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Continuous Cubic Formulations for Cluster Detection Problems in Networks

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Abstract The celebrated Motzkin-Straus formulation for the maximum clique problem provides a nontrivial characterization of the clique number of a graph in terms of the maximum value of a nonconvex quadratic function over a standard simplex. It was originally developed as a way of proving Turán's theorem in graph theory, but was later used to develop competitive algorithms for the maximum clique problem based on continuous optimization. Clique relaxations, such as s-defective clique and s-plex, emerged as attractive, more practical alternatives to cliques in network-based cluster detection models arising in numerous applications. This paper establishes continuous cubic formulations for the maximum s-defective clique problem and the maximum s-plex problem by generalizing the Motzkin-Straus formulation to the corresponding clique relaxations. The formulations are used to extend Turán's theorem and other known lower bounds on the clique number to the considered clique relaxations. Results of preliminary numerical experiments with the CONOPT solver demonstrate that the proposed formulations can be used to quickly compute high-quality solutions for the maximum s-defective clique problem and the maximum s-plex problem. The proposed formulations can also be used to generate interesting test instances for global optimization solvers.

Keywords Clique relaxations, maximum s-defective clique problem, maximum s-plex problem, Motzkin-Straus formulation, Turán's theorem, cubic optimization, fractional b-matching.

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1 Introduction

Let $G = (V, E)$ be a simple (undirected) graph with vertex set $V = \{1, 2, \dots, n\}$ and edge set $E \subseteq \binom{V}{2}$ consisting of m unordered pairs of adjacent vertices. A subset of vertices $C \subseteq V$ is called a clique if $\{i, j\} \in E$ for every pair of distinct vertices $i, j \in C$. The maximum clique problem is to find a clique of largest cardinality in a graph, and the clique number $\omega(G)$ of G is the cardinality of a maximum clique in G.

In 1941, Turán [44] established the following inequality between the number of edges m, the number of vertices n, and the clique number $\omega(G)$ of a simple graph G:

$$m \leq \left(1 - \frac{1}{\omega(G)}\right) \frac{n^2}{2}. \tag{1}$$

This inequality, known as Turán's theorem, is one of the most prominent results in extremal graph theory [2].

In 1965, Motzkin and Straus [32] discovered a nontrivial connection between the clique number of a simple graph G and the global optimal value of a quadratic program associated with G:

$$1 - \frac{1}{\omega(G)} = \max_{x \in \Delta^n} x^T A_G x, \tag{2}$$

where A_G is the adjacency matrix of G, $\Delta^n = \{x \in \mathbb{R}^n \mid e_n^T x = 1,\ x \geq 0\}$ is the standard simplex in $\mathbb{R}^n$, and e_n is the vector of n ones. Turán's theorem can be proved by setting $x = \frac{1}{n} e_n$ in the Motzkin-Straus formulation. This proof is among the "Proofs from THE BOOK" [3], containing some of the most elegant mathematical proofs.

In 1990, Pardalos and Phillips [35] proposed the first algorithmic approach for the maximum clique problem based on the Motzkin-Straus formulation. This inspired some interesting developments in the interface of discrete and continuous optimization, aiming to use properties of this (continuous) model in order to solve the (discrete) maximum clique problem [10, 13, 19, 20, 23]. In addition, the Motzkin-Straus formulation influenced several other research directions in mathematical optimization, including quadratic programming [12, 26], copositive programming [9, 11, 14], and complexity analysis in nonlinear optimization [1, 45].

In this paper, the Motzkin-Straus formulation is extended to two clique relaxation models, s-defective clique and s-plex, defined next. Given a simple graph $G = (V, E)$ and vertex subset $S \subseteq V$, denote by $G[S] = (S, E \cap \binom{S}{2})$ the subgraph induced by S in G. Let s be a fixed positive integer. A subset of vertices $S \subseteq V$ is

- an *s-defective clique* if $G[S]$ has at least $\binom{|S|}{2} - s$ edges;
- an *s-plex* if each vertex in S is adjacent to at least $|S| - s$ other vertices from S.

A clique is equivalent to a 0-defective clique and to a 1-plex. Given a graph G and an integer s, the maximum s-defective clique problem asks for an s-defective clique of maximum cardinality $\omega_s^d(G)$ in G, and $\omega_s^d(G)$ is called the s-defective clique number. The maximum s-plex problem and the s-plex number $\omega_s(G)$ are defined similarly.

These and other clique relaxations were introduced in the literature in order to overcome practical limitations of using cliques for modeling tightly knit clusters in networks [36]. In particular, s-defective cliques were introduced in the context of protein interaction networks [47] and s-plexes originally appeared in the social networks literature [39]. Existing approaches for the maximum s-defective clique problem and the maximum s-plex problem, as well as their analogues in the complement graph, include algorithms based on integer linear programming [6, 29, 41] and combinatorial branch-and-bound methods [22, 28, 31, 43]. In addition, several metaheuristics for the maximum s-plex problem have been proposed [30, 33, 48].

In this work, we show that the Motzkin-Straus formulation can be generalized to formulate the considered optimization problems in terms of maximizing a cubic function over a polyhedral set described by two types of decision variables, x – corresponding to the graph's vertices, and y – representing the edges of the complement graph $\bar{G}$. In both cases, the trilinear objective function is quadratic with respect to the vertex variables x and linear with respect to the auxiliary variables y. Also, the projection of the feasible set onto x is the standard simplex Δ^n, while the y variables indicate whether the corresponding missing edge is a part of the subgraph induced by the desired clique relaxation.

The proposed formulations can be thought of as a formalization of the following two-stage process. First, we pick a subset of missing edges that would be feasible to add to G with respect to the considered clique relaxation (i.e., up to s edges for s-defective clique and up to $s-1$ incident edges per vertex for s-plex). We will refer to such missing edges as *fake edges*. Next, we write the Motzkin-Straus formulation for the maximum clique problem in the graph obtained from G by including the fake edges picked in the first stage. The described process involves binary decisions concerning the missing edges, represented by y-variables. We show that the binary variables can be relaxed to obtain a continuous formulation for each problem. The correctness of the continuous formulation is easy to establish for s-defective clique, but is rather nontrivial for s-plex. In the latter case, we take advantage of a classical result concerning the half-integrality of the fractional b-matching polytope, given in Lemma 1 below.

Given a simple graph $G = (V, E)$ and a nonnegative integer vector $b \in \mathbb{Z}_+^n$, $M \subseteq E$ is called a (1-capacitated) b-matching in G if no vertex $i \in V$ is incident to more than b_i edges in M. The maximum b-matching problem, which is to find a b-matching with the largest number of edges in G (whose cardinality is denoted by $\mu_b(G)$), is polynomial-time solvable [18]. Note that for $b = e_n$ this problem becomes the maximum matching problem. Given a weight w_{ij} associated with each edge $\{i, j\} \in E$, the maximum weight b-matching problem is to find a b-matching with the largest total weight in G.

Let $N_G(i) = \{j \in V \mid \{i,j\} \in E\}$ denote the neighborhood of i in G. Then the maximum-weight b-matching problem can be formulated as the following 0-1 program, where y_{ij} and y_{ji} refer to the same variable and $w_{ij} = w_{ji}$:

$$\begin{aligned} \max \ & \sum_{\{i,j\}\in E} w_{ij} y_{ij} \\ \text{s.t.} \ & \sum_{j \in N_G(i)} y_{ij} \le b_i \quad && \forall i \in V \\ & y_{ij} \in \{0,1\} && \forall \{i,j\} \in E. \end{aligned} \tag{3}$$

Clearly, the linear programming (LP) relaxation of this formulation, obtained by replacing $y_{ij} \in \{0,1\}$ with $y_{ij} \in [0,1]$ in (3), may have a fractional optimal solution. Consider, for example, the maximum matching problem (i.e., the case where $b = e_n$ and $w_{ij} = 1$ for every edge $\{i,j\} \in E$) on $G = C_5$, the cycle on 5 vertices. Then the optimal solution of the LP relaxation is obtained by setting $y_{ij} = \frac{1}{2}$ for every edge $\{i,j\} \in E$. This observation led to the following well-known result (see, e.g., [25, pp. 44-46]).

Lemma 1 *Let P be the feasible region of the LP relaxation of* (3). *Any extreme point $\hat{y}$ of P is half-integral, i.e., $\hat{y}_{ij} \in \{0, \frac{1}{2}, 1\}$, $\forall \{i,j\} \in E$. Moreover, the edge-induced subgraph $G\langle F \rangle$, where $F = \{\{i,j\} \in E \mid \hat{y}_{ij} = \frac{1}{2}\}$, consists of disjoint odd cycles.*

Here, the *edge-induced subgraph* $G\langle F \rangle = (V_F, F)$ has F as its edge set while its vertex set $V_F \subseteq V$ includes all vertices incident to the edges of F.

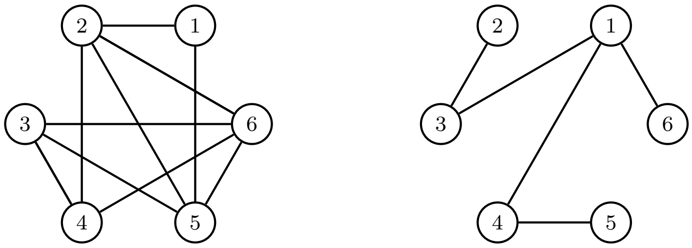
The remainder of this paper is organized as follows. Section 2 establishes the generalizations of Motzkin-Straus formulation to the maximum s-defective clique problem and to the maximum s-plex problem. Section 3 generalizes Turán's theorem and some known lower bounds on the clique number to s-defective clique and s-plex. Section 4 reports the results of numerical experiments. Finally, Section 5 concludes the paper.

2 Generalizations of the Motzkin-Straus formulation

Given a simple graph $G = (V, E)$, let $\bar{G} = (V, \bar{E})$ denote its complement and let $\bar{m} = |\bar{E}| = \binom{n}{2} - m$. For each missing edge $\{i,j\} \in \bar{E}$, we introduce a binary variable y_{ij}, indicating whether both i and j are included in the clique relaxation structure sought. Let $A_{\bar{G}}(y)$ be the matrix with the entry in the i^{th} row and j^{th} column given by y_{ij} if $\{i,j\} \in \bar{E}$, and 0, otherwise. That is, $A_{\bar{G}}(y)$ is obtained from the adjacency matrix $A_{\bar{G}}$ of $\bar{G}$ by replacing each 1 entry with the corresponding y_{ij}. See Figure 1 for an illustration. We refer to the variables y_{ij}, for $\{i,j\} \in \bar{E}$, as the *fake edge variables*.

2.1 Motzkin-Straus formulation for the maximum s-defective clique problem

Consider the following mixed integer optimization problem.



$$A_G = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 \end{bmatrix} \qquad A_{\bar{G}}(y) = \begin{bmatrix} 0 & 0 & y_{13} & y_{14} & 0 & y_{16} \\ 0 & 0 & y_{23} & 0 & 0 & 0 \\ y_{13} & y_{23} & 0 & 0 & 0 & 0 \\ y_{14} & 0 & 0 & 0 & y_{45} & 0 \\ 0 & 0 & 0 & y_{45} & 0 & 0 \\ y_{16} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Fig. 1 Illustration of $A_{\bar{G}}(y)$ construction.

$$f_s^d(G) = \max_{(x,y)\in\Delta^n\times D_s(G)} f_G(x,y), \tag{4}$$

where

$$f_G(x,y) = x^T(A_G + A_{\bar{G}}(y))x, \tag{5}$$

$\Delta^n = \{x \in \mathbb{R}^n \mid e_n^T x = 1,\ x \geq 0\}$ is the standard simplex in $\mathbb{R}^n$, and

$$D_s(G) = \{y \in \{0,1\}^{\bar{m}} \mid e_{\bar{m}}^T y \leq s\}. \tag{6}$$

Proposition 1 *Let $\omega_s^d(G)$ denote the s-defective clique number of G. Then*

$$1 - \frac{1}{\omega_s^d(G)} = f_s^d(G). \tag{7}$$

Proof First, we show that $1 - \frac{1}{\omega_s^d(G)} \leq f_s^d(G)$. Suppose that S is a maximum s-defective clique of cardinality $k = \omega_s^d(G)$, and define $(\hat{x}, \hat{y})$ as follows:

$$\hat{x}_i = \begin{cases} \frac{1}{k}, \text{ if } i \in S, \\ 0, \text{ otherwise;} \end{cases} \qquad \hat{y}_{ij} = \begin{cases} 1, \text{ if } i,j \in S \text{ and } \{i,j\} \in \bar{E}, \\ 0, \text{ otherwise.} \end{cases}$$

Then $(\hat{x}, \hat{y}) \in \Delta^n \times D_s(G)$ and

$$1 - \frac{1}{\omega_s^d(G)} = 2\binom{k}{2}\frac{1}{k^2} = f_G(\hat{x}, \hat{y}) \leq \max_{(x,y)\in\Delta^n\times D_s(G)} f_G(x,y) = f_s^d(G).$$

We prove $1 - \frac{1}{\omega_s^d(G)} \geq f_s^d(G)$ by contradiction. Suppose there exists $(\hat{x}, \hat{y}) \in \Delta^n \times D_s(G)$ such that $1 - \frac{1}{\omega_s^d(G)} < f_G(\hat{x}, \hat{y})$. Let $\hat{E} = \{\{i,j\} \in \bar{E} \mid \hat{y}_{ij} = 1\}$ and

$\hat{G} = (V, E \cup \hat{E})$. Then if we fix $y = \hat{y}$, equation (4) becomes the Motzkin-Straus formulation for the maximum clique problem in $\hat{G}$. We have

$$1 - \frac{1}{\omega_s^d(G)} < f_G(\hat{x}, \hat{y}) \leq \max_{x \in \Delta^n} f_G(x, \hat{y}) = 1 - \frac{1}{\omega(\hat{G})},$$

implying that $\omega_s^d(G) < \omega(\hat{G})$. However, since $(\hat{x}, \hat{y}) \in \Delta^n \times D_s(G)$, we have $|\hat{E}| \leq s$, hence any clique in $\hat{G}$ is an s-defective clique in G. Thus, $\omega_s^d(G) \geq \omega(\hat{G})$, a contradiction. □

Theorem 1 (Motzkin-Straus formulation for s-defective clique) *The s-defective clique number $\omega_s^d(G)$ of G can be expressed using a global maximum value of a continuous cubic program as follows:*

$$1 - \frac{1}{\omega_s^d(G)} = \max_{(x,y) \in \Delta^n \times D'_s(G)} f_G(x, y), \tag{8}$$

where $f_G(x, y)$ is as in (5), and $D'_s(G)$ is obtained from $D_s(G)$ by relaxing the integrality of y:

$$D'_s(G) = \{y \in [0,1]^{\bar{m}} \mid e_{\bar{m}}^T y \leq s\}. \tag{9}$$

Proof By Proposition 1, it suffices to prove that (8) has an optimal solution with binary y. Note that $f_G(x, y)$ is linear with respect to y and can be expressed as $f_G(x, y) = z(x) + \sum_{\{i,j\} \in \bar{E}} w_{ij}(x) y_{ij}$, where $z(x) = x^T A_G x$ and $w_{ij}(x) = 2x_i x_j$ for $\{i, j\} \in \bar{E}$. Let $(\hat{x}, \hat{y})$ be an optimal solution of (8), where $\hat{y}$ is fractional. Let $F = \{\{i, j\} \in \bar{E} \mid 0 < \hat{y}_{ij} < 1\}$ and $t = \sum_{\{i,j\} \in F} \hat{y}_{ij}$. Let F_t be the set of the first $\lceil t \rceil$ elements of the ordered set listing the edges $\{i, j\} \in F$ in nonincreasing order of $w_{ij}(\hat{x})$. For $\{i, j\} \in \bar{E}$, let

$$y^*_{ij} = \begin{cases} 1, & \text{if } \{i,j\} \in F_t, \\ 0, & \text{if } \{i,j\} \in F \setminus F_t, \\ \hat{y}_{ij}, & \text{if } \{i,j\} \in \bar{E} \setminus F. \end{cases}$$

Then,

$$e_{\bar{m}}^T y^* = \sum_{\{i,j\} \in F} y^*_{ij} + \sum_{\{i,j\} \in \bar{E} \setminus F} y^*_{ij} = \lceil t \rceil + \sum_{\{i,j\} \in \bar{E} \setminus F} \hat{y}_{ij} \leq s,$$

so $y^* \in D_s(G)$. Finally, let $x^* = \hat{x}$. Then $f_G(x^*, y^*) \geq f_G(\hat{x}, \hat{y})$, so (x^*, y^*) is optimal for (8) with binary y^*. □

2.2 Motzkin-Straus formulation for the maximum s-plex problem

Consider the following mixed integer optimization problem.

$$f_s(G) = \max_{(x,y) \in \Delta^n \times P_s(G)} f_G(x, y), \tag{10}$$

where $f_G(x, y)$ is defined in (5),

$$P_s(G) = \{y \in \{0,1\}^{\bar{m}} \mid B_{\bar{G}} y \leq (s-1) e_n\}, \tag{11}$$

and $B_{\bar{G}}$ is the $n \times \bar{m}$ incidence matrix of the complement graph $\bar{G}$.

Proposition 2 *Let $\omega_s(G)$ denote the s-plex number of G. Then*

$$1 - \frac{1}{\omega_s(G)} = f_s(G). \tag{12}$$

Proof The proof is nearly identical to that of Proposition 1. □

To obtain a generalization of the Motzkin-Straus formulation for s-plex, we need to show that the integrality constraints on y in (11) can be relaxed. The resulting optimization problem is

$$f'_s(G) = \max_{(x,y)\in \Delta^n \times P'_s(G)} f_G(x, y), \tag{13}$$

where

$$P'_s(G) = \{y \in [0, 1]^{\bar{m}} \mid B_{\bar{G}} y \leq (s - 1)e_n\}. \tag{14}$$

First, we establish some lemmata which require some new notation. For $S \subseteq V$, the notation $x[S]$ refers to the restriction of x to S, i.e., $x[S] = [x_i]_{i\in S}$. Also, $y[\bar{E}(S)]$ refers to the restriction of y to $\bar{E}(S) = \{\{i, j\} \in \bar{E} \mid i, j \in S\}$. Finally, the support of x is denoted by $\operatorname{supp}(x) := \{i \in V \mid x_i > 0\}$.

Lemma 2 *For every feasible solution $(\hat{x}, \hat{y})$ to (13), there is an alternative feasible solution $(\tilde{x}, \hat{y})$ whose objective value is no worse, $f_G(\tilde{x}, \hat{y}) \geq f_G(\hat{x}, \hat{y})$, and whose restriction to $S := \operatorname{supp}(\tilde{x})$ is strictly positive, $(\tilde{x}[S], \hat{y}[\bar{E}(S)]) > 0$. Moreover, the inclusion $\operatorname{supp}(\tilde{x}) \subseteq \operatorname{supp}(\hat{x})$ holds and is strict when $\hat{y} \not> 0$.*

Proof If the restriction of $(\hat{x}, \hat{y})$ to $\hat{S} := \operatorname{supp}(\hat{x})$ is strictly positive, i.e., $(\hat{x}[\hat{S}], \hat{y}[\bar{E}(\hat{S})]) > 0$, then the statement holds trivially by setting $\tilde{x} = \hat{x}$. So, suppose there is a fake edge $\{i, j\} \in \bar{E}(\hat{S})$ with $\hat{y}_{ij} = 0$. We modify $\hat{x}$ to obtain $\tilde{x}$ such that $f_G(\tilde{x}, \hat{y}) \geq f_G(\hat{x}, \hat{y})$, and $\operatorname{supp}(\tilde{x}) \subseteq \operatorname{supp}(\hat{x})$. For $k \in V$, let

$$\tilde{x}_k = \begin{cases} \hat{x}_k, & \text{if } k \neq i, j, \\ \hat{x}_k - \varepsilon, & \text{if } k = i, \\ \hat{x}_k + \varepsilon, & \text{if } k = j, \end{cases}$$

where ε is selected later. We have

$$f_G(\tilde{x}, \hat{y}) - f_G(\hat{x}, \hat{y}) = 2\varepsilon p,$$

where

$$p := \sum_{k\in N(j)} \hat{x}_k - \sum_{k\in N(i)} \hat{x}_k + \sum_{k\in \bar{N}(j)\setminus\{i\}} \hat{y}_{jk}\hat{x}_k - \sum_{k\in \bar{N}(i)\setminus\{j\}} \hat{y}_{ik}\hat{x}_k$$

and $\bar{N}(v) := N_{\bar{G}}(v)$. Note that p does not contain ε because $\hat{y}_{ij} = 0$. Setting

$$\varepsilon = \begin{cases} \hat{x}_i, & \text{if } p \geq 0, \\ -\hat{x}_j, & \text{if } p < 0 \end{cases}$$

yields $\tilde{x}$ such that $f_G(\tilde{x}, \hat{y}) \geq f_G(\hat{x}, \hat{y})$. Meanwhile, the restriction of $(\tilde{x}, \hat{y})$ to $\tilde{S} := \mathrm{supp}(\tilde{x})$, denoted $(\tilde{x}[\tilde{S}], \hat{y}[\bar{E}(\tilde{S})])$, has fewer zero entries than that of $(\hat{x}[\hat{S}], \hat{y}[\bar{E}(\hat{S})])$ in both its x and y portions. Also, $\tilde{S} \subsetneq \hat{S}$. So, if $(\tilde{x}[\tilde{S}], \hat{y}[\bar{E}(\tilde{S})])$ is strictly positive, then we are done. Otherwise, repeat this process recursively, by setting $\hat{x} = \tilde{x}$, until $\hat{y}[\bar{E}[\tilde{S}]]$ has no zero entries. □

Lemma 3 *If $(\hat{x}, \hat{y})$ is an optimal solution of* (13) *for G, then its restriction $(\hat{x}[S], \hat{y}[\bar{E}(S)])$ to $S = \mathrm{supp}(\hat{x})$ is an optimal solution of* (13) *for $G[S]$.*

Proof First, see that $\hat{x}[S] \in \Delta^{|S|}$ because $\hat{x} \in \Delta^n$ and $\hat{x}_i = 0$ for all $i \in V \setminus S$. Also, $\hat{y}[\bar{E}(S)]$ belongs to $P'_s(G[S])$ because every $i \in S$ satisfies

$$\sum_{j \in N_{\bar{G}[S]}(i)} \hat{y}_{ij} \leq \sum_{j \in N_{\bar{G}}(i)} \hat{y}_{ij} \leq s - 1.$$

For contradiction purposes, suppose there exists $(\tilde{x}, \tilde{y}) \in \Delta^{|S|} \times P'_s(G[S])$ such that $f_{G[S]}(\tilde{x}, \tilde{y}) > f_{G[S]}(\hat{x}[S], \hat{y}[\bar{E}(S)])$. Add zero entries to $(\tilde{x}, \tilde{y})$ for vertices $V \setminus S$ and fake edges $\bar{E} \setminus \bar{E}(S)$ to obtain $(\tilde{x}^+, \tilde{y}^+) \in \Delta^n \times P'_s(G)$. Then,

$$f_G(\tilde{x}^+, \tilde{y}^+) = f_{G[S]}(\tilde{x}, \tilde{y}) > f_{G[S]}(\hat{x}[S], \hat{y}[\bar{E}(S)]) = f_G(\hat{x}, \hat{y}),$$

contradicting that $(\hat{x}, \hat{y})$ is an optimal solution of (13) for G. □

Lemma 4 *If $(\hat{x}, \hat{y})$ is an optimal solution of* (13) *and $\hat{y}$ is a fractional extreme point of $P'_s(G)$, then at least one entry of $(\hat{x}, \hat{y})$ is zero.*

Proof For contradiction purposes, suppose that such an optimal solution $(\hat{x}, \hat{y})$ is strictly positive. Note that if we fix $x = \hat{x}$ in (13), we obtain the problem

$$\begin{aligned} \max \; & \sum_{\{i,j\} \in \bar{E}} \hat{w}_{ij} y_{ij} + \hat{z} & \\ \text{s.t.} \; & \sum_{j \in N_{\bar{G}}(i)} y_{ij} \leq s - 1 & \forall i \in V \\ & 0 \leq y_{ij} \leq 1 & \forall \{i, j\} \in \bar{E}, \end{aligned} \tag{15}$$

where $\hat{w}_{ij} = 2\hat{x}_i \hat{x}_j > 0$ for $\{i, j\} \in \bar{E}$, and $\hat{z} = 2\sum_{\{i,j\} \in E} \hat{x}_i \hat{x}_j$. This problem is equivalent to the LP relaxation of the maximum b-matching formulation (3) for graph $\bar{G}$ with $b = (s-1)e_n$ and the edge weights $\hat{w}_{ij}$, $\{i, j\} \in \bar{E}$.

Since $\hat{y}$ is fractional, $F := \{\{i, j\} \in \bar{E} \mid 0 < \hat{y}_{ij} < 1\}$ is nonempty. So, by Lemma 1, $\hat{y}_{ij} = \frac{1}{2}$, $\forall \{i, j\} \in F$, and there exists $H \subseteq F$ such that $\bar{G}\langle H \rangle = (V_H, H)$ is an isolated odd cycle in $\bar{G}\langle F \rangle$. Let $l = |V_H|$ and relabel the vertices in V so that $V_H = \{1, 2, \ldots, l\}$. We construct $(\tilde{x}, \tilde{y}) \in \Delta^n \times P'_s(G)$ such that $f_G(\tilde{x}, \tilde{y}) > f_G(\hat{x}, \hat{y})$, contradicting the optimality of $(\hat{x}, \hat{y})$.

Let $q = \lfloor l/3 \rfloor$ and $r = l - 3q \in \{0, 1, 2\}$ be the quotient and the remainder from the division of l by 3. That is, $l = 3q + r$ for some $r \in \{0, 1, 2\}$. Let

$$\hat{\sigma} := \sum_{i \in V_H} \hat{x}_i. \tag{16}$$

Note that $\hat{\sigma} > 0$ since $(\hat{x}, \hat{y})$ is strictly positive.

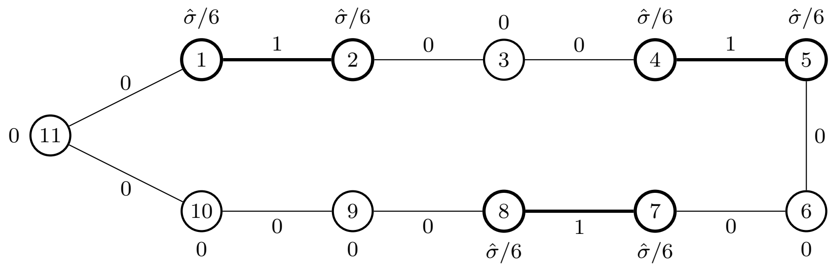


Fig. 2 An illustration of the proof of Lemma 4 for $l = 11$, i.e., $q = 3$ and $r = 2$.

First, assume $q > r$. Since $l = 3q + r$ and $r \in \{0, 1, 2\}$, this assumption is valid for all odd integers $l \geq 3$ except $l = 5$; this exceptional case will be addressed later. We define $(\tilde{x}, \tilde{y})$ as follows.

$$\tilde{x}_i = \begin{cases} \hat{\sigma}/(2q), & \text{if } i \in \{3k+1, 3k+2 \mid k = 0, 1 \ldots, q-1\}, \\ 0, & \text{if } i \in \{3k \mid k = 0, 1, \ldots, q-1\} \cup \{3q + j \mid j = 0, 1, \ldots, r\}, \\ \hat{x}_i, & \text{otherwise;} \end{cases} \tag{17}$$

$$\tilde{y}_{ij} = \begin{cases} 1, & \text{if } \{i, j\} \in H' := \{\{3k+1, 3k+2\} \mid k = 0, 1 \ldots, q-1\}, \\ 0, & \text{if } \{i, j\} \in H \setminus H', \\ \hat{y}_{ij}, & \text{otherwise.} \end{cases} \tag{18}$$

Figure 2 provides an illustration. Note that $2q$ of the first $l = 3q + r$ entries of $\tilde{x}$ defined above are equal to $\hat{\sigma}/(2q)$, and the remaining $q + r$ entries are zeros. Thus, $\sum_{i \in V_H} \tilde{x}_i = \hat{\sigma} = \sum_{i \in V_H} \hat{x}_i$ according to (16). Also, each $j \in V_H$ has exactly two incident edges in H. Denoting these edges by $\{j, j'\}$ and $\{j, j''\}$, we have $\tilde{y}_{jj'} + \tilde{y}_{jj''} \leq 1$ for all $j \in V_H$. Since $\hat{y}_{jj'} + \hat{y}_{jj''} = \frac{1}{2} + \frac{1}{2} = 1$, changing $\hat{y}$ to $\tilde{y}$ does not violate the s-plex constraints (14). Thus, $(\tilde{x}, \tilde{y}) \in \Delta^n \times P'_s(G)$.

Now, we show $f_G(\tilde{x}, \tilde{y}) > f_G(\hat{x}, \hat{y})$. Denote by

$$\begin{aligned} E(V_H) &= \{\{i, j\} \in E \mid i, j \in V_H\}, \\ \bar{E}(V_H) &= \{\{i, j\} \in \bar{E} \mid i, j \in V_H\}, \\ \delta(V_H) &= \{\{i, j\} \in E \mid i \in V_H,\ j \in V \setminus V_H\}, \\ \bar{\delta}(V_H) &= \{\{i, j\} \in \bar{E} \mid i \in V_H,\ j \in V \setminus V_H\}. \end{aligned}$$

Since $(\tilde{x}, \tilde{y})$ and $(\hat{x}, \hat{y})$ can only differ in the entries corresponding to the vertices and edges within $\bar{G}\langle H \rangle$, we can write

$$f_G(\tilde{x}, \tilde{y}) - f_G(\hat{x}, \hat{y}) = \Big(g(\tilde{x}, \tilde{y}) + h(\tilde{x}, \tilde{y}) \Big) - \Big(g(\hat{x}, \hat{y}) + h(\hat{x}, \hat{y}) \Big),$$

where

$$\begin{aligned}
g(x,y) &:= 2 \sum_{\{i,j\} \in E(V_H)} x_i x_j + 2 \sum_{\{i,j\} \in \bar{E}(V_H)} y_{ij} x_i x_j \\
&= 2 \sum_{\{i,j\} \in E(V_H) \cup \bar{E}(V_H)} x_i x_j - 2 \sum_{\{i,j\} \in \bar{E}(V_H)} (1 - y_{ij}) x_i x_j, && (19) \\
h(x,y) &:= 2 \sum_{\{i,j\} \in \delta(V_H)} x_i x_j + 2 \sum_{\{i,j\} \in \bar{\delta}(V_H)} y_{ij} x_i x_j \\
&= 2 \sum_{\{i,j\} \in \delta(V_H) \cup \bar{\delta}(V_H)} x_i x_j - 2 \sum_{\{i,j\} \in \bar{\delta}(V_H)} (1 - y_{ij}) x_i x_j. && (20)
\end{aligned}$$

The following equality will be used later.

$$2 \sum_{\{i,j\} \in E(V_H) \cup \bar{E}(V_H)} x_i x_j = \left(\sum_{i \in V_H} x_i \right)^2 - \sum_{i \in V_H} x_i^2. \tag{21}$$

By Lemma 1 and the assumption that $\hat{y}$ is strictly positive, we have $\hat{y}_{ij} = 1$ for every $\{i,j\} \in \bar{\delta}(V_H)$. So, by (20),

$$h(\hat{x},\hat{y}) = 2 \sum_{\{i,j\} \in \delta(V_H) \cup \bar{\delta}(V_H)} \hat{x}_i \hat{x}_j = 2 \sum_{i \in V_H} \hat{x}_i \sum_{j \in V \setminus V_H} \hat{x}_j = 2\hat{\sigma}(1 - \hat{\sigma}) = h(\tilde{x},\tilde{y}),$$

and so

$$f_G(\tilde{x},\tilde{y}) - f_G(\hat{x},\hat{y}) = g(\tilde{x},\tilde{y}) - g(\hat{x},\hat{y}).$$

By the construction of $(\tilde{x},\tilde{y})$ given in (17) and (18), every $\{i,j\} \in H$ satisfies $\tilde{y}_{ij}$=1 or $\tilde{x}_i \tilde{x}_j = 0$. Also, $\tilde{y}_{ij} = \hat{y}_{ij} = 1$ for every $\{i,j\} \in \bar{E}(V_H) \setminus H$. Thus,

$$\sum_{\{i,j\} \in \bar{E}(V_H)} (1 - \tilde{y}_{ij}) \tilde{x}_i \tilde{x}_j = 0.$$

So, by (19), (21), and (17),

$$g(\tilde{x},\tilde{y}) = 2 \sum_{\{i,j\} \in E(V_H) \cup \bar{E}(V_H)} \tilde{x}_i \tilde{x}_j = \hat{\sigma}^2 \left(1 - \frac{1}{2q} \right).$$

By Lemma 1 and the assumption that $\hat{y}$ is strictly positive, every $\{i,j\} \in H$ has $\hat{y}_{ij} = \frac{1}{2}$ and every $\{i,j\} \in \bar{E}(V_H) \setminus H$ has $\hat{y}_{ij} = 1$. So, by (19) and (21),

$$g(\hat{x},\hat{y}) = \left(\sum_{i \in V_H} \hat{x}_i \right)^2 - \sum_{i \in V_H} \hat{x}_i^2 - \sum_{\{i,j\} \in H} \hat{x}_i \hat{x}_j = \hat{\sigma}^2 - c(\hat{x}),$$

where $c(\hat{x}) := \sum_{i \in V_H} \hat{x}_i^2 + \sum_{\{i,j\} \in H} \hat{x}_i \hat{x}_j$ satisfies the following inequality:

$$c(\hat{x}) = \frac{1}{2} \sum_{\{i,j\} \in H} (\hat{x}_i + \hat{x}_j)^2 \geq \frac{1}{2l} \left(\sum_{\{i,j\} \in H} (\hat{x}_i + \hat{x}_j) \right)^2 = \frac{2\hat{\sigma}^2}{l}.$$

The inequality above is obtained by invoking the root mean square – arithmetic mean inequality. Therefore,

$$g(\hat{x}, \hat{y}) = \hat{\sigma}^2 - c(\hat{x}) \leq \hat{\sigma}^2 \left(1 - \frac{2}{l}\right).$$

By our assumption that $q > r$, we obtain

$$f_G(\tilde{x}, \tilde{y}) - f_G(\hat{x}, \hat{y}) = g(\tilde{x}, \tilde{y}) - g(\hat{x}, \hat{y}) \geq \hat{\sigma}^2 \left(\frac{2}{l} - \frac{1}{2q}\right) = \hat{\sigma}^2 \left(\frac{q - r}{2ql}\right) > 0.$$

Finally, in the exceptional case where $l = 5$ (and thus $q = 1$ and $r = 2$), the entries of $(\tilde{x}, \tilde{y})$ corresponding to $\bar{G}\langle H\rangle$ can be defined as follows:

$$\tilde{x}_1 = \tilde{x}_2 = \tilde{x}_4 = \hat{\sigma}/3 \qquad \tilde{x}_3 = \tilde{x}_5 = 0; \tag{22}$$

$$\tilde{y}_{12} = 1 \qquad \tilde{y}_{23} = \tilde{y}_{34} = \tilde{y}_{45} = \tilde{y}_{51} = 0. \tag{23}$$

Then, $g(\tilde{x}, \tilde{y}) = \left(\sum_{i \in V_H} \tilde{x}_i\right)^2 - \sum_{i \in V_H} \tilde{x}_i^2 = \frac{2}{3}\hat{\sigma}^2$, so

$$f_G(\tilde{x}, \tilde{y}) - f_G(\hat{x}, \hat{y}) = g(\tilde{x}, \tilde{y}) - g(\hat{x}, \hat{y}) \geq \hat{\sigma}^2 \left(\frac{2}{3} - 1 + \frac{2}{5}\right) = \frac{\hat{\sigma}^2}{15} > 0,$$

contradicting the optimality of $(\hat{x}, \hat{y})$. The proof is complete. □

Theorem 2 (Motzkin-Straus formulation for s-plex) *The s-plex number $\omega_s(G)$ of G can be expressed using a global maximum value of a continuous cubic program as follows:*

$$1 - \frac{1}{\omega_s(G)} = \max_{(x,y) \in \Delta^n \times P'_s(G)} f_G(x, y), \tag{24}$$

where $f_G(x, y)$ is as in (5), and $P'_s(G)$ is given in (14).

Proof By Proposition 2, it suffices to show that problem (24) always has an optimal solution (x^*, y^*) with $y^* \in \{0,1\}^{\bar{m}}$. We show this by constructing such an optimal solution, given an arbitrary optimal solution $(\hat{x}, \hat{y})$. The proof consists of the following steps.

1. Apply Lemma 2 to obtain an alternative optimal solution $(\tilde{x}, \hat{y})$ in which $\hat{y}[\bar{E}(\tilde{S})] > 0$ and $\tilde{S} \subseteq \hat{S}$, where $\tilde{S} := \text{supp}(\tilde{x})$ and $\hat{S} := \text{supp}(\hat{x})$.
2. By Lemma 3, $(\tilde{x}[\tilde{S}], \hat{y}[\bar{E}(\tilde{S})])$ is an optimal solution of the Motzkin-Straus formulation (24) for the maximum s-plex problem in $G[\tilde{S}]$.
3. Solve the b-matching LP obtained by fixing $x = \tilde{x}[\tilde{S}]$ to find an optimal solution $\tilde{y}$ that is an extreme point of $P'_s(G[\tilde{S}])$. This gives an alternative optimal solution $(\tilde{x}[\tilde{S}], \tilde{y})$ of (24) for $G[\tilde{S}]$.
4. If $\tilde{y}$ is not strictly positive, repeat steps 1-3 until obtaining an optimal solution $(\tilde{x}[\tilde{S}], \tilde{y})$ of (24) for $G[\tilde{S}]$ with $\tilde{y}$ being an extreme point of $P'_s(G[\tilde{S}])$. If $\tilde{y}$ is fractional, we obtain a contradiction with Lemma 4 for $G[\tilde{S}]$ and the optimal solution $(\tilde{x}[\tilde{S}], \tilde{y})$. We conclude that $\tilde{y}_{ij} = 1$ for all $\{i, j\} \in \bar{E}(\tilde{S})$.

5. Finally, extend $(\tilde{x}[\tilde{S}], \tilde{y})$ to $(x^*, y^*) \in \Delta^n \times P'_s(G)$ by adding zero entries for vertices in $V \setminus \tilde{S}$ and for fake edges in $\bar{E} \setminus \bar{E}(\tilde{S})$.

Every change applied during this procedure preserves optimality, so (x^*, y^*) is an optimal solution of (24) with binary y^*. $\square$

Observe that as a part of the above proof, we showed that we can find $x^* \in \Delta^n$ such that the LP relaxation (15) of the maximum weight b-matching problem has an integer optimal solution. Providing a complete description of the b-matching polytope (which is the convex hull of the solutions to the binary program (3)) generally requires adding the so-called blossom inequalities:

$$\sum_{\{i,j\} \in E(U)} y_{ij} + \sum_{\{i,j\} \in F} y_{ij} \le \left\lfloor \frac{b(U)+|F|}{2} \right\rfloor, \forall U \subseteq V, F \subseteq \delta(U) : b(U) + |F| \text{ odd},$$

to the degree inequalities and bound constraints [15], where $b(U) = \sum_{i \in U} b_i$, $E(U) = \{\{i,j\} \in E \mid i,j \in U\}$, and $\delta(U) = \{\{i,j\} \in E \mid i \in U,\ j \in V \setminus U\}$. However, no blossom inequalities are needed to find a binary optimal solution in our case.

In the proof of Theorem 2, we constructed an optimal solution (x^*, y^*) satisfying two intuitive properties:

1. $S^* := \mathrm{supp}(x^*)$ is a maximum s-plex in G, and
2. y^* is binary, with $y^*_{ij} = 1$ if and only if $\{i,j\} \in \bar{E}(S^*)$.

However, not all global optima satisfy these properties, as Example 1 shows.

Example 1 Any pair of vertices in the graph G from Figure 3 is a maximum 2-plex, and yet there is a global optimal solution (x', y') of (24) for which $S' := \mathrm{supp}(x') = \{1, 2, 3\}$ is not a 2-plex.

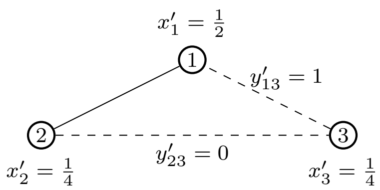


Fig. 3 An illustration to Example 1. The dashed lines show the missing edges.

We have seen that even though an optimal solution of (24) may not directly correspond to an s-plex, it can be easily converted into another optimal solution that does. In the next subsection, we show the same to be true for feasible (not necessarily optimal) solutions to the s-defective clique and s-plex formulations.

2.3 Computing clique relaxations from feasible solutions to multi-linear continuous formulations

One of the challenges associated with continuous optimization approaches to combinatorial optimization problems consists in developing effective and efficient strategies for converting a solution obtained for a continuous model into a feasible solution for the combinatorial problem. In particular, it is known that the original Motzkin-Straus formulation allows the so-called spurious local maxima, which do not correspond to characteristic vectors of cliques [37], and we have seen in Example 1 that spurious optima are also possible for the Motzkin-Straus formulation of the maximum s-plex problem. To overcome this issue, regularized versions of the Motzkin-Straus formulation for the maximum clique problem have been developed [8, 23], where every continuous local maximum is guaranteed to correspond to a maximal clique. These results can potentially be extended to the considered clique relaxations. However, one should keep in mind that all the known regularizations of the Motzkin-Straus formulation for the maximum clique problem result in the loss of the bilinear structure that the original formulation enjoys.

Alternatively, one could take advantage of the trilinear structure of the objective function of the proposed cubic formulations in order to extract an s-defective clique or an s-plex based on a feasible point of the corresponding cubic formulation. This approach essentially follows the logic of the proofs of Theorems 1 and 2. Each of these proofs constructs a global optimal solution (x^*, y^*) of the Motzkin-Straus formulation for the respective cluster detection problem, where y^* is guaranteed to be binary, starting from an arbitrary global maximum $(\hat{x}, \hat{y})$. The cardinality of a maximum s-defective clique (s-plex) is then given by $\lceil 1/(1 - f_G(x^*, y^*)) \rceil = \lceil 1/(1 - f_G(\hat{x}, \hat{y})) \rceil$. Since computing a global maximum of a Motzkin-Straus cubic program is extremely challenging (our results imply NP-hardness of both cubic problems), in practice we are interested in converting any feasible solution $(\hat{x}, \hat{y})$ of a Motzkin-Straus formulation into an s-defective clique or s-plex C of cardinality $|C| \geq \lceil 1/(1 - f_G(\hat{x}, \hat{y})) \rceil$. We break this task into two steps:

(i) Compute a feasible solution $(\tilde{x}, \tilde{y})$ to the respective Motzkin-Straus formulation such that $\tilde{y}$ is binary and $f_G(\tilde{x}, \tilde{y}) \geq f_G(\hat{x}, \hat{y})$.

(ii) Use $(\tilde{x}, \tilde{y})$ to construct a feasible solution $C \subseteq V$ of cardinality

$$|C| \geq \lceil 1/(1 - f_G(\tilde{x}, \tilde{y})) \rceil \geq \lceil 1/(1 - f_G(\hat{x}, \hat{y})) \rceil .$$

In the case of s-defective clique, the first step can be completed using the procedure outlined in the proof of Theorem 1. In the case of s-plex, the procedure in the proof of Theorem 2 uses the fact that $(\hat{x}, \hat{y})$ is a global optimal solution to obtain a contradiction in Lemma 4 and hence cannot be used directly. However, a slight modification of this procedure will lead to the desired outcome. Specifically, instead of obtaining a contradiction by Lemma 4 in step 4 of the procedure, we use the modification described in (17)-(18) or (22)-(23) to obtain $(\tilde{x}, \tilde{y})$ such that $\tilde{y}$ is binary and $f_G(\tilde{x}, \tilde{y}) > f_G(\hat{x}, \hat{y})$.

Given a feasible solution $(\tilde{x}, \tilde{y})$ with binary $\tilde{y}$, we can use the following process to obtain an s-defective clique (s-plex) with at least $\lceil 1/(1 - f_G(\tilde{x}, \tilde{y}))\rceil$ vertices. Let $\tilde{E} = \{\{i, j\} \mid \tilde{y}_{ij} = 1\}$ and $\tilde{G} = (V, E \cup \tilde{E})$. Let $\tilde{C} = \text{supp}(\tilde{x}_i)$. If $\tilde{C}$ is a clique in $\tilde{G}$, then it is an s-defective clique (s-plex) in G and we are done. Otherwise, if $\tilde{C}$ is not a clique in $\tilde{G}$, we use Lemma 2 to construct x' such that $f_G(x', \tilde{y}) \geq f_G(\tilde{x}, \tilde{y})$, and $C' = \text{supp}(x')$ is a clique in $\tilde{G}$. Furthermore, if $x'_i - x'_j > \epsilon > 0$ for some $i, j \in C'$, modifying x' by subtracting ϵ from x'_i and adding ϵ to x'_j will increase the value of $f_G(x', \tilde{y})$ by $(x'_i - \epsilon)(x'_j + \epsilon) - x'_i x'_j = \epsilon(x'_i - x'_j) - \epsilon^2 > 0$. So, by setting

$$\bar{x}_i = \begin{cases} \frac{1}{|C'|}, & \text{if } i \in C', \\ 0, & \text{if } i \in V \setminus C', \end{cases}$$

we have $C := \text{supp}(\bar{x}) = C'$ and $f_G(\bar{x}, \tilde{y}) \geq f_G(x', \tilde{y})$. Thus, we obtain an s-defective clique (s-plex) C in G such that

$$1 - \frac{1}{|C|} = f_G(\bar{x}, \tilde{y}) \geq f_G(x', \tilde{y}) \geq f_G(\tilde{x}, \tilde{y}),$$

implying that $|C| \geq \lceil 1/(1 - f_G(\tilde{x}, \tilde{y}))\rceil$.

3 Extending Turán's theorem and other lower bounds on the clique number to clique relaxations

In this section, we show that the formulations developed in Section 2 can be used to generalize Turán's theorem to s-defective clique and s-plex, as well as to extend some known lower bounds on the clique number to the considered clique relaxations.

First, recall Turán's bound (1):

$$m \leq \left(1 - \frac{1}{\omega(G)}\right) \frac{n^2}{2}. \tag{25}$$

Let λ_G be the maximum eigenvalue (spectral radius) of A_G, and let u_P be the Perron unit eigenvector of A_G ($u_P^T u_P = 1$). Also, let $s_P = e_n^T u_P$. In addition, denote by $d = (d_1, d_2, \ldots, d_n)^T$, where $d_i = |N_G(i)|$ is the degree of i in G, $\forall i \in V$. The following spectral lower bound on the clique number was established by Wilf [46]:

$$\omega(G) \geq \frac{s_P^2}{s_P^2 - \lambda_G}. \tag{26}$$

Finally, the following degree-based lower bound can be obtained from the Motzkin-Straus formulation by setting $x = d/(2m)$ [42]:

$$1 - \frac{1}{\omega(G)} \geq \frac{d^T A_G d}{(2m)^2}. \tag{27}$$

3.1 Bounds for the s-defective clique number

Theorem 3 (Turán's bound for s-defective clique) *Assume that $m \le \binom{n}{2} - s$. Then*

$$m \le \left(1 - \frac{1}{\omega_s^d(G)}\right)\frac{n^2}{2} - s. \tag{28}$$

Proof Let

$$\bar{x} = \frac{1}{n}e_n \text{ and } \bar{y} = \frac{s}{\bar{m}}e_{\bar{m}}. \tag{29}$$

Then, since $s \le \bar{m}$, $(\bar{x}, \bar{y})$ is feasible to (8), and from Theorem 1 we have

$$1 - \frac{1}{\omega_s^d(G)} \ge \frac{2(m+s)}{n^2},$$

which is equivalent to (28). □

When $s = 0$, the lower bound (28) is equivalent to Turán's classical bound (25). Next, we apply the Motzkin-Straus formulation to derive a spectral lower bound on the s-defective clique number.

Theorem 4 (Wilf's bound for s-defective clique) *Assume that $m \le \binom{n}{2} - s$. Then*

$$1 - \frac{1}{\omega_s^d(G)} \ge \frac{\lambda_G}{s_P^2} + \frac{s}{\binom{n}{2} - m}\left(1 - \frac{\lambda_G + 1}{s_P^2}\right), \tag{30}$$

Proof We substitute

$$\bar{x} = \frac{u_P}{s_P} \text{ and } \bar{y} = \frac{s}{\bar{m}}e_{\bar{m}} \tag{31}$$

in (8). Then it follows from Theorem 1 that

$$\begin{aligned}
1 - \frac{1}{\omega_s^d(G)} &\ge f_G(\bar{x}, \bar{y}) = \frac{u_P^T A_G u_P}{s_P^2} + \frac{s}{\bar{m}}\left(\frac{u_P^T A_{\bar{G}} u_P}{s_P^2}\right) \\
&= \frac{\lambda_G}{s_P^2} + \frac{s}{\bar{m}} \cdot \frac{1}{s_P^2} \cdot u_P^T(O_n - I_n - A_G)u_P \\
&= \frac{\lambda_G}{s_P^2} + \frac{s}{\bar{m}} \cdot \frac{1}{s_P^2} \cdot (s_P^2 - 1 - \lambda_G) = \frac{\lambda_G}{s_P^2} + \frac{s}{\binom{n}{2} - m}\left(1 - \frac{\lambda_G + 1}{s_P^2}\right),
\end{aligned}$$

where O_n is the $n \times n$ matrix with all ones and I_n is the $n \times n$ identity matrix. □

When $s = 0$, the lower bound (30) is equivalent to Wilf's bound (26).

Theorem 5 (Degree-based bound for s-defective clique) *Assume that $m \le \binom{n}{2} - s$. Then*

$$1 - \frac{1}{\omega_s^d(G)} \ge \frac{d^T A_G d}{(2m)^2} + \frac{s}{\binom{n}{2} - m} \cdot \frac{d^T A_{\bar{G}} d}{(2m)^2}. \tag{32}$$

Proof We substitute

$$\bar{x} = \frac{d}{2m} \text{ and } \bar{y} = \frac{s}{\bar{m}} e_{\bar{m}} \tag{33}$$

in (8) to obtain

$$1 - \frac{1}{\omega_s^d(G)} \geq f_G(\bar{x}, \bar{y}) = \frac{d^T A_G d}{(2m)^2} + \frac{s}{\binom{n}{2} - m} \cdot \frac{d^T A_{\bar{G}} d}{(2m)^2}.$$

□

When $s = 0$, the lower bound (32) is equivalent to the degree-based bound (27) for the clique number.

3.2 Bounds for the s-plex number

Theorem 6 (Turán's bound for s-plex)

$$m \leq \left(1 - \frac{1}{\omega_s(G)}\right) \frac{n^2}{2} - \mu_{s-1}(\bar{G}), \tag{34}$$

where $\mu_{s-1}(\bar{G})$ is the cardinality of a maximum (1-capacitated) b-matching in $\bar{G}$ with $b = (s-1)e_n$.

Proof We substitute

$$\bar{x} = \frac{1}{n} e_n \text{ and } \bar{y}_{ij} = \begin{cases} 1, \text{ if } \{i,j\} \in M, \\ 0, \text{ otherwise} \end{cases} \tag{35}$$

in (10), where $M \subseteq \bar{E}$ is a maximum b-matching with $b = (s-1)e_n$ in the complement graph $\bar{G}$. □

When $s = 1$, the lower bound (34) is equivalent to Turán's classical bound (25).

Theorem 7 (Wilf's bound for s-plex) *Assume that V is not an s-plex. Then*

$$1 - \frac{1}{\omega_s(G)} \geq \frac{\lambda_G}{s_P^2} + \frac{s-1}{n-1-\delta(G)} \left(1 - \frac{\lambda_G + 1}{s_P^2}\right), \tag{36}$$

where $\delta(G)$ denotes the minimum degree of G.

Proof We substitute

$$\bar{x} = \frac{u_P}{s_P} \text{ and } \bar{y} = \frac{s-1}{n-1-\delta(G)} e_{\bar{m}} \tag{37}$$

in (10). Since V is not an s-plex, we have $s \leq n - \delta(G) - 1$, so $\bar{y}_{ij} \in [0,1]$ for every $\{i,j\} \in \bar{E}$. Also, for every $i \in V$,

$$\sum_{j \in N_{\bar{G}}(i)} \bar{y}_{ij} = (s-1) \frac{n-1-d_i}{n-1-\delta(G)} \leq s-1,$$

so $(\bar{x}, \bar{y})$ is feasible. We have

$$\begin{aligned}1 - \frac{1}{\omega_s(G)} &\geq f_s(\bar{x}, \bar{y}) = \frac{u_P^T A_G u_P}{s_P^2} + \frac{s-1}{n-1-\delta(G)} \bar{x}^T A_{\bar{G}} \bar{x} \\ &= \frac{\lambda_G}{s_P^2} + \frac{s-1}{n-1-\delta(G)} \cdot \frac{1}{s_P^2} \cdot u_P^T (O_n - I_n - A_G) u_P \\ &= \frac{\lambda_G}{s_P^2} + \frac{s-1}{n-1-\delta(G)} \cdot \frac{1}{s_P^2} \cdot (s_P^2 - \lambda_G - 1) \\ &= \frac{\lambda_G}{s_P^2} + \frac{s-1}{n-1-\delta(G)} \left(1 - \frac{\lambda_G + 1}{s_P^2}\right),\end{aligned}$$

where O_n is the $n \times n$ matrix with all ones and I_n is the $n \times n$ identity matrix. □

When $s = 1$, the lower bound (36) becomes Wilf's bound (26) on the clique number.

Theorem 8 (Degree-based bound for s-plex) *Assume that V is not an s-plex. Then*

$$1 - \frac{1}{\omega_s(G)} \geq \frac{d^T A_G d}{(2m)^2} + \frac{s-1}{n-1-\delta(G)} \cdot \frac{d^T A_{\bar{G}} d}{(2m)^2}. \tag{38}$$

Proof We substitute

$$\bar{x} = \frac{d}{2m} \text{ and } \bar{y} = \frac{s-1}{n-1-\delta(G)} e_{\bar{m}} \tag{39}$$

in (10). □

When $s = 1$, bound (38) becomes the degree-based bound (27) on the clique number.

4 Computational experiments

Computing provable global optima of the cubic formulations developed in this paper is a difficult task, even for small-scale instances. However, a local maximum can be found fairly quickly starting from any feasible point, and then converting it into the desired clique relaxation structure, thus yielding a heuristic for the corresponding combinatorial optimization problem. In this section, we report the results of preliminary experiments for such an approach, with local optima computed using the CONOPT solver [4]. The experiments were conducted with the following objectives in mind.

– Assess the quality of the solutions for the maximum s-defective clique and the maximum s-plex problems corresponding to local maxima obtained starting from the different points used to establish the analytical lower bounds in Section 3.

– Evaluate the performance of the local optimization solver applied to the Motzkin-Straus formulation starting from random initial points under a specified time limit.

In Section 2.3, we explained how a feasible solution $(\hat{x}, \hat{y})$ of a Motzkin-Straus formulation can be converted to a feasible solution C for the graph problem of interest such that $|C| \geq \lceil 1/(1 - f_G(\hat{x}, \hat{y})) \rceil$. It is easy to construct graph instances where the solution C obtained using this combinatorial argument will have a much higher cardinality than the lower bound obtained from the Motzkin-Straus formulation. (Consider, for example, the complement of a graph consisting of many disjoint odd cycles as an input for the maximum s-plex problem.) As a result, the contribution of the combinatorial post-processing to the overall quality of the obtained solution could overshadow that of the initial solution given by a local maximum of the continuous formulation. Hence, to provide a fair assessment of the performance of the continuous approach, we focus primarily on the quality of local maxima obtained for the cubic formulations.

Experimental setting. All experiments were conducted on a Dell PC with 64 GB RAM, Intel® Xeon® CPU E5-2643 0 @ 3.30GHz processor, running a 64-bit Windows 7 Enterprise operating system. The cubic formulations were implemented in AMPL, with the CONOPT 3.17A solver used to produce local optima. The maximum b-matchings used to generate the Turán points for the maximum s-plex problem were computed using the CPLEX 12.9.0.0 solver. The corresponding running times are negligible and are not reported. The Perron eigenvectors used in the Wilf points were computed in MATLAB® R2018A using the `perron` function [40]. The results were recorded and used as inputs in the AMPL implementation.

Test instances and the comparison base. In our experiments, we use fifty graph instances from the Second DIMACS Implementation Challenge [24]. These graphs were originally proposed for testing algorithms for the maximum clique problem, but are also typically used as a standard testbed for clique relaxation detection algorithms [6, 22, 43]. The instances are described in Table 1, together with results from [22], which will be used to assess the performance of the proposed formulations. In this table, the column "Graph" contains the name of each instance used. The next three columns give the number of vertices ($|V|$) and edges ($|E|$) in the graph, and the number of edges in its complement ($|\bar{E}|$). The latter is important since $\bar{m} = |\bar{E}|$ gives the number of the fake edge variables in the considered formulations. The total number of variables is $n+\bar{m} = |V|+|\bar{E}|$. The fifth column of the table specifies the clique number $\omega(G)$ of the corresponding graph. The remaining columns present the s-defective clique number $\omega_s^d(G)$ (for $s = 1, 2, 3, 4$) and the s-plex number $\omega(G)$ (for $s = 2, 3, 4, 5$), respectively, according to [22]. The figures preceded by "≥" in these columns do not necessarily show the best known lower bound for the corresponding instance and graph invariant; instead, they report the value of the best solution obtained by Russian Doll Search (RDS) algorithm within a 600-second time limit in [22]. Notably, some of the solutions found by RDS within the specified time limit are of worse quality than those found by the same algorithm for smaller values of s (see, e.g., the results for brock200_1, for which RDS failed to match the size of the maximum clique for any of the considered s values). Even though better solutions were found by heuristic methods [30, 33, 48], we use the RDS results as a comparison base in our preliminary experiments since, similarly to [22], we simply assess the performance of a standard general-purpose algorithm (solver), without any additional problem-specific enhancements.

First set of experiments: Starting points used in the analytical bounds. Local optima computed by the CONOPT solver strongly depend on the starting point used. In the first set of experiments, we tried three different initial solution choices for both the maximum s-defective clique problem (with $s = 1, 2, 3, 4$) and the maximum s-plex problem (with $s = 2, 3, 4, 5$). Namely, the starting solutions correspond to the points used to obtain the analytical bounds in Section 3, described next.

1. *The Turán points*: The points employed in establishing the extensions of Turán's theorem, (29) for s-defective clique, and (35) for s-plex. The corresponding results are presented in Table 4 for s-defective clique and in Table 7 for s-plex.
2. *The Wilf points*: The points used to prove the generalizations of Wilf's bound, (31) for s-defective clique and (37) for s-plex. See Tables 5 and 8 for the results for s-defective clique and s-plex, respectively.
3. *The degree-based points*: The points used to obtain the degree-based bounds, (33) for s-defective clique and (39) for s-plex. Tables 6 and 9 show the corresponding results.

Table 2 presents a summary of results for the first set of experiments. More specifically, the table contains the results of pairwise comparisons between the solutions obtained using RDS and CONOPT applied to the cubic formulations with the three different starting points (Turán, Wilf, and degree-based). The diagonal entries in this table show the number of instances on which the corresponding method yielded the best result obtained. A non-diagonal entry a-b in row i and column j ($i, j \in$ {RDS, Turán,Wilf, Degree}) indicates that method i beat method j on a instances, and method j beat method i on b instances out of 200 (50 graphs $\times$ four different values of s); thus, the methods i and j were tied on the remaining $200 - (a + b)$ instances.

We observe that the Turán, Wilf, and degree-based points perform similarly for s-defective clique. Meanwhile, on the s-plex instances, there is a clear hierarchy, with the Wilf points outperforming the degree-based points, and the degree-based points outperforming the Turán points. One explanation for this phenomenon is the amount of information they exploit. For example, the Turán points, which use no instance-specific information (besides the number of vertices), perform the worst. One explanation for why the hierarchy is more

Table 1 Description of the graphs used in the experiments and the results obtained in [22] by running RDS with 600-second time limit.

Graph	$\lvert V\rvert$	$\lvert E\rvert$	$\lvert\bar{E}\rvert$	$\omega(G)$	$\omega_s^d(G)$ for $s = \ldots$				$\omega_s(G)$ for $s = \ldots$			
					1	2	3	4	2	3	4	5
brock200_1	200	14834	5066	21	≥20	≥20	≥19	≥19	≥20	≥20	≥19	≥19
brock200_2	200	9876	10024	12	12	12	13	≥13	13	≥15	≥16	≥16
brock200_3	200	12048	7852	15	15	16	≥15	≥15	17	≥18	≥18	≥20
brock200_4	200	13089	6811	17	17	≥17	≥16	≥16	≥19	≥20	≥21	≥21
brock400_1	400	59723	20077	27	≥22	≥20	≥19	≥19	≥23	≥25	≥26	≥26
brock400_2	400	59786	20014	29	≥20	≥20	≥18	≥18	≥22	≥23	≥23	≥26
brock400_3	400	59681	20119	31	≥19	≥20	≥20	≥19	≥23	≥24	≥26	≥28
brock400_4	400	59765	20035	33	≥19	≥20	≥19	≥18	≥23	≥22	≥24	≥27
c-fat200-1	200	1534	18366	12	12	12	12	12	12	12	12	14
c-fat200-2	200	3235	16665	24	24	24	24	24	24	24	24	24
c-fat200-5	200	8473	11427	58	58	58	58	58	58	58	58	58
c-fat500-1	500	4459	120291	14	14	14	14	14	14	14	14	15
c-fat500-2	500	9139	115611	26	26	26	26	26	26	26	26	26
c-fat500-5	500	23191	101559	64	64	64	64	64	64	64	64	64
c-fat500-10	500	46627	78123	126	126	126	126	126	126	126	126	126
hamming6-2	64	1824	192	32	32	32	32	32	32	32	40	48
hamming6-4	64	704	1312	4	4	5	6	6	6	8	10	12
hamming8-2	256	31616	1024	128	128	128	128	128	128	≥89	≥44	≥55
hamming8-4	256	20864	11776	16	16	16	16	≥15	16	≥16	≥18	≥16
hamming10-2	1024	518656	5120	512	512	512	512	512	512	≥89	≥44	≥55
hamming10-4	1024	434176	89600	40	≥17	≥18	≥18	≥15	≥22	≥16	≥18	≥16
johnson8-2-4	28	210	168	4	4	5	5	6	5	8	9	12
johnson8-4-4	70	1855	560	14	14	14	14	15	14	18	≥21	≥23
johnson16-2-4	120	5460	1680	8	8	9	≥9	≥10	≥10	≥15	≥18	≥20
johnson32-2-4	496	107880	14880	16	≥8	≥7	≥8	≥9	≥21	≥24	≥25	≥26
keller4	171	9435	5100	11	12	13	≥14	≥15	15	≥21	≥16	≥18
keller5	776	225990	74710	27	≥16	≥15	≥15	≥15	≥15	≥22	≥16	≥18
MANN_a9	45	918	72	16	17	18	19	20	26	36	36	45
MANN_a27	378	70551	702	126	≥21	≥19	≥18	≥18	≥235	≥351	≥351	≥351
MANN_a45	1035	533115	1980	345	≥21	≥19	≥18	≥18	≥661	≥990	≥990	≥990
p_hat300-1	300	10933	33917	8	9	9	10	10	10	12	≥13	≥14
p_hat300-2	300	21928	22922	25	26	≥22	≥23	≥22	≥29	≥27	≥27	≥28
p_hat300-3	300	33390	11460	36	≥26	≥26	≥24	≥24	≥31	≥32	≥31	≥31
p_hat500-1	500	31569	93181	9	10	11	≥11	≥11	12	≥13	≥14	≥14
p_hat500-2	500	62946	61804	36	≥32	≥28	≥27	≥24	≥34	≥31	≥29	≥30
p_hat500-3	500	93800	30950	50	≥30	≥28	≥28	≥28	≥35	≥35	≥33	≥35
p_hat700-1	700	60999	183651	11	12	12	≥11	≥11	13	≥13	≥13	≥13
p_hat700-2	700	121728	122922	44	≥26	≥25	≥25	≥23	≥31	≥30	≥29	≥25
p_hat700-3	700	183010	61640	62	≥29	≥28	≥25	≥24	≥32	≥29	≥29	≥30
san200_07_1	200	13930	5970	30	≥18	≥18	≥18	≥19	≥29	≥41	≥52	≥73
san200_07_2	200	13930	5970	18	≥15	≥15	≥15	≥16	≥24	≥34	≥46	≥56
san200_09_1	200	17910	1990	70	≥36	≥34	≥35	≥34	≥67	125	≥38	≥40
san200_09_2	200	17910	1990	60	≥30	≥28	≥27	≥28	≥42	≥47	≥43	≥46
san200_09_3	200	17910	1990	44	≥28	≥26	≥25	≥25	≥42	≥35	≥38	≥43
san400_0.5_1	400	39900	39900	13	≥9	≥10	≥11	≥11	≥14	≥20	≥26	≥31
san400_0.7_1	400	55860	23940	40	≥20	≥20	≥21	≥22	≥34	≥48	≥70	≥90
san400_0.7_2	400	55860	23940	30	≥17	≥18	≥18	≥19	≥28	≥41	≥51	≥56
san400_0.7_3	400	55860	23940	22	≥15	≥16	≥16	≥17	≥23	≥33	≥44	≥54
sanr200_07	200	13868	6032	18	≥19	≥18	≥17	≥17	≥20	≥21	≥22	≥24
sanr200_09	200	17863	2037	42	≥27	≥28	≥27	≥27	≥33	≥37	≥40	≥43

apparent on the s-plex instances than on the s-defective clique instances is that the s-plex numbers are themselves more varying; recall that the s-defective clique number satisfies $\omega(G) \leq \omega_s^d(G) \leq \omega(G) + s$, while the s-plex number satisfies $\omega(G) \leq \omega_s(G) \leq s\omega(G)$, see [7].

Table 2 Summary of results for the first set of experiments. The diagonal entries show the number of instances on which the corresponding method yielded the best result obtained. An entry a-b in row i and column j indicates that method i beat method j on a instances, and method j beat method i on b instances out of 200.

s-defective clique:

	RDS	Turán	Wilf	Degree
RDS	121	85-76	86-76	88-76
Turán	76-85	90	34-35	29-31
Wilf	76-86	35-34	89	34-35
Degree	76-88	31-29	35-34	88

s-plex:

	RDS	Turán	Wilf	Degree
RDS	131	107-55	95-64	98-63
Turán	55-107	51	22-94	27-63
Wilf	64-95	94-22	80	60-34
Degree	63-98	85-27	34-60	71

Table 3 Summary of results for the second set of experiments. An entry a-b in the first (second) row indicates that the best (average) solution found was better than that obtained by RDS on a instances, and worse on b instances.

	s-defective clique, $s = \ldots$					s-plex, $s = \ldots$				
	1	2	3	4	all	2	3	4	5	all
max	20-8	23-8	25-7	27-4	95-27	21-7	26-13	27-16	23-19	97-55
mean	18-28	20-28	22-26	24-25	84-107	20-30	23-27	19-30	18-32	70-119

As one would expect, RDS outperforms the cubic formulations in terms of quality of the solutions; however, the fact that the results obtained using CONOPT are better than those for RDS on many of the instances is rather encouraging. Moreover, the time limit used for RDS in [22] was 600 seconds, whereas the local optima of the cubic formulations were computed much quicker with CONOPT. This motivated the second set of experiments, described next.

Second set of experiments: Random starting points under a time limit. The second set of experiments evaluates the performance of the formulations by recording the quality of local maxima found by CONOPT within a 600-second time limit, starting from up to 100 randomly generated initial feasible solutions. The chosen time limit matches that used in [22] for RDS. Tables 10 and 11 give results for the maximum s-defective clique problem. Table 10 reports the values for the best solution found, the average quality of the solution found, as well as the standard deviation for the objective value, and Table 11 shows the number of runs performed within the 600-second time limit, as well as the average time per run and the standard deviation for the running times. Similarly, Tables 12 and 13 give results for the maximum s-plex problem.

Table 3 provides a comparison with RDS, where "max" and "mean" stand for the best and average solution found using the random starting points, respectively. An entry a-b in this table means that the best or average solution found in this set of experiments was better than that reported for RDS on a instances, and worse on b instances, out of 50 instances for each value of s, or out of 200 instances total for all considered s values. Clearly, the approach based on the cubic formulations outperforms RDS in terms of the best solution found within the allocated time limit. This advantage can be explained by the relatively high level of diversification achieved in the second set of experiments via randomization. The RDS approach favors intensification over diversification in search for the optimal solution. Its performance strongly depends on the ordering of vertices used, which is fixed once it has been decided. The method continues exploring the branch-and-bound tree without revisiting the selected ordering, even when little to no progress has been made for a while. On the other hand, the random starting points used in conjunction with a local optimization solver in our experiments allow to obtain a diverse set of local optima, which increases the chance of finding a high-quality solution. It is notable that even the average quality of the solutions found using random initial points for the cubic formulation is better than that of RDS solutions on a considerable number of instances.

We would like to conclude this section by remarking that the preliminary numerical experiments conducted here are by no means conclusive. Still, we hope that these initial experiments show sufficient promise to stimulate future work in this direction, including development of global optimization algorithms based on the proposed cubic formulations. While specialized algorithms for solving non-convex quadratic problems are gradually becoming an integral part of standard optimization engines [34, 38], research focusing on cubic programming is still rather scarce. We hope that the formulations developed in this paper will encourage work towards filling this gap. At the very least, the proposed formulations yield challenging and interesting cubic test instances for continuous global optimization solvers; also see [5, 16, 17].

5 Conclusion

The paper develops continuous cubic formulations for the maximum s-defective clique problem and the maximum s-plex problem, extending the well-known Motzkin-Straus quadratic formulation for the maximum clique to the considered clique relaxations. The proof of the formulation for the case of maximum s-plex establishes interesting connections to classical results regarding the fractional b-matching polytope. The proposed formulations are used to obtain analytical bounds on the s-defective clique number and the s-plex number of a graph, generalizing three of the standard bounds on the clique number. The numerical experiments conducted using the CONOPT solver demonstrate that the developed formulations can be used to quickly obtain high-quality lower bounds for the considered cluster detection problems.

The results presented in this paper invite several directions for future research. In particular, analyzing optimality conditions for the proposed formulations could lead to non-trivial continuous characterizations for the considered discrete problems, as was the case with the Motzkin-Straus formulation for the maximum clique problem [20]. The obtained local optima of the cubic formulations could likely be improved using tailored stochastic global optimization methods, such as a monotonic basin hopping strategy that was successfully used for several applications [21, 27]. In addition, the special structure of the proposed formulations could be exploited to develop methods based on bilevel optimization and decomposition techniques. Another direction to investigate is whether meaningful generalizations of the Motzkin-Straus formulation can be obtained for other important clique relaxation models, such as quasi-clique and s-club [36]. Finally, from a graph theory perspective, Turán's theorem is known to have several elegant proofs [3]. It would be interesting to explore whether the techniques used in each proof could be extended to obtain the generalizations of Turán's theorem presented here.

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Appendix A Tables with detailed results of experiments

Table 4 Results for the maximum s-defective clique problem starting from the Turán point.

Graph	$s=1$			$s=2$			$s=3$			$s=4$		
	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time
brock200_1	3.87	19	0.30	3.87	19	0.33	3.87	21	1.47	3.87	21	1.20
brock200_2	1.98	9	4.73	1.98	10	0.53	1.98	12	3.78	1.98	11	2.93
brock200_3	2.52	12	0.44	2.52	13	2.61	2.52	13	3.00	2.52	15	4.56
brock200_4	2.89	15	0.41	2.89	16	2.18	2.90	16	0.47	2.90	18	2.37
brock400_1	3.95	21	8.80	3.95	22	8.44	3.95	22	8.67	3.95	25	14.63
brock400_2	3.96	21	41.75	3.96	24	10.83	3.96	23	32.12	3.96	22	8.22
brock400_3	3.94	24	8.21	3.94	21	8.27	3.94	22	1.73	3.94	24	1.68
brock400_4	3.95	22	2.07	3.95	22	20.76	3.95	24	15.91	3.95	24	10.61
c-fat200-1	1.08	12	0.70	1.08	12	0.80	1.08	12	0.76	1.08	12	0.17
c-fat200-2	1.19	24	0.14	1.19	24	0.19	1.19	24	0.17	1.19	24	0.17
c-fat200-5	1.74	58	0.31	1.74	58	0.14	1.74	58	0.11	1.74	58	0.11
c-fat500-1	1.04	14	24.63	1.04	14	1.15	1.04	14	25.74	1.04	14	1.37
c-fat500-2	1.08	26	23.15	1.08	26	3.07	1.08	26	2.23	1.08	26	2.07
c-fat500-5	1.23	64	17.97	1.23	64	1.03	1.23	64	1.22	1.23	64	1.09
c-fat500-10	1.59	126	0.75	1.59	126	0.67	1.59	126	0.66	1.60	126	0.66
hamming6-2	9.18	9.18	0.03	9.23	9.23	0.02	9.27	9.27	0.02	9.31	9.31	0.00
hamming6-4	1.52	1.52	0.00	1.53	1.53	0.02	1.53	1.53	0.02	1.53	1.53	0.00
hamming8-2	28.47	28.47	0.05	28.49	28.49	0.05	28.52	28.52	0.06	28.54	28.54	0.05
hamming8-4	2.75	2.75	0.08	2.75	2.75	0.08	2.75	2.75	0.09	2.75	2.75	0.08
hamming10-2	93.11	93.11	0.76	93.12	93.12	0.76	93.14	93.14	0.83	93.16	93.16	0.76
hamming10-4	5.82	5.82	0.98	5.82	5.82	1.01	5.82	5.82	1.00	5.82	5.82	1.03
johnson8-2-4	2.17	2.17	0.00	2.18	2.8	0.00	2.19	2.19	0.00	2.20	2.20	0.00
johnson8-4-4	4.12	4.12	0.02	4.13	4.13	0.02	4.14	4.14	0.00	4.15	4.15	0.02
johnson16-2-4	4.14	4.14	0.02	4.14	4.14	0.02	4.15	4.15	0.03	4.15	4.15	0.02
johnson32-2-4	8.13	8.13	0.20	8.13	8.13	0.20	8.13	8.13	0.22	8.13	8.13	0.20
keller4	2.82	10	1.26	2.82	10	1.19	2.82	11	1.06	2.82	12	0.28
keller5	4.01	20	39.70	4.01	19	9.87	4.01	20	12.65	4.01	22	40.17
MANN_a9	10.83	14	0.00	10.95	15	0.02	11.07	14.27	0.02	11.19	16	0.03
MANN_a27	80.27	118	0.69	80.36	119	0.69	80.45	120	0.64	80.54	121	0.67
MANN_a45	214.55	331	5.90	214.63	332	8.78	214.728	333	6.79	214.80	334	5.97
p_hat300-1	1.32	7	1.92	1.32	9	18.92	1.32	9	25.96	1.32	8	0.76
p_hat300-2	1.95	23	1.03	1.95	26	20.34	1.95	26	7.69	1.95	27	1.05
p_hat300-3	3.88	34	6.36	3.88	36	6.46	3.88	35	7.64	3.88	36	6.46
p_hat500-1	1.34	7	2.93	1.34	8	4.23	1.34	9	3.28	1.34	9	32.23
p_hat500-2	2.01	35	4.13	2.01	36	2.48	2.01	36	162.65	2.01	37	165.74
p_hat500-3	4.01	48	45.71	4.01	50	46.80	4.01	50	45.68	4.01	51	2.18
p_hat700-1	1.33	7	9.09	1.33	9	307.21	1.33	9	146.02	1.33	10	207.25
p_hat700-2	1.99	44	6.60	1.99	45	10.37	1.99	46	66.86	1.99	46	7.83
p_hat700-3	3.95	60	5.10	3.95	61	31.75	3.95	61	195.02	3.95	62	211.79
san200_0.7_1	3.30	16	1.76	3.30	17	1.70	3.30	18	1.70	3.30	19	1.73
san200_0.7_2	3.30	13	1.68	3.30	14	1.64	3.30	15	1.59	3.30	15	1.61
san200_0.9_1	9.57	46	0.37	9.58	47	0.41	9.58	48	0.44	9.59	49	0.44
san200_0.9_2	9.57	36	0.42	9.58	37	0.44	9.58	38	0.50	9.59	39	0.47
san200_0.9_3	9.57	28	0.44	9.58	30	0.42	9.58	30	0.51	9.59	32	0.48
san400_0.5_1	2.00	8	2.34	2.00	8	62.59	2.00	9	62.96	2.00	11	63.85
san400_0.7_1	3.31	21	26.33	3.31	22	26.43	3.31	23	25.99	3.31	24	27.07
san400_0.7_2	3.31	16	26.47	3.31	17	25.57	3.31	18	26.07	3.31	19	26.61
san400_0.7_3	3.31	13	25.35	3.31	13	25.93	3.31	15	26.27	3.31	16	26.08
sanr200_0.7	3.26	15	0.33	3.26	16	0.30	3.26	17	0.37	3.268	20	1.78
sanr200_0.9	9.36	39	0.45	9.37	41	0.44	9.37	41	0.58	9.38	42	0.48

Table 5 Results for the maximum s-defective clique problem starting from the Wilf point.

Graph	$s=1$			$s=2$			$s=3$			$s=4$		
	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time
brock200_1	3.91	18	1.48	3.91	19	1.58	3.91	21	1.65	3.91	20	0.34
brock200_2	1.99	9	0.53	1.99	10	0.51	1.99	11	0.59	1.99	11	4.01
brock200_3	2.54	12	0.47	2.54	13	2.40	2.54	14	3.74	2.54	14	3.98
brock200_4	2.92	14	2.79	2.92	16	0.55	2.92	17	0.41	2.92	16	3.87
brock400_1	3.96	21	8.72	3.96	22	8.21	3.96	22	1.79	3.96	23	8.36
brock400_2	3.97	23	19.69	3.98	22	21.47	3.98	23	9.69	3.98	24	1.95
brock400_3	3.96	22	20.36	3.96	21	8.31	3.96	22	20.26	3.96	23	1.40
brock400_4	3.97	23	1.84	3.97	23	14.45	3.97	23	20.94	3.97	23	20.81
c-fat200-1	1.23	12	0.41	1.23	12	0.17	1.23	12	0.23	1.23	12	0.20
c-fat200-2	1.24	24	0.61	1.24	24	0.14	1.24	24	0.17	1.24	24	0.12
c-fat200-5	1.74	58	0.36	1.74	58	0.09	1.74	58	0.09	1.74	58	0.11
c-fat500-1	1.17	14	18.77	1.17	14	2.06	1.17	14	1.61	1.17	14	19.27
c-fat500-2	1.16	26	3.56	1.16	26	1.47	1.16	26	1.15	1.16	26	1.59
c-fat500-5	1.24	64	13.81	1.24	64	0.94	1.24	64	1.08	1.24	64	1.12
c-fat500-10	1.60	126	0.89	1.60	126	0.98	1.60	126	0.73	1.60	126	0.75
hamming6-2	9.18	9.18	0.00	9.23	9.23	0.00	9.27	9.27	0.00	9.31	9.31	0.00
hamming6-4	1.52	1.52	0.02	1.53	1.53	0.02	1.53	1.53	0.02	1.53	1.53	0.02
hamming8-2	28.47	128	0.56	28.49	128	0.42	28.52	128	0.36	28.54	124	0.50
hamming8-4	2.75	2.75	0.09	2.75	2.75	0.08	2.75	2.75	0.08	2.75	2.75	0.08
hamming10-2	93.11	93.11	0.73	93.12	93.12	0.75	93.14	93.14	0.76	93.16	93.16	0.75
hamming10-4	5.82	5.82	1	5.82	5.82	1.01	5.82	5.82	1.01	5.82	5.82	1
johnson8-2-4	2.17	2.17	0.00	2.18	2.18	0.00	2.19	2.19	0.00	2.20	2.20	0.00
johnson8-4-4	4.12	4.12	0.00	4.13	4.13	0.02	4.14	4.14	0.02	4.15	4.15	0.02
johnson16-2-4	4.14	4.14	0.02	4.14	4.14	0.02	4.15	4.15	0.02	4.15	4.15	0.02
johnson32-2-4	8.13	8.13	0.20	8.13	8.13	0.20	8.13	8.13	0.22	8.13	8.13	0.20
keller4	2.86	8	0.23	2.86	10	1.15	2.86	10	0.27	2.86	12	0.25
keller5	4.04	18	125.22	4.04	18	39.20	4.04	19	7.66	4.04	10.89	23.32
MANN_a9	10.85	14	0.02	10.97	15	0.02	11.09	15	0.02	11.21	17	0.02
MANN_a27	80.88	118	0.66	80.97	119	0.66	81.06	120	0.66	81.16	121	0.69
MANN_a45	215.85	331	5.97	215.94	332	6.61	216.02	333	7.16	216.11	334	6.65
p_hat300-1	1.41	7	1.72	1.41	8	1.40	1.41	9	1.98	1.41	9	43.76
p_hat300-2	2.30	23	1.12	2.30	23	0.94	2.30	27	16.18	2.30	27	7.55
p_hat300-3	4.11	34	4.34	4.11	35	6.41	4.11	36	6.41	4.11	35	6.75
p_hat500-1	1.42	10	3.01	1.42	10	4.40	1.42	11	50.09	1.42	9	2.82
p_hat500-2	2.39	35	179.95	2.39	36	26.88	2.39	37	165.44	2.39	38	21.33
p_hat500-3	4.26	48	45.82	4.26	49	2.22	4.26	49	46.24	4.26	51	48.73
p_hat700-1	1.41	10	97.16	1.41	10	290.12	1.41	10	9.86	1.41	12	71.42
p_hat700-2	2.38	43	5.23	2.38	46	13.29	2.38	45	10.14	2.38	47	8.44
p_hat700-3	4.21	60	189.07	4.21	61	4.35	4.21	62	27.66	4.21	62	4.52
san200_0.7_1	3.32	16	1.79	3.32	17	1.70	3.32	18	1.78	3.32	19	1.78
san200_0.7_2	3.76	13	1.73	3.76	14	1.72	3.76	14	1.73	3.76	15	1.75
san200_0.9_1	9.79	46	0.41	9.80	47	0.50	9.80	48	0.42	9.80	48	0.42
san200_0.9_2	9.66	36	0.42	9.67	37	0.42	9.67	38	0.44	9.68	39	0.48
san200_0.9_3	9.64	30	0.45	9.64	29	0.45	9.65	30	0.48	9.65	34	0.51
san400_0.5_1	2.10	8	65.18	2.10	9	64.62	2.10	10	64.82	2.10	11	64.41
san400_0.7_1	3.32	21	25.54	3.33	22	25.91	3.33	23	26.24	3.33	24	26.19
san400_0.7_2	3.33	16	25.63	3.33	17	25.79	3.33	18	27.13	3.33	18	27.07
san400_0.7_3	3.35	13	29.03	3.35	14	27.07	3.35	15	27.30	3.35	16	26.94
sanr200_0.7	3.29	14	0.34	3.29	16	2.15	3.29	16	2.53	3.29	16	0.76
sanr200_0.9	9.46	41	0.50	9.47	41	0.53	9.47	43	0.64	9.47	43	0.67

Table 6 Results for the maximum s-defective clique problem starting from the degree-based point.

Graph	$s=1$			$s=2$			$s=3$			$s=4$		
	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time
brock200_1	3.91	19	1.48	3.91	18	0.30	3.91	19	0.30	3.91	22	2.28
brock200_2	1.99	10	4.56	1.99	10	2.90	1.99	11	3.12	1.99	11	0.70
brock200_3	2.54	12	0.47	2.54	13	0.41	2.54	13	0.45	2.54	13	0.30
brock200_4	2.92	16	0.45	2.92	16	2.90	2.92	15	2.95	2.92	17	0.19
brock400_1	3.96	20	42.03	3.96	21	8.28	3.96	21	10.25	3.96	23	8.63
brock400_2	3.98	23	19.95	3.98	21	9.13	3.98	23	1.67	3.98	24	35.54
brock400_3	3.96	24	9.34	3.96	22	8.22	3.96	23	42.92	3.96	24	28.45
brock400_4	3.97	22	42.32	3.97	23	8.58	3.97	25	14.41	3.97	23	10.76
c-fat200-1	1.09	12	0.70	1.09	12	1.53	1.09	12	0.87	1.09	12	0.28
c-fat200-2	1.19	23	0.59	1.19	24	0.17	1.19	24	0.14	1.19	24	0.17
c-fat200-5	1.74	58	2.48	1.74	58	0.12	1.74	58	0.09	1.74	58	0.09
c-fat500-1	1.04	14	21.75	1.04	14	1.62	1.04	14	1.19	1.04	14	4.90
c-fat500-2	1.08	26	22.74	1.08	26	24.27	1.08	26	1.19	1.08	26	1.59
c-fat500-5	1.23	64	16.44	1.23	64	0.87	1.23	64	1.33	1.23	64	1.31
c-fat500-10	1.60	126	0.95	1.60	126	0.66	1.60	126	1.00	1.60	126	0.75
hamming6-2	9.18	9.18	0.02	9.23	9.23	0.03	9.27	9.27	0.00	9.31	9.31	0.00
hamming6-4	1.52	1.52	0.02	1.53	1.53	0.02	1.53	1.53	0.00	1.53	1.53	0.02
hamming8-2	28.47	28.47	0.05	28.49	28.49	0.05	28.52	28.52	0.05	28.54	28.54	0.03
hamming8-4	2.75	2.75	0.08	2.75	2.75	0.08	2.75	2.75	0.08	2.75	2.75	0.08
hamming10-2	93.11	93.11	0.76	93.12	93.12	0.75	93.14	93.14	0.76	93.16	93.16	0.75
hamming10-4	5.82	5.82	1.01	5.82	5.82	1.00	5.82	5.82	1.01	5.82	5.82	1.00
johnson8-2-4	2.17	2.17	0.02	2.18	2.18	0.00	2.19	2.19	0.00	2.20	2.20	0.02
johnson8-4-4	4.12	4.12	0.00	4.13	4.13	0.02	4.14	4.14	0.02	4.15	4.15	0.00
johnson16-2-4	4.14	4.14	0.03	4.14	4.14	0.02	4.15	4.15	0.02	4.15	4.15	0.02
johnson32-2-4	8.13	8.13	0.20	8.13	8.13	0.20	8.13	8.13	0.22	8.13	8.13	0.22
keller4	2.87	9	0.25	2.87	10	1.15	2.87	11	0.33	2.87	13	1.17
keller5	4.04	20	181.57	4.04	18	44.63	4.04	20	41.01	4.04	20	7.21
MANN_a9	10.85	14	0.02	10.97	15	0.02	11.09	16	0.02	11.21	16	0.02
MANN_a27	80.88	118	0.66	80.97	119	0.64	81.06	120	0.75	81.15	121	0.64
MANN_a45	215.85	331	6.01	215.94	332	6.55	216.02	333	7.16	216.11	334	6.55
p_hat300-1	1.41	8	12.57	1.41	8	1.20	1.41	8	1.34	1.41	9	26.97
p_hat300-2	2.34	24	1.06	2.34	25	7.60	2.34	26	1.37	2.34	28	31.39
p_hat300-3	4.12	34	6.47	4.12	36	8.24	4.12	36	7.38	4.12	37	6.52
p_hat500-1	1.42	9	3.21	1.42	10	4.68	1.42	10	293.75	1.42	11	52.60
p_hat500-2	2.43	37	165.75	2.43	35	161.32	2.43	37	24.30	2.43	38	22.60
p_hat500-3	4.27	48	46.44	4.27	48	1.97	4.27	50	1.89	4.27	51	48.86
p_hat700-1	1.42	10	10.87	1.42	10	8.07	1.42	9	8.27	1.42	12	39.73
p_hat700-2	2.42	43	6.18	2.42	44	46.33	2.42	46	8.33	2.42	46	8.27
p_hat700-3	4.21	60	30.72	4.21	60	4.17	4.21	61	5.38	4.21	62	197.56
san200_0.7_1	3.32	16	1.68	3.32	17	1.76	3.32	18	1.73	3.32	19	2.76
san200_0.7_2	3.62	13	1.78	3.63	14	1.73	3.63	15	1.76	3.63	15	1.76
san200_0.9_1	9.78	46	0.44	9.78	47	0.42	9.79	48	0.42	9.79	49	0.44
san200_0.9_2	9.66	36	0.44	9.67	37	0.39	9.67	38	0.47	9.68	39	0.41
san200_0.9_3	9.64	28	0.47	9.64	33	0.47	9.65	30	0.50	9.65	35	0.53
san400_0.5_1	2.02	8	63.94	2.02	8	3.78	2.02	9	67.55	2.02	11	67.08
san400_0.7_1	3.33	21	26.75	3.33	22	26.40	3.33	23	26.80	3.33	24	26.52
san400_0.7_2	3.33	16	29.34	3.33	17	26.85	3.33	17	26.35	3.33	19	27.86
san400_0.7_3	3.34	13	26.36	3.34	14	25.82	3.34	15	26.27	3.34	16	26.10
sanr200_0.7	3.29	15	0.34	3.29	16	0.36	3.29	17	0.37	3.29	18	2.93
sanr200_0.9	9.46	39	0.50	9.47	40	0.64	9.47	43	0.62	9.47	41	0.61

Table 7 Results for the maximum s-plex problem starting from the Turán point.

Graph	$s=2$			$s=3$			$s=4$			$s=5$		
	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time
brock200_1	3.95	18	0.31	4.03	22	0.22	4.11	21	0.20	4.20	22	0.34
brock200_2	2.00	11	0.56	2.02	11	0.33	2.04	11	0.33	2.06	10	0.44
brock200_3	2.55	13	0.27	2.58	15	0.41	2.61	15	1.58	2.65	15	0.39
brock200_4	2.94	16	2.70	2.98	16	0.47	3.03	16	0.22	3.07	16	0.20
brock400_1	3.98	21	1.19	4.02	22	0.86	4.07	24	1.50	4.11	21	1.23
brock400_2	4.00	25	1.47	4.04	26	2.23	4.08	25	1.25	4.12	26	11.64
brock400_3	3.98	24	1.44	4.02	23	2.04	4.06	22	2.23	4.10	25	1.65
brock400_4	3.99	26	1.75	4.03	25	1.22	4.07	24	1.12	4.12	25	2.29
c-fat200-1	1.09	12	0.37	1.09	12	0.37	1.10	10	0.51	1.11	12	0.31
c-fat200-2	1.20	24	0.20	1.21	24	0.17	1.21	24	0.22	1.22	24	0.22
c-fat200-5	1.75	58	0.16	1.77	58	0.12	1.78	58	0.14	1.80	58	0.14
c-fat500-1	1.04	14	3.85	1.04	14	2.40	1.04	14	1.84	1.05	14	1.68
c-fat500-2	1.08	26	2.04	1.08	26	2.45	1.09	26	2.39	1.09	17	4.80
c-fat500-5	1.23	64	1.29	1.23	64	1.37	1.24	64	1.95	1.24	64	1.54
c-fat500-10	1.60	126	0.81	1.61	126	0.86	1.61	126	1.01	1.62	126	1.12
hamming6-2	10.67	10.67	0.00	12.80	12.80	0.00	16	16	0.02	21.33	21.33	0.02
hamming6-4	1.56	1.56	0.02	1.60	1.60	0.02	1.64	1.64	0.02	1.68	1.68	0.02
hamming8-2	32.00	32	0.06	36.57	36.57	0.06	42.67	42.67	0.05	51.20	51.20	0.06
hamming8-4	2.78	2.78	0.12	2.81	2.81	0.09	2.84	2.84	0.11	2.88	2.88	0.11
hamming10-2	102.40	102.40	0.84	113.78	113.78	0.75	128	128	0.80	146.29	146.29	0.80
hamming10-4	5.85	5.85	1.20	5.89	5.89	1.20	5.92	5.92	1.20	5.95	5.95	1.22
johnson8-2-4	2.33	2.33	0.02	2.55	2.55	0.00	2.80	2.80	0.02	3.11	3.11	0.02
johnson8-4-4	4.38	4.38	0.00	4.67	4.67	0.00	5.00	5	0.02	5.38	5.38	0.02
johnson16-2-4	4.29	4.29	0.03	4.44	4.44	0.02	4.62	4.62	0.02	4.80	4.80	0.02
johnson32-2-4	8.27	8.27	0.25	8.41	8.41	0.25	8.55	8.55	0.25	8.70	8.70	0.25
keller4	2.87	12	0.33	2.92	14	0.20	2.97	14	0.28	3.02	13	0.17
keller5	4.03	25	13.20	4.05	28	6.33	4.07	33	12.87	4.09	35	147.70
MANN_a9	13.78	24	0.02	20.45	36	0.00	32.14	36	0.02	45.00	45	0.02
MANN_a27	95.64	233	0.22	139.26	351	1.97	155.65	351	0.34	165.37	351	0.37
MANN_a45	252.35	660	8.75	366.23	990	39.56	390.25	990	1.65	403.47	990	1.70
p_hat300-1	1.33	8	1.06	1.33	8	1.17	1.34	9	1.26	1.34	7	0.94
p_hat300-2	1.96	26	7.94	1.98	26	1.34	1.99	23	1.33	2.00	24	1.06
p_hat300-3	3.93	36	0.66	3.98	37	1.37	4.03	38	1.28	4.09	37	1.15
p_hat500-1	1.34	9	42.76	1.35	9	2.95	1.35	8	3.88	1.35	9	3.09
p_hat500-2	2.02	36	4.87	2.03	34	5.23	2.04	39	38.27	2.05	41	11.34
p_hat500-3	4.04	53	22.98	4.07	55	38.77	4.11	60	12.46	4.14	58	23.09
p_hat700-1	1.33	8	4.70	1.34	8	4.35	1.34	9	7.21	1.34	9	4.77
p_hat700-2	1.99	39	3.99	2.00	41	12.85	2.00	43	107.69	2.01	44	68.94
p_hat700-3	3.97	65	13.20	4.00	66	11.14	4.02	66	64.85	4.04	68	69.95
san200_0.7_1	3.35	29.50	1.53	3.41	32	0.44	3.47	36	2.32	3.53	41	1.98
san200_0.7_2	3.35	24	0.25	3.41	32	1.54	3.47	34	2.45	3.53	38	1.51
san200_0.9_1	10.05	89.50	3.26	10.58	108	1.90	11.17	113	1.70	11.83	124	0.48
san200_0.9_2	10.05	67	3.15	10.58	71	2.36	11.17	71	2.26	11.83	76	2.15
san200_0.9_3	10.05	43.50	2.29	10.58	51	0.87	11.17	48	0.97	11.83	53	1.25
san400_0.5_1	2.01	14	1.44	2.02	17	17.97	2.03	20	4.20	2.04	21	4.51
san400_0.7_1	3.34	40	2.37	3.37	44	26.05	3.40	55	31.50	3.43	61	3.48
san400_0.7_2	3.34	29	1.50	3.37	41	4.34	3.40	45	30.45	3.43	47	4.66
san400_0.7_3	3.34	24	1.79	3.37	30	13.15	3.40	36	2.95	3.43	36	14.62
sanr200_0.7	3.32	17	0.42	3.37	16	0.33	3.43	16	0.23	3.49	18	1.19
sanr200_0.9	9.82	45	0.45	10.33	48	0.44	10.89	51	1.03	11.51	49	0.50

Table 8 Results for the maximum s-plex problem starting from the Wilf point.

Graph	$s=2$			$s=3$			$s=4$			$s=5$		
	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time
brock200_1	3.96	23	0.50	4.02	23	0.23	4.08	24	0.27	4.14	24	0.23
brock200_2	2.01	11	0.76	2.03	12	0.51	2.04	12	0.45	2.06	12	0.36
brock200_3	2.56	14	0.58	2.59	16	0.75	2.61	15	0.34	2.64	14	0.30
brock200_4	2.95	16	0.53	2.99	17	0.30	3.02	18	0.28	3.06	17	0.27
brock400_1	3.99	24	3.29	4.03	25	2.28	4.06	26	2.09	4.09	25	2.04
brock400_2	4.01	25	2.85	4.04	27	2.45	4.07	29	4.46	4.10	28	2.61
brock400_3	3.99	23	2.04	4.02	29	3.98	4.05	26	1.53	4.09	25	1.67
brock400_4	4	26	4.49	4.04	25	2.12	4.07	25	1.75	4.10	27	1.79
c-fat200-1	1.23	12	0.22	1.24	12	0.23	1.25	12	0.23	1.25	12	0.25
c-fat200-2	1.25	24	0.25	1.26	24	0.23	1.26	24	0.14	1.27	24	0.17
c-fat200-5	1.75	58	0.14	1.77	58	0.11	1.78	58	0.12	1.80	58	0.11
c-fat500-1	1.17	14	2.07	1.18	14	2.89	1.18	14	2.57	1.18	14	2.62
c-fat500-2	1.16	26	3.88	1.17	26	2	1.17	26	1.98	1.17	26	1.87
c-fat500-5	1.24	64	1.11	1.25	63	1.15	1.25	63	1.44	1.25	64	1.25
c-fat500-10	1.60	126	1.14	1.61	126	0.95	1.61	126	1.42	1.62	126	1.20
hamming6-2	10.67	10.67	0.02	12.80	12.80	0.02	16	16	0.00	21.33	21.33	0.00
hamming6-4	1.56	1.56	0.02	1.60	1.60	0.02	1.64	1.64	0.02	1.68	1.68	0.02
hamming8-2	32	32	0.05	36.57	36.57	0.06	42.67	42.67	0.06	51.20	51.20	0.06
hamming8-4	2.78	2.78	0.08	2.81	2.81	0.08	2.84	2.84	0.08	2.88	2.88	0.08
hamming10-2	102.40	102.40	0.78	113.78	113.78	0.78	128	128	0.80	146.29	146.29	0.78
hamming10-4	5.85	5.85	1.08	5.89	5.89	1.06	5.92	5.92	1.05	5.95	5.95	1.03
johnson8-2-4	2.33	2.33	0.02	2.55	2.55	0.00	2.80	2.80	0.00	3.11	3.11	0.00
johnson8-4-4	4.38	4.37	0.00	4.67	4.67	0.02	5	5	0.02	5.38	5.38	0.00
johnson16-2-4	4.29	4.29	0.03	4.44	4.44	0.02	4.62	4.62	0.03	4.80	4.80	0.02
johnson32-2-4	8.27	8.27	0.23	8.41	8.41	0.22	8.55	8.55	0.22	8.70	8.70	0.27
keller4	2.90	12	0.48	2.95	15	0.51	2.99	15	0.33	3.04	23	0.73
keller5	4.06	30	102.26	4.08	32	62.42	4.10	38	120.20	4.11	35	20.87
MANN_a9	13.26	22.50	0.02	17.33	31	0.02	25.03	36	0.00	45	45	0.00
MANN_a27	85.99	175.50	6.71	91.91	351	1.36	98.70	351	0.12	106.58	351	0.12
MANN_a45	223.82	495.50	13.57	232.49	986	62.68	241.87	990	1.03	252.04	990	1.11
p_hat300-1	1.41	9	2.50	1.42	9	2.31	1.42	9	1.03	1.43	8	1.06
p_hat300-2	2.31	27	2.51	2.32	30	1.25	2.33	28	0.84	2.34	28	0.92
p_hat300-3	4.14	41	2.12	4.17	41	0.97	4.21	51	1.73	4.24	44	0.64
p_hat500-1	1.42	9	3.68	1.42	10	7.66	1.43	9	4.95	1.43	11	3.88
p_hat500-2	2.40	39	10.53	2.41	40	5.02	2.41	41	3.67	2.42	42	3.43
p_hat500-3	4.28	55	7.96	4.30	57	3.49	4.32	58	2.12	4.35	58	1.75
p_hat700-1	1.41	10	25.35	1.42	9	15.62	1.42	11	14.46	1.42	9	7.85
p_hat700-2	2.38	49	42.46	2.39	49	12.23	2.39	49	6.68	2.40	51	6.75
p_hat700-3	4.22	72	28.70	4.24	71	12.90	4.25	80	9.36	4.26	72	3.81
san200_0.7_1	3.36	29	2.06	3.41	41	2.46	3.46	47	2.53	3.51	60	3.06
san200_0.7_2	3.80	22	2.07	3.84	33	2.09	3.88	42	2.25	3.92	48	2.46
san200_0.9_1	10.02	77.50	0.51	10.27	123	0.56	10.54	124	0.31	10.81	123	0.16
san200_0.9_2	9.97	68.50	1.15	10.31	80	1.81	10.67	88	1.17	11.06	86	0.76
san200_0.9_3	9.92	49	0.47	10.22	61	0.50	10.55	69	0.34	10.89	69	0.27
san400_0.5_1	2.11	12.50	69.17	2.12	21	71.25	2.13	25	65.80	2.14	27	73.85
san400_0.7_1	3.35	39.50	36.10	3.37	54	30	3.40	64	43.63	3.42	79	42.39
san400_0.7_2	3.35	28.50	32.53	3.37	42	33.65	3.40	47	34.96	3.42	60	33.46
san400_0.7_3	3.37	23	28.39	3.39	33	29.17	3.42	42	28.14	3.44	43	37.85
sanr200_0.7	3.33	16	0.39	3.37	20	0.44	3.42	19	0.23	3.46	19	0.22
sanr200_0.9	9.74	47	0.25	10.04	48	0.19	10.35	50	0.16	10.69	47	0.16

Table 9 Results for the maximum s-plex problem starting from the degree-based point.

Graph	$s = 2$			$s = 3$			$s = 4$			$s = 5$		
	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time	Bound	Sol	Time
brock200_1	3.96	23	0.50	4.02	23	0.25	4.08	23	0.22	4.14	21	0.28
brock200_2	2.01	11	0.94	2.03	11	0.41	2.04	12	0.45	2.06	12	0.36
brock200_3	2.56	14	0.53	2.59	14	0.36	2.61	13	0.41	2.64	14	0.23
brock200_4	2.95	15	0.42	2.99	18	0.28	3.02	17	0.23	3.06	18	0.28
brock400_1	3.99	25	4.23	4.03	24	2.29	4.06	24	1.20	4.09	25	1.12
brock400_2	4.01	25	2.96	4.04	25	1.81	4.07	24	1.62	4.10	28	1.64
brock400_3	3.99	24	3.74	4.02	24	2.34	4.05	26	2.56	4.09	25	1.56
brock400_4	4.00	25	3.28	4.04	23	0.97	4.07	30	2.64	4.10	26	1.19
c-fat200-1	1.09	12	0.16	1.10	12	0.16	1.10	12	0.22	1.11	12	0.20
c-fat200-2	1.20	24	0.22	1.21	24	0.17	1.21	24	0.16	1.22	24	0.16
c-fat200-5	1.75	58	0.14	1.77	58	0.11	1.78	58	0.14	1.80	58	0.12
c-fat500-1	1.04	14	1.51	1.04	14	1.98	1.04	14	1.83	1.05	14	1.68
c-fat500-2	1.08	26	1.54	1.08	26	1.65	1.09	26	1.75	1.09	26	1.67
c-fat500-5	1.23	64	1.39	1.23	64	1.44	1.24	64	1.06	1.24	64	1.06
c-fat500-10	1.60	126	1.09	1.61	126	0.95	1.61	126	0.69	1.62	126	0.92
hamming6-2	10.67	10.67	0.00	12.80	12.80	0.00	16.00	16	0.02	21.33	21.33	0.02
hamming6-4	1.56	1.56	0.02	1.60	1.60	0.00	1.64	1.64	0.00	1.68	1.68	0.02
hamming8-2	32	32	0.05	36.57	36.57	0.05	42.67	42.67	0.05	51.20	51.20	0.05
hamming8-4	2.78	2.78	0.08	2.81	2.81	0.09	2.84	2.84	0.08	2.88	2.88	0.08
hamming10-2	102.40	102.40	0.76	113.78	113.78	0.78	128	128	0.75	146.29	146.29	0.76
hamming10-4	5.85	5.85	1.05	5.89	5.89	1.03	5.92	5.92	1.05	5.95	5.95	1.01
johnson8-2-4	2.33	2.33	0.00	2.55	2.55	0.00	2.80	2.80	0.00	3.11	3.11	0.02
johnson8-4-4	4.38	4.37	0.02	4.67	4.67	0.00	5.00	5	0.02	5.38	5.38	0.02
johnson16-2-4	4.29	4.29	0.02	4.44	4.44	0.03	4.62	4.62	0.02	4.80	4.80	0.02
johnson32-2-4	8.27	8.27	0.22	8.41	8.41	0.22	8.55	8.55	0.22	8.70	8.70	0.22
keller4	2.91	14	0.64	2.95	16	0.53	2.99	16	0.41	3.04	16	0.30
keller5	4.06	29.50	62.73	4.08	31	50.19	4.10	37	74.43	4.12	33	36.33
MANN_a9	13.26	22.50	0.02	17.33	29	0.02	25.03	36	0.02	45.00	45	0.02
MANN_a27	85.99	187	1.20	91.91	349	3.49	98.70	351	0.14	106.57	351	0.53
MANN_a45	223.82	495	10.20	232.49	990	13.70	241.87	990	0.98	252.03	990	1.00
p_hat300-1	1.42	8	2.22	1.42	8	1.09	1.43	8	0.98	1.43	8	0.86
p_hat300-2	2.35	26	2.17	2.36	26	1.05	2.37	29	0.78	2.38	29	0.73
p_hat300-3	4.15	40	2.18	4.18	41	0.97	4.21	40	0.51	4.24	44	0.47
p_hat500-1	1.43	9	3.90	1.43	9	7.75	1.43	9	4.12	1.44	9	3.15
p_hat500-2	2.44	39	12.36	2.44	40	6.27	2.45	40	3.43	2.46	41	2.73
p_hat500-3	4.29	57	7.47	4.31	56	4.15	4.33	56	1.59	4.35	67	2.50
p_hat700-1	1.42	10	11.67	1.42	9	15.09	1.43	11	25.79	1.43	10	10.72
p_hat700-2	2.42	48	36.33	2.43	49	15.01	2.43	50	6.57	2.44	51	5.99
p_hat700-3	4.22	71	27.77	4.24	71	12.12	4.25	77	10.50	4.27	72	4.43
san200_0.7_1	3.36	27.50	2.11	3.41	38	2.23	3.45	46	2.65	3.50	59	2.37
san200_0.7_2	3.66	22.50	2.06	3.70	34	2.26	3.74	42	2.11	3.78	48	2.32
san200_0.9_1	10.01	77.50	0.51	10.26	123	0.48	10.53	114	0.23	10.80	122	0.23
san200_0.9_2	9.97	68	1.25	10.31	85	1.12	10.67	87	0.81	11.06	96	0.90
san200_0.9_3	9.92	47.50	0.42	10.22	64	0.53	10.55	68	0.33	10.89	75	0.27
san400_0.5_1	2.03	12.50	63.55	2.04	19	64.99	2.04	23.50	44.57	2.05	24	25.13
san400_0.7_1	3.35	38	30.83	3.37	56	36.04	3.40	70	40.67	3.42	81	37.13
san400_0.7_2	3.35	29	31.96	3.37	45	30.86	3.40	51	38.06	3.42	59	35.47
san400_0.7_3	3.36	22	28.31	3.38	34	32.18	3.41	40	33.68	3.43	43	34.27
sanr200_0.7	3.33	19	0.66	3.38	19	0.31	3.42	19	0.23	3.46	17	0.22
sanr200_0.9	9.74	45	0.37	10.04	50	0.25	10.35	53	0.27	10.69	45	0.17

Table 10 Results for the maximum s-defective clique problem starting from random points.

Graph	$s = 1$			$s = 2$			$s = 3$			$s = 4$		
	max	mean	std	max	mean	std	max	mean	std	max	mean	std
brock200_1	21	18.56	1.12	21	19.45	0.97	22	20.17	0.95	23	20.81	0.90
brock200_2	12	9.89	0.65	12	10.37	0.68	12	10.67	0.75	13	11.18	0.76
brock200_3	14	12.17	0.75	15	12.82	0.85	16	13.43	0.78	16	13.76	0.88
brock200_4	17	14.26	1.07	18	14.92	1.01	18	15.68	0.89	18	16.15	0.89
brock400_1	25	21.47	1.18	25	22.32	1.23	25	22.84	1.09	25	23.38	1.09
brock400_2	24	21.60	1.16	25	22.09	1.17	25	22.78	0.98	26	23.50	1.20
brock400_3	25	21.48	1.23	25	22.00	1.24	26	22.75	1.22	25	22.92	1.04
brock400_4	25	21.82	1.08	25	22.55	1.22	26	23.51	1.10	26	24.00	0.97
c-fat200-1	12	12.00	0.00	12	12.00	0.00	12	12.00	0.00	12	11.94	0.31
c-fat200-2	24	23.02	0.84	24	22.88	0.89	24	23.07	1.21	24	23.12	0.82
c-fat200-5	58	57.59	0.59	58	57.51	0.66	58	57.51	0.69	58	57.51	0.72
c-fat500-1	14	13.95	0.23	14	14.00	0.00	14	14.00	0.00	14	14.00	0.00
c-fat500-2	26	25.73	0.47	26	25.77	1.35	26	23.50	5.00	26	23.86	3.76
c-fat500-5	64	63.44	0.89	64	63.46	0.78	64	63.14	0.87	64	63.45	0.76
c-fat500-10	126	125.54	0.66	126	125.50	0.72	126	125.57	0.72	126	125.35	0.78
hamming6-2	32	29.96	4.26	32	31.23	2.77	32	30.66	3.44	32	30.54	3.73
hamming6-4	4	4.00	0.00	5	4.86	0.35	6	4.93	0.41	6	5.27	0.68
hamming8-2	128	103.33	17.09	128	104.50	16.37	128	106.13	16.13	128	108.61	16.42
hamming8-4	16	15.80	0.84	16	15.60	1.29	16	15.67	1.15	16	15.86	0.79
hamming10-2	512	390.74	60.60	512	394.03	59.46	503	401.03	65.34	496	398.91	52.73
hamming10-4	33	31.75	1.50	33	32.50	0.58	35	33.33	1.53	36	36.00	0.00
johnson8-2-4	4	4.00	0.00	5	4.64	0.48	5	4.59	0.49	6	4.69	0.56
johnson8-4-4	14	13.81	0.84	14	13.80	0.74	14	13.85	0.74	15	13.97	0.30
johnson16-2-4	8	8.00	0.00	9	8.83	0.38	9	8.93	0.26	10	9.13	0.66
johnson32-2-4	16	16.00	0.00	17	16.89	0.32	17	17.00	0.00	18	17.51	0.54
keller4	11	8.91	0.81	11	10.01	0.81	12	10.83	0.89	13	11.82	0.85
keller5	21	18.00	1.47	21	19.33	1.15	22	20.07	1.10	23	20.44	1.74
MANN_a9	17	15.39	0.90	18	16.54	0.87	19	17.39	0.76	20	18.14	0.89
MANN_a27	118	118.00	0.00	119	119.00	0.00	120	120.00	0.00	121	121.00	0.00
MANN_a45	331	331.00	0.00	332	332.00	0.00	333	333.00	0.00	334	333.97	0.17
p_hat300-1	9	7.72	0.59	9	8.00	0.46	9	8.32	0.61	10	8.56	0.62
p_hat300-2	26	25.00	0.60	27	25.93	0.57	28	26.67	0.82	29	27.00	0.60
p_hat300-3	37	33.96	1.25	37	34.38	1.15	38	35.33	1.11	38	35.98	1.06
p_hat500-1	10	8.88	0.49	10	9.15	0.69	10	9.90	0.32	10	8.74	0.81
p_hat500-2	37	35.73	1.51	38	36.50	0.96	39	37.40	0.84	39	37.73	1.49
p_hat500-3	50	48.41	0.82	51	49.00	1.06	51	49.39	1.04	52	51.24	1.03
p_hat700-1	10	9.00	0.58	10	9.12	0.83	11	10.17	0.75	12	10.43	0.98
p_hat700-2	45	44.08	0.29	46	44.54	1.05	46	45.71	0.49	46	46.00	0.00
p_hat700-3	60	59.18	0.88	61	60.29	0.76	62	61.75	0.50	64	62.75	1.26
san200_0.7_1	16	16.00	0.00	17	16.98	0.14	18	17.95	0.22	20	18.99	0.17
san200_0.7_2	13	13.00	0.00	14	13.89	0.31	15	14.89	0.31	16	15.79	0.41
san200_0.9_1	46	46.00	0.00	47	47.00	0.00	48	47.97	0.17	49	48.95	0.22
san200_0.9_2	40	36.68	0.96	51	37.92	1.71	43	38.72	1.07	51	39.69	1.50
san200_0.9_3	38	31.50	3.01	37	32.10	2.71	38	33.62	2.17	39	34.48	2.43
san400_0.5_1	8	8.00	0.00	9	8.98	0.15	10	9.56	0.50	11	10.47	0.57
san400_0.7_1	22	21.01	0.11	22	21.96	0.21	23	22.92	0.28	24	23.87	0.34
san400_0.7_2	16	16.00	0.00	18	16.99	0.21	19	17.90	0.40	19	18.94	0.25
san400_0.7_3	13	13.00	0.00	14	13.93	0.25	15	14.82	0.39	16	15.53	0.50
sanr200_0.7	19	16.23	0.99	19	16.80	1.15	20	17.57	1.14	20	17.92	1.04
sanr200_0.9	42	38.34	1.55	42	39.15	1.49	43	39.56	1.58	44	40.48	1.59

Table 11 Running times (in CPU seconds) for the maximum s-defective clique problem experiments starting from random points.

Graph	$s=1$			$s=2$			$s=3$			$s=4$		
	runs	mean	std	runs	mean	std	runs	mean	std	runs	mean	std
brock200_1	100	0.73	0.55	100	1.05	0.53	100	1.37	0.53	100	1.56	0.42
brock200_2	100	1.13	1.02	100	1.72	1.20	100	1.72	1.22	100	2.28	1.22
brock200_3	100	1.03	0.87	100	1.52	1.10	100	1.90	1.07	100	2.14	1.01
brock200_4	100	0.84	0.69	100	1.32	0.84	100	1.64	0.88	100	1.87	0.86
brock400_1	100	5.64	5.46	66	9.18	6.46	45	13.59	8.46	37	16.58	7.14
brock400_2	94	6.49	5.10	68	8.85	6.08	54	11.38	6.25	40	15.12	7.39
brock400_3	83	7.29	5.61	62	9.70	6.60	53	11.35	6.44	37	16.48	5.85
brock400_4	88	6.84	5.24	64	9.38	6.45	49	12.51	8.10	37	16.39	7.23
c-fat200-1	100	1.24	0.35	100	1.17	0.53	100	0.92	0.37	100	1.20	1.85
c-fat200-2	100	0.74	0.28	100	0.64	0.95	100	0.64	1.14	100	0.55	1.02
c-fat200-5	100	0.38	0.73	100	0.29	0.68	100	0.28	0.64	100	0.18	0.04
c-fat500-1	19	32.06	11.22	25	24.45	12.55	24	25.78	11.40	34	17.87	9.67
c-fat500-2	11	66.84	158.04	35	17.26	10.84	4	225.33	270.52	7	96.20	220.46
c-fat500-5	27	22.38	82.56	52	12.88	56.96	74	9.31	50.66	56	10.78	60.30
c-fat500-10	67	9.70	37.05	98	7.99	34.57	61	9.84	43.81	100	1.62	0.67
hamming6-2	100	0.02	0.01	100	0.02	0.01	100	0.01	0.01	100	0.02	0.01
hamming6-4	100	0.03	0.01	100	0.04	0.01	100	0.04	0.02	100	0.05	0.02
hamming8-2	100	0.41	0.09	100	0.44	0.11	100	0.43	0.13	100	0.41	0.14
hamming8-4	100	0.88	0.72	100	1.08	1.45	100	1.05	1.48	100	1.02	1.53
hamming10-2	35	17.60	2.41	34	17.98	2.87	34	17.87	2.11	34	17.89	2.62
hamming10-4	4	217.72	197.48	4	150.23	178.68	3	258.63	176.96	2	468.06	23.04
johnson8-2-4	100	0.01	0.01	100	0.01	0.01	100	0.01	0.01	100	0.01	0.01
johnson8-4-4	100	0.02	0.01	100	0.02	0.01	100	0.02	0.01	100	0.02	0.01
johnson16-2-4	100	0.11	0.03	100	0.13	0.05	100	0.14	0.05	100	0.15	0.05
johnson32-2-4	60	10.02	4.08	54	11.25	4.30	50	12.02	3.58	49	12.42	4.50
keller4	100	0.40	0.31	100	0.51	0.37	100	0.60	0.39	100	0.69	0.39
keller5	14	44.13	50.62	12	50.73	35.01	15	42.28	29.72	9	70.84	75.04
MANN_a9	100	0.01	0.01	100	0.01	0.01	100	0.01	0.00	100	0.01	0.01
MANN_a27	100	0.76	0.14	100	0.78	0.15	100	0.72	0.14	100	0.72	0.15
MANN_a45	77	7.86	1.49	76	7.93	1.42	75	8.02	1.91	72	8.39	2.12
p_hat300-1	100	5.63	3.41	66	9.20	7.16	68	8.91	5.94	61	9.97	7.54
p_hat300-2	100	3.38	2.80	91	6.71	5.31	58	10.39	6.52	40	15.03	6.55
p_hat300-3	100	2.59	2.18	100	4.22	2.35	100	5.25	2.03	96	6.29	1.86
p_hat500-1	17	35.63	28.04	13	46.78	38.63	10	60.87	38.96	19	32.51	13.37
p_hat500-2	26	23.35	25.16	22	30.11	30.19	10	67.68	55.21	11	63.80	30.41
p_hat500-3	34	18.02	17.28	26	23.11	18.36	18	35.55	16.16	17	36.37	11.26
p_hat700-1	7	88.01	36.28	8	76.11	26.36	6	104.00	39.66	7	109.02	43.92
p_hat700-2	12	51.37	17.62	13	48.18	8.47	7	88.64	24.95	3	236.38	283.48
p_hat700-3	17	35.82	56.40	7	86.70	74.60	4	159.66	62.32	4	162.03	42.90
san200_0.7_1	100	0.59	0.45	100	0.72	0.33	100	0.94	0.32	100	1.09	0.28
san200_0.7_2	100	0.65	0.36	100	0.90	0.21	100	1.17	0.27	100	1.37	0.23
san200_0.9_1	100	0.49	0.08	100	0.48	0.11	100	0.47	0.07	100	0.47	0.06
san200_0.9_2	100	0.36	0.09	100	0.44	0.06	100	0.48	0.09	100	0.48	0.06
san200_0.9_3	100	0.39	0.10	100	0.45	0.07	100	0.47	0.06	100	0.50	0.07
san400_0.5_1	63	10.06	11.06	43	14.08	14.90	45	13.50	11.28	32	19.01	19.06
san400_0.7_1	90	6.77	7.06	69	8.76	7.46	49	12.29	8.23	45	13.35	7.37
san400_0.7_2	80	7.55	7.88	67	8.99	7.25	60	10.33	6.94	47	12.98	7.19
san400_0.7_3	94	6.41	6.94	59	10.20	8.37	50	12.40	7.75	55	11.10	5.77
sanr200_0.7	100	0.80	0.64	100	1.16	0.71	100	1.59	0.67	100	1.66	0.65
sanr200_0.9	100	0.41	0.10	100	0.49	0.07	100	0.55	0.06	100	0.57	0.07

Table 12 Results for the maximum s-plex problem starting from random points.

Graph	$s = 1$			$s = 2$			$s = 3$			$s = 4$		
	max	mean	std	max	mean	std	max	mean	std	max	mean	std
brock200_1	23	21.45	0.99	24	21.74	1.13	25	21.88	1.14	25	21.86	1.24
brock200_2	12	10.91	0.77	13	11.20	0.79	13	11.17	0.77	12	11.09	0.79
brock200_3	16	13.79	0.80	16	14.01	0.86	16	13.98	0.89	17	14.12	1.05
brock200_4	19	16.39	0.91	20	16.69	1.01	20	16.41	1.10	19	16.46	0.97
brock400_1	27	24.53	1.18	28	24.94	1.26	30	25.23	1.56	30	24.98	1.36
brock400_2	28	24.50	1.13	29	24.68	1.45	31	25.05	1.62	30	25.21	1.34
brock400_3	27	24.56	1.36	28	24.93	1.22	33	25.12	1.51	29	25.13	1.24
brock400_4	28	25.15	1.28	30	25.90	1.49	32	25.84	1.48	33	25.86	1.78
c-fat200-1	12	11.99	0.10	12	11.95	0.30	12	12.00	0.00	12	11.99	0.10
c-fat200-2	24	23.16	0.83	24	22.93	0.78	24	22.93	0.86	24	22.82	0.87
c-fat200-5	58	57.50	0.70	58	57.46	0.70	58	57.56	0.67	58	57.53	0.67
c-fat500-1	14	13.98	0.14	14	13.96	0.40	14	13.99	0.10	14	13.98	0.14
c-fat500-2	26	25.96	0.20	26	25.96	0.20	26	25.98	0.14	26	25.93	0.52
c-fat500-5	64	63.13	0.90	64	63.20	0.85	64	63.42	0.77	64	63.41	0.79
c-fat500-10	126	125.37	0.77	126	125.34	0.79	126	125.25	0.78	126	125.37	0.77
hamming6-2	32	30.71	3.32	32	30.76	3.20	32	30.39	3.58	32	31.09	2.66
hamming6-4	6	4.07	0.36	6	4.19	0.51	7	4.35	0.78	8	4.37	0.80
hamming8-2	128	101.85	13.99	128	107.72	10.37	128	112.97	8.77	128	115.97	10.09
hamming8-4	16	15.85	0.74	16	15.93	0.50	20	16.13	0.87	23	16.32	1.36
hamming10-2	420	352.89	31.51	500	407.92	40.46	488	413.18	42.87	454	407.71	21.27
hamming10-4	39	38.00	1.00	42	39.38	1.41	52	42.44	4.72	55	44.50	5.21
johnson8-2-4	5	4.03	0.17	7	4.34	0.83	7	4.12	0.46	7	4.29	0.73
johnson8-4-4	14	13.84	0.68	15	13.96	0.35	19	14.03	0.87	23	14.28	1.39
johnson16-2-4	10	8.33	0.57	14	11.13	2.22	16	12.35	3.07	20	13.73	4.51
johnson32-2-4	19	16.71	0.94	28	22.28	3.94	31	25.12	5.80	36	29.46	6.90
keller4	15	14.32	0.76	17	14.82	0.73	19	15.37	1.04	22	15.55	1.51
keller5	31	28.06	1.77	35	31.46	1.41	37	32.10	1.82	44	34.14	3.57
MANN_a9	26	24.53	0.80	30	25.85	1.75	33	26.17	1.94	32	26.05	1.79
MANN_a27	230	226.03	2.47	345	336.43	4.01	350	339.48	5.37	350	339.31	6.36
MANN_a45	646	637.10	9.77	960	947.37	8.38	987	981.21	5.07	988	981.08	3.78
p_hat300-1	10	8.45	0.59	10	8.18	0.69	10	8.09	0.65	10	8.28	0.73
p_hat300-2	29	27.85	0.74	31	28.06	0.80	31	28.02	0.72	33	28.20	0.99
p_hat300-3	42	39.38	1.34	45	40.34	1.39	50	41.85	2.57	53	41.80	2.72
p_hat500-1	12	9.54	0.76	11	9.26	0.81	11	9.44	0.83	11	9.24	0.73
p_hat500-2	40	39.13	0.81	43	39.86	0.97	47	40.13	1.34	51	40.51	1.86
p_hat500-3	58	56.06	1.03	64	57.14	1.56	69	58.32	2.58	70	59.01	3.00
p_hat700-1	11	10.33	0.84	13	10.51	0.95	14	10.64	1.45	13	10.57	1.06
p_hat700-2	50	48.57	0.68	50	48.65	0.72	56	49.27	1.39	59	49.63	1.98
p_hat700-3	72	70.21	1.25	78	70.85	1.55	84	72.35	3.47	90	73.96	4.86
san200_0.7_1	30	29.54	0.61	45	42.80	1.35	58	49.39	3.21	72	56.33	5.67
san200_0.7_2	24	23.75	0.50	36	34.09	1.36	44	41.20	1.96	52	47.38	2.19
san200_0.9_1	90	88.13	1.13	121	114.28	3.98	122	112.38	5.06	122	112.17	4.13
san200_0.9_2	71	66.48	5.98	96	83.10	10.02	98	82.31	8.08	97	82.93	8.02
san200_0.9_3	53	45.72	3.30	69	51.50	7.76	77	52.54	9.71	82	53.31	10.34
san400_0.5_1	14	13.93	0.27	21	20.08	1.00	25	22.55	2.02	27	25.09	1.30
san400_0.7_1	40	39.32	0.89	59	56.68	1.62	75	67.20	4.60	89	76.75	6.23
san400_0.7_2	30	29.75	0.44	45	42.95	1.16	57	51.33	3.15	62	57.14	2.50
san400_0.7_3	24	23.96	0.21	36	34.48	1.03	42	38.90	1.33	49	45.42	1.68
sanr200_0.7	21	18.45	1.14	22	18.74	1.25	25	18.93	1.58	22	18.71	1.23
sanr200_0.9	48	44.40	1.45	54	46.28	2.37	58	47.21	3.02	57	47.22	2.84

Table 13 Running times (in CPU seconds) for the maximum s-plex problem experiments starting from random points.

Graph	$s = 1$			$s = 2$			$s = 3$			$s = 4$		
	runs	mean	std	runs	mean	std	runs	mean	std	runs	mean	std
brock200_1	100	0.41	0.08	100	0.24	0.06	100	0.25	0.29	100	0.22	0.04
brock200_2	100	0.60	0.16	100	0.30	0.08	100	0.28	0.05	100	0.27	0.05
brock200_3	100	0.54	0.12	100	0.29	0.08	100	0.28	0.06	100	0.26	0.04
brock200_4	100	0.47	0.11	100	0.27	0.07	100	0.24	0.04	100	0.23	0.05
brock400_1	100	3.24	0.77	100	1.79	2.00	100	1.31	0.28	100	1.21	0.23
brock400_2	100	3.30	0.71	100	1.62	0.51	100	1.28	0.33	100	1.21	0.27
brock400_3	100	3.48	0.80	100	1.52	0.44	100	1.63	2.61	100	1.24	0.24
brock400_4	100	3.31	0.78	100	1.57	0.54	100	1.25	0.31	100	1.30	0.32
c-fat200-1	100	0.28	0.06	100	0.26	0.04	100	0.26	0.04	100	0.25	0.04
c-fat200-2	100	0.22	0.04	100	0.22	0.08	100	0.22	0.04	100	0.22	0.02
c-fat200-5	100	0.17	0.02	100	0.23	0.28	100	0.17	0.02	100	0.16	0.02
c-fat500-1	100	4.12	5.75	100	3.72	6.83	100	3.58	4.84	100	2.78	0.84
c-fat500-2	100	3.32	4.55	100	4.19	10.58	100	4.75	10.83	100	3.87	11.09
c-fat500-5	100	4.22	14.45	100	5.38	20.66	100	3.52	12.01	100	5.21	15.80
c-fat500-10	100	1.40	0.15	100	1.40	0.16	100	2.50	10.91	100	2.48	10.37
hamming6-2	100	0.02	0.01	100	0.02	0.01	100	0.02	0.01	100	0.02	0.01
hamming6-4	100	0.03	0.01	100	0.03	0.01	100	0.02	0.01	100	0.02	0.01
hamming8-2	100	0.47	0.22	100	0.49	0.34	100	0.48	0.33	100	0.48	0.31
hamming8-4	100	0.47	0.60	100	0.34	0.14	100	0.52	0.82	100	0.51	0.78
hamming10-2	9	66.91	54.80	13	48.85	44.80	11	58.75	48.84	7	89.40	81.68
hamming10-4	5	128.88	152.56	8	80.62	136.71	16	49.07	87.61	8	118.80	176.14
johnson8-2-4	100	0.01	0.01	100	0.01	0.01	100	0.01	0.01	100	0.01	0.01
johnson8-4-4	100	0.02	0.01	100	0.02	0.01	100	0.02	0.01	100	0.02	0.01
johnson16-2-4	100	0.12	0.04	100	0.15	0.06	100	0.14	0.05	100	0.14	0.06
johnson32-2-4	95	6.32	3.93	54	11.28	6.85	51	11.80	6.69	41	14.93	7.18
keller4	100	0.43	0.07	100	0.27	0.08	100	0.21	0.06	100	0.19	0.05
keller5	16	37.69	6.85	24	25.60	14.31	48	12.84	8.63	59	10.25	7.49
MANN_a9	100	0.02	0.00	100	0.02	0.00	100	0.02	0.00	100	0.02	0.00
MANN_a27	100	0.89	0.09	100	1.22	0.17	100	0.59	0.09	100	0.60	0.12
MANN_a45	48	12.55	0.93	35	17.46	1.96	96	6.31	0.91	96	6.26	0.85
p_hat300-1	100	2.26	0.84	100	1.20	0.53	100	0.98	0.22	100	0.97	0.22
p_hat300-2	100	1.91	0.42	100	0.91	0.24	100	0.83	0.11	100	0.82	0.13
p_hat300-3	100	1.35	0.29	100	0.76	0.17	100	0.66	0.15	100	0.58	0.12
p_hat500-1	56	10.75	4.57	100	4.17	1.85	100	3.48	0.94	100	3.26	0.69
p_hat500-2	79	7.64	2.15	100	3.85	1.82	100	2.90	0.99	100	2.56	0.48
p_hat500-3	100	5.54	0.97	100	2.79	0.83	100	2.00	0.54	100	1.72	0.32
p_hat700-1	18	33.87	11.87	59	10.34	7.96	75	8.01	3.09	79	7.66	1.61
p_hat700-2	21	30.44	15.91	65	9.26	3.33	83	7.23	2.29	100	6.03	1.70
p_hat700-3	34	17.66	3.62	97	6.42	2.98	100	5.13	2.04	100	3.98	0.83
san200_0.7_1	100	2.01	0.16	100	2.39	2.04	100	2.09	0.32	100	2.09	0.22
san200_0.7_2	100	2.38	0.21	100	2.37	0.28	100	2.17	0.26	100	2.07	0.19
san200_0.9_1	100	0.46	0.03	100	0.48	0.05	100	0.16	0.03	100	0.16	0.02
san200_0.9_2	100	0.47	0.06	100	0.43	0.08	100	0.19	0.03	100	0.19	0.04
san200_0.9_3	100	0.38	0.07	100	0.34	0.38	100	0.21	0.05	100	0.17	0.03
san400_0.5_1	14	43.56	4.16	12	50.39	2.36	11	55.92	3.08	11	55.44	3.30
san400_0.7_1	22	28.14	4.49	22	28.43	1.77	20	31.09	2.24	20	30.95	2.54
san400_0.7_2	24	25.66	1.91	21	28.88	3.73	21	28.82	1.90	21	29.63	1.66
san400_0.7_3	23	26.58	2.36	21	29.28	1.50	20	31.12	1.45	19	31.83	2.12
sanr200_0.7	100	0.45	0.09	100	0.27	0.06	100	0.25	0.06	100	0.25	0.13
sanr200_0.9	100	0.29	0.05	100	0.21	0.04	100	0.18	0.03	100	0.17	0.03