Exploring Extensions of Maximum Clique Problems

from 2-Graphs to k-Uniform Hypergraphs

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Introduction

- My end-of-study internship took place from the 1st pf May to the 20th of October at the University of Padua, department of applied mathematics.
- I was guided by Mr. Francesco Rinaldi, with support from Mr. Damiano Zeffiro (a former Ph.D. student).
- The objective was to generalize several techniques for solving clustering problems in hypergraphs, focusing on the Maximum Clique Problem (MCP) and related relaxations.

Definitions

- We work on graphs represented as G = (V, E) where V is a list of vertices and E is a list of edges.
- An hypergraph generalizes traditional graphs by allowing edges to connect more than two vertices. Here we are interested in k-uniform hypergraphs where all of the hyperedges connect the same number of vertices.
- In a graph G = (V, E), a clique is a subset $S \subseteq V$ such that every two distinct vertices in S are adjacent, i.e., $\{u, v\} \in E$ for all $u, v \in S$.
- The MCP is the search of the largest clique in an arbitrary graph. It is an NP-hard problem.

First Part: A Continuous Formulation for the Maximum s-Defective Clique Problem

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- The first part of my internship focused on developing a continuous formulation for the Maximum s-Defective Clique Problem (MsdCP) in hypergraphs.
- This formulation was inspired by existing formulations for the simpler case k=2, and its equivalence with the combinatorial problem was proven.
- We then generalized results about variants of the Frank-Wolfe (FW) algorithm applied to this problem.

Motivation

- Since the strict requirement that every two elements have a direct relation is often not satisfied in practice (e.g., due to experimental errors in protein research), relaxations of the clique model have been proposed.
- Here we are interested in the concept of *s*-defective cliques, allowing up to *s* missing links.

Turán's theorem states:

$$\max_{x \in \Delta} x^T A x = 1 - \frac{1}{\omega(G)} \tag{5}$$

where $\Delta = \{x \in \mathbb{R}^n \mid x \geq 0 \text{ and } 1^T x = 1\}$, A is the adjacency matrix, and $\omega(G)$ is the size of the maximum clique.

To address spurious solutions (continuous solutions that has no interpretation in terms of set), regularization was introduced:

$$\max_{x \in \Delta} x^T A x + \alpha \|x\|_2^2 \tag{6}$$

with $\alpha \in (0,1)$. Global and local maximizers are in one-one correspondence with characteristic vectors of maximum and maximal cliques.

The continuous unregularized formulation for the MCP was generalized to the MsdCP:

$$\max_{(x,y)\in\Delta\times D_s(G)} x^T (A + A(y)) x \tag{7}$$

where $\Delta=\{x\in\mathbb{R}^n\mid x\geq 0 \text{ and } 1^Tx=1\}$, and $D_s(G)=\{y\in\{0,1\}^{\overline{E}|1^Ty\leq s\}}$. x corresponds to the node chosen in the s-defective clique, and y corresponds to the missing edges in the s-defective clique.

The formulation can be seen as two nested problems: first, finding the best *s* edges to add to the graph in order to have the largest clique in the augmented graph, and then finding this clique.

Regularization was added to suppress spurious maxima, ensuring full equivalence with the discrete problem:

$$\max_{(x,y)\in\Delta\times D_s(G)} x^T (A + A(y)) x + \alpha ||x||_2^2 + \beta ||y||_2^2$$

where $0 < \alpha < 2$ and $\beta > 0$.

The regularized maximum clique formulation was generalized to k-uniform hypergraphs:

$$\min_{x \in \Delta} \underbrace{\sum_{e \in \overline{E}} \prod_{i \in e} x_i + \tau \|x\|_k^k}_{L_{\overline{G}}(x)}$$

where $0 < \tau \le \frac{1}{k(k-1)}$ (strict inequality when k=2). Note that this formulation searches for a minimum on the complement of the graph.

Formulation for the MsdCP on hypergraphs

We came up with the following formulation :

$$\min_{\text{s.t. } (x,y) \in \mathcal{P}_s} L_{\overline{G}}(x) - \underbrace{L_{G(y)}(x)}_{\sum_{e \in \overline{E}} y_e \prod_{i \in e} x_i} + \alpha \|x\|_k^k - \beta \|y\|_2^2$$

where $0 < \alpha \le \frac{1}{k(k-1)}$ (strict inequality for k = 2) and $\beta > 0$.

Remark

To explain the origin of the formulation, combining the ideas of the MsdCP on 2-graphs and the MCP on k-graphs, we come to this starting point:

$$\min_{s.t.\ (x,y)\in\mathcal{P}_s} L_{\overline{G\cup G(y)}}(x) + \alpha \|x\|_k^k \pm \beta \|y\|_I^I$$

Then it seems natural to write

$$L_{\overline{G \cup G(y)}}(x) = L_{\overline{G} \setminus G(y)}(x) = L_{\overline{G}}(x) - L_{G(y)}(x).$$

Formal Equivalence between the Discrete and the Continuous Problems

Denoting $h(x,y) := L_{\overline{G}}(x) - L_{G(y)}(x) + \alpha ||x||_k^k - \beta ||y||_2^2$.

Proposition

The following are equivalent :

- (i) $p = (x, y) \in \mathcal{P}_s$ is a local minimizer for h(x, y)
- (ii) p is a strict local minimizer
- (iii) $p = (x^{(C)}, y^{(p)})$, where $s \ge I = \mathbf{1}^T y^{(p)} \in \mathbb{N}$, with C an I-defective clique in G which is also a maximal clique in $G \cup G(y^{(p)})$, and $y^{(p)} \in \{0,1\}^{\overline{E}}$ such that $y_e^{(p)} = 1$ for every $e \in {C \choose k} \cap \overline{E}$ and with $supp(y^{(p)})$ of maximum cardinality under these constraints.

In either of these equivalent cases, we have $h(p) = \alpha |C|^{1-k} - \beta I$.

Frank-Wolfe Algorithm Overview

- The Frank-Wolfe (FW) algorithm is an optimization scheme suitable for problems with a search space represented as a polytope, as it is in our case.
- At each step, the algorithm moves the argument towards a vertex of the polytope in order to maximize a first-order local approximation of the objective function.
- The convexity of the search space ensures that the updated position x_{k+1} is feasible without the need for a costly projection step into the feasible domain.

FW algorithm

- 1: Initialize x^0 within the feasible polytope $\mathcal{P} = \operatorname{conv}(\mathcal{Q})$ with $|\mathcal{Q}| < \infty$.
- 2: **for** t = 1, 2, ... **do**
- 3: Compute the gradient: $\nabla f(x^t)$.
- 4: Find the vertex $v \in \mathcal{Q}$ that maximizes $\nabla f(x^t)^T v$.
- 5: Determine the step size: γ_t .
- 6: Update the solution: $x^{t+1} = x^t + \gamma_t(v x^t)$.
- 7: end for

FDFW

- 1: Initialize: $w_0 \in \mathcal{Q}, k = 0$
- 2: **if** w_k is stationary **then**
- 3: **STOP**
- 4: end if
- 5: Find $s_k \in \arg\max_{y \in \mathcal{Q}} \nabla f(w_k)^T y$ and $d_k^{\mathcal{FW}} = s_k w_k$.
- 6: Find $v_k \in \arg\min_{y \in \mathcal{F}(w_k)} \nabla f(w_k)^T y$ and $d_k^{\mathcal{FD}} = w_k v_k$.
- 7: if $\nabla f(w_k)^T d_k^{\mathcal{FW}} \ge \nabla f(w_k)^T d_k^{\mathcal{FD}}$ then
- 8: $d_k = d_k^{\mathcal{F} \mathcal{W}}$
- 9: **else**
- 10: $d_k = d_k^{\mathcal{FD}}$
- 11: end if
- 12: Choose the step size $\alpha_k \in (0, \alpha_k^{\text{max}}]$ using a suitable criterion.
- 13: Update $w_{k+1} = w_k + \alpha_k d_k$.
- 14: Set k = k + 1 and go to step 2.



Motivation for the FWdc

- The convergence of the previous optimization scheme applied to our objective can be slow and inefficient, due to the structural differences between *x* and *y*.
- Since the two variables are tied, it is difficult to efficiently adjust the regularization parameters. The algorithm may either ignore x if the penalty coefficient on the y variable is large or ignore y if this coefficient is small.
- This limitation motivated the introduction of the following FW variant, named FWdc.

FWdc

- 1: Initialize: $z_0 = (x_0, y_0) \in \Delta \times \mathcal{D}_s(G), k = 0$
- 2: **if** z_k is stationary **then**
- 3: **STOP**
- 4: end if
- 5: Compute x_{k+1} by applying one step of the previous algorithm with $w_0 = x_k$ and $f(w) = \tilde{h}(w, y_k)$.
- 6: Find $y_{k+1} \in \arg\max_{y \in \mathcal{D}_s(G)} \nabla_y h_G(x_{k+1}, y_k)^T y$.
- 7: Set k = k + 1 and go to step 2.

Rationale

- The FWdc algorithm exploits the cross-product structure of the search space by splitting the update rules for x and y.
- This allows for a more efficient adjustment of the regularization parameters since the updates for x and y are decoupled.
- As the convergence for y is extremely slow (due to its high dimensionality), its update step is replaced by a full FW step.

FDFW Local Identification and Convergence

Theorem

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Let p := (x^{(C)}, y^{(p)}) be a strict minimizer, let z_k be a sequence generated by the FDFW. Then under certain conditions there exists a neighborhood U(p) of p such that if K := \min\{k \in \mathbb{N} | z_k \in U(p)\} we have the following properties : (a) if \tilde{h}(z_k) is monotonically increasing, then \sup(z_k) = C and y_k = y^{(p)} for every k \geq K + \dim \mathcal{F}(w_k) (b) under additional conditions, then z_k \to p.
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FDFW Global Convergence

Corollary

Let $\{z_k\}$ be a sequence generated by the FDFW, and assume that there are no saddle points in the limit set of $\{z_k\}$. Then under certain conditions on the step size we have $z_k \to p := (x^{(C)}, y^{(p)})$ with p a strict minimizer such that $supp(x_k) \subset C$ and $y_k = y^{(p)}$ for k large enough.

Limited Changes in FWdc Variant

Proposition

In the FWdc variant, if $\tilde{h}(z_k)$ is increasing at each separate update of x_k and y_k , then $\{y_k\}$ can change at most $I + \frac{|\overline{E}| + \alpha \left(1 - |C^*|^{1-k}\right)}{\beta}$ times, with C^* a maximum I-defective clique if we consider the MsdCP.

Explicit Bound in FWdc for Local Identification

Proposition

Let C be a clique in $G \cup G(\overline{y})$ and δ_{\max} be the maximum eigenvalue of the adjacency tensor $\mathcal{A}(\overline{G \cup G(\overline{y})})$, and define :

$$m_{\alpha}(C, G \cup G(\overline{y})) := \min_{v \in V \setminus C} E^{C}(v) - \alpha k$$

Let K be a fixed index in $\mathbb N$ and I^c be the components of $supp(x_K)$ with index not in C, and $L:=\frac{1}{(k-2)!}\delta_{\max}+k(k-1)\alpha$. Assume that y is stationary, and that

$$\|x_{\mathcal{K}}-x^{(C)}\|_1 \leq \frac{m_{\alpha}(C,G \cup G(\overline{y}))}{m_{\alpha}(C,G \cup G(\overline{y})) + 2|C|^{k-1}\left(\frac{1}{(k-2)!}\delta_{\mathsf{max}} + k(k-1)\alpha\right)}$$

Then
$$supp(x_{K+|I^c|}) = C$$
.

Failure

Theorem

Let $\{z_k\}$ be a sequence generated by the FDFW, with regularization coefficient $\alpha=1$. Under certain conditions on the step sizes, $\{z_k\}$ converges to a stationary point and identifies its support infinite time.

Second Part : Study of the Regularizer in the Continuous MCP Formulation

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The second part of the internship focused on generalizing the study of the regularizer function. For k=2, the MCP formulation was relaxed to :

$$\max_{\mathsf{s.t.}} x^\mathsf{T} \mathsf{A} x + \phi(x)$$

where ϕ satisfies the following conditions :

- $\nabla^2 \phi(x) > 0$ i.e. ϕ is strictly convex
- $\|\nabla^2 \phi(x)\|_2 < 2$
- $\phi(x)$ is invariant by permutation of x

Examples of Regularizers

Examples of regularizers satisfying these conditions:

- $\phi(x) = \frac{1}{2} ||x||_2^2$
- $\phi(x) = \alpha_2 \sum_{i=1}^n (e^{-\beta x_i} 1)$, with $\beta > 0$ and $0 \le \alpha_2 \le \frac{2}{\beta^2}$ (approximation of $-\alpha_2 ||x||_0$)

Generalized Relaxed Formulation

We generalized the relaxed formulation to :

$$\min_{\text{s.t. } x \in \Delta} L_{\overline{G}}(x) + \Phi(x) \tag{1}$$

where Φ satisfies the three following assumptions :

- $\Phi \in C^2(\mathbb{R}^n)$ and for all face S of Δ , $\nabla^2 \Phi_S(x) > 0$ for all $x \in \Delta^{(S)}$ i.e. the restriction of Φ to any face of Δ is strictly convex
- $\Phi(\overline{x}) = \Phi(x)$ for all \overline{x} permutation of the indices of x i.e. Φ is symmetric / permutation invariant
- $(\mathbf{e}_i \mathbf{e}_j)^T \nabla^2 \Phi(x) (\mathbf{e}_i \mathbf{e}_j) < x_i^{k-2} + x_j^{k-2}$ for every $x \in \Delta$, $i, j \in supp(x)$ with $i \neq j$

Sum of Real Functions

For a regularizer that is a sum of real functions (i.e. $\phi(x) = \sum_i q(x_i)$), the conditions can be equivalently expressed as:

Equivalent Conditions

- $q \in C^2(\mathbb{R})$ and q''(y) > 0 when y > 0.
- $q''(y) < y^{k-2} \text{ for } 0 < y \le \frac{1}{2} \text{ and } q''(y) \le y^{k-2} \text{ for } \frac{1}{2} < y \le 1.$
- $q''(y) < y^{k-2}$ for $0 < y \le \frac{1}{2}$ and $q''(y) \le y^{k-2}$ for $\frac{1}{2} < y \le 1$, ensuring strict convexity and symmetry.

Generalization of the Regularizers

- Original regularizers :
 - $\phi(x) = \frac{1}{2} ||x||_2^2$
 - 2 $\alpha_1 \|x + \varepsilon_1\|_p^p$ with $\varepsilon \ge 0$, $p \ge 2$, and $0 \le \alpha_1 \le \frac{2}{p(p-1)(1+\varepsilon)p-2}$
 - 3 $\phi(x) = \alpha_2 \sum_{i=1}^n (e^{-\beta x_i} 1)$ with $\beta > 0$ and $0 \le \alpha_2 \le \frac{2}{\beta^2}$ (approximation of $-\alpha_2 ||x||_0$)
- Generalizations:
 - **1** $\Phi_B(x) = \alpha ||x||_k^k$ with $0 < \alpha < \frac{1}{k(k-1)}$
 - 2 $\Phi_1(x) = \alpha_1 \|x + \varepsilon_1\|_p^p \frac{n}{2}\alpha_1 p(p-1)\varepsilon^{p-2}x^2$ with $\varepsilon > 0$, $p \ge k$, and $0 < \alpha_1 \le \frac{1}{p(p-1)(1+\varepsilon)p-2}$
 - 3 More complicated, so no easy generalization

Third Part: Lovász Extensions

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Given a function $f: P(V) \to \mathbb{R}$, its Lovász extension extends the domain of f to \mathbb{R}^n :

Denote $x=(x_1,\ldots,x_n)\in\mathbb{R}$, and let $\sigma:V\cup\{0\}\to V\cup\{0\}$ be a permutation such that $x_{\sigma(1)}\leq x_{\sigma(2)}\leq \ldots \leq x_{\sigma(n)}$ and $\sigma(0):=0$ where we add $x_0:=0$ to x. The Lovász extension is defined as:

$$f_L(x) = \sum_{i=0}^{n-1} (x_{\sigma(i+1)} - x_{\sigma(i)}) \cdot f(V_{\sigma(i)}(x))$$

where $V^0 := V$ and $V_{\sigma(i)}(x) := \{ j \in V : x_i > x_{\sigma(i)} \}.$

Key Properties of Lovász Extension

Proposition

- For a set S, denoting its characteristic vector $1_S \in \{0,1\}^n$, $f_L(1_S) = f(S)$.
- f_L is the unique function that is affine on each polyhedral cone $R_{\sigma}^n := \{x \in R^n, x_{\sigma(1)} \le x_{\sigma(2)} \le \ldots \le x_{\sigma(n)}\}$ and for which $f_L(1_S) = f(S)$ for every set S.
- f_L is positively one-homogeneous, piecewise-linear, and Lipschitzian continuous.
- f is submodular $\Leftrightarrow f_L$ is convex $\Leftrightarrow f_L$ is submodular.

Theorem

Given set functions $f_1, \ldots, f_n : A \to \mathbb{R}^+$ and a zero-homogeneous function $H : (\mathbb{R}^+)^m \setminus \{0\} \to \mathbb{R} \cup \{+\infty\}$ with $H(a+b) \ge \min(H(a), H(b))$ for all $a, b \in (\mathbb{R}^+)^m \setminus \{0\}$, we have $\min_{S \in A'} H(f_1(S), \ldots, f_n(S)) = \inf_{x \in D'} H(f_L^1(x), \ldots, f_L^n(x))$ where $A' = \{S \in A : (f_1(S), \ldots, f_n(S)) \in Dom(H)\}$, $D' = \{x \in DA \cap (\mathbb{R}^+)^V : (f_L^1(x), \ldots, f_L^n(x)) \in Dom(H)\}$, and $Dom(H) = \{a \in (\mathbb{R}^+)^m \setminus \{0\} : H(a) \in \mathbb{R}\}$.

Theorem

Given two set functions $f,g:A\to [0,\infty)$, let $\tilde{f},\tilde{g}:DA\to \mathbb{R}$ satisfying $\tilde{f}\geq f_L$, $\tilde{g}\leq g_L$, $\tilde{f}(1_S)=f(S)$, and $\tilde{g}(1_S)=g(S)$. Then

$$\min_{S \in A \cap supp(g)} \frac{f(S)}{g(S)} = \inf_{\Psi \in DA \cap supp(\tilde{g})} \frac{\tilde{f}(\Psi)}{\tilde{g}(\Psi)}$$

If we replace the conditions by $\tilde{f} \leq f_L$, $\tilde{g} \geq g_L$, then

$$\max_{S \in A \cap supp(g)} \frac{f(S)}{g(S)} = \sup_{\Psi \in DA \cap supp(\tilde{g})} \frac{\tilde{f}(\Psi)}{\tilde{g}(\Psi)}$$

Theorem

Let $f,g:A\to [0,+\infty)$ be two set functions with decompositions $f=f_1-f_2$ and $g=g_1-g_2$ as differences of submodular functions. Let \tilde{f}_2, \tilde{g}_1 be the restrictions of positively one-homogeneous convex functions onto DA, with $f_2(S)=\tilde{f}_2(1_S)$ and $g_1(S)=\tilde{g}_1(1_S)$. Define $\tilde{f}=f_L^1-\tilde{f}_2$ and $\tilde{g}=\tilde{g}_1-g_L^2$. Then,

$$\min_{S \in A \cap supp(g)} \frac{f(S)}{g(S)} = \min_{x \in DA \cap supp(\tilde{g})} \frac{\tilde{f}(S)}{\tilde{g}(S)}$$

Piecewise Multilinear Extensions

For now, Lovász extensions satisfy the property $(f+g)^L=f^L+g^L$, and homogeneous and piecewise multilinear extensions extend this property to $(gf)^L=g^Lf^L$, sacrificing the equalities between the discrete and continuous problems and replacing them by inequalities, the reverse inequalities having to be proved on a case-by-case basis.

Piecewise Multilinear Extension

Given $V_i := \{1, ..., n_i\}$ and the power set $P(V_i)$ for i = 1, ..., k, for a discrete function $f : P(V_1) \times ... \times P(V_k) \to \mathbb{R}$, its piecewise multilinear extension is defined on $\mathbb{R}^{n_1} \times ... \times \mathbb{R}^{n_k}$ by

$$f^{M}(x_{1},...,x_{k}) := \sum_{i_{1} \in V_{1},...,i_{k} \in V_{k}} \prod_{l=1}^{k} (x_{l}^{\sigma_{l}(i_{l})} - x_{l}^{\sigma_{l}(i_{l}-1)}) f(V_{i_{1}}(x_{1}),...,V_{i_{k}}(x_{k}))$$

where $V_i(x_l) := \{j \in V_l \mid x_{l,j} > x_{l,l-1}\}$ for $i \ge 2$, $V_1(x_l) := V_l$, σ_l is a permutation of indices sorting x_l by non-decreasing order, and we add $x_{l,0} := 0$ to each x_l .

Theorem

Given $f: A \to \mathbb{R}$ and $g: A \to [0, +\infty)$, we have

$$\sup_{A \in A \cap supp(g)} \frac{f(A)}{g(A)} \le \sup_{x \in D \cap supp(g^M)} \frac{f^M(x)}{g^M(x)} \le \sup_{A \in \tilde{A}} \frac{f(A)}{g(A)}$$

whenever $\{1_A : A \in A\} \subset D$ and $A(D) \subset \tilde{A}$. The above inequality still holds replacing \sup and \le by \inf and \ge . If we further assume that (A,D) is a perfect domain pair, and $\sup p(f) \subset \sup p(g)$, then

$$\max_{A \in A \cap supp(g)} \frac{f(A)}{g(A)} = \max_{x \in D \cap supp(g^M)} \frac{f^M(x)}{g^M(x)}$$

and the same holds replacing max with min.

Theorem

Let $H: \mathbb{R}_+^* \to \mathbb{R} \cup \{+\infty\}$ be a zero-homogeneous and quasi-concave function. For any function $f_1, \ldots, f_n: A \to \mathbb{R}^+$, we have

$$\min_{A\in\mathcal{A}}H(f_1(A),\ldots,f_n(A))=\inf_{x\in\mathcal{D}}H(f_1^M(x),\ldots,f_n^M(x))$$

where (A, D) forms a perfect domain pair w.r.t. the piecewise multilinear extension.

In addition, if $H: \mathbb{R}_+^* \to \mathbb{R} \cup \{-\infty\}$ is a zero-homogeneous and quasi-convex function, for any function $f_1, \ldots, f_n: A \to \mathbb{R}^+$, we have

$$\max_{A \in A} H(f_1(A), \dots, f_n(A)) = \sup_{x \in D} H(f_1^M(x), \dots, f_n^M(x))$$

Recovering the Classical MCP in 2-graphs

We have

$$\max_{\substack{S \in P(V) \setminus \{\emptyset\}}} \underbrace{\frac{|E(S,S)|}{|S|^2}}_{\substack{\text{Maximized when} \\ \text{S is a maximum clique}}} = \max_{\mathbf{x} \neq \mathbf{0}} \frac{2 \sum_{(i,j) \in E} x_i x_j}{\|\mathbf{x}\|_2^2}$$

where P(V) is the power set of V, E(S,S) denotes the set of edges between vertices in set S.

Recovering the MCP for Hypergraphs

We have:

$$\min_{S \in P(V) \setminus \{\emptyset\}} \underbrace{\frac{|E(S, \dots, S)| + \tau |S|}{|S|^k}}_{\substack{\text{Maximized when} \\ S \text{ is a maximum clique}}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{k! \sum_{e \in E} \prod_{i \in e} x_i + \tau \|\mathbf{x}\|_k^k}{\|\mathbf{x}\|_k^k}$$

where $0 < \tau < \frac{1}{|V|(|V|^{k-1}-1)}$, P(V) is the power set of V and $E(S, \ldots, S)$ represents the set of hyperedges with all vertices in set S.

Starting Point for the MsdcP

I suggested starting from the following function :

$$h(S) := (s+2)^{|S|} \left(s+1 - \left(\frac{|S|(|S|-1)}{2} - |E(S,S)| \right) \right)$$
 (2)

Conclusion

The internship work progressed along three main directions:

- Developed a novel continuous formulation for MsdCP in hypergraphs, studied algorithm convergence, and provided implementation.
- Extended the continuous formulation of MCP in hypergraphs to a broader class of regularizers.
- Laid the groundwork for using continuous extensions to find formulations for discrete problems within the MCP family.