Domain-Reduction Matheuristics for Bilinear Programming

Master's Dissertation Proposal

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Abstract

This dissertation proposes domain-reduction matheuristics for solving bilinear programming problems, with applications spanning protein synthesis, mechanical design, and switching strategies for power converter. Bilinear programming poses challenges due to its nonlinear nature, often requiring complex optimization strategies. The research aims to develop innovative algorithms combining domain reduction and convexification approaches to efficiently tackle bilinear optimization. These algorithms will be implemented in modern programming languages and applied to real-world problems. Comparative analyses with state-of-the-art optimization solvers will assess the performance of the proposed matheuristic algorithms. The findings will be disseminated through reports, publications, and presentations, contributing to advancements in bilinear optimization and promoting practical applications.

Key-words: Bilinear programming, matheuristics, convexification, MINLP.

1) Introduction

Optimization problems from different domain applications have nonlinearities that can be modeled with bilinear terms, which are functions consisting of the product of two variables, for instance, f(x,y) = xy. Bilinear terms can be used to model the condition that the concentration of products in an outflow from a tank is the same concentration in the volume stored in the tank. This is a typical constraint that appears in the transfer operations between tanks and processing units, like column distillation units (CDUs), in petrochemical plants and refineries (Assis et al., 2019), (Rocha, 2021).

In protein design, the Protein Structure Prediction (PSP) problem involves predicting a protein's three-dimensional structure from its amino acid sequence, which is inherently nonlinear due to the complex energy landscape governing protein folding (Khalatbari et al., 2019), (Almeida Paiva et al., 2022). However, recent research has shown that the nonlinearities can be formulated with bilinear terms, rendering a bilinear optimization problem. Reframing the traditionally nonlinear protein structure prediction problem into a bilinear optimization represents a significant advancement in the field, establishing a baseline formulation that can be solved by global optimization algorithms. Figure 1 illustrates the process of protein folding.

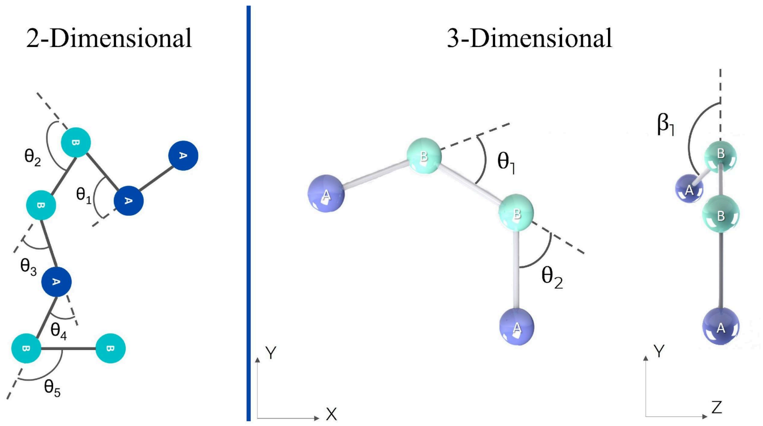

Figure 1. Example of the protein folding model showing different types of angles.

The optimal operation of multilevel power converters is critical for improving performance in various industrial applications. Multilevel converters, which can operate with more than three voltage levels, benefit from optimized modulation strategies to minimize the weighted total harmonic distortion and reduce the number of commutations. Recent research has proposed a bilinear programming formulation for the problem of designing such multilevel converters without relying on trigonometric functions but rather introducing bilinear terms that represent the decision space in the Cartesian space (Camponogara, Seman & Gili, 2019). Such a reformulation enabled the application of global optimization strategies.

The above domain applications are three problems that can be formulated as bilinear programming problems. One key advantage of bilinear programming is the existence of convexification strategies for the bilinear terms. The tightest convexification is obtained with McCormick envelopes, which consist of two linear underestimators and two linear overestimators for a bilinear function (McCormik, 1976). Figure 2 depicts the McCormick envelope of a bilinear function. Such envelopes can be further tightened by dividing the domain of the variables and introducing binary variables to select the domain, leading to MILP relaxation problems. This strategy is known as piecewise McCormick when the domain of one variable is divided, and bivariate piecewise McCormick if the domain of both variables is divided (Rocha 2021), (Castro, 2015). Figure 3 illustrates the piecewise McCormick envelope of a bilinear function. Other convexification strategies for bilinear functions include multiparametric disaggregation (Kolodziej, Castro & Grossmann, 2013) and reformulation linearization (Sherali & Tuncbilek, 1992), (Sherali & Adams, 1999).

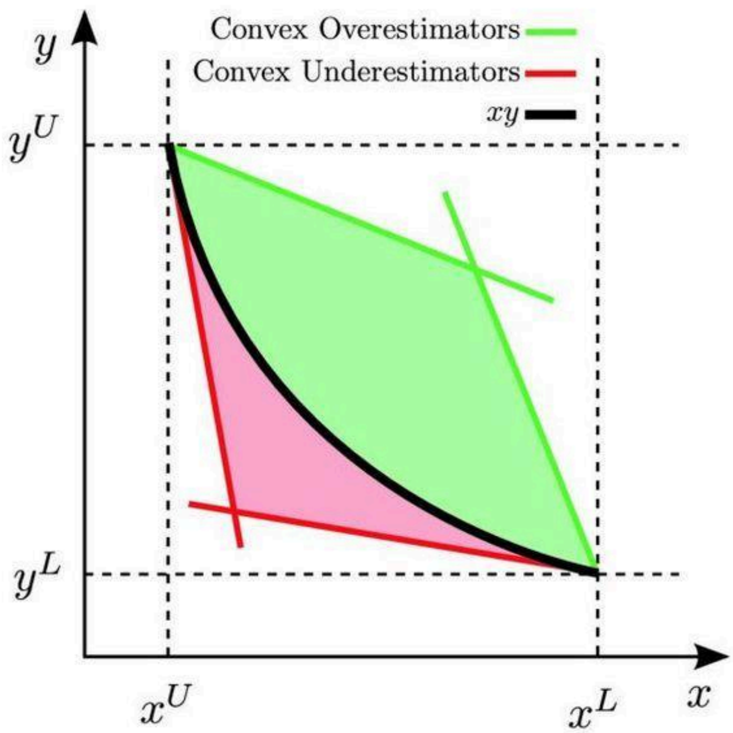

Figure 2. McCormick envelope.

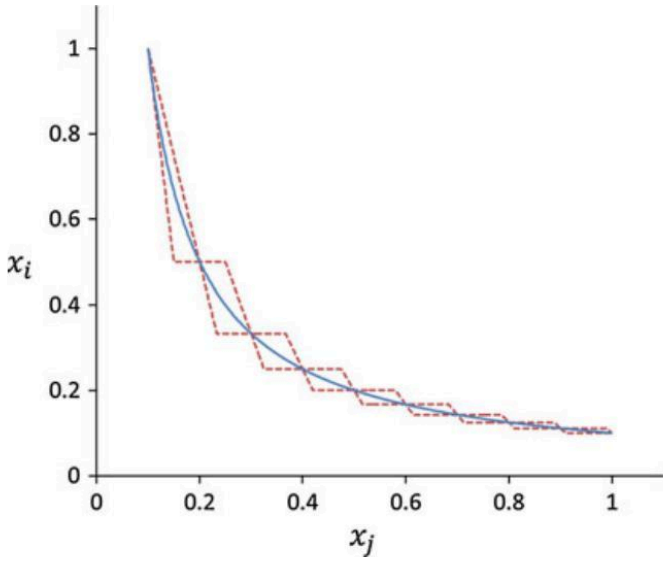

Figure 3. Piecewise McCormick envelope.

Despite the theory on bilinear terms, convexification strategies, and algorithms, the global solution of bilinear programming problems is extremely hard. Global solvers are not likely to solve large or complex bilinear problems; they can solve relatively small problems and take considerable computational resources. To this end, this dissertation will propose and apply matheuristics based on domain-reduction and convexification approaches that can reach nearly-optimal solutions within a reduced computational time. A matheuristic is a heuristic algorithm that combines heuristic decisions and mathematical optimization to obtain an approximate solution to a problem.

2) Objectives

This dissertation aims to advance the state-of-the-art approximation algorithms for solving bilinear programming problems, with a focus on metaheuristics that combine convexification approaches and domain-reduction strategies to obtain nearly optimal solutions in a short computational time. The specific objectives are:

Design matheuristics combine domain reduction with convexification approaches for bilinear functions, particularly McCormick envelopes, piecewise McCormick envelopes, and reformulation linearization strategies.

Implement the matheuristics in a modern programming language, such as Julia/JuMP or Python/Pyomo, for general application to bilinear programming problems.

Apply the matheuristics to representative bilinear programming problems found in protein design, angle switching strategies for power converters, and mechanical design, among others.

Compare the quality of the solutions obtained with the domain-reduction matheuristic against state-of-the-art global solvers, possibly Gurobi nonlinear, Couenne, SCIP and Baron.

3) Methodology

The research is organized in steps to gradually advance the knowledge of the problem and related topics, through problem formulation and towards its effective solution. This is a systematic approach is structured as follows:

1. *Literature Review (Months 1-6):* Conduct a comprehensive review of existing literature on bilinear programming problems, convexification strategies, domain reduction techniques, global optimization algorithms, and matheuristic approaches. Analyze relevant studies in application domains such as protein design, power converters, mechanical design, and others. Identify challenges and opportunities for advancing approximation algorithms and matheuristics for solving bilinear programming problems.
2. *Algorithm Design (Months 5-10):* Design matheuristic combining domain reduction with convexification approaches, possibly including McCormick envelopes, piecewise McCormick envelopes, and reformulation linearization strategies. Explore innovative combinations of these techniques to approach global solutions to bilinear programming problems. In the design, account for algorithm flexibility, scalability, and robustness to handle diverse problem characteristics and complexities.
3. *Implementation (Months 6-13):* Implement the designed algorithms in a suitable programming language, such as Julia/JuMP or Python/Pyomo, to facilitate general application to bilinear programming problems. Develop modular and well-documented code to promote integration with existing optimization frameworks and software packages. Conduct rigorous testing and validation to ensure the soundness of the implemented algorithms.
4. *Application (Months 11-15):* Apply the developed matheuristic algorithms to representative bilinear programming problems across different domains, possibly to protein design problems to predict protein structure and protein folding, design power converters by identifying optimal switching strategies, synthesis of mechanical systems.
5. *Performance Evaluation (Months 13-16):* Conduct comprehensive performance evaluation of the proposed matheuristic algorithms in terms of the solution quality in comparison with global optimal solutions obtained from state-of-the-art solvers (e.g., Gurobi nonlinear, Couenne, SCIP, Baron). Evaluate computational time and resource requirements of the matheuristics,

including scalability analysis for large-scale problem instances. Investigate the robustness and reliability of the matheuristics under different problem settings and input variations.

6. *Documentation and Reporting (Months 14-18):* The project's findings will be shared through technical reports, papers submitted to journals, and papers presented at conference, allowing both academics and practitioners to use the models developed in the dissertation. We aim to advance knowledge in bilinear optimization and streamline practical applications.

In summary, the dissertation research will systematically review progress and make necessary adjustments to follow the planned schedule. Collaboration among team members, including advisors and the master's student, will be paramount. By fostering an environment of open communication and shared expertise, we aim to leverage diverse perspectives and collective efforts to ensure the project's success. Through regular feedback, proactive problem-solving, and mutual support, we will navigate challenges and achieve our research objectives effectively.

4) Expected Results

The expected contributions resulting from this dissertation are:

1. Novel matheuristic algorithms for solving bilinear programming problems.
2. Implementation of the developed matheuristics in modern programming languages for easy integration, such as Julia/JuMP and Python/Pyomo.
3. Application of the matheuristics to real-world problems in protein design, design of switching strategies for power converters, and mechanical design.
4. Comparative analysis of the matheuristic with state-of-the-art solvers to assess performance.
5. Dissemination of findings through reports, publications, and presentations.

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