminology of Héctor Cancela and Louis Petingi [10]. An analogous expression of (2) for the case of homogeneous links holds:

$$R^d_{K,G}(p) = \sum_{i=0}^{n} F_i^{(K,d)} p^{m-i}(1-p)^i, \tag{4}$$

where now $F_i^{(K,d)}$ is the number of d-K-connected subgraphs $H = (V, E')$ for G such that $|E'| = m - i$, and the terminals are linked by paths with d hops or less. Since DCR is a generalization of CLR (the CLR occurs when $d \geq |V| - 1$), the general DCR problem is $\mathcal{NP}$-Hard as well. Special care is needed to adapt Expression 3 for the diameter constrained measure, since the node-contraction operation does not preserve distances. The reader can find an adaptation of factorization the diameter-constrained measure in [10]. There, the authors need to identify all paths that include the selected link.

Observe that if a link $e \in E$ fails, the DCR event corresponds to network $G - e$, where all link reliabilities are kept the same (but $p_e = 0$). On the other hand, if e operates, we should find the DCR of network G^e, that is precisely G but $p_e = 1$. A similar factorization formula for the DCR is the following:

$$R^d_{K,G} = p_e R^d_{K,G^e} + (1 - p_e)R^d_{K,G-e} \tag{5}$$

It is worth to notice that the recursion provided by Equation (5) iteratively *deletes* or *consolidate* links. As a consequence, the iterative procedure finishes in non-connected instances, or, on the other hand, in "strong" networks, where all links are perfect. In the latter, the network is either d-K-connected (and the DCR equals 1) or not (where the DCR equals 0). Future work is required to test exact DCR computations in polynomial time using this novel factorization technique.

5. DCR IN SPECIAL GRAPHS

So far, an efficient (polynomial-time) computation of the DCR is available only for special graphs, to know, paths, cycles, ladders, generalized ladders and spanish fans [25]. The reader can appreciate from Figure 2 that an efficient computation is also feasible for diameter $d = 2$ and a fixed number of input terminals k [6]. An explicit expression for $R^d_{K,G}(p)$ is provided by [7].

In this article, we will extend the previous list, adding Weak graphs, Monma graphs, Tree graphs and Arborescence graphs.

DEFINITION 1. *Let $G = (V, E)$ a simple graph, $K \subseteq V$ and d a positive integer. The graph G is d-K-r weak if $G - U$ is d-K disconnected, for every set $U \subseteq E$ with $|U| \geq r$.*

In words, "r-weakness" states the network fails (i.e. is not d-K connected) whenever we remove an arbitrary set of r links (or more).

THEOREM 3. *Let $G = (V, E)$ a d-K-r weak graph, for some r independent of n. Then, the DCR can be found in polynomial time in n.*

PROOF. Given an arbitrary configuration $G' = (V, H) \subseteq G$, we can decide in polynomial time whether G' is d-K-connected or not. Let us denote $\mathcal{O}^r$ to the set of all configurations (V, H), with $|H| \geq m - r$, where $m = |E|$. Since G' is d-K-r weak, summing the probability of disjoint events with positive probability we get that

$$R^d_{K,G} = \sum_{G' \in \mathcal{O}^r} 1_{\{G' \in \mathcal{O}^K_D(G)\}} \prod_{e \in E(G')} p(e) \prod_{e \notin E(G')} (1 - p(e)), \tag{6}$$

where $1_{\{x\}} = 1$ if x is true, and $1_{\{x\}} = 0$ otherwise. It suffices to show that the number of terms in the sum is polynomial with respect to n. In fact, by Sum-rule, the cardinality $|\mathcal{O}^r|$ is precisely:

$$|\mathcal{O}^r| = \sum_{i=0}^{r-1} \binom{m}{m-i} \sim m^{r-1}, \tag{7}$$

where the symbol $\sim$ means that both real sequences are equivalent when m tends to infinity. Observe that $m < n^2$ holds for all connected graphs. Therefore, $|\mathcal{O}^r| \sim m^{r-1} \leq n^{2r-2}$, and the number of terms from Expression (7) is bounded by a polynomial in n. Thus, $R^d_{K,G}$ can be found in a polynomial number of elementary operations in n. ♠ □

COROLLARY 1. *The DCR in connected graphs $G = (V, E)$ with bounded co-rank $c(G) = m - n + 1$ can be found in polynomial time in n.*

PROOF. Consider a simple graph $G = (V, E)$, with bounded co-rank $c(G)$, a terminal set $K \subseteq V$ and diameter d. If we delete an arbitrary link set $U \subseteq E$ of cardinality $c(G) + 1$, the resulting subgraph has less links than a tree. Then, $G - U$ us disconnected, and G is d-K-$(c(G)+1)$ weak. Since $c(G)+1$ is a constant bound, Theorem 3 applies, and the DCR can be found in polynomial time in n. ♠ □

COROLLARY 2. *If the number of faces of a connected graph G of genus g has a constant bound, the diameter-constrained reliability can be computed in polynomial time.*

PROOF. Follows from the fact that the number of faces f of a graph of genus g is $f = m - n + 2 - 2g = c(G) - (2g - 1)$. Then, the co-rank $c(G) = f + 2g - 1$ has a constant bound. ♠ □

COROLLARY 3. *Consider a graph G with genus g and a constant bound on its faces. Then, if we consider an arbitrary arborescence for G, its diameter-constrained reliability can be computed in polynomial time.*

PROOF. Trees do not add faces, and Corollary 2 holds for any arborescence of G. ♠ □

The relevance of the following corollary comes from the fact that most telecommunication networks are planar.

COROLLARY 4. *If the number of faces of a planar graph G has a constant bound, the diameter-constrained reliability can be computed in polynomial time.*

PROOF. A planar graph has genus 0. ♠ □

The property is unaffected by elementary subdivisions of a graph:

COROLLARY 5. *If a family of graphs $\mathcal{F}$ has all its elements homeomorphic to a fixed graph, its diameter-constrained reliability can be computed in polynomial time with respect to its order.*

PROOF. Homeomorphic graphs have the same co-rank. ♠ □

Now we focus on a distinguished family of graphs coming from robust network design. Specifically, Clyde Monma et. al. studied the minimum cost two-connected network design problem, for the metric case spanning all nodes in the set V [19]. There, the authors prove that there exists a solution $G' = (V, H) \subseteq G$ such that every vertex in G' has degree 2 or 3, and the deletion of one or two links from G' leaves one bridge in one of the resultant connected components. Moreover, those graphs are either a Hamiltonian cycle in G or contain a *Monma graph* as an induced subgraph. The term Monma graph was introduced in later works with this family of graphs [8]. Figure 3 sketches a general Monma graph.

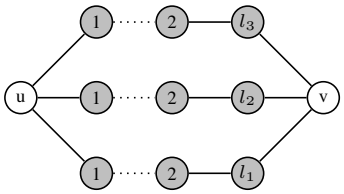

Figure 3: Monma's graph structure.

The following corollary provides the dimension of reliability in the study of Monma graphs:

COROLLARY 6. *The diameter-constrained reliability of Monma graphs can be computed in polynomial time respect to its order.*

PROOF. Monma graphs are those homeomorphic to the general graph consisting in two vertices and three edges joining them. ♠ □

Observe that Monma graphs are 3-K-weak for every selection of the terminal set K. Therefore, Theorem 3 also proves Corollary 6. All sub-trees in a Monma graph are obtained removing two links from different u-v-paths (see Figure 3). If we delete more than three links, the resulting subgraph is disconnected. In Appendix A we count the number of spanning trees in an arbitrary Monma graph. Also, trees are 1-K-weak for every subset of terminals K, and Theorem 3 states that the DCR computation in trees is feasible in polynomial time. Indeed, we show in Appendix B that it is linear in the order of the tree.

6. CONCLUSIONS

In this paper we address the diameter-constrained reliability. This measure joints is the probability that all distinguished terminals $K \subseteq V$ in a network $G = (V, E)$ remain connected by d hops or less, where links $e \in E$ may fail with certain probabilities $q_e = 1 - p_e$.

The DCR is $\mathcal{NP}$-Hard, since it subsume the probability that a random graph is connected. We summarize the computational complexity of DCR sub-problems in terms of the number of terminals $k = |K|$ and diameter d. It remains $\mathcal{NP}$-Hard in all cases but $d \leq 2$ and k finite.

Deletion-contraction formulas are available for the classical reliability problem (CLR). However, contractions modify the diameter. Therefore, we adapted this recursive technique with the introduction of a different factorization methodology.

An efficient (polynomial time) DCR computation is possible in special graphs. Indeed, from prior literature we know that the DCR in paths, cycles, ladders, generalized ladders and spanish fans can be found efficiently [25].

In this paper we extended the previous list, including weak and strong graphs, some graphs with bounded genus, arborescences, graphs with bounded co-rank and special classes, to know, Monma graphs and trees.

The best design (minimum cost) 2-node-connected metric network must be either Hamiltonian or it has a Monma graph a an induced subgraph. Then, this work connects reliability aspects of network design in a probabilistic context with robust network design.

As a future work, we wish to find the DCR in Halin graphs, which play a key role in robust network design (specially in 3-connected minimum cost network design). Furthermore, we will analyze local properties of the DCR (node contraction, link deletion and other local movements) that will enrich our understanding in this measure that connects quality (in hop-constrained applications) with reliability. A hint for this study is DCR factorization.

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APPENDIX

A

The complexity of a simple graph G is its number of spanning trees, denoted by $\kappa(G)$. Gustav Kirchhoff provided an efficient way to count $\kappa(G)$, by means of a determinant [17]. Indeed, $\kappa(G)$ is an arbitrary minor of the Laplacian matrix $L = A_G - \Delta$, being A_G de adjacency matrix of G (i.e. $A = (a_{i,j}) : a_{i,j} = 1$ if $\{i, j\} \in E$; or 0 otherwise) and Δ_G a diagonal matrix with the degrees of the vertices. The result is known as "Matrix-Tree Theorem", and it is a seminar result in the field called Algebraic Graph Theory [3].

In this appendix, we will study the complexity of Monma graphs, $\kappa(M_{l_1,l_2,l_3})$. To the best of our knowledge, even its simplicity this is the first place where a closed expression for $\kappa(M_{l_1,l_2,l_3})$ is available.

We invite the reader to see Figure 3. All Monma graphs have co-rank 2. As a consequence, in order to find spanning trees it is required to delete precisely two links. If both links are removed from the same independent path between nodes u and v, the resulting subgraph is disconnected. On the other hand, if two links from different paths are removed, a tree is obtained. Then, the complexity of M_{l_1,l_2,l_3} is:

$$\kappa(M_{l_1,l_2,l_3}) = l_1l_2 + l_1l_3 + l_2l_3 \tag{8}$$

Expression (8) has the following combinatorial interpretation: it is the number of ways to remove two balls from different bins, where we have exactly l_i balls in bin i, where $i \in \{1, 2, 3\}$.

It is clear that $l_1 + l_2 + l_3 = m$, the number of links from Monma graph, and that $\kappa(M_{l_1,l_2,l_3}) \leq \binom{m}{2}$, since some deletion of pairs of links result in a tree. Now, we will find a tighter bound for the complexity of Monma graphs. For that purpose, we will study the structure of Monma graphs with m links that maximize the complexity. Consider the following combinatorial optimization problem:

$$\begin{aligned} \max_{l_1,l_2,l_3} f(l_1, l_2, l_3) &= l_1l_2 + l_1l_3 + l_2l_3 \\ s.t. & \\ l_1 + l_2 + l_3 &= m \\ l_1, l_2, l_3 &\in \mathbb{N} \end{aligned}$$

By the symmetry of function f, we will assume that $l_1 \geq l_2 \geq l_3$ without loss of generality. We will prove that the maximum is attained when $l_1 = l_2 = l_3$ if $m = 3k$ for some $k \geq 1$, $l_1 = l_2 = l_3 - 1$ if $m = 3k-2$, for some $k \geq 1$, or $l_3 = l_2 = l_1 + 1$ otherwise. In the combinatorial interpretation is the following: "the number of ways to remove two balls from different bins is maximized when the number of balls in each bin is balanced".

Indeed, if $l_1 \geq l_2 - 2$ then $f(l_1 - 1, l_2 + 1, l_3) = f(l_1, l_2, l_3) + l_1 - l_2$. Therefore, we subtract a unit from l_1 and it to l_2, and the objective is increased, respecting the constraint $l_1 + l_2 + l_3 = m$. Therefore, the integers l_1, l_2 and l_3 that achieve the maximum cannot differ in more than one unit. The reader can appreciate that if we choose (w.l.o.g.) $l_1 \geq l_2 \geq l_3$ then $l_1 = l_2 = l_3$ if m is a multiple of 3, or they differ in one unit, as mentioned before.

A graph reading is the following: "the complexity of Monma graphs with a fixed size is maximized when the three independent paths have roughly the same length". This maximum is roughly $3(\frac{m}{3})^2 = \frac{m^2}{3} < \binom{m}{2}$. In this case, roughly two-thirds of all pair deletion of links are trees.

B

We already know that trees are 1-weak (i.e. an arbitrary link deletion disconnects them). In this paragraph, we will reinforce this result:

PROPOSITION 2. *The DCR of a tree can be computed in linear time with its order.*

PROOF. Let $T = (V, E)$ be a tree and $K \subseteq E$ the terminal set. Since T is a tree, given two terminals $u, v \in K$ there is precisely one path P_{uv} that connects them. All those links must be operational, and the length of P_{uv} must be smaller than d. The links not included the set $P = \cup_{u,v \in K} P_{uv}$ are irrelevant. Let d' be the diameter of P. Therefore:

$$R^d_{K,T} = 1_{\{d' \leq d\}} \prod_{e \in P} p_e, \tag{9}$$

being p_e the probability of operation of link e, $1_{\{x\}}$ equals one if x is true and 0 otherwise. The set P can be found linearly in $|V|$ using breadth first search (BFS) with an arbitrary terminal $u \in K$ as the root node (the process finishes when all terminals are reached). Let $x \in K$ be the terminal that is farthest away from u during the BFS process. If we apply BFS again starting from x as the root node and y is farthest away we get $d' = d(x, y)$. So, the diameter d' can be obtained in linear time with $|V|$. Since the number of products in Expression (9) is $|P| \leq |E| \leq |V|$, the whole computation of $R^d_{K,T}$ be obtained in order $|V|$ elementary operations. ♠ □

Chapter 3

Recursive Variance Recursion Method in Stochastic Monotone Binary Systems

The reliability analysis is described in more abstract structures. We consider stochastic binary systems, where its components either fail or operate with independent probabilities, and a rule determines whether the whole system works or not.

If the rule is monotonous with respect to failures, a stochastic monotone binary system (SMBS) is obtained as a particular case. The reliability evaluation of arbitrary SMBS belongs to the class of $\mathcal{NP}$-Hard computational problems. Therefore, we develop approximation methods for the reliability.

In a first stage, an outstanding method for network reliability analysis called Recursive Variance Reduction (RVR) is extended to general SMBS. Again, RVR method presents lower variance than Crude Monte Carlo (CMC). Finally, RVR is tested over three different SMBS, and compared with two Monte Carlo methods (based on statistical and counting methods).

Recursive Variance Reduction Method in Stochastic Monotone Binary Systems

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***Abstract*—A multi-component system is usually defined over a ground set S with $m = |S|$ components that work (or fail) stochastically and independently, ruled by the probability vector $p \in [0,1]^m$, where p_i is the probability that component i works. We study systems which can be either in "up" or "down" state, according to their ability to comply with their stated mission given the subset of components under operation, through a function $\phi : \mathcal{P}(S) \to \{0,1\}$, called structure. A stochastic binary system (SBS) is the triad (S, p, ϕ), and the reliability r of an SBS is the probability that the system is up. The reliability evaluation of an arbitrary SBS belongs to the class of $\mathbb{NP}$-Hard computational problems. Therefore, there is no polynomial time algorithm to find r for every SBS, unless $\mathbb{P} = \mathbb{NP}$.**

The goal of this paper is to study approximation algorithms to accurately estimate the reliability of a stochastic monotone binary system, or SMBS, where its structure is monotonous. First, two Monte Carlo approaches are discussed. Then, the Recursive Variance Reduction (RVR) method (designed originally for the particular case of network reliability) is generalized to estimate the reliability of an SBMS.

The performance of these algorithms under different SMBS (inspired mainly in network design and k-out-of-m structures) is illustrated numerically. Hints and challenges for future work are discussed in the conclusions.

***Index Terms*—Stochastic Binary System, Recursive Variance Reduction, Network Reliability, Monte Carlo.**

I. Introduction

In real-life, the correct operation of a complex system (e.g., a car, a train, a plane, a bridge) depends on the operation of its components. Usually, it is hard to know deterministically when a certain component will fail. Thus, a natural way to model the system is probabilistically, where the probability of operation of each component can be estimated by historical information.

This paper is structured in the following manner. Section II formally presents the problem and its related terminology. The computational complexity is analyzed in Section III. There, it is proved that the reliability evaluation of an SMBS belongs to the class of $\mathbb{NP}$-Hard computational problems. Therefore, it seems natural to define efficient approximation algorithms for the reliability of an SMBS. Consequently, two straightforward Monte Carlo approaches and a generalization of the Recursive Variance Recursion (RVR) method are described in Section IV. In Section V, the behavior of these algorithms is explored on different SMBS, related to network reliability and k-out-of-m systems. Finally, Section VI contains the main conclusions and ideas for future research.

II. Problem and Terminology

A. Stochastic Monotone Binary Systems

In this section, we will follow the terminology in Ball [1]. Consider a system composed of m components arbitrarily ordered. The set of components is $S = \{1, \ldots, m\}$. For convenience, we translate every subset $T \subseteq S$ into a binary word, using the indicator vector $\varphi(T) = \mathbb{1}_T \in \{0,1\}^m$, such that $\mathbb{1}_T(i) = 1$ if and only if $i \in T$. Its inverse function $\varphi^{-1} : \{0,1\}^m \to \mathcal{P}(S)$ is denoted by $\varphi^{-1}(x) = S_x \subseteq S$.

We will use equivalently subsets of S or binary words, using the translation φ. A *stochastic binary system* (SBS for short) is a triad (S, p, ϕ), where $p \in [0,1]^m$ is a probability vector and $\phi : \{0,1\}^m \to \{0,1\}$ a structure function, such that $\phi(x) = 1$ ($\phi(x) = 0$) means that when S_x operates and the other components fail, the system is up (respectively, down). We have $p_i = P(\text{component } i \text{ is up})$, and $q_i = 1 - p_i$. If $x, y \in \{0,1\}^m$, we consider the relation $x \leq y$ whenever $x_i \leq y_i$ for all i, and $x < y$ when $x \leq y$ and $x_j < y_j$ for some

j. A *stochastic monotone binary system* (SMBS) is an SBS such that the structure function is monotonous, that is, when $\phi(x) \leq \phi(y)$ whenever $x \leq y$.

A set $T \subseteq S$ is a pathset if $\phi(\mathbb{1}_T) = 1$. A minpath is a minimal pathset under inclusion. A subset $T \subseteq S$ is a cutset if the system is down whenever all the components from T fail. Formally, T is a cutset when $\phi(\mathbb{1}_{S-T}) = 0$. A mincut is a minimal cutset under inclusion. The number of failed components is a function $f : \{0,1\}^m \to \mathbb{N}$ such that $f(x) = m - \sum_{i=1}^{m} x_i$. A minimum cardinality cutset is a cutset $T \subseteq S$ such that $f(\mathbb{1}_T)$ is a global minima of f. Consider a random binary vector $X = (X_1, \ldots, X_m)$ such that $X_1, \ldots, X_m$ are independent Bernoulli random variables with $P(X_i) = p_i$. The *reliability* of an SBS is the probability that the system is up:

$$r = P(\phi(X) = 1) \ = E(\phi(X)). \tag{1}$$

B. Computational Complexity

The class $\mathbb{NP}$ is the set of problems polynomially solvable by a non-deterministic Turing machine [2]. A problem is $\mathbb{NP}$-Hard if it is at least as hard as every problem in the set $\mathbb{NP}$ (formally, if every problem in $\mathbb{NP}$ has a polynomial reduction to the former). It is widely believed that $\mathbb{NP}$-Hard problems are intractable (i.e., there is no polynomial-time algorithm to solve them). An $\mathbb{NP}$-Hard problem is $\mathbb{NP}$-Complete if it is inside the class $\mathbb{NP}$. Stephen Cook proved that the joint satisfiability of an input set of clauses in disjunctive form is an $\mathbb{NP}$-Complete decision problem; in fact, this is the first known problem of this class [3]. In this way, he provided a systematic procedure to prove that a certain problem is $\mathbb{NP}$-Complete. Specifically, it suffices to prove that the problem is inside the class $\mathbb{NP}$, and that it is at least as hard as an $\mathbb{NP}$-Complete problem. Richard Karp followed this idea and presented the first 21 combinatorial problems inside this class [4]. Leslie Valiant defines the class $\#\mathbb{P}$ of counting problems, such that testing whether an element should be counted or not can be accomplished in polynomial time [5]. A problem is $\#\mathbb{P}$-Complete if it is in the set $\#$-$\mathbb{P}$ and it is at least as hard as any problem of that class.

III. Reliability Evaluation of an SMBS: Computational Complexity

In this section we outline the computational complexity aspect of the problem of computing r for any SBS. The intractability is a trivial corollary of two classical results.

Proposition 1: Recognition and counting minimum cardinality mincuts/minpaths are at least as hard as computing the reliability of a SMBS.

Proof: See [1]. ∎

Proposition 2: The reliability computation of an arbitrary SMBS belongs to the class of $\mathbb{NP}$-Hard problems.

Proof: It suffices to prove that computing the reliability of class of SMBS belongs to the class $\mathbb{NP}$-Hard. The result follows by inclusion.

Given an arbitrary connected graph $G = (V, E)$ with $|V| > 1$, $|E| \geq 1$, and a subset $K \subseteq V$, we define the structure $\phi : \mathcal{P}(E) \to \{0,1\}$ such that $\phi(H) = 1$ if and only if the nodes in the set K are connected by paths in the subgraph (V, H) (and $\phi(H) = 0$ otherwise). Let $p_e \in [0,1]$ where p_e is an arbitrary probability of operation for link $e \in E$. Arnon Rosenthal proved that the reliability computation of the SMBS $(\phi, E, (p_e)_{e \in E})$ is $\mathbb{NP}$-Hard [6], showing that the minimum cardinality mincut recognition is precisely the Steiner-Tree problem, included in Richard Karp's list. Therefore, the computation of the reliability of this particular family of SMBS, called *K-terminal reliability*, belongs to the class of $\mathbb{NP}$-Hard problems. The conclusion then follows. ∎

By means of an exhaustive enumeration of cutsets (or pathsets), exact expressions for the reliability of an SMBS can be obtained:

$$\begin{aligned} r &= \sum_{x \in \{0,1\}^m : \phi(x) = 1} P(X = x) \\ &= 1 - \sum_{x \in \{0,1\}^m : \phi(x) = 0} P(X = x). \end{aligned}$$

However, the cardinality of the set of all cutsets (pathsets) is in general exponential in the size m, which is computationally prohibitive. Furthermore, Lemma 2 supports the development of Monte Carlo algorithms, which usually trade accuracy for computational effort. This is the main reason that lead us to study statistical approximation for the reliability of arbitrary SMBS.

Lemma 1 is in contrast with Proposition 2, and will be used in Section IV in order to define a generalization of Recursive Variance Reduction (RVR).

Lemma 1: Given an arbitrary SMBS (S, p, ϕ), we can find a mincut $S' \subseteq S$ in a quadratic order of evaluations with respect to $m = |S|$.

Proof: Without loss of generality, we assume S is a cutset (otherwise, by monotonicity we get that $\phi \equiv 1$ and there are no mincuts in this system). We look for the first component such that $S - \{i\}$ is not a cutset. If there is no such component, S is itself a mincut (found applying m structure evaluations), and S is the evidence of the truth of the statement. Otherwise, a new stage of the same process takes place for the cutset $S_1 = S - \{i\}$. Since m is finite, each stage requires less than m evaluations, and there are at most m stages, the whole process requires not more than m^2 evaluations. ∎

Lemma 2 formally states that monotonicity is preserved under conditional failure and/or operation of some components in an arbitrary SMBS:

Lemma 2: Consider an SMBS (S, p, ϕ) and an arbitrary subset of components C, where some components in C fail and others operate, arbitrarily. Then, the sub-system $(S - C, p', \phi')$ is an SMBS, where p' is the original vector with the corresponding indices from C being deleted, and $\phi' = \phi|_{S-C}$ is the sub-structure that sets the bits from C correspondingly (i.e., setting to 1 components under operation and to 0 the ones under failure).

Proof: Monotonicity is inherited from the original SMBS, since the partially ordered set $(\{0,1\}^m, \leq)$ holds for an arbitrary subset of $\{0,1\}^m$. ∎

Definition 1: Under the conditions of Lemma 2, the substructure of ϕ associated to the subset C is denoted by ϕ_C.

The recursive aspect of RVR method is strongly based on the efficient computation of a cutset (Lemma 1) and the analysis of smaller subsystems (inspired in Lemma 2 and Definition 1).

IV. Algorithms

Monte Carlo simulation is a noteworthy computational tool for approximating measures whose exact evaluation is not feasible. In a macroscopic point of view, the idea is to represent the behavior of a complex system (or a part of it), and consider N independent realizations of that simulation, in order to statistically estimate the performance of the system (or subsystem) and assist decision making.

Monte Carlo has been widely applied to a great diversity of problems, including counting, numerical integration, discrete-event (and rare event) simulation. The reader can find a generous variety of applications in [7], and a thorough analysis of rare event simulation using Monte-Carlo methods in [8].

We are also inspired by a method originally designed for network reliability evaluation, called Recursive Variance Reduction or RVR for short [9]. There, the authors introduce a statistical method to estimate the K-terminal reliability, which is more efficient than Crude Monte Carlo (CMC) when the quantity to estimate is small. In this section, we present Monte Carlo approaches and a generalization of RVR to find the reliability of an arbitrary SMBS.

A. Crude Monte Carlo (CMC)

In the simplest Monte Carlo method (sometimes called Crude Monte Carlo, CMC), N independent replicas $X^1, \ldots, X^N$ of a random variable with finite mean $E(X)$ are carried out. By Kolmogorov's strong law, the unbiased average $\overline{X}_N$ converges almost surely to $E(X)$. Its variance (and therefore its mean square error) is $Var(\overline{X}_N) = Var(X)/N$.

In this context, we need to pick N independent copies $X^1, \ldots, X^N$ of the random vector $X = (X_1, \ldots, X_m)$, such that $P(X_i = 1) = p_i$. Then, the CMC estimation is

$$r_{CMC} = \frac{1}{N} \sum_{i=1}^{N} \phi(X^i). \tag{2}$$

It is unbiased, with variance $Var(r_{CMC}) = r(1-r)/N$. Observe that CMC can be used in general SBS.

B. F-Monte Carlo (FMC) in the homogeneous case

The reliability computation of an SMBS with identical probabilities of operation $p_i = p$ is a combinatorial problem. Consider the following partition of $\{0,1\}^m$:

$$S_i = \{x \in \{0,1\}^m : f(x) = i, \phi(x) = 1\},\ \forall i = 0, \ldots, m.$$

Consider the numbers $F_i = |S_i|$. If we find the *F-vector* $F = (F_0, F_1, \ldots, F_m)$, then we can deduce the reliability of the SMBS. In fact:

$$\begin{aligned} r &= \sum_{T \in \mathcal{P}(S):\phi(T)=1} P(X = T) \\ &= \sum_{i=0}^{m} \sum_{T \in S_i} P(X = T) \\ &= \sum_{i=0}^{m} \sum_{T \in S_i} p^{m-i}(1-p)^i \\ &= \sum_{i=0}^{m} |S_i| p^{m-i}(1-p)^i \\ &= \sum_{i=0}^{m} F_i p^{m-i}(1-p)^i. \end{aligned}$$

In this case (under identical probabilities), the reliability $r = r(p)$ is a polynomial in the here scalar variable $p \in [0,1]$. The function $r(p)$ is called *reliability polynomial* of the SMBS. Therefore, the reliability polynomial computation is a counting problem.

The key idea of F-Monte Carlo (FMC) is to pick random states $x \in \{0,1\}$ such that $f(x) = i$. Then, we count the ones that belong to the set S_i in order to estimate F_i. Let us consider independent, identically distributed samples $X_i^1, \ldots, X_i^N$ with exactly $m - i$ elements up, and take the mean sample:

$$\widehat{\phi}_i = \frac{1}{N} \sum_{j=i}^{N} \phi(X_i^j).$$

There are $\binom{m}{i}$ states with $m-i$ elements up. Therefore, $\widehat{F}_i = \binom{m}{i}\widehat{\phi}_i$ is an unbiased estimation for F_i. Finally, an unbiased estimation for the reliability polynomial $r(p)$ is:

$$r_{FMC}(p) = \sum_{i=0}^{m} \hat{F}_i p^{m-i}(1-p)^i.$$

This method has been designed first in network reliability analysis. The reader is invited to see [10] for its performance in a network reliability context.

Algorithm 1 $r_{CMC} = CMC(\phi, S, p)$

```
Sum ← 0
for i = 1 to N do
    X_i ← ∅
    for j = 1 to m do
        if Rand < p_j then
            X_i ← X_i ∪ {x_j}
        end if
    end for
    Sum ← Sum + φ(X_i)
end for
return r_CMC = Sum/N
```

Fig. 1. Pseudocode for CMC method.

Algorithm 2 $r_{FMC}(p) = FMC(\phi, S)$

for $i = 0$ to m **do**
  $Sum_i \leftarrow 0$
  for $j = 1$ to N **do**
    $X_i^j \leftarrow Subset(m - i, S)$
    $Sum_i \leftarrow Sum_i + \phi(X_i^j)$
  end for
  $\widehat{F}_i \leftarrow \binom{m}{i} Sum_i / N$
end for
$r_{FMC}(p) \leftarrow \sum_{i=0}^{m} \widehat{F}_i p^{m-i}(1-p)^i$
return r_{FMC}

Fig. 2. Pseudocode for FMC method.

Algorithm 3 $Q = RVR(\phi, S, p)$

if $\phi \equiv 1$ **then**
  return $q_{RVR} = 0$
end if
if $\phi \equiv 0$ **then**
  return $q_{RVR} = 1$
end if
$C \leftarrow MinCut(\phi, S)$
$q_C \leftarrow \prod_{j=1}^{|C|}(1 - p_j)$
$(V, B_i, A_i, p') \leftarrow SampleCut(C, p)$
return $Q = q_C + (1 - q_C) \times RVR(\phi_{B_i}, S - A_i, p')$

Fig. 3. Pseudocode for RVR method.

C. Recursive Variance Reduction (RVR)

This method has been widely applied in network reliability problems, with good results [9], [11]. The key idea is to work with conditional probability measures, using the presence or absence of a specific cutset.

The probability of ocurrence of the cutset event (all the components in the cutset are down) is included as a term to be added to the unreliability estimator. Additionally, using an arbitrary ordering of the components of the cutset in each replication it is possible to sample the first component that is up (conditional to the absence of this specific cutset). Applying a recursion over the corresponding sybsytems (and using conditional probabilities), we can sample the system and compute an estimator of its reliability (or unreliability). The sampling respects the probability of the events that correspond to those subsystems, weighting the relevance of those subsystems according to the probability of the conditional event.

More specifically, consider a random vector $X = (X_1, \ldots, X_m)$ such that $X_1, \ldots, X_m$ are independent Bernoulli variables and $P(X_i = 1) = p_i$. We will stick to the original notation from Cancela and El Khadiri [9], adapted to this context of general SMBS.

1) A mincut $C = (a_1, \ldots, a_{|C|})$ is found using Lemma 1.
2) A_C denotes the event "all the components in C fail".
3) $q_C = P(A_C) = \prod_{j \in C}(1 - p_j)$.
4) $A_i = \{a_1, \ldots, a_i\}$
5) B_i is the event "a_i is up but a_j fails for all $j < i$".
6) $P(B_i) = p_i \prod_{j<i}(1 - p_j)$.
7) V is a discrete random variable such that $P(V = i) = P(B_i | \bar{A}_C) = P(B_i)/(1 - q_C)$, where $\bar{A}_C$ is the complement of A_C.
8) $Y_i = 1 - \phi_{B_i}$ is the unreliability of the system, conditional on the event B_i.

Consider now the following random variable:

$$Z = q_C + (1 - q_C) \sum_{i=1}^{|C|} 1_{\{V=i\}} Y_i. \tag{3}$$

By Lemma 2, the subsystems ϕ_{B_i} are SMBS as well. By direct calculation, we can check that Z is an unbiased estimator of the unreliability $q = 1 - r$. What is more, a mean sample of Z has smaller variance than CMC, therefore it is more accurate (since both are unbiased estimators). The proofs are similar to the ones offered in the paper [9], substituting SMBS instead of networks. We invite the reader to observe that they do not exploit any specificity of the particular K-terminal structure other than monotonicity.

Without any loss of generality, our target is $q = 1 - r$, known as the unreliability of an SMBS. Expression (3) suggests the following recursive operator Q as the unreliability estimator:

$$Q(X) = \begin{cases} 1, & \text{if } \phi \equiv 0; \\ 0, & \text{if } \phi \equiv 1, \text{ or} \\ q_{C_{S'}} + (1 - q_{C_{S'}}) & \sum_{i=1}^{|C_{S'}|} 1_{\{V=i\}} Q_{B_i}(X). \end{cases} \tag{4}$$

where the mincut $C_{S'}$ is recursively found for each subsystem using Lemma 1 over the whole component-set S'. Observe that the recursion fixes some elements that are down from the cutset and the first element i that is up as well. In other words, the historical information during the recursion is recorded in the conditional measure. It is worth to remark that the successive subsystems have less components, and the termination is guaranteed.

An unbiased estimator for q is:

$$q_{RVR} = \frac{1}{N} \sum_{i=1}^{N} Q_i, \tag{5}$$

being $\{Q_1, \ldots, Q_N\}$ and independent and identically distributed sample of $Q(X)$.

V. Performance Analysis on different SMBS

The number of SBS with m components is 2^{2^m}. If we further reduce the space, the number of SMBS is called Dedekind number $D(m)$ (i.e., the number of nondecreasing boolean functions $\{0,1\}^m \to \{0,1\}$). The sequence respects the asymptotic behavior $log_2 D(n) \sim \binom{n}{n/2}$, and, to the best of our knowledge, it is only known for values of $m \leq 8$ [12].

Therefore, a statistically meaningful selection of SMBS is not feasible. Instead, we choose a sample of three outstanding SMBS that showed to have relevant applications in network reliability and survivability. Consider a simple graph $G = (V, E)$, terminal set $K \subseteq V$, $p_e \in [0, 1]$ for each $e \in E$ and a positive integer d.

1 K-Terminal Reliability: $S = E$, $p = (p_e)_{e \in E}$, $\phi(H) = 1$ if and only if all pairs in K are reachable in the partial graph (V, H).
2 Diameter-Constrained Reliability: $S = E$, $p = (p_e)_{e \in E}$, $\phi(H) = 1$ iff all pairs $u, v \in K$ satisfy $d(u, v) \leq d$ in the partial graph (V, H).
3 k-out-of-m: $S = \{1, \ldots, m\}$, $p = (p_1, \ldots, p_m)$, $\phi(x) = 1$ if and only if $\sum_{i=1}^{m} x_i \geq k$.

We invite the reader to verify that these three models are examples of SMBS. In order to highlight the effectiveness of the different algorithms, we apply CMC, FMC and RVR (defined in Section IV) to the selected examples of SMBS. Since FMC estimates the reliability polynomial, it is only suitable for homogeneous scenarios (i.e., with identical probabilities of operation p in all components). Finding this polynomial is trivial for k-out-of-m systems; $F_i = 0$ for all $i > m - k$ and $F_i = \binom{m}{i}$ for all $i \leq k$.

Observe that CMC, FMC and RVR return unbiased estimators of the reliability. Therefore, a fair comparison should consider both mean square error (i.e, variance) and computational effort. Suppose we have two methods A and B that provide an unbiased estimation of the reliability. The relative efficiency of A with respect to B is the ratio $t_B V(B)/(t_A V(A))$, where t_A and t_B are the respective mean computational times (in the same units), and $V(A)$ and $V(B)$ the variances (or mean square error) of the estimators of the respective methods A and B.

We carried out the following three tests, using the Dodecahedron graph depicted in Figure 4:

1 K-Terminal Reliability with $K = \{0, 11, 13, 15\}$, $p_e = 0,99$ (homogeneous system).
2 DCR with All-Terminal, $d = 5$ and $p_e = 0,999$ (homogeneous system).
3 3-out-of-29 with $p_i = 0.1 - 0.8 \times (i - 1)/29$ (heterogeneous system).

The three algorithms are useful for the first two structures. However, as said before, FMC is not defined for heterogeneous systems, and the third instance just compares CMC versus RVR.

The exact reliability of the first two tests is not available. However, we will see that the discrepancy between the current estimations is vanishingly small. Let us look more in depth at the third case. The number of components under operation in a k-out-of-m system is a sum of independent Bernoulli variables with different success probabilities. This is a Poisson-Binomial distribution, and a closed formula is provided in [13]. If $p = (p_1, \ldots, p_m)$ denotes the probability of operation for each component, $p(h) = P(\sum_{i=1}^{m} X_i = h)$ represents the probability mass function of the number of components under operation and $Q(x) = \sum_{j=x}^{m} p(j)$ is the cumulative probability of the tail, then the exact reliability of a k-out-of-m system is precisely [13]:

$$r = Q(k) = 1 - \frac{k}{m+1} - \frac{1}{m+1} \sum_{i=1}^{m} \frac{1 - \mathrm{e}^{-j2\pi ik/(m+1)}}{1 - \mathrm{e}^{-j2\pi i/(m+1)}} \times \prod_{h=1}^{m} \left[p_h \mathrm{e}^{j2\pi i/(m+1)} + 1 - p_h \right],$$

with $j^2 = -1$.

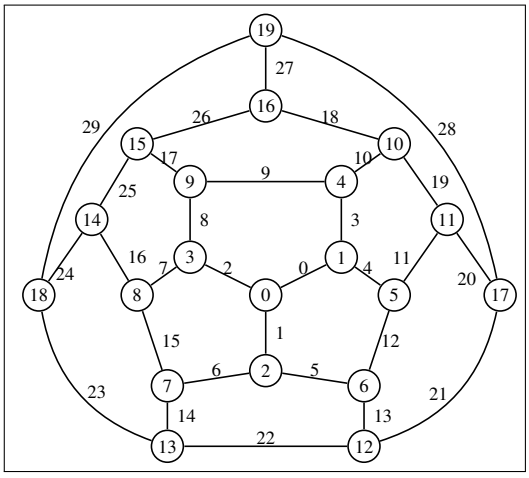

Fig. 4. Dodecahedron network

In Tests 1 and 2 we set high values for p (0.99 and 0.999) since in real networks links are usually highly reliable, and the unreliability is thus a rare event. The application of Monte Carlo methods in rare-event contexts has been extensively studied [8]. Variance-reduction methods like RVR outperform CMC as network failures become rarer.

In our first test, an average among one-hundred independent runs of both CMC and RVR are carried out, using sample sizes $N = 10^6$ and $N = 10^4$ respectively. An average over thirty independent runs of FMC is also considered (using $N = 10^5$ as the CMC sample size for estimating each F_i). The same runs take place for Test 2, setting $p = 0.999$. Finally, CMC versus RVR under equal conditions of $N = 10^6$ samples are studied in Test 3.

Tables I, II and III present the average reliability, computing time, sampling variance and relative efficiency (using RVR as algorithm A and CMC as algorithm B) respectively, in different rows.

Metric	CMC	RVR	Ratio	FMC
Reliability	0.9999956	0.9999958	1	0.9999944
Variance	4.9070E-12	1.1400E-13	43.043	5.28841E-11
Avg. Time (ms)	6509	6480	1.004	17586
Rel. Efficiency	B	A	***43.233***	

TABLE I
TEST 1: RESULTS

Metric	CMC	RVR	Ratio	FMC
Reliability	0.999949	0.999941	1	0.999940
Variance	5.3525E-09	7.5224E-11	71.154	2.57166E-13
Avg. Time (ms)	591	42677	0.014	17586
Rel. Efficiency	B	A	***0.985***	

TABLE II
TEST 2: RESULTS

Metric	CMC	RVR	Ratio
Reliability	0.99999995	0.999999971	1
Variance	4.7980E-14	2.2243E-16	215.708
Avg. Time (ms)	291	3161	0.092
Rel. Efficiency	B	A	***19.877***

TABLE III
TEST 3: RESULTS

It can be appreciated from Tables I and II that RVR has lower variance than CMC, as predicted from the classical literature [9], [8]. This variance reduction is even better when the unreliability becomes rarer (Test 2). In terms of relative efficiency, RVR clearly outperforms CMC in Test 1, while they present similar relative efficiency for Test 2, due to the more complex processing that RVR performs for each sample.

Further analysis is required to choose mincuts during the RVR process in a general SMBS, in order to improve its computational effort. On the other hand, FMC provides accurate reliability estimations. However, it typically takes longer times since it performs several CMC estimations to return a polynomial (it requires computing and averaging N CMC calls for each coefficient F_i). It showed poor relative efficiency in Test 1, but surprisingly its relative efficiency is approximately 320 versus RVR and CMC for Test 2. The causes of this outstanding performance of FMC under a rare event scenario should be explored as a part of future work.

In Test 3, RVR again outperforms CMC in terms of relative efficiency; its gain is close to 20. CMC presents lower computational time, but higher variance. They are both accurate estimators in this scenario. We remark that this is the first test where RVR has been carried out in a context other than network reliability.

VI. CONCLUSIONS

The object under study is the reliability computation of stochastic monotone binary systems (SMBS). The exact computation of the associated metrics belongs to the class of $\mathbb{NP}$-Hard computational problems. As a corollary, the literature offers exact algorithms for reliability computations in exponential time (for instance, based on a summation of all possible pathsets), and approximation techniques.

When the system failure is a rare event, Recursive Variance Reduction method (RVR) presents excellent performance studying connectivity properties in graphs. This paper explains why RVR can be used to find the reliability of arbitrary SMBS. The key point is to show how to build mincuts in these systems. The termination and application of RVR is guaranteed by monotonicity.

RVR provides an unbiased estimator for the reliability, and has lower variance than Crude Monte Carlo (CMC). The performance of RVR and CMC has been compared to an alternative approach called F-Monte Carlo (FMC), when the model is homogeneous, that is, when its components have identical probabilities of operation.

The performance analysis was carried out choosing three different SMBS: two coming from network reliability and one from survivability under redundancy, specifically, a k-out-of-m system. As expected, RVR outperforms CMC in non-network contexts as well, at least for special structures. On the other hand, the counting technique called F-Monte Carlo (FMC) provides accurate estimations of the whole reliability polynomial $r(p)$ for homogeneous SMBS.

Several aspects not considered here should be covered in future work. The selection of mincuts in arbitrary SMBS for the RVR process should be studied. A thorough comparison of the presented methods should be considered. Some trade-offs have to be evaluated. E.g., even in cases where the relative efficiency favors RVR or CMC versus FMC, once known $r(p)$, it can be effortless applied to estimate the reliability of any homogeneous system. What is the subset $A \subseteq [0, 1]$ of probability values for which the estimation $r(p)$ offered by FMC outperforms both RVR and CMC? Furthermore, we would like to perform an in-depth analysis of rare events in SMBS, using RVR, FMC and Importance Sampling as well, which presented outstanding results in network reliability [14].

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Part II

Resilence in Dynamic Systems

Chapter 4

Node-Immunization Strategies in a Stochastic Epidemic Model

A great source of inspiration in epidemic modeling is classical SIR (Susceptible - Infected - Removed) model. However, the major shortcomings in SIR model are its assumptions (random contacts in a fully-mixed population).

In this paper we consider an epidemic propagation as a dynamic multiclass system in an underlying graph topology. A stochastic process counts the number of infected individuals. Then, a Node Immunization Problem (NIP) is presented, where the goal is to minimize the epidemic outbreak by a correct choice of nodes for immunization.

By numerical simulation, we show that a Greedy node immunization heuristic is not optimal.

Node-Immunization Strategies in a Stochastic Epidemic Model

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Abstract. The object under study is an epidemic spread of a disease through individuals. A stochastic process is first introduced, inspired in classical Susceptible, Infected and Removed (SIR) model. In order to jeopardize the epidemic spread, two different immunization strategies are proposed. A combinatorial optimization problem is further formalized. The goal is to minimize the effect of the disease spread, choosing a correct immunization strategy, subject to a budget constraint. We are witness of a counter-intuitive result: in non-virulent scenarios, it is better to immunize common individuals rather than communicative ones. A discussion is provided, together with open problems and trends for future work.

Keywords: Epidemic Model, Susceptible, Infected and Removed Model, Stochastic Process, Combinatorial Optimization Problem

1 Introduction

Ironically, a cornerstone in the mathematical analysis of epidemiology has not been published in the scientific literature. The work by Lowell Reed and Wade Frost on Susceptible, Infected and Removed (SIR) model was considered by its authors as too slight a contribution [4]. The most valuable aspects of SIR model is its simplicity: closed formulas are met, an epidemic spread can easily be carried out on a computer, and it connects deterministic and stochastic models in an elegant fashion. For those reasons, SIR model is the starting point in teaching and understanding epidemic propagation. However, it assumes a full-mixed population with random contacts. Several subsequent authors in the field believe a more realistic model is inspired by networks, where nodes represent individuals, and the epidemic spread takes places in the links [14]. The interest of the topic is increased with the current threaten of bioterrorism as a letal weapon over an induced pandemia [13]. The reader can find other authoritative works about SIR epidemics on graphs in the related literature [12, 10, 11]. Simulations carried-out on small-world networks confirm that there exists an extinction threshold [12, 10, 11, 15]. There, the epidemic propagation is carried out through graphs with either potential or exponential degree distribution as distinguished characteristics. However, for social network applications an asymmetric right-tailed distribution

shows to be more suitable. Specifically, if nodes represent people and links are contacts, most individuals have a reduced number of neighbors, that keep in contact daily. Aspects such as network awareness and node-ageing has been suggested by Barabasi in order to define realistic evolutionary network models [1]. Explicit characterizations of extinction and probability distribution of the epidemic outbreak are currently available by means of percolation theory. Kena and Robins use percolation techniques and random mixing using classical SIR model [7]). An empirical study using SIR model is performed by Macdonald and Shakarian. They find centrality measures and detect main spreaders of a disease [9]. The goal of this work is to develop immunization methods to cope with an epidemic propagation. As a mathematical framework, a realistic stochastic process for epidemic propagation is here introduced, together with a score for different immunization strategies. This process is more realistic than classical SIR model.

This article is organized in the following manner. In Section 2, classical SIR model is described as a reference to study epidemic propagation. In order to introduce a more realistic model for disease propagation, a stochastic process is introduced in Section 3. A combinatorial problem is formally presented in Section 4. There, the goal is to choose among a set of feasible immunization strategies, in order to minimize the peak of the epidemic spread. There, the precise meaning of "peak"will be formalized in terms of the underlying stochastic process. Two extremal immunization strategies are proposed. On one hand, we consider a *greedy* immunization notion, were nodes with the highest degree are immunized first, called $HighDegree$. On the other, we pick nodes with low degree uniformly at random, called $LowFirst$. Section 5 introduces classical random graphs as opposite to lattices, as well as efficiency measures for simple graphs. Two random graphs are generated in this work as a case study for disease propagation. Section 6 introduces two massive random graphs used in the simulation of the stochastic process. Then, the performance of strategies $HighDegree$ and $LowDegree$ is analyzed on the lights of these graphs. Finally, Section 7 contains concluding remarks and trends for future work.

The main contributions of this article are summarized in the following items:

- We propose a realistic stochastic process to simulate and understand the evolution of an disease spread.
- A combinatorial optimization problem is formally presented, where the decision variable involves a set of immunization strategies, and the goal is to minimize the infection in the population subject to a budget constraint.
- A greedy notion for the previous combinatorial problem is introduced, where nodes with high degree are immunized first.
- We explicitly show that greedy is not the best option; indeed, a better result is achieved when nodes with low degree are immunized in some scenarios (precisely, in two graphs with 2000 nodes). We will discuss how this counter-intuitive result is possible, in terms of the underlying topology and different virus-types.
- Open problems are presented, arising from the stochastic process and the global optimum for the combinatorial problem.

2 SIR Model

Probably the most-studied class of epidemic models is classical SIR model. There, individuals are Susceptible (S), Infected (I), or Removed (R). The last category represents those individuals that are immune after being recovered of the disease. Iinfected individuals have random contacts with others (from any of the three states) at a mean rate β. They are removed (recovered) at a mean rate γ. If a susceptible receives a contact, it turns infected.

If we consider a big population of n individuals, SIR epidemic model can be described by the following system of non-linear differential equations:

$$\frac{ds}{dt} = -\beta is, \frac{di}{dt} = \beta is - \gamma i, \frac{dr}{dt} = \gamma i,$$

being $s(t) = S(t)/n, i(t) = I(t)/n, r(t) = R(t)/n$ the respective proportions of classes at time t. The last equation can be omitted, since $s + i + r = 1$ [5]. The model assumes standard incidence and recover (I-output) at a rate $\gamma I/n$. This represents a waiting time (or residence time in class I) of $e^{-\gamma t}$ time units, with mean $1/\gamma$. Since such period is small, the model lacks of a vital dynamics (i.e., natural death and birth). Therefore, it is suitable just to describe diseases with fast propagation and conclusion. Furthermore, they provide immunity to infected individuals, for instance, influenza. In computer viruses, we can interpret this as an antivirus program that, once updated, infection is no longer allowed.

SIR model is suitable for a completely-mixed population, where the assumption of uniformly random contact selection is plausible. All individuals have the same number of contacts in a given time unit, and those contacts are equally likely to propagate the disease. However, in real-life applications, we rarely meet all the requirements that must be fulfilled to apply SIR model. Individuals do not contact randomly, and full-mixtures should be replaced by networks [12, 10, 11]. Links represent those pair of individuals with a potential epidemic spread between them. Neighboring nodes represent individuals that potentially contact during the disease (i.e. in real life, partners, mates, friends, people that travel together occasionally, among others). The approach from Percolation Theory gives us information about asymptotic size of infected population, usually under some assumptions such that random mixing or same types of mixing [7]. An overview of mixing and its relation with percolation theory can be found at [6].

It is neither consistent nor realistic to assume the infection probability between pairs of nodes to be identical. It is possible to find some pairs that have higher probability of infection than others. Furthermore, it is not realistic to assume that an infectious-susceptible contact is equivalent to an infection. The capacity of the infectious to spread susceptible with which it has contact may vary over time. The existence of a link between infected and susceptible nodes is not a guaranteed contagion of the susceptible one. The time-window during which an infected node can spread has a non-deterministic (nor fixed) length. In fact, an infected node does not have to contact all its susceptible neighbors at a time. This is our motivation to propose a more realistic stochastic process for disease propagation, in the sense that includes the previous concerns.

3 Stochastic Process

We are given a simple graph $G = (V, E)$, where nodes represent individuals and links are relation between nodes (i.e., possible infection channels). Time is slotted, and the starting point ($t = 0$) is defined as follows:

- Certain selected nodes $V^* \subset V$, called *immunized nodes*, are removed, and the process takes place in the subgraph induced by $V' = V - V^*$, denoted by G'. Observe that $V^* = \emptyset$ implies no immunization at all.
- A single *infected node* $x_0 \in V'$ is chosen uniformly at random (the zero case). All nodes from V' but x_0 are *susceptible nodes*.

Infected nodes might affect neighboring nodes from G' over time, and then susceptible nodes may become infected ones. If a node is infected at time t_i, it can affect neighboring susceptible nodes during a random time-window $[t_i, t_i']$. It is reasonable to assume that although this time-window is random and this length varies from an infected node to another, it fluctuates around a mean value. Therefore, we represent the time-window picking a normal distribution with parameters (μ, σ), where $\mu > 0$ represents the mean length of the time-window and σ denotes its standard deviation. Time t_i' is then picked using the rule $t_i' = t_i + |X_i|$, being X_i a normally distributed random variable, $X_i \sim N(\mu, \sigma)$. The parameters (μ, σ) are called the *virus-type of the disease*. Once t_i' is reached, that infected node is in removed state. When an infected node contacts a susceptible one, the probability of spread varies over time, depending on the state of the infected node. An infected node will affect a susceptible neighboring node at $t \in [t_i, t_i']$ if and only if its *infectivity profile* $f(t) > u$, being $f(t) = \exp\left\{-\frac{1}{(t_i'-t)(t-t_i)}\right\}$ a *bump function* and u a random number in the compact set $[0, 1]$. Function f represents the capacity of the node to spread the disease. This is in agreement with real life, where the infectivity is first monotonically increasing, then it presents a maximum, and later it is monotonically dicreasing.

Definition 1 *The number of infected nodes* $\{X_t\}_{t\in\mathbb{N}}$ *is the stochastic process under study.*

We want to minimize the overall effect of the disease spread. Formally:

Definition 2 *The peak of the disease spread in graph* G *with immunization set* V^* *and virus-type* (μ, σ) *is the first moment of the maximum achieved by the process:* $p(G, V^*, \mu, \sigma) = E(\max_{t\in\mathbb{N}}\{X_t\})$

4 Node Immunization Problem and Heuristics

In this paper, we formulate the performance of different immunization strategies by means of a combinatorial optimization problem. Given a simple graph $G = (V, E)$ and virus-type (μ, σ), we want to minimize the peak of the epidemic spread $p(G, V^*, \mu, \sigma)$ among all feasible immunization sets V^*. The Node Immunization Problem is formulated as follows:

$$\min_{V^*} p(G, V^*, \mu, \sigma) \tag{1}$$

$$s.t.$$

$$|V^*| \leq N \tag{2}$$

The reasons leading to include Constraint (2) in the combinatorial problem are twofold. The first reason is related with a real budget constraint. Even though the desease is propagated through links, the protection takes place in the nodes. The second is related with a requirements associated with immunization heuristics: In order to fix the constraint N, let C be the number of nodes that can be immunized with the available resources.

The critical degree is the first degree g^* such that an epidemic spread occurs (the peak exceeds the 5% of total population), once we remove all nodes from the set $V^* = \{v \in V : deg(v) \geq g^*\}$. Now, let us focus on the development of naive immunization strategies suitable for the combinatorial problem. A small number of individuals with a big link action will have a higher impact than a highly populated group with a sparse number of links. If we immunized these nodes, we would remove its edges of the graph. At first glance, the best nodes to protect should be those with the highest degree.

Nevertheless, the link density is not the only matter, but the quality of those links. This means that if a node-group has several links but they are mostly locally defined (like a clique or quasi-clique), then the immunization of those nodes will not mine the link structure, in the sense that it should be better to immunize a set of nodes V^* with large amount of external links. This suggests another approach: instead of immunizing nodes of higher degree, immunize randomly chosen nodes (those likely to have low degree, since these nodes are the majority of the population). In order to have a strong contrast with the greedy notion, we will choose nodes with low degree. Specifically, the following immunization strategies will be considered in this article:

- *HighDegree*: the greedy notion, where nodes are sort in terms of degree (nodes with the same degree are sort randomly). The immunization takes place in nodes with the highest degree, meeting at the same time Constraint (2).
- *LowDegree*: analogously, but nodes with the lowest degree are selected first, meeting Constraint (2).
- *Raw*: when no immunization takes place ($V^* = \Phi$), we have Raw immunization strategy, which is the cheapest one in practice (but naturally, its performance is low as we will see in Section 6).

5 Random Graphs and Efficiency

Let $G = (V, E)$ a graph with $|V| = n, |E| = m$. There are $C^m_{n(n-1)/2}$ possible spanning subgraphs with m edges in the complete graph K_n. In Erdös-Rënyi rule for random graph generation, a number $t < \frac{n(n-1)}{2}$ is fixed, and a subgraph with t edges is selected uniformly at random. This type of random graphs have typically low diameter, since the random connection between nodes connects every pair of nodes with the same probability [3]. Also, the number of clusters is small, because if a is connected to b and b is connected to c, the probability of the $a-c$ connection is the same that for every pair of nodes. This kind of graph is the example of networks with purely random connections, leading to homogeneous Random Mixing. On the other hand we have Lattices: highly regular graphs with high diameter where the connection $a - c$ has higher probability provided a is connected to b and b is connected to c. From Lattices we can obtain other kind of random graphs (by "rewiring "pairs of nodes at random) that inherits these properties. In order to measure the presence of clusters the concepts of *Global and Local Efficiency* are introduced in [8]. Let us consider a simple graph $G = (V, E)$ with adjacency matrix $A = (a_{i,j})$ and distance matrix $D = (d_{i,j})$.

Definition 3 *The efficiency between nodes v_i and v_j is $e_{i,j} = \frac{1}{d_{i,j}}$.*

Definition 4 *The mean efficiency $Eff(G)$ is the normalized expected value over all node pairs: $Eff(G) = \frac{1}{n(n-1)} \sum_{i \neq j} \frac{1}{d_{i,j}}$.*

The mean efficiency $Eff(G)$ is maximized when $G = K_n$ is the complete graph.

Definition 5 *The global $GEff(G)$ is the ratio between the mean efficiency of G and K_n: $GEff(G) = \dfrac{Eff(G)}{Eff(K_n)}$.*

Note that $0 \leq GEff(G) \leq 1$ and $GEff(G)$ makes sense even if G is not connected. An analogous notion is considered locally for single nodes.

Definition 6 *Let v_i be a node, N_i its neighbor set and G_i the subgraph induced by N_i. The Local Efficiency is the mean of $GEff(G_i), i = 1, \ldots, n$:*

$$LEff(G) = \frac{1}{n} \sum_{i=1}^{n} GEff(G_i)$$

This concept measures the fault tolerance of the graph G. In other terms, it represents the efficiency of the communication between neighbors of a node i when it is removed. On one hand, random graphs present low diameters and then low values of $d_{i,j}$. This implies high values of Global Efficiency. The low probability of clusters implies low Local Efficiency. On the other, Lattices present low values of Global Efficiency (high diameters) but high values of Local Efficiency.

6 Performance Analysis

In order to test the effectiveness of different immunization strategies, two graphs with 2000 nodes have been generated. These graphs were built choosing a predetermined node-degree distribution, and using Havel-Hakimi theorem. To avoid the pure exponential or potential node-degree distributions, we use Gamma distribution (rounded to closest integer values). Let us consider the candidate degrees $(d_1 \geq d_2 \geq \cdots \geq d_{2000})$ of a graph. Havel-Hakimi theorem helps to determine whether such graph exists:

Theorem 1. *the sequence* $d_1 \geq d_2 \geq \cdots \geq d_{2000}$ *is graphic if and only if the sequence is graphic* $d_2 - 1 \geq d_3 - 1 \cdots \geq d_{d_1+1} - 1 \geq d_{d_1+2} \cdots \geq d_p$ *is graphic.*

Once we have a graphic sequence, a recursive method to produce the graph is offered by the work from Bayati [2]. This method generates a graph chosen uniformly at random from the set of all graphic graphs with 2000 nodes and prescribed degrees. In this way, we generated two graphs with 2000 nodes, called $2000A$ and $2000B$. These graphs present low values of Global Efficiency as Lattices, and low values of Local Efficiency, as Random Graphs:

$$\begin{aligned} GEff(2000A) &= 0.2564, \\ LEff(2000A) &= 0.0079, \\ GEff(2000B) &= 0.2158 \\ LEff(2000B) &= 0.0043. \end{aligned}$$

Both graphs are sketched in Figure 1.

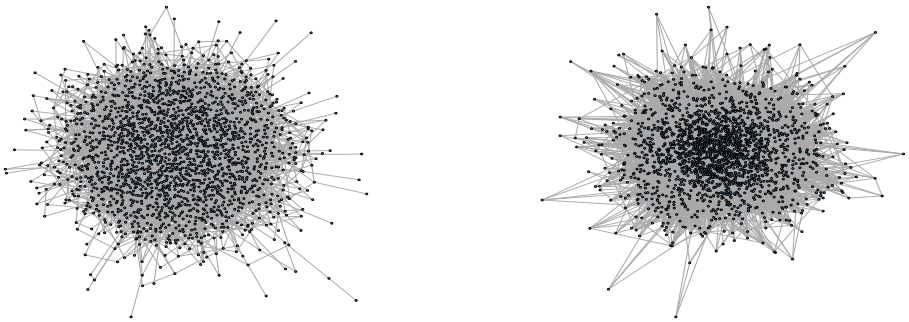

Fig. 1: Left: Graph $2000A$. Right: Graph $2000B$

Simulations were carried-out for different virus-types (μ, σ) in both graphs. In order to perform a faithful comparison of both strategies, one-hundred independent simulations were considered with $t_f = 100$ time slots for each graph, using Crude Monte Carlo. The time-window is generated using a normal distribution with parameters (μ, σ), with mean $\mu \in \{3, 5, 10, 20\}$ and standard deviation $\sigma = 1$. Higher values for μ imply that an infected individual will have more time to infect contacted susceptible individuals. When μ is extremely large, the existence of a link will practically guarantee a positive infection if the neighbor node is susceptible. Figure 2 presents the temporal evolution of X_t in a 100-run average (or mean-epidemic), for $HighDegree$ (red) and $LowDegree$ (blue), with Raw as a reference (green) for the set of virus types $(\mu, \sigma) \in \{(3, 1), (5, 1), (10, 1), (20, 1)\}$ in Graph 2000A.

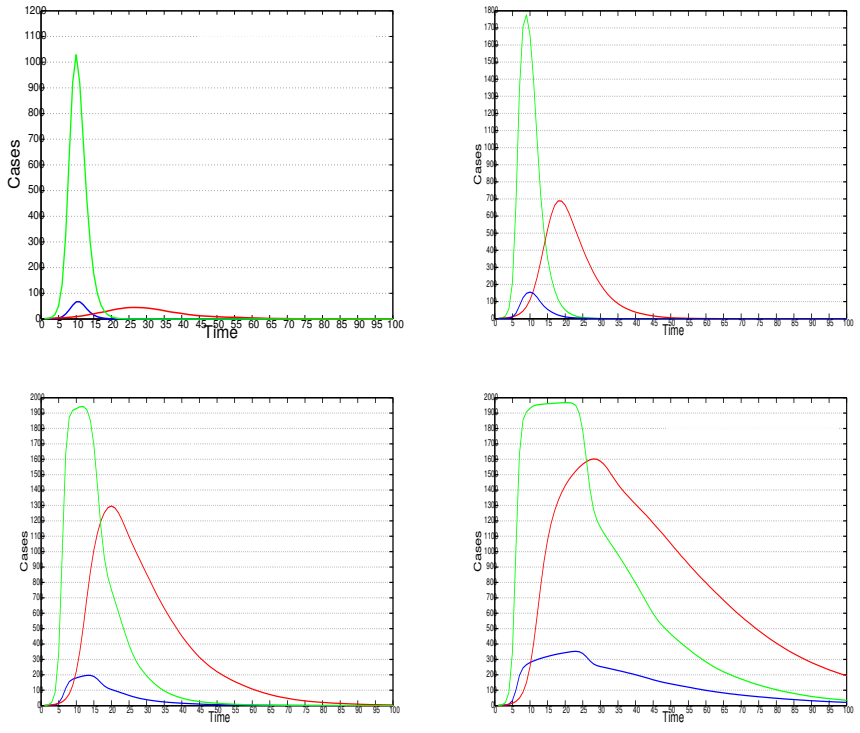

Fig. 2: Performance in Graph 2000A for Virus Types $(3, 1)$, $(5, 1)$, $(10, 1)$ and $(20, 1)$. $HighDegree$ (red), $LowDegree$ (blue), Raw (green).

All simulations for $HighDegree$ were carried out using the critical node set V^* for the set of removed nodes. Analogously, $LowDegree$ is performed choosing nodes whose degree is below the critical one g^* (see Section refcop).

Curiously enough, $LowDegree$ outperforms both $HighDegree$ and Raw heuristics for virus type $(20, 1)$. Therefore, the graph connectivity has low sensibility to a high-degree node-deletion via immunization. This fact suggests that nodes with higher degree tend to connect each other. Therefore, the deletion of their links do not undermine the link-structure of the graph as much if we eliminate the links of the N low degree nodes. For virus-type $(10, 1)$,an epidemic spread takes place in $HighDegree$ if we remove all nodes with degree $d \geq 7$. With virus type $(5, 1)$ the situation is similar to the previous case, as it could be expected if the topology is in fact relevant. For less virulent diseases it is expected to get a lower influence in the underlying network topology. As the disease is less virulent and the topological influence is decreased, $HighDegree$ tends to be more effective.

An analogous performance analysis is carried out in Graph $2000B$.

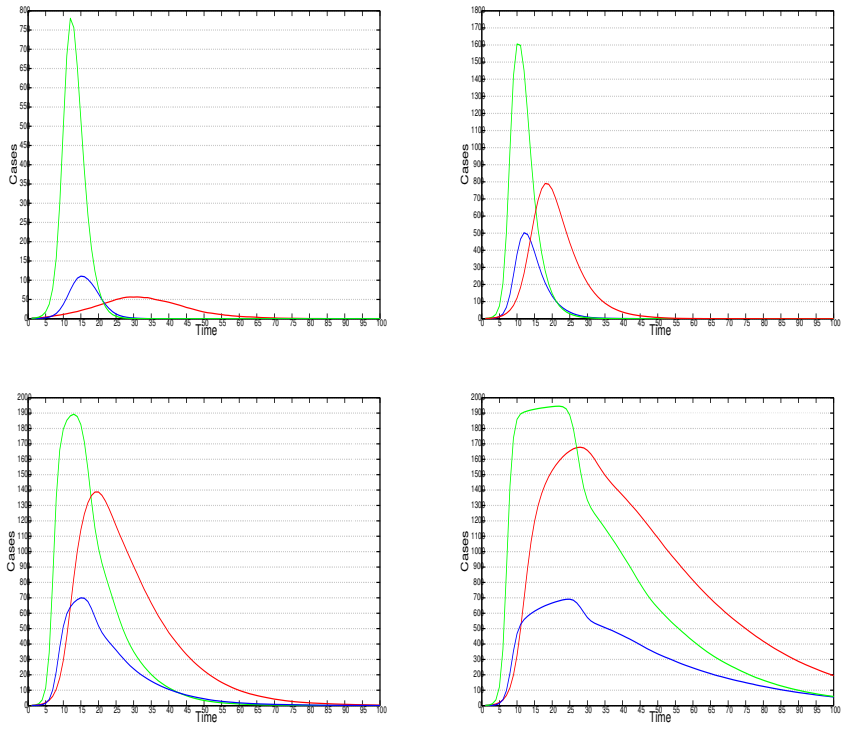

Fig. 3: Performance in Graph 2000B for Virus Types $(3, 1)$, $(5, 1)$, $(10, 1)$ and $(20, 1)$. $HighDegree$ (red), $LowDegree$ (blue), Raw (green).

Figures 3 presents the temporal evolution X_t of infected individuals in a 100-run average (or mean-epidemic). As in previous instances, the difference between both strategies tends to vanish when the disease is less virulent (less influence of the underlying topology). This points out a huge amount of internal links between nodes with the highest degree.

7 Concluding Remarks

The effects of an epidemic propagation under two different immunization heuristics has been discussed. For that purpose, we built two massive random graphs (with Gamma degree distribution and using the strength of Havel-Hakimi theorem), and develop a SIR-based model simulations with different virulence levels.

Two "opposite" heuristics have been proposed. On one hand a *greedy* notion, called $HighDegree$ heuristic, immunizes N nodes with the highest degree first. The intuition here is that they could infect more neighbors in the same time-window. On the other hand, $LowDegree$ heuristic picks N nodes with lower degree uniformly at random, and immunizes them. They are computationally efficient, since the number of elementary operations is linear with the order of the input graph. If we do not immunize nodes we have Raw heuristic. As expected, both heuristics outperform Raw.

A counter-intuitive result is that $LowDegree$ heuristic outperforms $HighDegree$ in some scenarios. A possible explanation would be the following: when we have low values of μ, the number of infected individuals from the neighbor-set N_i is small, and only infected nodes of high degree have a chance to spread disease, since they have a number of contacts many times greater than low-degree nodes and this compensate the low number of trials (time). So, deletion of high-degree nodes is more effective and $HighDegree$ is better.

On the other hand, when we have high values of μ low degree nodes ended by infecting all its neighbors further nodes of high degree, because they have comparatively few neighbors and more time to each one. Graph with a low local efficienct are highly sensible to node deletions, regardless of the degree (see Section 5). The deletion of low-degree nodes disconnects the graph more effectively, and $LowDegree$ is better. As real social networks are adequately modeled by random graphs, simulations will assist in order to study virtual versions of real epidemics. This tool provides a systematic way to produce essays of control and disease prevention, which is an essential element to design adequate strategies to cope with epidemics.

As a future work, we will develop a greedy randomized heuristics in order to find outstanding immunization strategies. More sophisticated ideas should be considered in order to detect high-performance immunization strategies, understanding the underlying graph topology as an input of the heuristic. It is worth to remark that the problem is purely combinatorial when the virus-type is increased without bound, and can be expressed in terms of graph theory and network connectivity. The complexity of this combinatorial problem is still open.

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Chapter 5

A counter-intuitive result on SIR-based Node-immunisation Heuristics

Here we go one step further in epidemic modeling and node immunization strategies. The Node Immunization Problem is revisited. We mathematically prove that Greedy heuristic is not optimal.

A counter-intuitive result on SIR-based Node-immunisation Heuristics

Abstract: We introduce a combinatorial optimisation problem whose goal is to minimize the effect of an epidemic spread, by choosing adequately a number of individuals (limited by external constraints) for immunisation. The epidemic spread is governed by a stochastic process and takes effect in a graph.

Surprisingly, immunisation applied to nodes with the highest degree is not always the best practice. In addition, vaccinating more nodes does not always guarantee a better result. These results are first illustrated empirically through simulations carried-out over random graphs, and finally a mathematical proof is provided.

Keywords: Epidemic Models, SIR, Random graphs.

Reference to this paper should be made as follows: < List of authors > (xxxx) 'A counter-intuitive result on SIR-based Node-immunisation Heuristics', *Int. Journal of Metaheuristics*, Vol. x, No. x, pp.xxx–xxx.

1 Introduction

Ironically, a cornerstone in the mathematical analysis of epidemiology has not been published in the scientific literature. According Fine (1977), the work by Lowell Reed and Wade Frost on Susceptible, Infected and Removed (SIR) model was considered by its authors as too slight of a contribution.

The most valuable aspect of SIR model is its simplicity: closed formulas are met, an epidemic spread can easily be carried out on a computer, and it connects deterministic and stochastic models in an elegant manner. For those reasons, SIR model is the starting point in teaching and understanding an epidemic process. However, it assumes a full-mixed population with random contacts, identical contagion probabilities for all individuals, etc.

Santhanam et al. (2011) propose a more realistic model inspired by networks, where nodes represent individuals and the epidemic spread takes place across the links. Newman et al. (2001); Newman (2002, 2003); Ball et al. (2010) reinforces this idea, since individuals do not contact randomly, and full-mixtures should be replaced by networks.

Andersson (1998) studied the spread of a disease under SIR model in large closed homogeneous populations with fixed friendship circles for each individual. Britton et al. (2007) studied random graphs with pre-specified degree distribution assuming constant probability of contagion. In those articles, the authors studied two different vaccination heuristics: random vaccination versus acquaintance vaccination (the vaccination of all friends of a randomly chosen individual). Ball and Sirl (2013) extended the above analysis considering imperfect vaccines and nonconstant infectious period distributions. Ball et al. (2010) use SIR model for

the spread of an epidemic among a population with a random network of social contacts partitioned into households.

The approach from Percolation Theory gives us information about asymptotic size of infected population, usually under some assumptions such as random mixing or some types of mixing. Kenah and Robins (2007) use percolation techniques and random mixing in the classical SIR model. Keeling and Eames (2005) includes an overview of mixing and its relation with percolation theory.

Aspects such as network awareness and node-aging have been suggested by Barabasi (2002) in order to define realistic evolutionary network models.

Newman et al. (2001); Newman (2002, 2003); Shirley and Rushton (2005) show through simulations carried-out on small-world networks (graphs with either potential or exponential degree distribution) that there exists an extinction threshold. However, for social network applications, an asymmetric right-tailed distribution shows to be more suitable. Specifically, if nodes represent people and links are contacts, most individuals have a reduced number of neighbours which whom they keep in contact daily. Ye Sun (2014) studies epidemic propagation in weighted complex networks, using the edge weights to represent multi-role relations. They perform detailed analysis of two representative metrics: outbreak threshold and epidemic prevalence, on SIS and SIR models.

The literature in epidemic models and simulation is vast, ranging from node aging to outstanding spreaders, transmission rates and underlying topological network. Here we just scratch the surface of literature in epidemic propagation.

The goal of this work is to investigate and explain some counter-intuitive results. They arise when comparing (through simulations) the effectiveness of two different vaccination heuristics in networks with right-tailed degree distributions. We will use the terms immunisation or vaccination indistinctly. The main contributions of this article are summarized in the following items:

1. A combinatorial optimisation problem is presented. Two counter-intutive results arise from it.

2. The first is that *Random* outperforms *Greedy* in some scenarios. We discuss how this is possible, providing mathematical proof and an example. This implies that the belief about it is better to focus on vaccinating high degree nodes is not necessarily true.

3. The second result is that vaccinating more nodes does not always guarantee a better result. We provide a mathematical proof and an example.

This article is organized in the following manner.

- In Section 2 we describe the classical SIR model as a reference to study epidemic propagation.
- In Section 3 we define a SIR-based stochastic process, where contacts do not necessarily mean transmission of the disease, allowing the probability of contagion and the number of contacts between an infected node and its neighbours change over time. We define the underlying optimisation problem, to minimize the peak of the curve cases vs. time, under certain restrictions.
- In Section 4 we introduce two well-known immunisation heuristics. On one hand, we consider the *Greedy* immunisation notion, where nodes with the highest degree are immunised. We contrast this greedy heuristic against *Random*, where the same number of nodes to immunise are (uniformly) chosen at random. We build random graphs and right-tailed graphs with two thousand nodes. These graphs will serve as the underlying network topology.
- In Section 5 we analise the performance of both heuristics on the light of the previous graphs.
- In Section 6 we theoretically prove that Greedy is suboptimal, and the counterintuitive result that sometimes it is better not to immunize more individuals.
- Section 7 contains concluding remarks and trends for future work.

2 SIR Model

Probably the most-studied class of epidemic models is classical SIR model. There, individuals are Susceptible (S), Infected (I), or Removed (R). The last category represents those individuals that are immune after being recovered from the disease.

Infected individuals have random contacts with others (from any of the three states) at a mean rate β. They are removed (recovered) at a mean rate γ.
If a susceptible has contact with an infected, the susceptible becomes infected.

If we consider a big population of n individuals, SIR epidemic model can be described by the following system of non-linear differential equations:

$$\frac{ds}{dt} = -\beta is, \frac{di}{dt} = \beta is - \gamma i, \frac{dr}{dt} = \gamma i, \tag{1}$$

being $s(t) = S(t)/n, i(t) = I(t)/n, r(t) = R(t)/n$ the respective proportions of classes at time t.

Following Hethcote (2000), the last equation in (1) can be omitted, since $s + i + r = 1$. The model assumes standard incidence and recovery (I-output) at a rate $\gamma I/n$. This represents a waiting time (or residence time in class I) of $e^{-\gamma t}$ time units, with mean $1/\gamma$. Since such period is small, the model lacks of a vital dynamic (i.e., natural death and birth).

Therefore, it is suitable just to describe diseases with fast propagation and conclusion. Furthermore, they provide immunity to infected individuals, for instance, influenza. In computer viruses, we can interpret this as an anti-virus program in which, once updated, infection is no longer allowed.

SIR model is suitable for a completely-mixed population, where the assumption of uniformly random contact selection is plausible. All individuals have the same number of contacts in a given time unit, and those contacts are equally likely to propagate the disease.

However, as Newman et al. (2001); Newman (2002, 2003); Ball et al. (2010) remark, in real-life applications we rarely meet all the requirements that must be fulfilled to apply SIR model. Individuals do not contact randomly, and full-mixtures should be replaced by networks.

The links represent pairs of individuals through which an epidemic may spread. neighbour nodes represent individuals who can potentially contact during illness (partners, colleagues, friends, people who travel together occasionally, etc.).

As Fromont et al. (1996) points, in real populations the graph structure is strongly heterogeneous. Andersson (1997) shows that even small heterogeneous levels (both social and spacial) can have huge effects in epidemic propagation.

Indeed, in real-life we find constraints that regulate networks. Each link has a cost; then, it is progressively harder to add links to a given node. This in turn leads to the fact that each node has a maximum degree. The resulting networks are neither random nor fully-regular.

Furthermore, it is not realistic to assume that an infectious-susceptible contact is equivalent to an infection. The spread capacity varies dynamically with time and may differ from one node to another. The time-window during which an infected node can spread has a stochastic length. The number of potential contacts from an infected node during this period is stochastic as well.

3 Stochastic Process

Let $G = (V, E)$ be a simple graph where nodes represent individuals, and links the relations between nodes (i.e., possible infection channels). Time is slotted , and at start ($t = 0$) we have:

- Certain selected nodes $V^* \subset V$, called *immunised nodes*, are removed, and the process takes place in the subgraph induced by $V' = V - V^*$, denoted by G'. Observe that $V^* = \emptyset$ implies no immunisation at all.

- A single *infected node* $x_0 \in V'$ is chosen uniformly at random (the case zero). All nodes from V' but x_0 are *susceptible nodes*.

Infected nodes might affect a random number of neighbouring nodes from G' through time, and then susceptible nodes may become infected ones with a certain time-varying probability. If a node is infected at time t_i, it can affect a random number of neighbouring susceptible nodes during a random time-window $[t_i, t_i']$.

It is reasonable to assume that although this time-window is random and its length varies from an infected node to another, it fluctuates around a mean value. Therefore, we represent the time-window picking a suitable non-negative

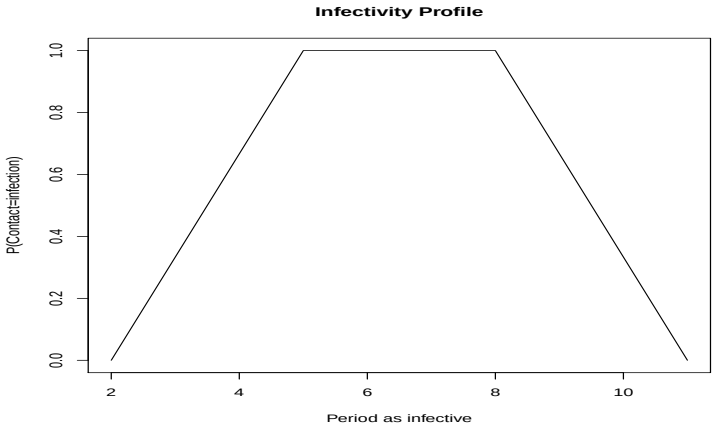

Figure 1 : Typical infectivity profile

distribution F with parameters (μ, σ), where $\mu > 0$ represents the mean length of the time-window and σ denotes its standard deviation.

Time t_i' is then picked using the rule $t_i' = t_i + X_i$, being X_i a random variable, $X_i \sim F_{(\mu,\sigma)}$. The parameters (μ, σ) are called the *virus-type of the disease*. Once t_i' is reached, that infected node is in removed state.

When a susceptible-infected contact occurs, the probability of contagion depends on the state of the infected node at this time: An infected node will affect a susceptible neighbouring node at $t \in [t_i, t_i']$ if and only if its *infectivity profile* $f(t) > u$, being $f(t)$ a trapezoidal function and u a random number in the compact set $[0, 1]$.

Function f represents the capacity of the node to spread the disease.

Figure 1 shows an example with $a_i = 2$ and $b_i = 11$.

Definition 1 *The stochastic process under study is the number of infected nodes* $\{X_t\}_{t\in\mathbb{N}}$.

We want to minimize the overall effect of the spread of the disease. Formally:

Definition 2 *The peak of the spread of the disease in graph* G *with immunisation set* V^* *and virus-type* (μ, σ) *is the first moment of the maximum achieved by the process:* $p(G, V^*, \mu, \sigma) = E(\max_{t\in\mathbb{N}}\{X_t\})$

We want to minimize the peak of the spread of the epidemic $p(G, V^*, \mu, \sigma)$ among all feasible immunisation sets V^*, subject to a budget constraint N.
The Node immunisation Problem is formulated as follows:

$$\min_{V^*} p(G, V^*, \mu, \sigma)$$

$$s.t.$$

$$|V^*| \leq N$$

4 Heuristics

Let us focus on two naive immunisation heuristics suitable for the combinatorial problem. From a structural viewpoint, a way to protect nodes is to eliminate a certain amount of their links.

Following Britton et al. (2007), the best nodes to protect seem to be those with the highest link contribution in the graph. It seems reasonable to assume that a small number of individuals with a large link action will have a higher impact than a highly populated group with a sparse number of links.

As Britton et al. (2007) said, in practice this implies knowledge of the degree-distribution of the network. Alternatively, the same authors analysed a different heuristic (acquaintance vaccination): chose random individuals and vaccinated them and their friends.

As Ball and Sirl (2013) notes, this heuristic has the effect that vaccinated individuals tend to have a higher degree and this targeting of well-connected individuals increases the efectiveness of vaccination. Specifically, the following immunisation heuristics will be considered in the simulations:

- *Greedy*: the immunisation takes place in N nodes with the highest degree.
- *Random*: N nodes are selected uniformly at random.
- *Raw*: no immunisation takes place ($V^* = \Phi$).

Let us define:

Definition 3 *The critical degree is the first degree d such that an epidemic spread occurs when $V^* = \{v \in V : deg(v) > d\}$.*

First, given a graph G we found the critical degree d and $N = |V^*|$. For this, let D be the highest degree of G. Then for $d = D-1, D-2, \ldots, 1$ take the corresponding V^* and run several times the SIR-based simulation over G, V^*.

For each run we have a curve of cases vs. time. If the peak of the mean curve is less than *Threshold*, repeat using next value of d until an epidemic occurs (in the mean sense).

Once we found the critical degree d and let $N = |V^*|$, the *Greedy* heuristics immunise the N nodes with degree $> d$, while *Random* immunise N nodes chosen at random.

About the graphs in which heuristics will be tested: Let us consider a social network $G = (V, E)$ with $m = |E|$ contacts and $|V| = n$ individuals.
In the complete graph K_n all contacts are possible, and $m = n(n-1)/2$.

This graph represents the closest case to a fully mixed population. Gilbert (1959) propose a link selection rule for random graphs.

In this rule, each link (contact) belongs to the graph with identical probability $p \in [0, 1]$.

These graphs are suitable to model Homogeneous Random Mixing.
The diameter of Gilbert graphs is $d = 2$ almost surely when the size tends to infinity for every fixed probability $p < 1$.
The reader can find a proof in the classical book authored by Bollobás (1985).

The intuition behind this small diameter of random graphs is that random links connect all parts of the network with equal probability.
We build ten random graphs called $G_1, \ldots, G_{10}$ following Gilbert model with different choices for $0 \leq p \leq 1$.

Also, we design ten graphs called $R_1, \ldots, R_{10}$ with right-tailed degree distribution. These graphs represent a model where there are few nodes with high degree, several nodes with low degree and the distribution is not monotonically decreasing. All these graphs were generated using the IGraph package developed by Csardi and Nepusz (2006). Figures 2 and 3 show the node-degree distributions of both graph sets.

5 Performance Analysis

In this section we study the performance of both heuristics, on the lights of graphs $R_1, \ldots, R_{10}$ and $G_1, \ldots, G_{10}$. In order to develop a faithful comparison, we run Function $Performance$.

It receives a graph G, number of iterations $iter$, virus-type parameters (μ, σ), number of slots T in $SirBased$ simulation and a $Threshold$, that allows to determine whether $SIRBased$ simulation is declared an epidemic case or not. Runs $iter$ times a SIR-based simulation and test if the peak of the mean curve is less than $Threshold$.

It returns all the parameters required to understand the performance of both heuristics, to know, *Greedy* and *Random*. Specifically, G^d and $n_d = |V^*|$ represent the output network in *Greedy* and the number of immunised nodes following this heuristic.

Additionally, a "Raw" heuristic is defined with no node-immunisation, in order to have a comprehensive understanding of the advantages of both *Random* and *Greedy* heuristics.

We call Function $Performance$ for graphs $R_1, \ldots, R_{10}, G_1, \ldots, G_{10}$,
$iter = 200$, $Threshold = 0,05$, $T = 120$ time slots and two different virus-types (μ, σ): $(5, 1)$ and $(10, 2)$.

The heuristics induce a subgraph in which the epidemic process takes place.
A measure of the process strength is the proportion of infected nodes at the subgraph in the worst moment (the peak of cases vs time in the mean curve).
Some of the results from simulations seem to run contrary to expectations.

Figure 4 shows the percentage of infected nodes as a function of time for the heuristics *Raw*, $Random(G, d+1)$ and $Greedy(G, d+1)$ for virus-types $(5, 1)$ and $(10, 2)$ in the right-tailed graph R_8.

Note that the confidence interval for *Random* contains the zero. This means that in several of the runs epidemics did not happen. Even though the average is shifted toward positive values, *Random* becomes competitive with *Greedy*, being comparable or even better than *Greedy* in some cases.

Figures 5 and 6 show the results for the heuristics *Raw*, $Random(G, d+1)$ and $Greedy(G, d+1)$ for virus-types $(5, 1)$ and $(10, 2)$ in the Gilbert graphs G_3 and G_4. *Random* is again competitive or better than *Greedy*. This counter-intuitive fact will be explained in Subsection 6.1.

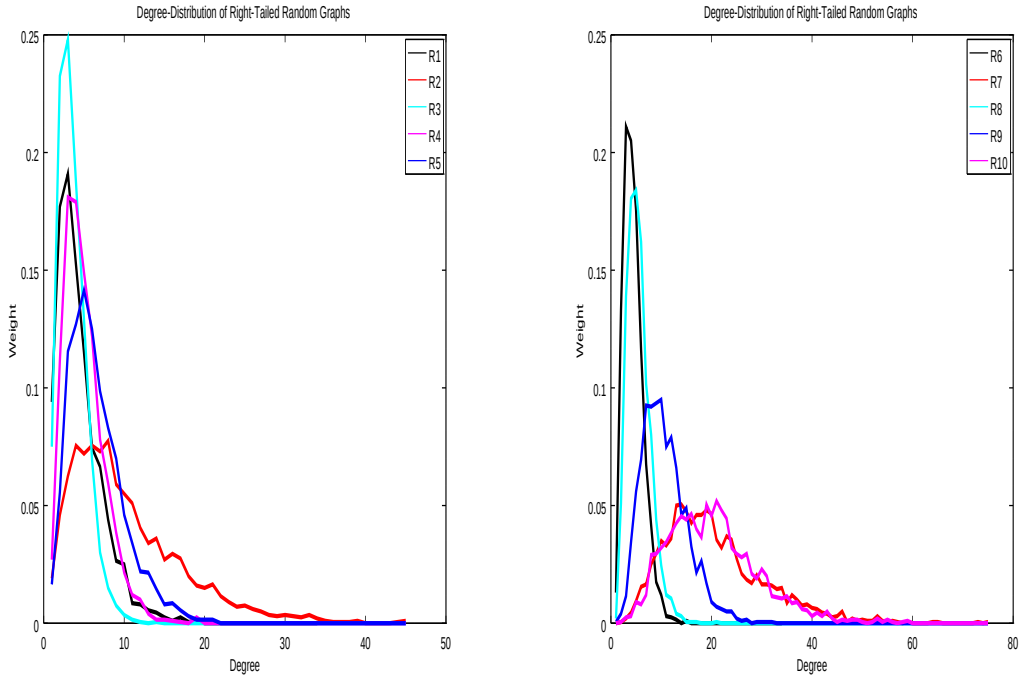

Figure 2 : Degree-Distribution for graphs $R_1, \ldots, R_{10}$

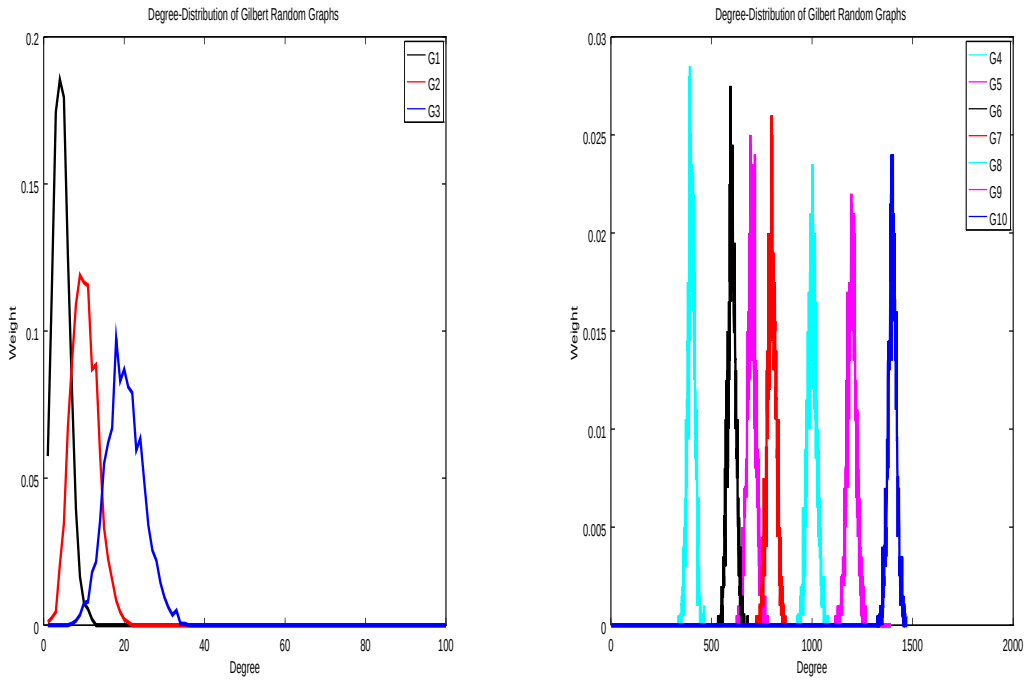

Figure 3 : Degree-Distribution in Gilbert graphs $G_1, \ldots, G_{10}$

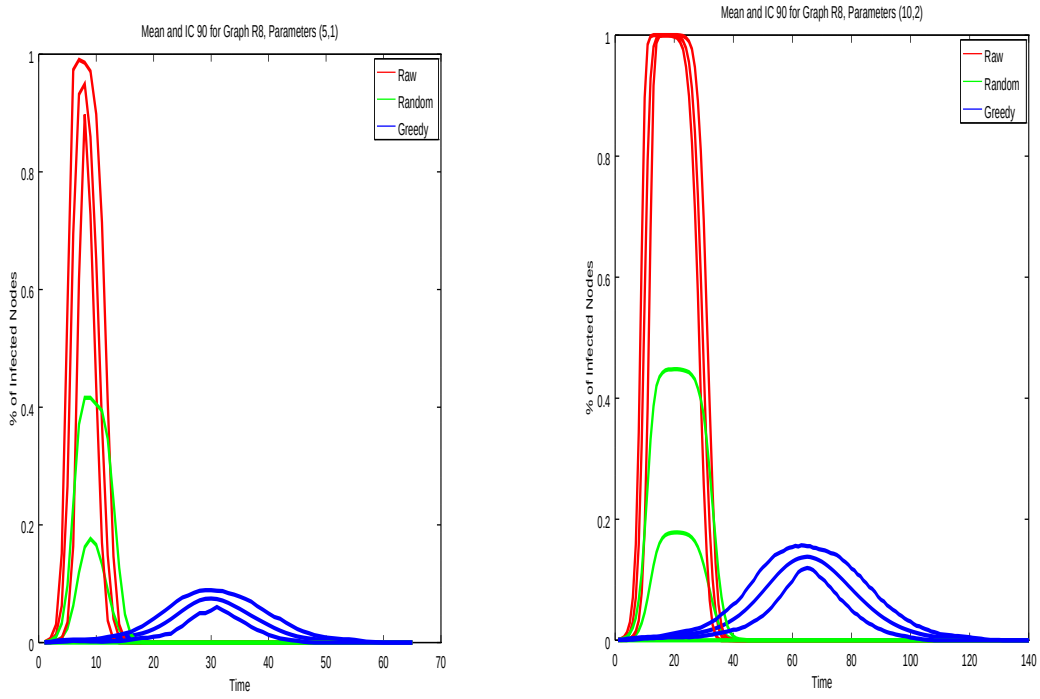

Figure 4 *Raw*, *Greedy*$(d+1)$ and *Random*$(d+1)$ in graph R_8, parameters $(5,1)$ and $(10,2)$

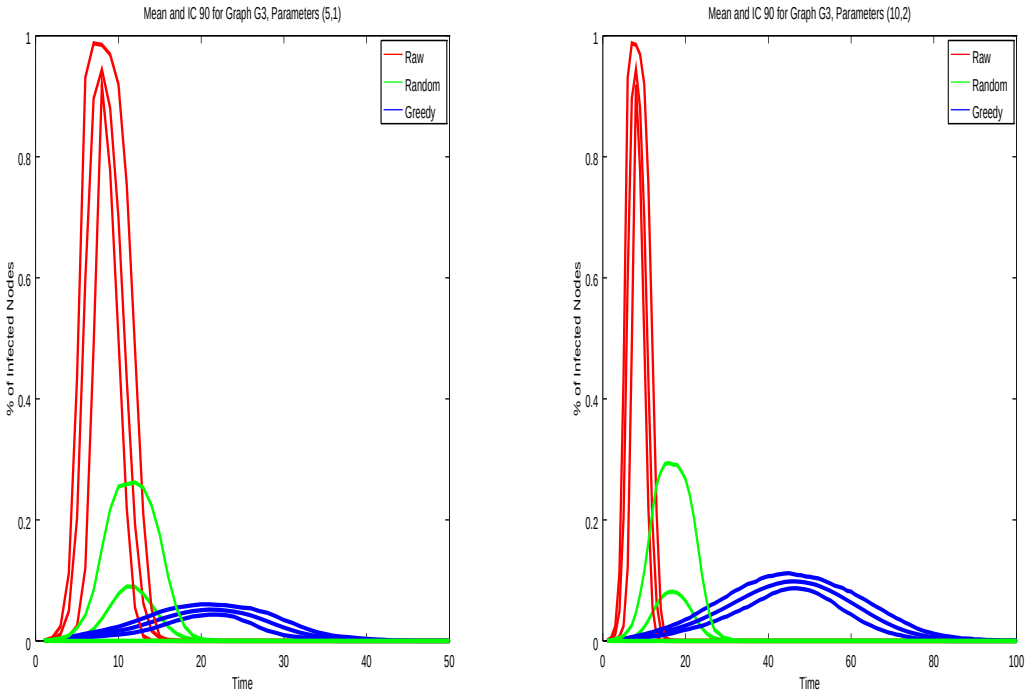

Figure 5 *Raw*, $Greedy(d+1)$ and $Random(d+1)$ in graph G_3, virus-types $(5,1)$ and $(10,2)$

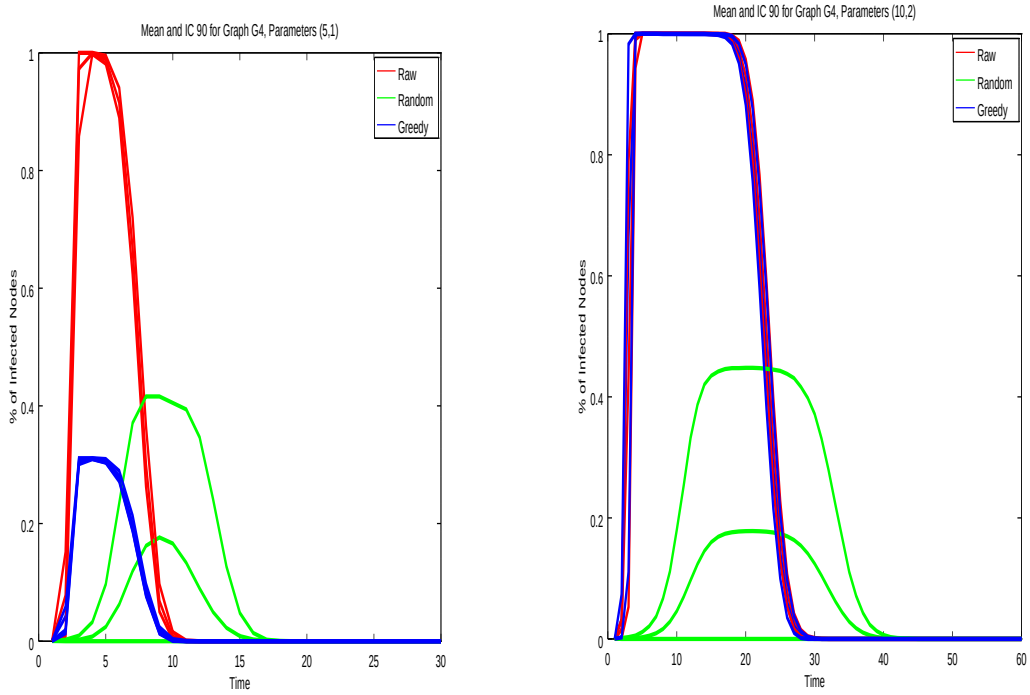

Figure 6 *Raw*, $Greedy(d+1)$ and $Random(d+1)$ in graph G_4, virus-types $(5,1)$ and $(10,2)$

This suggests that the graph connectivity has low sensitivity to the elimination of the highest degree nodes. Their immunisation does not sufficiently undermine the link structure of the graph, and the immunisation of a set of nodes with a lot of external links can be competitive, and presumably is what occurs under *Random* removal.

In all heuristics the fraction of infected nodes at the worst moment (peak) grows when μ is increased. The more the degree-distribution shifts to the right, the greater the impact of the epidemic, no matter the virus-type.

6 Main Results

6.1 Greedy is sub-optimal

If we consider $\mu \to \infty$, a pandemia is spread over the whole component that corresponds to x_0. Consider a set V^* such that $V - V^* = V' = \bigcup_{i=1}^{k} V_i$ is a partition into connected components from G'. The event $x_0 \in V_i$ has probability $\frac{|V_i|}{|V|}$, and the number of infections in that case equals $|V_i|$. In this extremal situation, the objective function is the expected number of infected nodes or expected loss, and it can be found analytically:

$$E = \sum_{i=1}^{k} \frac{|V_i|^2}{|V|} \tag{2}$$

Consider $M >> N > 2$, and a ground graph G that consists of two complete graphs K_M linked by a single node v with degree 2. Specifically, some nodes v_1 and v_2 from each K_M are connected to v. Since $M >> 2$, *Greedy* heuristic removes $N/2$ nodes in each complete graph.

The graph is connected, and all nodes will be affected. The score under *Greedy* heuristic is $E = M + 1 - N$ the worst possible, do to the fact that an extinction takes place. Nevertheless, if only v is immunised, the score is better, as the reader can verify.

6.2 Vaccinating more is not always better

Suppose we have vaccinated $c-1$ nodes, being $V' = \bigcup_{i=1}^{k} V_i$ (disjoint union) with expected loss $E_{c-1} = \dfrac{\sum_{i=1}^{k} |V_i|^2}{|V| - c + 1}$.
Let us vaccinate another node, the c-th. We have two cases:

1. The removal of c -th node maintains the number of connected components.
2. The removal of c -th node increases the number of connected components.

For our purposes, it is enough to prove the first case. Let V_j be the component from which the c-th node is removed. The expected loss is

$$E_c = \sum_{i \neq j}^{k} \frac{|V_i|^2}{|V| - c} + \frac{(|V_j| - 1)^2}{|V| - c} = A_c + B_c$$

Write E_{c-1} following the same criteria, then

$$E_{c-1} = \sum_{i \neq j}^{k} \frac{|V_i|^2}{|V| - c + 1} + \frac{|V_j|^2}{|V| - c + 1} = A_{c-1} + B_{c-1}$$

So, $E_c < E_{c-1}$ if and only if $B_{c-1} - B_c > A_c - A_{c-1}$ or

$$B_{c-1} - B_c > \frac{A_{c-1}}{|V| - c} \tag{3}$$

Let $X = |V_j|$ and $u = |V| - c$. Equation (3) turns into $\frac{X^2}{u+1} - \frac{(X-1)^2}{u} > \frac{A_{c-1}}{u}$. After some algebra, we obtain

$$P(X) = X^2 - 2(u+1)X + (u+1)(1 + A_{c-1}) < 0 \tag{4}$$

It can be proved that P has positive real roots in the interval

$$[(u+1) \pm \sqrt{(u+1)(u - A_{c-1})}]$$

This tells us that if we remove a node when we have already removed $c-1$ nodes and this extra node does not break the component V_j, the expected loss E_c will be less than E_{c-1} if and only if

$$|V_j| > |V| - c + 1 - \sqrt{(|V| - c + 1)(|V| - c - A_{c-1})} \tag{5}$$

As an example where equation 5 does not hold, consider a graph $G = C_3 \cup C_8$.

Then the expected loss for G is $E = \frac{64}{11} + \frac{9}{11} = \frac{73}{11} = 6.36$. If we vaccinate one node from C_3, then $E = \frac{64}{10} + \frac{4}{10} = \frac{68}{10} = 6.8$, which is worse than before.

7 Concluding Remarks

In this paper, an epidemic spread is modeled by a SIR-based stochastic process. Then, a combinatorial optimisation problem is formalized. The goal is to minimize the overall impact of the epidemic spread, by means of node-immunisation.

A *Greedy* notion is to immunise nodes with the highest degree. On the other hand, *Random* heuristic picks nodes at random, and immunises them. Both heuristics are computationally efficient, since the number of elementary operations is linear with the order of the input graph. We provide both mathematical proofs and examples of two counterintuitive results:

- *Random* heuristic outperforms *Greedy* in some specific scenarios. This means that vaccinating the nodes with highest degree is not always better than a random vaccination heuristic.
- Vaccinating more nodes is not necessarily the best choice.

The network topology should be considered in the selection of node resilience heuristics. Currently, we are working in order to develop a topology-aware GRASP heuristic for the combinatorial problem here presented. As future work, we also aim to study the interplay between epidemic propagation models and network reliability analysis under scenarios of dependent failures.

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Part III

Combinatorics in Epidemic Models

Chapter 6

Graph Fragmentation Problem

A new combinatorial problem is intoduced, called Graph Fragmentation Problem (GFP). The GFP can be seen as a particular case of the Node Immunization Problem (NIP) when the level of virulence is infinite. A sufficient condition for the optimality in the GFP is provided. As a corollary, we again derive the fact that Greedy is suboptimal.

It is worth to remark the fact that the GFP is at least as hard as the NIP. We suspect that the GFP belongs to the class of $\mathcal{NP}$-Hard computational problems.

Graph Fragmentation Problem

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Abstract: A combinatorial optimization problem called Graph Fragmentation Problem (GFP) is introduced. The decision variable is a set of protected nodes, which are deleted from the graph. An attacker picks a non-protected node uniformly at random from the resulting subgraph, and it completely affects the corresponding connected component. The goal is to minimize the expected number of affected nodes or Score S. The GFP finds applications in fire fighting, epidemiology and robust network design among others. A Greedy notion for the GFP is presented. Then, we develop a GRASP heuristic enriched with a Path-Relinking post-optimization phase. Both heuristics are compared on the lights of graphs inspired by a real-world fire fighting application.

1 INTRODUCTION

In robust network design, the major cause of concern is connectivity. The goal is to find a minimum cost design, meeting high connectivity requirements. Network connectivity is a rich field of knowledge, and the related literature is vast (Monma et al., 1990; Stoer, 1993). However, in several real-world applications a malfunctioning or affection of a single element is immediately propagated to neighboring elements. This is the case of fire fighting, electric shocks, epidemic propagations, etc., where an incorrect protection scheme might have catastrophic effects. In this paper, an abstract setting of the previous problems is presented as a combinatorial optimization problem.

The reader can find problems related with graph partitioning, which are similar in nature to ours in ((Borgatti, 2006), (Ortiz-Arroyo, 2010)). In ((Borgatti, 2006)), the author adress the combinatorial problem of the identification of key players in a network for the purpose of disrupting or fragmenting the network by removing the key nodes. In ((Ortiz-Arroyo, 2010)), an entropy-based method is proposed to the same problem. The main difference with respect to the problem covered in this article is that we prove mathematically a set of desirable properties for solutions. These properties are then used as part of a GRASP heuristic. The document is organized in the following manner. Section 2 formally presents the Graph Fragmentation Problem. Desired properties of candidate solutions are included in Section 3. A Greedy notion and a more sophisticated heuristic for the GFP is developed in Section 4. Section 5 shows the results of both heuristics in a real-world application, while Section 6 presents concluding remarks.

2 GRAPH FRAGMENTATION PROBLEM

We are given a simple graph $G = (V,E)$ and a budget constraint B. The decision variable is a subset V^*, called *protected nodes*, which will be deleted from the graph. The result is an induced subgraph $G' = (V',E(V'))$, with $V' = V - V^*$. A node $v \in V'$ is uniforlmy chosen at random, and the full component from G' that contains v is affected, this is, damaged by an atacker or an accident that starts at v.

The goal is to choose the set $V^* : |V^*| \leq B$ in order to minimize the expected value (or *Score*) of affected nodes. If the resulting graph G' is partitioned into k connected components with orders $n_1, \ldots, n_k$ such that $n = |V'|$, then the Graph Fragmentation Problem (GFP) is the following combinatorial optimization problem:

$$\min_{V^*} Sc(G') = \sum_{i=1}^{k} p_i n_i, \quad (1)$$

$$s.t. |V^*| \leq B, \quad (2)$$

being $p_i = \frac{n_i}{n}$ the probability of the event $v \in V_i$, being v the node uniformly chosen at random.

3 PROPERTIES

In this section, we study properties of the FGP. Observe that the best case occurs when only a singleton is affected, so $Sc(G') \geq 1$. The equality is achieved if and only if G' consists of isolated nodes. Furthermore, if n_{max} denotes the number of nodes from the largest component, then $Sc(G') \leq n_{max}$ by its definition.

Recall that the union between graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is the graph $G = (V_1 \cup V_2, E_1 \cup E_2)$, and it is denoted $G = G_1 \cup G_2$. A counterintuitive result is that a uniformly random node protection strategy might lead to a worse solution. In fact, let us consider $G = K_2 \cup K_4$, being K_n the complete graph with n nodes. The score is $Sc(G) = \frac{2}{6} \times 2 + \frac{4}{6} \times 4 = \frac{10}{3}$. However, if we pick $v \in K_2$ then $Sc(G - v) = \frac{1}{5} \times 1 + \frac{4}{5} \times 4 = \frac{17}{5}$, so $Sc(G-v) > Sc(G)$.

The intuition suggests that it is better to disconnect the graph whenever possible, this is, to protect nodes in such a way that the resulting subgraphs has as many components as possible. Then, only few nodes will be affected. This property explains the name of the problem. These results are mathematically formalized in the following paragraphs.

Proposition 1 (Load Balancing)**.** *The best resulting graph G' among all feasible graphs with k components and identical order n should have balanced components: $n_i = n/k, \forall i = 1, \ldots, k$.*

Proof. The score is precisely $Sc(G') = \frac{\|x\|_2^2}{\|x\|_1}$, being $x = (n_1, \ldots, n_k)$, $\|x\|_2$ and $\|x\|_1$ the respective Euclidean and 1-norm for vector x. We should minimize the Euclidean distance in the hyperplane $\|x\|_1 = n$ constant, whose normal vector is $\overrightarrow{1} \in \mathbb{R}^k$, with all unit coordinates. The optimum is found in the orthogonal projection of the null vector onto the polyhedra: $x_{opt} = \overrightarrow{0} + \frac{n}{\|\overrightarrow{1}\|_2} \frac{\overrightarrow{1}}{\|\overrightarrow{1}\|_2} = \overrightarrow{1} \frac{n}{k}$. □

Now, let us determine whether it is better to protect an additional node. Let G be an arbitrary graph with k components and cardinalities $n_1, \ldots, n_k$, and $n = \sum_{j=1}^{k} n_i$. If we delete some node v from the first component (observe that the labels are not relevant for analysis), there are two cases:

a) The number of connected components is the same.

b) The number of connected components is increased.

First, assume that Condition [a] holds. Then:

$$Sc(G-v) - Sc(G) = \sum_{i=2}^{k} \frac{(n_i)^2}{n} \frac{1}{n-1} + \frac{(n_1-1)^2}{n-1} - \frac{(n_1)^2}{n}$$
$$= \frac{A}{n-1} + B_v - B,$$

being $A = 1/n \sum_{i=2}^{k} (n_i)^2$, $B_v = (n_1-1)^2/(n-1)$ and $B = n_1^2/n$. As a consequence, $Sc(G-v) < Sc(G)$ if and only if n_1 meets the following inequality:

$$P(n_1) = (n_1)^2 - 2nn_1 + (1+A)n < 0 \qquad (3)$$

Observe that the minimum (or the highest score reduction) is achieved when $n_1 = n$, this is, when G is connected. In that case $Sc(G-v) - Sc(G) = 1$. We have proved the following

Proposition 2 (Best Singleton)**.** *If there is no cut-node, the best node protection belongs to the highest connected component.*

Proof. The polynomial P is monotonically decreasing with respect to n_1. □

Let n_{max} be the size of the highest connected component. Studying the sign of $P(n_{max})$, there is a positive score reduction if and only if:

$$n_{max} \geq n - \sqrt{n(n-1-A)}. \qquad (4)$$

We will see that this inequality always holds:

Proposition 3 (Single Balancing)**.** *If G does not present a cut-node, then there exists v such that $Sc(G-v) < Sc(G)$.*

Proof. Inequality 4 occurs if and only if $nA + n_{max}^2 \leq n(2n_{max} - 1)$. But $nA + n_{max}^2 = \sum_i n_i^2 = nSc(G)$, so Inequality 4 holds if and only if $Sc(G) \leq 2n_{max} - 1$. But $Sc(G) \leq n_{max} \leq 2n_{max} - 1$ always holds. □

Let us now focus our study to Condition [b], and denote by v a cut-node in G. First of all, observe that a node-protection in a balanced way always produces a score reduction. However, in some cases, the deletion of a cut node is not a good idea. Consider for instance $G = C_9 \cup P_3$, being C_9 an cycle with 9 nodes and P_3 an elementary path with 3 nodes, and v the central node from P_3. Then, we have that $Sc(G) = \frac{9^2}{12} + \frac{3^2}{12} = \frac{90}{12} = \frac{15}{2}$, but $Sc(G-v) = \frac{9^2}{11} + 2 \times \frac{1^2}{11} = \frac{83}{11} = 7 + \frac{6}{11}$, so $Sc(G-v) > Sc(G)$. However, if we choose a cut-node v from a component with n_j nodes, such that $P(n_j) < 0$, then the score is decreased. Furthermore, the score reduction is even better than in the case of no cut-node.

Proposition 4 (Fragmentation)**.** *If G presents a cut-node $v \in V_j$ where $|V_j| = n_j$ and $P(n_j) < 0$, then $Sc(G-v) < Sc(G)$. Furthermore, if $v' \in V$ is not a cut-node, then $Sc(G-v) < Sc(G-v') < Sc(G)$.*

Proof. If $V_j - \{v\} = V_a \cup V_b$, $n_a + n_b = n_j - 1$, then $(n_a)^2 + (n_b)^2 < (n_j - 1)^2$. This implies that the score reduction is even larger than in a non cut-node deletion. A similar argument is met when the cut node produces more than two components. As a consequence, the score reduction is even larger than the protection of a non-cut-node from V_j. By Proposition 3, a score reduction is achieved if v' is not a cut-node. □

Theorem 1 (Score Reduction)**.** *Consider an arbitrary graph $G = (V,E)$. There is some $v \in V$ such that $Sc(G-v) < Sc(G)$, unless G consists of isolated nodes.*

Proof. This is a Corollary of Single Balancing and Fragmentation. We always pick a node v from the largest connected component with n_{max} nodes. If v is not a cut node, by Proposition 4 we have $Sc(G-v) < Sc(G)$. Otherwise, by Proposition 3 the score reduction is even larger, so $Sc(G-v) < Sc(G)$ again. In both cases a score reduction is produced. □

4 HEURISTICS

Combinatorial optimization problems arise in several real-world problems (economics, telecommunication, transport, politics, industry), were human beings have the opportunity to choose among several options. Usually, that number of options cannot be exhaustively analyzed, mainly because its number increases exponentially with an input size of the system. Much work has been done over the last six decades to develop optimal seeking methods that do not explicitly require an examination of each alternative, giving shape to the field of *Combinatorial Optimization* (Papadimitriou and Steiglitz, 1982). Several combinatorial problems belong to the $\mathcal{NP}$-Hard class, or the search space is sufficiently large to admit an exact algorithm, and a smart search technique should be considered exploiting the real structure of the problem via heuristics. Optimality is not guaranteed, but compromised at the cost of computational efficiency. Metaheuristics are an abstraction of search methodologies which are widely applicable to optimization problems. The most promising are Simulated Annealing (Kirkpatrick, 1984), Tabu Search (Glover, 1989), Genetic Algorithms (Goldberg, 1989), Variable Neighborhood Search (Hansen and Mladenovic, 2001), GRASP (Feo and Resende, 1989), Ant Colony Optimization (Dorigo, 1992) and Particle Swarm Optimization (Kennedy and Eberhart, 1995), among others. The interested reader can find a list of metaheuristics and their details in the Handbook of Metaheuristics (Gendreau and Potvin, 2010).

In this section, we develop a Greedy notion and a Grasp heuristic enriched with a Path Reliking post-optimization stage. First, we review basic elements of Grasp and Path Relinking.

4.1 GRASP

Greedy Randomized Adaptive Search Procedure (GRASP) is a multi-start or iterative process (Lin and Kernighan, 1973), where feasible solutions are produced in a first phase, and neighbor solutions are explored in a second phase. The best overall solution is returned as the result. The first implementation is due to Tomas Feo and Mauricio Resende, were the authors address a hard set covering problem arising for Steiner triple systems (Feo and Resende, 1989). They introduce adaptation and randomness to the classical Greedy heuristic for the set covering problem (where $P_1, \ldots, P_n$ cover the set $J = \{1, \ldots, m\}$ and the objective is to find the minimum cardinality set $I \subset \{1, \ldots, n\}$ such that $\cup_{i \in I} P_i = J$).

It is a powerful metaheuristic to address hard combinatorial optimization problems, and has been succesfully implemented in particular to several telecommunications problems, such as Internet Telephony (Srinivasan et al., 2000), Cellular Systems (Amaldi et al., 2003a; Amaldi et al., 2003b), Cooperative Systems (Romero, 2012), Connectivity (Canuto et al., 2001) and Wide Area Network design (Robledo Amoza, 2005). Here we will sketch the GRASP metaheuristic based on the work from Mauricio Resende and Celso Ribeiro, which is useful as a template to solve a wide family of combinatorial problems (Resende and Ribeiro, 2003; Resende and Ribeiro, 2014). Consider a ground set $E = \{1, \ldots, n\}$, a feasible set $F \subseteq 2^E$ for the optimization problem $\min_{A \subseteq E} f(A)$, and an objective function $f : 2^E \to \mathbb{R}$. The Pseudo-code 1 illustrates the main blocks of a GRASP procedure for minimization, where *Max_Iterations* iterations are performed, $\alpha \in [0,1]$ is the quantity of randomness in the process and $\mathcal{N}$ is a neighborhood structure of solutions (basically, a rule that defines a neighbor of a certain solution). The cycle includes Lines $1-5$, and the best solution encountered during the cycle is finally returned in Line 6. Lines 2 and 3 represent respectively the Construction and Local Search phases, whereas the partially best solution is updated in Line 4.

Algorithm 1 $S = GRASP(MaxIterations, \mathcal{N})$

1: **for** $k = 1$ **to** $Max\_Iterations$ **do**
2: $S \leftarrow Greedy\_Randomized(\alpha)$
3: $S \leftarrow Local\_Search(S, \mathcal{N})$
4: $Update\_Solution(S)$
5: **end for**
6: **return** S

A general approach for the Greedy Randomized Construction is specified in Pseudo-code 2. Solution S is empty at the beginning, in Line 1, and an auxiliary set C has the potential elements to be added to S. A carefully chosen element from C is picked up during each iteration of the While loop (Lines $3-9$), which is finished once a feasible solution is met. A Greedy construction would choose c^{min}, which is the element with the lowest cost to be added to the partial non-feasible solution (Line 4). On the other hand, c^{max} is the most expensive element to be added (Line 5). The *Restricted Candidate List* RCL is defined in Line 6, and has all the elements whose cost are below a certain threshold (see Line 6). In Line 7, an element from the RCL is uniformly picked at random and added to the solution S. The process is repeated until a feasible solution S is found. It is worth to notice the effect of the input parameter $\alpha \in [0,1]$. When $\alpha = 0$, the Greedy construction is retrieved. On the contrary, $\alpha = 1$ means a completely random construction. Therefore, the parameter α imposes a trade-off between diversification and greediness.

Algorithm 2 $S = Greedy\_Randomized(\alpha)$

1: $S \leftarrow \emptyset$
2: $C \leftarrow E$
3: **while** $C \neq \emptyset$ **do**
4: $c^{min} \leftarrow \min_{c \in C} f(S \cup \{c\})$
5: $c^{max} \leftarrow \max_{c \in C} f(S \cup \{c\})$
6: $RCL \leftarrow \{c \in C : f(S \cup \{c\}) \leq f(S \cup \{c^{min}\}) + \alpha(f(S \cup \{c^{max}\}) - f(S \cup \{c^{min}\}))\}$
7: $S \leftarrow S \cup Random(RCL)$
8: $Update(C)$
9: **end while**
10: **return** S

The Greedy Randomized Construction does not provide guarantee of local optimality. For that reason, a Local Search phase is finally introduced, in order to return a locally optimal solution (which could be incidentally globally optimal). In order to define this phase, a rule to define neighbors of a certain solution is mandatory, called a *neighborhood structure*. A better neighbor solution is iteratively picked until no improvement is possible. A general local search phase is presented in pseudo-code 3.

Algorithm 3 $S = Local\_Search(S, \mathcal{N})$

1: $H(S) = \{X \in \mathcal{N}(S) : f(X) < f(S)\}$
2: **while** $H(S) \neq \emptyset$ **do**
3: $S \leftarrow ChooseIn(H)$
4: $H(S) = \{X \in \mathcal{N}(S) : f(X) < f(S)\}$
5: **end while**
6: **return** S

The success of the local search phase strongly depends on the quality of the starting solution, the computational cost for finding a better local solution, and naturally, on the richness of the neighborhood structure. The interested reader can find valuable literature and GRASP enhancements in (Resende and Ribeiro, 2003; Festa and Resende, 2002) and references therein.

4.2 GREEDY FOR THE GFP

Usually, once we face a new combinatorial optimization problem, a Greedy notion is developed. In specific combinatorial structures, Greedy produces the globally optimum solution. Greedy heuristic builds a solution in a stepwise manner. The best step is chosen whenever possible. Therefore, Greedy tries to build the global optimum by means of the best local steps. Naturally, Greedy rarely produces the best solution (see for instance its performance in the celebrated Traveling Salesman Problem).

In our problem, Greedy iteratively applies the best node protection. Function *ChooseBestNode* finds v such that $v = arg\min_w\{Sc(G-w)\}$. Greedy is supported by Theorem 1, and the score reduction is guaranteed for the GFP.

Algorithm 4 $G_{out} = Greedy(G, B)$

1: **for** $i = 1 : B$ **do**
2: $v \leftarrow ChooseBestNode(G)$
3: $G \leftarrow G - v$
4: **end for**
5: $G_{out} \leftarrow G$
6: **return** G_{out}

A linear search among all nodes $w \in V$ is developed in order to find the best node protection in Greedy. Observe that if there is no cut node, a node is picked uniformly at random from the largest connected component, since they produce the same score reduction. In order to trade computational effort, we propose an alternative algorithm that always improves the score. It is supported by Proposition 3.

Algorithm 5 $G_{out} = Balance(G,B)$

```
1: for i = 1 : B do
2:    V_max ← LargestComponent(G_out)
3:    v ← ChooseRandom(V)
4:    G ← G − {v}
5: end for
6: G_out ← G
7: return G_out
```

Balance iteratively picks nodes from the largest connected component. Observe that no score evaluation is required, hence, the computational effort is below that of *Greedy*.

4.3 GRASP FOR THE GFP

We already have a Greedy notion for the GFP, and a Balance heuristic. Both reduce the score in each iteration. A key point is to note that a fragmentation in large components always improves the score. Therefore, *Separator* function finds the node-connectivity for a given connected graph. It returns a node separator set V_{aux} of the largest component V_{max}.

Algorithm 6 $G_{out} = Grasp(G,B,\alpha)$

```
1: G_out ← G
2: Counter ← B
3: LocalImprove ← True
4: while Counter > 0 do
5:    if random < α then
6:       v = RandomNode(G)
7:       G_out ← G_out − v
8:    else
9:       V_max ← LargestComponent(G_out)
10:      V_aux ← Separator(G, V_max)
11:      if Counter ≥ |V_aux| then
12:         G_out ← G_out − V_aux
13:         Counter ← Counter − |V_aux|
14:      end if
15:   end if
16: end while
17: while Improve(G) = True do
18:   (G_out, LocalImprove) ← Swap(G_out, G)
19: end while
20: return G_out
```

The construction phase is first applied (Lines 1-15) and then, a Local Search phase takes place (Lines 16-18). The graph (G_{out}) and number of remaining nodes to protect (*Counter*) are initialized in Lines 1-2. Nodes are protected in a While loop (Lines 3-15). If a uniform random variable over the compact set $[0,1]$ is greater than the input α (Line 4), a random node v is then picked and removed (Lines 5-6). Otherwise, the largest component is selected (Line 8), and the node separator in that component is found (Line 9). If it is feasible, that node separator is removed from the graph (Lines 10-12). Finally, a Local Search phase takes place. It guarantees a local optimum solution. The core is *Swap* function, explained in the following lines.

Algorithm 7 $(G_{out}, Improve) = Swap(G_1, G_2)$

```
1: {v_1, ..., v_{n−B}} ← V(G_1)
2: {v_{n−B+1}, ..., v_n} ← V(G_2) − V(G_1)
3: Improve ← False
4: G_out ← G_1
5: for i = 1 : B do
6:    for j = 1 : n − B do
7:       G_aux ← (G_out + v_{n−B+i}) − v_j
8:       reduction ← E(G) − E(G_aux)
9:       if reduction > 0 then
10:         G_out ← G_aux
11:         Improve ← True
12:         break
13:      end if
14:   end for
15: end for
16: return (G_out, Improve)
```

Non-protected nodes are those from the first argument G_1 (Line 1), while the remaining nodes belong to the difference $V(G_2) - V(G_1)$ (see Line 2). A Boolean constant determines whether there exists some improvement or not (Line 3). Iteratively, all (protected,non-protected) pairs are considered and switched to see whether there is some improvement or not (block of Lines 5-15). If there is some improvement, *LocalImprovement* is set to True (Line 11) and iterative process is finished (Line 12). The pair $(G_{out}, Improve)$ is returned. It is worth to remark that $G_{out} = G_1$ if and only if G_1 is a local optimum. Otherwise, the best first movement is produced.

4.4 PATH RELINKING

Thanks to the randomization introduced to the Grasp heuristic, new solutions are obtained with different runs. Then, once we consider a pool $\{G_1, \ldots, G_s\}$ of s elite solutions (they are the best solutions obtained using $N >> s$ runs), new solutions could be found via elementary paths in the graph $\mathcal{G}$ of solutions. In this case, the node set of $\mathcal{G}$ is the induced subgraph of G with precisely $n-B$ nodes. Two solutions G_1 and G_2 are incident if and only if there is a single swap that moves one solution into the other (i.e., if they differ in one node).

Algorithm 8 $Pool = Relinking(G_1, G_2, \ldots, G_r)$

1: $S \leftarrow (G_1, G_2, \ldots, G_r)$
2: **for all** $(u, v) \in Pool$ **do**
3: $\quad Path \leftarrow ShortestWalk(u, v)$
4: $\quad S_{u,v} \leftarrow Best(Path)$
5: $\quad S \leftarrow S \cup \{S_{u,v}\}$
6: **end for**
7: $Pool \leftarrow SelectBest(r, S)$
8: **return** $Pool$

Relinking receives a pool of r solutions and returns another pool of r solutions, with better score.New candidate solutions $S_{u,v}$ are found for every pair of elite solutions u and v. The best r solutions are returned.

4.5 MAIN ALGORITHM

The main algorithm combines Grasp strength and a Path relinking post-optimization stage, in a straightforward fashion.

Algorithm 9 $G_{out} = Main(G, B, N_1, N_2)$

1: $S \leftarrow \emptyset$
2: **for** $i = 1 : N_1$ **do**
3: $\quad G_i \leftarrow Grasp(G, B)$
4: $\quad S \leftarrow S \cup G_i$
5: **end for**
6: $(G_1, \ldots, G_r) \leftarrow Best(r, S)$
7: **for** $i = 1 : N_2$ **do**
8: $\quad (G_1, \ldots, G_r) \leftarrow Relinking(G_1, \ldots, G_r)$
9: **end for**
10: $G_{out} \leftarrow SelectBest(1, \{G_1, G_2, \ldots, G_r\})$
11: **return** G_{out}

5 RESULTS

In order to highlight the effectiveness of our three heuristics, we introduce *Greedy*, *Balance* and *Main* to three real-life graphs. These graphs G_{USA}, G_{FON} and G_{PEG} represent respectively the neighborhood of the states from USA, a real Fiber Optic Network and a part of a real Power Electric Grid. In all cases, it is highly desirable to minimize the risk of the neighboring elements, once a failure or catastrophic event occurs. Thanks to the randomization effect during *Balance* call, the performance of different runs is variable. Figures 1, 2 and 3 show the score of *Greedy* (solid line) and the scores of 30-runs of *Balance* (dashed lines) versus *Main* with $N_1 = N_2 = 30$, $r = 6$, $\alpha = 0.5$. The score for the different heuristics is expressed as a function of the budget B. Red point's

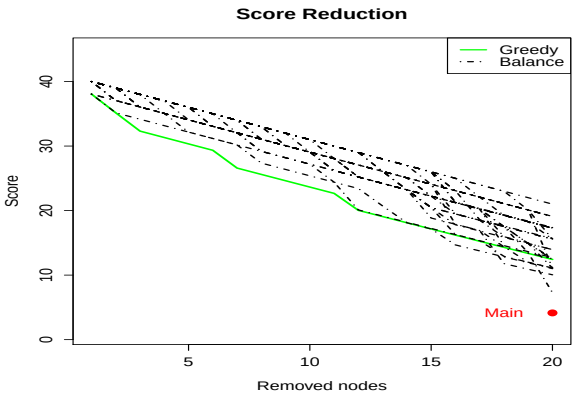

Figure 1: Greedy (solid) vs. 30 Balance runs (dashed) for the Neighborhood Graph

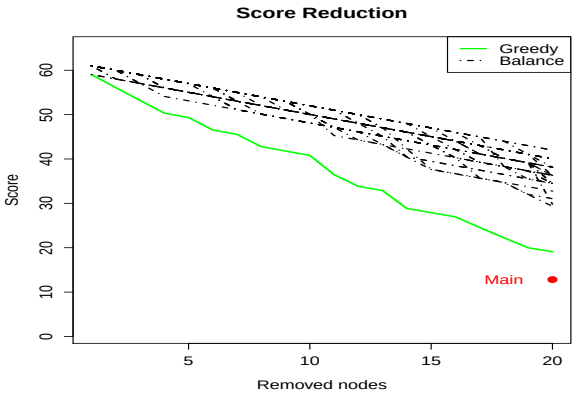

Figure 2: Greedy (solid) vs. 30 Balance runs (dashed) for the Fiber Optic Graph

abcissa is the cost reached by *Main* after removing 20 nodes. Runs were made on a computer Dell Inspiron-N4010 with 1.8 GiB of memory, proccesor Intel Core i3 CPU M380 @ 2.53 GHz x 4, 64 bit's OS. CPU times are 0.924 min. for G_{USA}, 1.065 min. for G_{FON} and 13.021 min. for G_{PEG}.

It can be appreciated that our *Main* heuristic outperforms both naive solutions *Greedy* and *Balance*, under all possible budgets. Even though *Balance* has a reduced computational cost, its performance presents a large gap with respect to *Greedy* heuristic. Figures 4, 5 and 6 show the pruning result for the different heuristics and graphs under study.

6 CONCLUSIONS

The Graph Fragmentation Problem (GFP) has been introduced. The goal is to protect (remove) B nodes from a graph G, in such a way that a random attack to an arbitrary node v affects the lowest expected

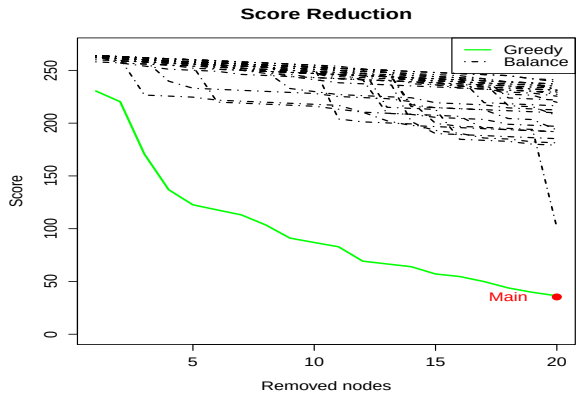

Figure 3: Greedy (solid) vs. 30 Balance runs (dashed) for the IEEE 300 Graph

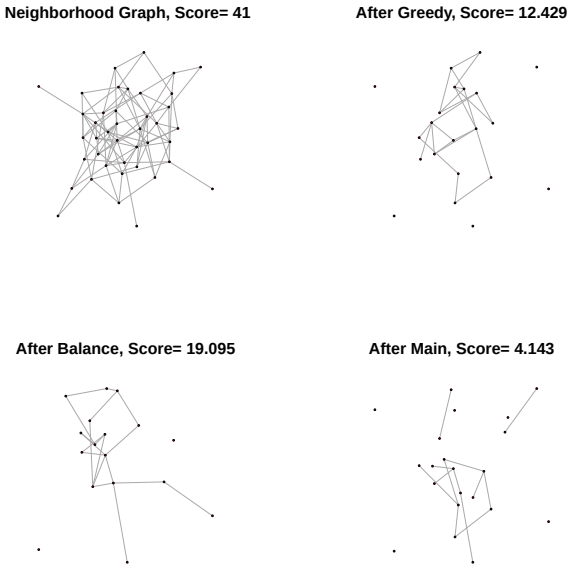

Figure 4: Graph G_{USA} when $\alpha = 1/2$

number of nodes (where the whole connected component from v is affected). The GFP finds applications to fire fighting, highly virulent epidemic propagations and electric shocks, among others.

In this paper, elementary properties of the GFP were studied. Specifically, graph fragmentation and balancing are good strategies. Together, they define a Greedy notion for the problem. Furthermore, we proved that Greedy achieves improvement in each iteration (i.e., in each node protection). A more sophisticated Grasp heuristic enriched with a Path Relinking post-optimization scheme has been developed. The effectiveness of our more sophisticated heuristic has been tested on a real-life networks.

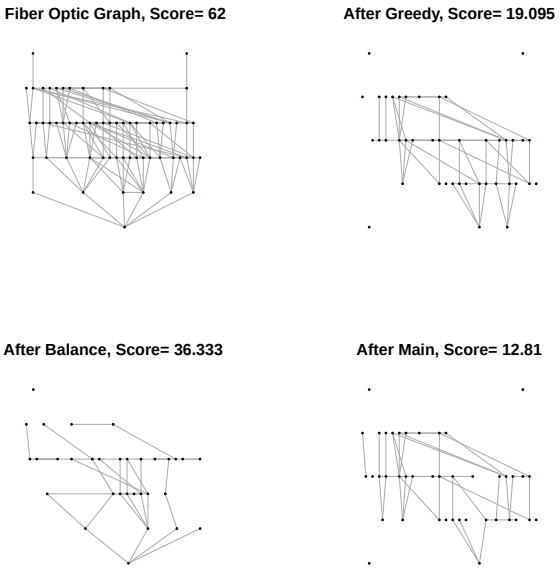

Figure 5: Graph G_{FON} when $\alpha = 1/2$

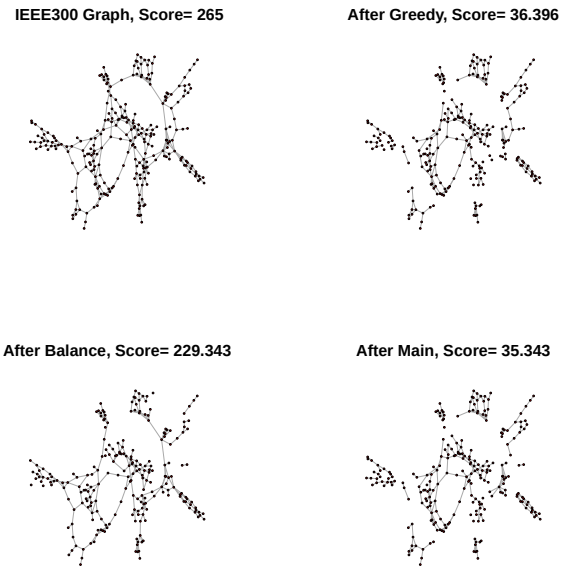

Figure 6: Graph G_{PEG} when $\alpha = 1/2$

As a future work, we would like to establish the intractability of GFP and incorporate different scores.

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