Convex Recoloring through Integer Programming: Formulations, Valid Inequalities, and Computational Experiments

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Let G be an undirected graph, and let $V(G)$ and $E(G)$ denote its sets of vertices and edges, respectively. A *(partial) coloring* of G is a function $C\colon V(G) \to \mathcal{C} \cup \{\emptyset\}$ that assigns to each vertex a color from a set of colors $\mathcal{C}$, or $\emptyset$, which represents the absence of color. A vertex v in $V(G)$ is said to be *uncolored* if $C(v) = \emptyset$. If every vertex in $V(G)$ has a color, then the coloring is called a *total coloring*. For each $c \in \mathcal{C}$, the *color class* of c (denoted by $C^{-1}(c)$) is the set of vertices that are assigned color c. Notice that, unlike in the standard definition of coloring where adjacent vertices must have different colors, a coloring here is any (partial) assignment of colors to the vertices.

A *colored graph* is a pair (G, C) consisting of a graph G and a coloring C of its vertices. A coloring C is said to be *convex* if the color class of c induces a connected subgraph of G for every $c \in \mathcal{C}$, that is, $G[C^{-1}(c)]$ is connected for every $c \in \mathcal{C}$. Given a colored graph (G, C), any other coloring $C'\colon V(G) \to \mathcal{C} \cup \{\emptyset\}$ is called a *recoloring* of (G, C). A vertex $v \in V(G)$ is *recolored* by C' if $C'(v) \neq C(v)$ and $C(v) \neq \emptyset$. The convex recoloring problem is defined as follows.

Convex Recoloring Problem (CR).
Instance: *A connected graph G, a coloring $C\colon V(G) \to \mathcal{C} \cup \{\emptyset\}$ and a weight function $w\colon V(G) \to \mathbb{Q}_{\geq}$.*
Find: *A convex recoloring C' of (G, C).*
Goal: *Minimize $\sum_{v \in R(C')} w(v)$, where $R(C') := \{v \in V(G)\colon C(v) \neq \emptyset \text{ and } C(v) \neq C'(v)\}$ is the set of vertices recolored by C'.*

Note that any partial convex recoloring can be extended in polynomial time to a total convex recoloring of same cost. There are several applications of Convex Recoloring in phylogenetic networks [6], protein-protein interaction [3], and communication and transportation networks [7]. In each of these domains, enforcing connectivity of vertices with the same attribute captures important structural or functional requirements.

Convex recoloring was originally motivated by the study of phylogenetic trees in Bioinformatics [9], and it is known to be NP-hard even on paths [8]. Most research on CR has focused on trees, with only limited results available for general graphs. Two integer programming formulations for CR on general graphs have previously been proposed in the literature: the vertex cut formulation [1] and the connected subgraph formulation [2]. However, the accompanying exact methods (branch-and-cut in [1] and branch-and-price in [2]) are implemented only for trees. This work advances this direction by designing and implementing exact solution methods for CR on general graphs.

We first derive a structural property that allows us to only consider optimal solutions in which each color class contains a vertex that retains its initial color. We use this property to restrict the solution space without changing the optimal value, and we observe improved computational performance in our experiments.

We further propose two new mixed-integer linear programming formulations for CR: a compact flow-based model, which is the first compact formulation for CR on general graphs, and a representatives model, which avoids explicitly encoding the original colors of the vertices in the decision variables.

We also present a comparison of the polytopes associated with the linear relaxation of some of the new and existing formulations for CR. Moreover, we describe classes of valid inequalities for the representatives formulation naturally derived from known inequalities for the connected subpartiton polytope devised by Moura et al. [10], and design heuristics for the corresponding separation problems.

Finally, we report on computational experiments with four algorithms: branch-and-cut approaches based on the vertex cut formulation (C) and the representatives formulation (R), a branch and price for the

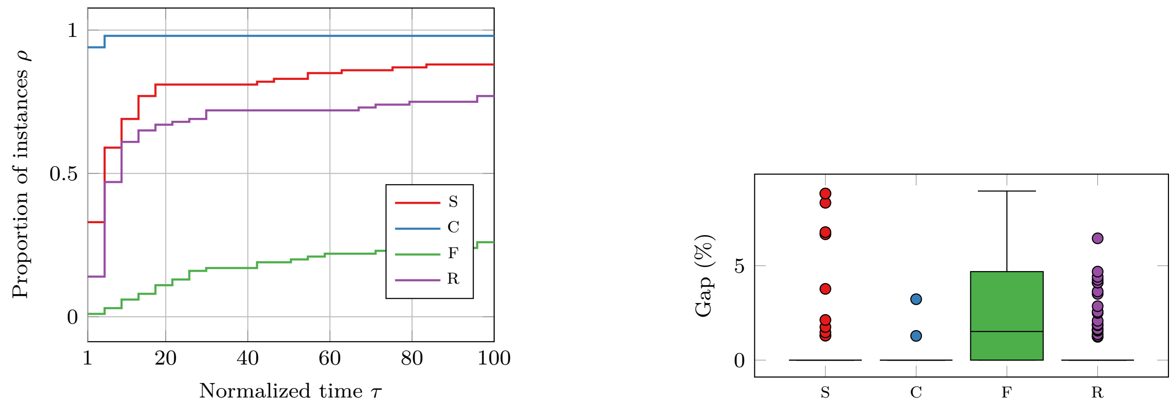

Figure 1: Performance profiles [5] and gaps (box plots) for the random instances.

connected subgraph formulation (S), and a branch-and-bound approach using the flow formulation (F). To the best of our knowledge, the proposed algorithms are the first exact solving methods in the literature described for convex recoloring on general graphs. The performance of the algorithms is evaluated on 100 random connected graph instances, sampled from the benchmark set introduced by Dantas et al. [4]. The results in Figure 1 indicate that the the vertex cut formulation is the fastest overall, and the flow formulation is the slowest.

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