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Resumo:

Quadratizations of pseudo-Boolean functions have been established in recent years as a very successful tool in the solution of very large binary optimization problems. Despite some good efforts and some nice results published about the structure and complexity of quadratizations, many of their theoretical aspects remain poorly understood. This is even more so regarding the class of Submodular pseudo-Boolean functions, where fewer results are known. Due to the vast importance of submodular functions in discrete optimization, we propose the beginning of a systematic investigation of submodular quadratizations of submodular functions and their extensions.

Declaração de Interesse por Bolsa

Declaro que a/o candidata/o, nos termos do edital 04/2022, deseja participar do programa de iniciação científica como **bolsista**.

Nota: Este projeto de iniciação científica está inserido no contexto de um projeto de pesquisa que estuda aspectos estruturais e ramificações algorítmicas em espaços dotados de convexidades não euclidianas.

Quadratizations of Submodular Pseudo-Boolean Functions

Abstract

Quadratizations of pseudo-Boolean functions have been established in recent years as a very successful tool in the solution of very large binary optimization problems. Despite some good efforts and some nice results published about the structure and complexity of quadratizations, many of their theoretical aspects remain poorly understood. This is even more so regarding the class of Submodular pseudo-Boolean functions, where fewer results are known. Due to the vast importance of submodular functions in discrete optimization, we propose the beginning of a systematic investigation of submodular quadratizations of submodular functions and their extensions.

1 Introduction and Problem Setting

A **pseudo-Boolean function** (pBf) in $n \geq 0$ variables is any real-valued mapping of the form $\{0,1\}^n \mapsto \mathbb{R}$. A pBf is **Boolean** if the binary set $\{0,1\}$ is used in place of $\mathbb{R}$. Pseudo-Boolean functions are closely related to **finite-set functions** – mappings of the form $2^S \mapsto \mathbb{R}$, for a finite **ground** sets S – since any subset $T \subseteq S$ can be identified with its *support* binary vector in $\{0,1\}^S$.

It is well known (cf. [11, 17]) that any pBf f in variables $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ can be uniquely represented by a multi-affine polynomial P_f in the same variables, namely as

$$P_f(\boldsymbol{x}) := \sum_{a \in \{0,1\}^n} f(a) \cdot \prod_{a_i = 1} x_i \cdot \prod_{a_j = 0} (1 - x_j) = \sum_{S \subseteq [n]} a_S \prod_{i \in S} x_i.$$

The **degree** of f is defined as $d(f) := \max\{|S \subseteq [n]| : a_S \neq 0\}$, the degree of its polynomial representation. Henceforth, we shall identify f with P_f and simple write f when talking about the function or its polynomial indiscriminately.

Given a pBf f in variables $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ and an integer $m \geq 0$, an ***m*-quadratization** for f is a degree-2 pBf $g : \{0,1\}^{n+m} \to \mathbb{R}$ in variables $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ and $\boldsymbol{y} = (y_1, y_2, \ldots, y_m)$ such that

$$f(\boldsymbol{x}) = \min \left\{ g(\boldsymbol{x}, \boldsymbol{y}) : \boldsymbol{y} \in \{0,1\}^m \right\} \qquad \text{for all} \qquad \boldsymbol{x} \in \{0,1\}^n.$$

The variables $\boldsymbol{y} = (y_1, y_2, \ldots, y_m)$ are **auxiliary**. The quadratization g is ***y*-linear** if products of the form $y_i y_j$ do not occur, and is **regular** otherwise.

Quadratizations were introduced in [44] as a way to lift high-degree pseudo-Boolean functions into quadratic ones and unify the study of the following **pseudo-Boolean Optimization** problem (PBO).

Problem 1. *Given a pseudo-Boolean function $f : \{0,1\}^n \to \mathbb{R}$ in multi-affine polynomial form, determine*

$$f(\boldsymbol{x}^*) = \min\big\{f(\boldsymbol{x}) : \boldsymbol{x} \in \{0,1\}^n\big\}.$$

As it turns out, Problem 1 is NP-hard (cf. [17]) even when f has degree 2, as it encompasses many optimization models such as *maximum cuts in graphs*, *facility location problems*, and *maximum satisfiability of Boolean formulae*. Moreover, the quadratization technique of [44] is based on the introduction of *penalty terms*, with rather large constants multiplying them, requires an excessive amount of auxiliary variables, and does not produce good results.

A different quadratization for degree-3, negative monomials was developed in [33] and generalized for any degree in [21]. These quadratizations avoided the penalty method and required only a single auxiliary variable (per negative monomial). The authors were then able to leverage on the *roof duality* machinery developed by [26, 10, 12, 13] and approximately solve Problem 1 to pBfs with tens of thousands of variables – those pBfs stemmed from imaging processing and computer vision problems and were highly *sparse*.

The positive results spawned a string of ad-hoc methods for quadratizing pBfs, some of which can be found in [28, 29, 46, 45, 54, 42]. A systematic study of quadratizations was initiated in [9, 18, 19, 1, 2, 7, 8], where many different algorithms for general (non term-wise) quadratizations were introduced, lower bounds on the number of required auxiliary variables were given, and connections ranging from extremal combinatorics to circuit complexity were shown. Despite all those efforts, the structure and properties of quadratizations are just fairly understood and many open questions remain. In the sequel, we describe some of those open questions that are the focus of this project.

1.1 Quadratizations of Submodular Functions

A pseudo-Boolean function $f : \{0,1\}^n \to \mathbb{R}$ is **submodular** if

$$f(\boldsymbol{x}) + f(\boldsymbol{y}) \geq f(\boldsymbol{x} \wedge \boldsymbol{y}) + f(\boldsymbol{x} \vee \boldsymbol{y}) \qquad \text{for all} \qquad \boldsymbol{x}, \boldsymbol{y} \in \{0,1\}^n,$$

with the operations $\wedge$ and $\vee$ performed component-wise. Submodularity fully captures the *diminishing returns property* used for indivisible goods in Economics and thus, in a sense, is the discrete analog of *convexity*[1]. For a glimpse of their relevance in optimization problems, see next section.

The main questions to be investigated in this project can be stated as follows:

Question 1.1. *What are some necessary and/or sufficient conditions for a submodular pBf f, given by its multi-affine polynomial, to possess submodular quadratizations? How many auxiliary variables are necessary and/or sufficient? How efficiently can a submodular quadratization of f be obtained?*

It is well known that a quadratic pBf f is submodular if and only if all quadratic terms of f are non positive [36]. Hence, deciding if a quadratic pBf is submodular can be done in linear time in the number of its terms. A similar, slightly more involved result [3] is known for cubic, submodular pBfs. For degree-4 and higher, no characterization is believed to exist, since the following theorem is known.

[1]A function $f : \mathbb{R}^n \to \mathbb{R}$ is **convex** if $f(\lambda\boldsymbol{x} + (1-\lambda)\boldsymbol{y}) \leq \lambda f(\boldsymbol{x}) + (1-\lambda)f(\boldsymbol{y})$ for all $\boldsymbol{x}, \boldsymbol{y} \in \mathrm{dom}(f)$ and $\lambda \in [0,1]$. Convex functions are know to have a single, global minimum that can be determined in polynomial time in n.

Theorem 1.2 (Crama [16], Nemhauser, Wolsey e Fisher [37]). *It is* coNP*-hard to determine if a degree-*4 *or higher pBf* f *is submodular, even if* f *is given by its multi-affine polynomial representation.*

Clearly, it is not possible for non-submodular functions to possess submodular quadratizations. Hence, Theorem 1.2 implies that not all higher-degree submodular pBfs can be quadratized in polynomial time unless $\mathsf{P} = \mathsf{coNP}$. Moreover, the theorem hints at the possibility that some higher-degree submodular functions may require an exponential number of variables to be quadratized.

On the positive side, it is known that the quadratization techniques of [21] and of [54] can produce submodular quadratizations for three small subclasses of submodular pBfs. However, no lower bounds on the numbers of auxiliary variables required by such classes are known.

On the negative side, it is known that the product substitution of [44], the symmetric approximation of [28, 29], the splitting technique of [9], the factoring method of [18, 19], the *universal sets* and *attractive partitions* of [2], the linear algebraic plus shifting procedure of [1], and the zero-in pattern approach of [7, 8] all lead to highly non-submodular quadratizations of submodular pBfs. Moreover, it was shown in [52, 53] the existence of a degree-4 submodular pBf in 4 variables that do not admit submodular quadratizations.

The result of [52, 53] was however, partly obtained thorough exhaustive enumeration and barely sheds a dim light into the structure of non-quadratizable submodular pBfs. Furthermore, the computational enumeration carried out seems unavoidable in the used approach.

It is clear then that Question 1.1 remains largely open, and that new, ingenious insights and methods will have to be developed in order to give it a proper answer.

The definition of quadratization provided in the previous section is exact, in the sense that

$$\min\big\{f(\boldsymbol{x}) : \boldsymbol{x} \in \{0,1\}^n\big\} = \min\big\{g(\boldsymbol{x},\boldsymbol{y}) : \boldsymbol{x} \in \{0,1\}^n,\, \boldsymbol{y} \in \{0,1\}^m\big\},$$

for g being a quadratization of f. Three different flavors of approximate quadratizations can be defined. For a pBf f in n variables, given by its multi-affine polynomial, a quadratic pBf g in $n+m$ variables can be an approximate quadratization of f if:

$$f(\boldsymbol{x}) \leq \min\big\{g(\boldsymbol{x},\boldsymbol{y}) : \boldsymbol{y} \in \{0,1\}^m\big\} \leq \rho f(\boldsymbol{x}) \qquad \text{for all} \qquad \boldsymbol{x} \in \{0,1\}^n,$$

for $f(x) > 0$ and some constant $\rho \geq 1$; or if

$$\big\| f(\boldsymbol{x}) - \min\big\{g(\boldsymbol{x},\boldsymbol{y}) : \boldsymbol{y} \in \{0,1\}^m\big\}\big\|_\ell \leq \delta,$$

for some integer $\ell \geq 1$ and some small constant $\delta > 0$, or still if

$$\frac{1}{2^n}\left|\left\{\boldsymbol{x} \in \{0,1\}^n : f(\boldsymbol{x}) \neq \min\big\{g(\boldsymbol{x},\boldsymbol{y}) : \boldsymbol{y} \in \{0,1\}^m\big\}\right\}\right| = \mathbb{P}\mathsf{r}_{\boldsymbol{x}\sim\{0,1\}^n}\left(f(\boldsymbol{x}) \neq \min_{\boldsymbol{y}\in\{0,1\}^m} g(\boldsymbol{x},\boldsymbol{y})\right) \leq \varepsilon,$$

for some small constant $\varepsilon > 0$ (preferably bounded away from 1).

We can then state another question of interest to this project.

Question 1.3. *Under what conditions can a higher-degree submodular pBf f be approximately quadratized? What are necessary and sufficient bounds on the number of auxiliary variables to approximate quadratize f? For those submodular pBfs that can be (exactly) quadratized, are the approximate counterparts any better (e.g., require smaller amounts of auxiliary variables)?*

To the adviser's best knowledge, Question 1.3 has never been investigated.

1.2 Application: Minimization of Submodular Functions

Due to its diminishing returns characteristic, submodular functions have many applications in areas as diverse as Algebra (vector space and lattice rankings [40]), Combinatorics (matroids and polymatroids [22, 48]), Computer Vision (image segmentation [4]), Economics (inventory problems [14]), Engineering (rigidity and electrical flows [43, 35]), Game Theory (cooperative games [38]), Graph Theory (packing and covering [41]), Statistics (discrete entropy [49]), and Theoretical Computer Science (constraint satisfaction problems [5]).

Minimization of quadratic, submodular pBf was shown to be achievable is strongly polynomial time through maximum-flow techniques in [27]. That result was later improved in [10, 12] using the *roof duality* machinery of [26]. Extensions to degree-3 submodular pBfs were given in [3] and in [51] – the latter using multi-flow techniques. Higher degree pBfs were addressed in [6], where roof-duality-type results were obtained. However, no combinatorial algorithms were given.

In a different setting, the so-called value-oracle[2] model, submodular function minimization (any degree) was shown to be achievable in strongly polynomial time in [23, 24, 25] through the use of the *ellipsoid method* (a polynomial time, albeit highly convoluted and impractical, solver for the broad class of *linear programming* problems). Strongly polynomial-time combinatorial algorithms were later, simultaneously introduced in [47] and [32], with running times $O(n^8 + \gamma n^7)$ and $O(\gamma n^7 \log n)$, respectively, where γ means the running time of an oracle call and n the cardinality of the ground set. A sequence of improvements [50, 20, 31, 30] culminated in a $O(n^6 + \gamma n^5)$ running time [39]. Despite being impressive achievements themselves, the n^6 running-time dominant term is too high for modern applications – especially, those inside the *big data* and computer vision realms – and pales in comparison to the $O(n^3)$ cost of flow-based techniques. Furthermore, since they are all value-oracle-based algorithms, they completely neglect the fact that an algebraic expression for the function is / may be available.

In face of the above, the study of submodular quadratizations of submodular pBfs becomes a good, viable alternative for the solution of very large submodular optimization problems and therefore, worthy of pursuit.

We end this section mentioning that recently, two new algorithms (and two extra variations) to submodular function minimization were introduced in [34, 15], one of which attains an additive ε-approximation for functions with domain $[-1, 1]^n$ in $O(\gamma n^{5/3}/\varepsilon^2)$ time. While this is no less than extraordinary, the results of [15] still assume the value-oracle model and make use of a very different set of continuous-based techniques and methods. Despite continuous optimization being beyond the scope of this project, we cannot help ourselves but wonder whether better results can be achieved in the multi-affine polynomial setting.

[2]A **value-oracle** is any procedure for a function f that, given $\boldsymbol{x} \in \mathrm{dom}(f)$, returns $f(\boldsymbol{x})$ and no extra information about f.

2 Goals

This project assumes the student has minimal to no research experience whatsoever. Its general goals are then to expose the student to a research environment: the mindset of a researcher; some of the techniques and methodologies commonly used; how to detect roadblocks and how to (try to) bypass them; how to carefully check the validity of one's results; how to read (and possibly write) academic papers; how to research in an ethical manner, to back up one's claims with proofs or evidence, to avoid sheer speculations and plagiarism.

The project will focus on Questions 1.1 and 1.3 stated in Section 1.1. The adviser anticipate the following specific goals to be achieved: the strengthening of the student's ability to think in a clear, concise, and formal way; the increase in the student's abilities to navigate through more abstract settings; the acquisition, from the student's perspective, of fundamental results in combinatorics, computational complexity, optimization, and theory of Boolean functions; the improvement of the student's coding skills, and the finding of some answers to the questions proposed.

Furthermore, the student will have the opportunity to interact with other advisees, some of which are working on related aspects of submodularity. It is expected for this interaction to be highly beneficial to the student.

3 Methodology

The methodology of this project will be the one compatible with the mathematical nature of the subject:

(1) Adviser and student will have office meetings – at first, every other week; later, on a weekly basis – to discuss the papers or book chapters read by the latter since the last meeting. The adviser will provide clarifications and suggest new material and/or directions to be worked upon.

(2) The student will write about the topics learned in order to develop their writing skills. Focus will be given to precise definitions, correct contextualization, clear and concise proofs of the main results, and the correctness and quality of any computer code that may be written. The final report will be made available under an open-access policy.

(3) At the adviser's discretion, the student may be asked to give a talk of her results in a seminar series run by the center. Any new result will be submitted to publication in conferences and/or international journals.

4 Student's Previous Exposure to the Topic

The student contacted the adviser for a research experience for undergraduates project halfway through the third term of 2021. Since then, under the adviser's guidance, the student:

- became familiar with the topics of pseudo-Boolean functions and quadratizations, working his way through the surveys Boros and Hammer [11], and Boros and Gruber [9];

- conducted his 'Projeto Dirigido' coursework at UFABC on the subject of this proposal.

Both activities provide a welcome warm-start and advance the initial stages of the project.

5 Schedule

Already taking into account the aforementioned exposure of the student to the topic.

Topic	Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Ago
Pseudo-Boolean Functions	*	*										
Submodularity		*	*	*	*	*	*	*	*	*	*	
Discrete Convexity					*	*	*	*	*	*	*	
Quadratizations			*	*	*	*	*	*	*	*	*	
Coding and Testing				*	*	*	*	*	*	*	*	
Writing		*	*	*	*	*	*	*	*	*	*	*

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