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Evolution towards the Maximum Clique

IMMANUEL M. BOMZE
Department of Statistics, Operations Research and Computer Science, University of Vienna, Vienna, Austria

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Abstract. As is well known, the problem of finding a maximum clique in a graph is NP-hard. Nevertheless, NP-hard problems may have easy instances. This paper proposes a new, global optimization algorithm which tries to exploit favourable data constellations, focussing on the continuous problem formulation: maximize a quadratic form over the standard simplex. Some general connections of the latter problem with dynamic principles of evolutionary game theory are established. As an immediate consequence, one obtains a procedure which consists (a) of an iterative part similar to interior-path methods based on the so-called replicator dynamics; and (b) a routine to escape from inefficient, locally optimal solutions. For the special case of finding a maximum clique in a graph where the quadratic form arises from a regularization of the adjacence matrix, part (b), i.e. escaping from maximal cliques not of maximal size, is accomplished with block pivoting methods based on (large) independent sets, i.e. cliques of the complementary graph. A simulation study is included which indicates that the resulting procedure indeed has some merits.

Key words: indefinite quadratic programming; replicator dynamics; evolutionary game; independent set

1. Introduction

Denote by $\#\mathcal{A}$ the number of elements of a finite set $\mathcal{A}$. Consider an undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with $\#\mathcal{V} = n$ vertices. A *clique* σ is a subset of the vertex set $\mathcal{V}$ which corresponds to a complete subgraph of $\mathcal{G}$ (i.e., any pair of vertices in σ is an edge in $\mathcal{E}$, the edge set). A clique σ is said to be *maximal* if there is no larger clique containing σ. A (maximal) clique is said to be a *maximum* clique if it contains most elements among all cliques. The search for such a maximum clique is an NP-hard problem, see, e.g. [17]; a comprehensive survey is provided in [25].

Methods termed "continuous-based heuristics" in [14] attack this problem by considering closely related nonlinear optimization problems. Most of them go back to the idea of Motzkin and Straus [21] who showed that $(1 - f^*)^{-1}$ is the size of a maximum clique if f^* denotes the optimal objective value of the indefinite quadratic program (QP)

$$f(x) = x' A_{\mathcal{G}} x \to \text{max!} \quad \text{subject to } x \in S^n, \tag{1.1}$$

where $A_{\mathcal{G}}$ denotes the adjacency matrix of the graph $\mathcal{G}$; a $'$ denotes transposition; and S^n is the standard simplex in n-dimensional Euclidean space $\mathbb{R}^n$,

$$S^n = \{x \in \mathbb{R}^n : x_i \geq 0 \quad \text{for all } i \in \mathcal{V}, e'x = 1\}.$$

Here and in the sequel, the letter e is reserved for a vector of appropriate length, consisting of unit entries exclusively. Note that to improve readability, the letters o and O (not 0) designate zero vectors and zero matrices of suitable size.

In [24], the Motzkin–Straus approach is used directly in a QP algorithm to determine maximum clique sizes, and to obtain sharp *a priori* lower bounds for this size. However, since the (local) solutions of (1.1) lack strictness, it is difficult to identify a maximum clique from the optimal objective value f^* of (1.1). In [27] and [15], this point is further elaborated. In particular, strategies are discussed to avoid spurious solutions to the Motzkin–Straus program (1.1), while [14] deals with a related approach using optimization of a quadratic function over the positive part of the Euclidean ball centered at zero with radius $1/\sqrt{k}$, to determine whether or not a clique with size at least k exists. The authors of [14] report that good cliques are obtained by relaxing from positivity, rounding, and estimating k.

In the present paper, we follow a different, evolutionary approach, as such seemingly novel in mathematical programming, but motivated by a textbook exercise [12, p. 300]. There the regularized version $\widehat{A_{\mathcal{G}}} = A_{\mathcal{G}} + \frac{1}{2} I_n$ is used instead of $A_{\mathcal{G}}$ in (1.1), where I_m denotes the $m \times m$ identity matrix. To be more precise, let $\widehat{A_{\mathcal{G}}} = [a_{ij}]_{i,j \in \mathcal{V}}$ with

$$a_{ij} = \begin{cases} \frac{1}{2} & \text{if } i = j \\ 1 & \text{if } (i,j) \in \mathcal{E}, \\ 0 & \text{else.} \end{cases} \tag{1.2}$$

Denote the face of S^n corresponding to a subset $\tau \subseteq \mathcal{V}$ of vertices by

$$S_\tau = \{x \in S^n : x_i = 0 \quad \text{if } i \notin \tau\};$$

its relative interior by

$$S_\tau^o = \{y \in S_\tau : y_i > 0 \quad \text{if } i \in \tau\};$$

and the barycentre of S_τ by

$$b_\tau = \frac{1}{\#\tau} \sum_{i \in \tau} e_i \in S_\tau,$$

where e_i denotes the i-th standard basis vector in $\mathbb{R}^n$, so that the i-th coordinate of b_τ is positive if and only if $i \in \tau$, in which case it equals $1/\#\tau$. As we will show in Section 3, x is a local solution to the problem

$$\hat{f}(x) = x' \widehat{A_{\mathcal{G}}} x \to \max! \quad \text{subject to } x \in S^n, \tag{1.3}$$

if and only if $x = b_\sigma$ for some maximal clique σ, in which case $\widehat{f}(x) = 1 - (2\#\sigma)^{-1}$. Hence the maximum clique corresponds to the global maximizer of (1.3). In sharp contrast to the methods using (1.1), where maximizers are usually not isolated, which creates difficulties in interpreting the result of a maximization routine in

terms of cliques, every local solution of (1.3) is isolated, see Section 3. While $A_{\mathcal{G}}$ can be used to obtain a sharp lower *a priori* bound for the size of the maximum clique [24, Corollary 1], the same arguments for $\widehat{A_{\mathcal{G}}}$ yield a lower bound which is not sharp.

The algorithm proposed works also for the more general problem

$$x'Ax \to \max! \quad \text{subject to } x \in S^n, \tag{1.4}$$

where A is an arbitrary symmetric $n \times n$ matrix, not necessarily of adjacency form (1.2). Note that the maximizers of (1.4) remain the same if A is replaced with $A + \gamma ee'$ where γ is an arbitrary constant. So without loss of generality assume henceforth that all entries of A are non-negative.

Of course, quadratic optimization problems like (1.4) are NP-hard [17], so it remains a challenging task to devise algorithms for solving this. The iterative procedure proposed in this paper consists of two parts. At first, a local solution of (1.4) will be generated very quickly; in the second step we escape from an inefficient local maximizer in a way such that improvement in the objective is guaranteed.

We start studying this general case in Section 2. Section 3 is devoted to the special case of finding the maximum clique, while in Section 4 some simulations are presented. In the Appendix, we prove a helpful inequality between powers of a quadratic form and the quadratic form of the respective power matrix.

2. Evolutionary Approach to Quadratic Programming on the Standard Simplex

Let us first consider the problem (1.4) of maximizing a general quadratic form over S^n. Most of the following results seem to be folklore in theoretical biology. However, the proofs appear to be somehow scattered in the literature, so that for the convenience of members of the optimization community the most important arguments will be repeated here in a concise way. To this end, we need some notions and notations. First consider the *generalized Lagrangian* $L(x; \lambda, \mu) = \frac{1}{2}x'Ax + \lambda'x + \mu(e'x - 1)$ of problem (1.4) where the multipliers λ_i (and μ) may have arbitrary sign. A critical point $x \in S^n$ of the generalized Lagrangian is said to be a *generalized* Karush–Kuhn–Tucker point if $L(x; \lambda, \mu) = \frac{1}{2}x'Ax$; i.e. if

$$\nabla_x L(x; \lambda, \mu) = o \quad \text{and} \quad \lambda'x = 0 \quad \text{for some } \lambda \in \mathbb{R}^n, \mu \in \mathbb{R}. \tag{2.1}$$

Now consider the following dynamical systems which operate on S^n:

$$\dot{x}_i(t) = x_i(t)[(Ax(t))_i - x(t)'Ax(t)], \quad i \in \mathcal{V}, \tag{2.2}$$

where a dot signifies derivative w.r.t. time t, and a discrete time version

$$x_i(t+1) = x_i(t)\frac{(Ax(t))_i}{x(t)'Ax(t)}, \quad i \in \mathcal{V}. \tag{2.3}$$

The *stationary points* under these dynamics, i.e. the points satisfying $\dot{x}_i(t) = 0$ for (2.2) or $x_i(t+1) = x_i(t)$ for (2.3), are the solutions of the equations

$$x_i[(Ax)_i - x'Ax] = 0, \quad i \in \mathcal{V}. \tag{2.4}$$

Hence the stationary points for both dynamics coincide, and it will turn out below that all local solutions of (1.4) are among these. Of course, there are quite many stationary points, e.g. all vertices e_i of S^n. However, only those which can be approximated by all nearby starting trajectories are serious candidates for strict local solutions: a stationary point x is said to be *asymptotically stable* if every solution to (2.2) or (2.3) which starts close enough to x, will converge to x as $t \nearrow \infty$.

Both (2.2) and (2.3) are called *replicator dynamics* in theoretical biology, since they are used to model evolution over time of relative frequencies $x_i(t)$ of interacting, self-replicating entities. Interaction is here described by the help of an $n \times n$-matrix A, which is not necessarily symmetric. The same dynamics arise in population genetics under the name *selection equations* where they are used to model time evolution of haploid genotypes, A being the fitness matrix here which is always symmetric.

From an optimization point of view, the difference between symmetric and non-symmetric matrices A is also crucial. Indeed, in the symmetric case the quadratic form $x(t)'Ax(t)$ is increasing along trajectories of the replicator dynamics (2.2) and (2.3) – this is the Fundamental Theorem of Selection going back to R. A. Fisher, J. B. S. Haldane, and S. Wright, see, e.g. [13] or [16].*

THEOREM 1. *If $A = A'$ then the function $x(t)'Ax(t)$ is strictly increasing with increasing t along any non-stationary trajectory $x(t)$ under (2.2) and (2.3). Furthermore, any such trajectory converges to a stationary point.*

Proof. First we deal with the continuous time dynamics (2.2): the time derivative of the objective is

$$\begin{aligned} \frac{d}{dt}[x(t)'Ax(t)] &= 2\dot{x}(t)'Ax(t) = \sum_{i \in \mathcal{V}} x_i(t)[Ax(t)]^2 - [x(t)'Ax(t)]^2 \\ &= \mathrm{Var}_{x(t)}(f) \geq 0, \end{aligned}$$

the variance of the quantity $f_i = [Ax(t)]_i$ if $x(t)$ is interpreted as a probability distribution over $\mathcal{V}$. Clearly, this variance is zero if and only if f_i does not depend on i almost surely w.r.t. $x(t)$, i.e. if and only if $x(t)$ satisfies (2.4). For dynamics (2.3), we make use of Lemma 13 – deferred to the Appendix – by choosing $m = 3$ and $B = [\sqrt{x_i(t)}a_{ij}\sqrt{x_j(t)}]_{i,j \in \mathcal{V}}$ as well as $p_i = \sqrt{x_i(t)}$. Then $x(t)'Ax(t) = p'Bp$ so

* However, this phenomenon is absent if A is not symmetric, which has been interpreted as supporting individual selection against the questionable theory of group selection in behavioural sciences.

that

$$[x(t)'Ax(t)]^3 = [p'Bp]^3 \le p'B^3p = \sum_{i,j,k,l} x_i(t)a_{ij}x_j(t)a_{jk}x_k(t)a_{kl}x_l(t)$$
$$= \sum_{j,k} x_j(t)[Ax(t)]_j a_{jk}x_k(t)[Ax(t)]_k$$
$$= [x(t)'Ax(t)]^2 x(t+1)'Ax(t+1),$$

whence the desired inequality $x(t)'Ax(t) \le x(t+1)'Ax(t+1)$ results. Equality holds only if $x_i(t) = 0$ or else if $[Ax(t)]_i$ does not depend on i, which means that (2.4) is satisfied by $x(t)$. In [19] it is shown that every trajectory converges to a stationary point. □

Under replicator dynamics in continuous time, the trajectory approaches its limit most efficiently in the sense that (2.2) is a gradient system if one uses the (non-Euclidean) Shahshahani metric [28], which for any point $p \in S^n$ is defined by

$$d_p(x,y) = \sum_{i:p_i>0} x_i y_i / p_i, \quad x, y \in S^n.$$

Note, however, that the limiting stationary point need not be a local solution of (1.4). This is clear when looking at the vertices of S^n which always constitute stationary points due to (2.4), or at any other non-minimizing stationary point. Moreover, there are even non-constant trajectories starting in the relative interior of s^n which end up in a (critical) saddle-point. See phase portrait No. 22 in [3] where

$$A = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 1 \\ -1 & 1 & 0 \end{bmatrix}.$$

Here, a trajectory in the relative interior exists which converges to $x = [\frac{1}{2}, \frac{1}{2}, 0]'$. However, $x'Ax = 0 < 6\varepsilon^2 = (x+\varepsilon u)'A(x+\varepsilon u)$ where $u = [-2, 1, 1]'$, and $x + \varepsilon u \in S^3$ if $0 < \varepsilon < \frac{1}{4}$. Hence we need for this (admittedly rare) case an *a priori* estimate for the maximum distance by which we could disturb a point like x without losing too much of the previously obtained improvement, i.e. to obtain a point nearby an improving stationary point which also improves the objective:

LEMMA 2. *For any symmetric $n \times n$ matrix A and $\sigma \subseteq \mathcal{V}$, denote by $\rho(A_\sigma)$ the spectral radius of A_σ, the matrix A restricted to $\sigma \times \sigma$. Assume that $z \in S_\sigma^o$ is a stationary point of (2.2) or (2.3) and let $x \in S^n$ be an arbitrary point with $\varepsilon = z'Az - x'Ax > 0$. Then any point $\tilde{x} \in S_\sigma$ with $\|\tilde{x} - z\| < \sqrt{\varepsilon/\rho(A_\sigma)}$ satisfies $\tilde{x}'A\tilde{x} > x'Ax$.*

Proof. Since both $\tilde{x}$ and z belong to S_σ, we may and do replace A with A_σ in the following estimation. Furthermore, due to (2.4) we have $\tilde{x}'Az = z'Az$ and

hence $|\tilde{x}'A\tilde{x} - z'Az| = |(\tilde{x}-z)'A(\tilde{x}-z)| \le \rho(A_\sigma)\|\tilde{x}-z\|^2$. Thus

$$\begin{aligned}\tilde{x}'A\tilde{x} - x'Ax &= \tilde{x}'A\tilde{x} - z'Az + z'Az - x'Ax \\ &> -|\tilde{x}'A\tilde{x} - x'Ax| + \varepsilon \\ &\ge \varepsilon - \|\tilde{x}-z\|^2\rho(A_\sigma) > 0,\end{aligned}$$

which shows the assertion. □

Now we provide the main characterization result which links optimization theory to the qualitative theory of dynamical systems.

THEOREM 3. *Let $A = A'$ be an arbitrary symmetric $n \times n$ matrix and $x \in S^n$. Consider the following properties:*

(a1) *x is an asymptotically stable stationary point of (2.2) and (2.3);*
(a2) *x is a strict local solution of (1.4);*
(b1) *x is a stationary point under (2.2) or (2.3), i.e. satisfies (2.4);*
(b2) *x is a generalized Karush–Kuhn–Tucker point for (1.4).*

Then (a1) $\Leftrightarrow$ (a2) $\Rightarrow$ (b1) $\Leftrightarrow$ (b2).

Proof. The implication (a1) $\Rightarrow$ (b1) is trivial. Hence we only have to show the equivalences.

(a1) $\Rightarrow$ (a2): Let x be asymptotically stable and choose a neighbourhood U of x in S^n such that any trajectory starting in a point $y \in U$ will converge to x. Then evidently $y'Ay < x'Ax$ for all $y \in U\backslash\{x\}$ due to Theorem 1.

(a2) $\Rightarrow$ (a1): Assume that x is a strict local solution to (1.4). Now put $v = x - y$ for any $y \in S^n$. Since $x'Ax - y'Ay$ can be written as $c'v - v'Av$ with $c'v \ge 0$ for all such v and $v'Av < 0$ if $c'v = 0$, straightforward compactness and continuity arguments entail that there is an $\varepsilon > 0$ and a $\rho > 0$ such that $x'Ax - y'Ay \ge \rho\|y - x\|$ if $y \in S^n$ and $\|y - x\| \le \varepsilon$. Choosing $\delta = \rho\varepsilon$ we thus see that the compact neighbourhood

$$U_\varepsilon = \{y \in S^n : y'Ay \ge x'Ax - \delta, \|y - x\| \le \varepsilon\}$$

of x in S^n is forward invariant, since Theorem 1 guarantees $y(t)'Ay(t) \ge y'Ay$ and thus $\|y(t) - x\| \le \varepsilon$ if $y(t)$ starts in $y \in U_\varepsilon$. Furthermore, Theorem 1 implies that the limit point $z = \lim_{t\nearrow\infty} y(t)$ exists and has to be stationary. But any stationary point $z \in U_\varepsilon$ has to satisfy (2.4) and thus $x'Ax = z'Ax = x'Az = z'Az$ if $\varepsilon > 0$ is so small that $x_i > 0$ implies $y_i > 0$ for all $y \in U_\varepsilon$. Therefore x is the only stationary point in U_ε, and hence the limit point of any trajectory starting in U_ε, which proves asymptotic stability of x.

(b1) $\Rightarrow$ (b2): since $\nabla_x L(x;\lambda,\mu) = Ax + \lambda + \mu e$ and because of (2.4), one may choose $\lambda = (x'Ax)e - Ax$ and $\mu = -x'Ax$ in order to satisfy both $\nabla_x L(x;\lambda\mu) = o$ and $L(x;\lambda,\mu) = \frac{1}{2}x'Ax$.

(b2) $\Rightarrow$ (b1): from $L(x;\lambda,\mu) = \frac{1}{2}x'Ax$ it follows $\lambda'x = 0$ and hence from $\nabla_x L(x;\lambda,\mu) = o$ we get

$$0 = x'o = x'Ax + x'\lambda + \mu = x'Ax + \mu,$$

which entails relation (2.4), using again $\nabla_x L(x;\lambda,\mu) = o$. □

In order to show finiteness of the complete algorithm presented below we need some further knowledge which guarantees that jamming cannot occur. To that end we need an auxiliary result due to Nachbar [23]:

LEMMA 4. *Suppose that a trajectory $y(t)$ under (2.2) or (2.3) converges to a point $z \in S^n$ as $t \to \infty$. Then $[Az]_i \leq z'Az$ for all i such that $y_i(0) > 0$.*

Proof. Assume that $[Az]_i > z'Az$. Then $U = \{y \in S^n : [Ay]_i > y'Ay\}$ is a neighbourhood of z in S^n, and therefore $y(t) \in U$ for all $t \geq T$ if T is large enough. But then $y_i(t) \geq y_i(T) > 0$ for all $t \geq T$ irrespective whether $y(t)$ is a trajectory under (2.2) or (2.3), which follows by $\dot{y}_i(t) > 0$ or $y_i(t+1)/y_i(t) > 1$, respectively. Hence $z_i = \lim_{t\to\infty} y_i(t) > 0$, which is absurd in view of (2.4) and of the fact that z is necessarily a stationary point. □

THEOREM 5. *For $x \in S^n$ let $\sigma = \{i \in \mathcal{V} : x_i > 0\}$. Assume that x satisfies* (a1) *(or* (a2)*, equivalently) of Theorem 3. Then*

(a) *$x'Ax > y'Ay$ for all $y \in S_\sigma$ with $y \neq x$;*

(b) *S_σ^o is contained in the basin of attraction of x.*

Proof. (a) For all $y \in S_\sigma$ we have, by (2.4),

$$y'Ax = \sum_{i\in\sigma} y_i[Ax]_i = e'y(x'Ax) = x'Ax$$

and hence $y'Ay < x'Ax$ follows from (a2) by considering the objective of $(1-\epsilon)x + \epsilon y$ for small $\epsilon > 0$.

(b) Suppose $y \in S_\sigma^o$ is the starting point of a trajectory under (2.2) or (2.3). Theorem 1 tells us that $y(t)$ converges to some point $z \in S_\sigma$, and hence $[Az]_i \leq z'Az$ for all $i \in \sigma$ due to Lemma 4. But then $x'Az \leq z'Az$. On the other hand, we have as in (a) $x'Az = z'Ax = x'Ax$. Hence property (a) guarantees $z = x$, which proves the claimed assertion. □

The algorithm proposed here (a) employs the maximization feature of the replicator dynamics; and (b) uses an escape procedure described below, if the trajectories are in the basin of attraction of an inefficient local solution of (1.4). This escape procedure consists of a finite check for global optimality, and delivers a globally improving feasible direction, if the current point is not the global solution.

For general non-convex quadratic minimization problems, a global optimality criterion has been proposed in [4]. This criterion has been used in [7] for an algorithm to obtain global solutions of the general quadratic problem. However, here we face the problem (1.4) with a special structure which we can exploit systematically to facilitate the above mentioned escape procedure.

THEOREM 6. *Suppose that $x \in S^n$ is a local solution to (1.4), and denote by $\sigma = \{i \in \mathcal{V} : x_i > 0\}$ the set of its positive coordinates (hence $x \in S^o_\sigma$). Then x is a global solution of (1.4) if and only if for all $i \in \sigma$, the $n \times n$-matrix*

$$Q_i = e_i(Ax)' + (Ax)e_i' - x_i A \tag{2.5}$$

is copositive with respect to the polyhedral cone

$$\Gamma_i = \{v \in \mathbb{R}^n : e'v = 0, v_r \geq 0 \text{ if } r \notin \sigma \text{ and } v_i/x_i \leq v_j/x_j \text{ for all } j \in \sigma\}, \tag{2.6}$$

which means that

$$v'Q_i v \geq 0 \quad \text{for all} \quad v \in \Gamma_i. \tag{2.7}$$

If there is a direction $v \in \Gamma_i$ such that $v'Q_i v < 0$, then $v_i < 0$ and

$$\tilde{x} = x - \frac{x_i}{v_i} v \in S^n$$

is a strictly improving feasible point.

Proof. see, e.g. [7]. □

While the above result is a specialization of the general criterion for global optimality in quadratic programming, and as such involves as many copositivity checks as there are non-binding constraints, it may be interesting to note that due to the special structures of objective and feasible set, there is a global optimality criterion which involves only one copositivity check:

THEOREM 7. *Let M be a simplicial polytope, i.e. there are some $h \in \mathbb{R}^n$, $\gamma > 0$, and an $m \times n$-matrix D such that $M = \{x \in \mathbb{R}^n : h'x = \gamma, Dx \geq o\}$ and $\Gamma = \mathbb{R}_+ M$ if $\Gamma = \{v \in \mathbb{R}^n : Dv \geq o\}$. Assume that $\overline{x} \in M$ is a feasible point of the problem*

$$f(x) = x'Ax \to \max! \quad \text{subject to } x \in M. \tag{2.8}$$

Then $\bar{x}$ is a global solution to (2.8) if and only if

$$Q_{\bar{x}} = f(\bar{x})hh' - \gamma^2 A$$

is Γ-copositive. If there is a direction $v \in \Gamma$ such that $v'Q_{\bar{x}}v < 0$, then for some $\alpha > 0$, the feasible point $\tilde{x} = \alpha v \in M$ improves the objective: $f(\tilde{x}) > f(\bar{x})$.

Proof. Evident from $x'Q_{\bar{x}}x = \gamma^2[f(\bar{x}) - f(x)]$. □

Thus the proposed algorithm runs as follows:

1. Initialisation: put $x = \frac{1}{n}e \in S^n$, or some other point in the relative interior of S^n if $\frac{1}{n}e$ satisfies (2.4);

2. follow the trajectory $y(t)$ under (2.3) – or under some faster discretization of (2.2), e.g., that in [10] – starting in $y(0) = x$ for a suitably long time, to obtain $z = \lim_{t\to\infty} y(t)$; denote by $\varepsilon = z'Az - x'Ax > 0$ the obtained improvement and by $\sigma = \{i : z_i > 0\}$;
3. if z is not asymptotically stable, pick a point $\tilde{x} \in S_\sigma$ with $\|z - \tilde{x}\| \leq \sqrt{\varepsilon/\rho(A_\sigma)}$ such that the trajectory $y(t)$ starting in $\tilde{x}$ converges to the relative boundary of S_σ (generically*, a randomly chosen starting point in S_σ^o within this range will satisfy this with probability one), and go to step 5; else z is asymptotically stable, i.e. a strict local solution;
4. to check whether or not z is the global solution, apply one of the escape procedures described in Theorems 6 or 7; if z is inefficient, an improving point $\tilde{x}$ is obtained;
5. $\tilde{x}$ improves the objective: $\tilde{x}'A\tilde{x} > x'Ax$, replace x with $\tilde{x}$ and go to step 2.

If the effort for all copositivity checks were more or less the same, one should of course prefer the criterion in Theorem 7. In the following section we shall see why the method of Theorem 6 may become important for large problems.

THEOREM 8. *Assume that all principal minors of A do not vanish. Then the above algorithm is almost surely finite in the sense that it uses finitely many steps in which a particular trajectory of (2.2) is followed.*

Proof. See [6]. □

Now let us sketch how to obtain from the preceding findings a global improvement strategy for general QPs of the form

$$g(x) = \frac{1}{2}x'Ax + c'x \to \text{max!} \quad \text{subject to} \quad x \in S^n. \tag{2.9}$$

Suppose that x is a local solution of (2.9), and we want to improve the current objective value $g(x)$. Without loss of generality, we may and do assume that $c_j > 0$, and as above $a_{ij} > 0$ for all i, j. Now consider the problem (1.4), where A is replaced with the positive matrix

$$A(x) = A + \frac{2}{c'x}cc',$$

and denote by $g(y : x) = \frac{1}{2}y'A(x)y$. then of course $g(x : x) = g(x)$ for all $x \in S^n$. Starting with x, employ the algorithm above to obtain a point $\tilde{x} \in S^n$ with $g(\tilde{x} : x) > g(x : x)$. Now if $c'\tilde{x} \leq c'x$, then obviously

$$g(\tilde{x}) = g(\tilde{x} : \tilde{x}) \geq g(\tilde{x} : x) > g(x : x) = g(x),$$

and we are done. On the other hand, if $c'\tilde{x} > c'x$, and if in addition $\tilde{x}'A\tilde{x} \geq x'Ax$, then we are done either since now we obtain directly $g(\tilde{x}) > g(x)$. But,

* A sufficient condition is that A_σ is nonsingular [6].

if unfortunately $\tilde{x}'A\tilde{x} < x'Ax$, then we can abandon the hope that there is an improvement possible along the direction of $\tilde{x} - x$. Nevertheless, we can now consider the problem (1.4) with the original A, and obtain via the same procedure a point $\hat{x}$ with $\hat{x}'A\hat{x} > x'Ax$. Joining the points $\hat{x}$ and $\tilde{x}$ by, e.g. a segment or another path, there thus is a fair chance to obtain an improving point $\bar{x}$ which satisfies $g(\bar{x}) > g(x)$. For instance, one can employ a-priori disturbance bounds from $\hat{x}$ as in Lemma 2, and proceed similarly for the linear part $c'(\tilde{x} - x)$. Then any point $\bar{x}$ in the intersection of the resulting discs improves the objective g.

3. Evolution towards the Maximum Clique

Now we adapt the general findings of the preceding section to the maximum clique problem, where $A = \widehat{A_{\mathcal{G}}}$ is given as in (1.2).

THEOREM 9. *Let $\mathcal{G}$ be a graph and consider problem (1.3). Then the following assertions are equivalent:*
(a) $x = b_\sigma = \frac{1}{k}\sum_{i\in\sigma} e_i$, where σ is a maximal clique of size $k = \#\sigma$;
(b) x is an asymptotically stable stationary point of (2.3) and (2.4);
(c) x is a strict local maximizer of $x'\widehat{A_{\mathcal{G}}}x$ over S^n, i.e., a strict local solution to (1.3).
(d) x is a local maximizer of $x'\widehat{A_{\mathcal{G}}}x$ over S^n, i.e., a local solution to (1.3).
If one of the above conditions (and therefore all) is met, the objective is $x'\widehat{A_{\mathcal{G}}}x = 1 - \frac{1}{2k}$. Hence σ is a maximum clique of $\mathcal{G}$ if and only if x is the global solution to (1.3).

Proof. (a) $\Rightarrow$ (b): if σ is a maximal clique, then for all $r \in \mathcal{V}\backslash\sigma$ we have $(i, r) \notin \mathcal{E}$ for at least one $i \in \sigma$ and hence

$$(\widehat{A_{\mathcal{G}}}x)_r = \frac{1}{k}\sum_{i\in\sigma} a_{ir} \leq \frac{k-1}{k}.$$

On the other hand completeness of σ yields, denoting by $M = \{(i, j) \in \sigma \times \sigma : i \neq j\}$,

$$x'\widehat{A_{\mathcal{G}}}x = \frac{1}{k^2}\left[\sum_{i\in\sigma}\frac{1}{2} + \sum_{(i,j)\in M} 1\right] = \frac{1}{2k} + \frac{k-1}{k} = (\widehat{A_{\mathcal{G}}}x)_i$$

for all $i \in \sigma$. Now suppose that $y \in S^n$ satisfies $y'\widehat{A_{\mathcal{G}}}x = x'\widehat{A_{\mathcal{G}}}x$. Then the strict inequalities $(\widehat{A_{\mathcal{G}}}x)_r < x'\widehat{A_{\mathcal{G}}}x$ for all $r \notin \sigma$ entail $y_r = 0$ for all such r, and hence

$$x'\widehat{A_{\mathcal{G}}}y = y'\widehat{A_{\mathcal{G}}}x = \sum_i y_i(x'\widehat{A_{\mathcal{G}}}x) = x'\widehat{A_{\mathcal{G}}}x = 1 - \frac{1}{2k}$$

while the Cauchy–Schwarz inequality yields $\frac{1}{k^2} = (y'x)^2 \leq (y'y)(x'x) = \frac{1}{k}(y'y)$ and hence

$$y'\widehat{A_{\mathcal{G}}}y = y'(ee' - \tfrac{1}{2}I_n)y = 1 - \tfrac{1}{2}y'y \leq 1 - \tfrac{1}{2k} = x'\widehat{A_{\mathcal{G}}}y$$

with equality only if $y = x$, which means that x is an evolutionarily stable strategy, the central solution concept of evolutionary game theory. From general principles in this field it follows that x has to be asymptotically stable; see, e.g. [32].

(b) $\Rightarrow$ (c) follows from Theorem 3 while (c) $\Rightarrow$ (d) is trivial.

(d) $\Rightarrow$ (a): let $\sigma = \{i \in \mathcal{V} : x_i > 0\}$ and suppose that σ is not complete, i.e. there is an edge $(i, j) \in M\backslash\mathcal{E}$. Then choose a suitably small $\delta > 0$ and put $y = x + \delta(e_i - e_j)$. Due to Theorem 3 we have $(\widehat{A_\mathcal{G}}x)_i = (\widehat{A_\mathcal{G}}x)_j$ since both i and j belong to σ. Hence

$$y'\widehat{A_\mathcal{G}}y = x'\widehat{A_\mathcal{G}}x + \delta^2 > x'\widehat{A_\mathcal{G}}x,$$

contradicting local optimality of x. Hence σ is complete. Therefore $B = ee' - \frac{1}{2}I_k$ if B is the modified adjacency matrix of $\mathcal{G}_\sigma$ and $k = \#\sigma$. Let $p = [x_i]_{i\in\sigma}$. Then $Bp = \mu e$ due to (2.4) and Theorem 3. On the other hand $e'p = 1$ whence $Bp = e - \frac{1}{2}p$ results. Therefore $p = \frac{1}{k}e$ and thus

$$x = \frac{1}{k}\sum_{i\in\sigma} e_i$$

as asserted. Now consider a node $r \in \mathcal{V}\backslash\sigma$. Since x is a local solution to (1.4) which has linear constraints, it has to satisfy the Karush–Kuhn–Tucker conditions, whence

$$o = \nabla_x L(x; \lambda, \mu) = \widehat{A_\mathcal{G}}x + \lambda + \mu e$$

results. Now $\lambda_r \geq 0$ and $\lambda' x = 0$ entails $(\widehat{A_\mathcal{G}}x)_r = -\lambda_r - \mu \leq -\mu = x'\widehat{A_\mathcal{G}}x$. On the other hand, $x'\widehat{A_\mathcal{G}}x = 1 - \frac{1}{2k}$ as established above, and so

$$\sum_{i\in\sigma} a_{ri} = k(\widehat{A_\mathcal{G}}x)_r \leq kx'\widehat{A_\mathcal{G}}x = k - \frac{1}{2} < k,$$

which shows that there must be an $i \in \sigma$ such that $(r, i) \notin \mathcal{E}$. Hence σ is a maximal clique. □

Since every local solution x of (1.3) is strict, there is no problem in identifying the clique σ from x. This is in sharp contrast to the emergence of spurious solutions to the Motzkin–Straus program (1.1) and thus avoids elaborate strategies to deal with this nuisance as in [15], [27]. See Section 4 for numerical evidence of this gain in reliability.

Essentially the same proof shows that a point $x \in S_\sigma^o$ is internally stable in either sense (e.g. is a local maximizer of $x'\widehat{A_\mathcal{G}}x$ on S_σ) if and only if $x = b_\sigma$, the barycenter of a face where σ is a clique. Furthermore, we can also gain some additional information if a trajectory stops at the barycenter b_τ of some face S_τ, even if τ is not a clique (note that by Lemma 4, every limit point z of a trajectory starting in the relative interior of S^n is a *Nash strategy*, i.e. satisfies $[Az]_i \leq z'Az$ for all $i \in \mathcal{V}$):

THEOREM 10. *Suppose τ contains at least a clique of size two. Then the following holds:*

(a) The barycenter b_τ is stationary under (2.2) or (2.3) if and only if the vertices in τ constitute a regular subgraph $\mathcal{G}_\tau$ of $\mathcal{G}$;

(b) b_τ is a Nash strategy if and only if $\mathcal{G}_\tau$ is regular but $\mathcal{G}_{\tau\cup\{r\}}$ is not for all $r \notin \tau$;[⋆]

(c) if b_τ is the limit point of a trajectory starting in the relative interior of S^n, then τ is either a maximal clique, or can contain subcliques of size at most $\frac{m}{2}$ if $m > 1$ is the size of τ.

Proof. (a) is evident from (2.4) and the observation that $[\widehat{A_\mathcal{G}} b_\tau]_i = \frac{1}{2m} + \frac{1}{m} d_\tau(i)$ for all $i \in \tau$, where

$$d_\tau(i) = \sum_{j\in\tau, j\neq i} a_{ij}$$

is the degree of i in $\mathcal{G}_\tau$. Indeed, (2.4) is here equivalent to the requirement that $d_\tau(i)$ does not depend on i for all $i \in \tau$, which means regularity of $\mathcal{G}_\tau$.

(b) is due to the fact that for any $r \notin \tau$, we have

$$\frac{1}{m} d_\tau(r) = [\widehat{A_\mathcal{G}} b_\tau]_r \leq b_\tau' \widehat{A_\mathcal{G}} b_\tau = \frac{1}{2m} + \frac{1}{m} d_\tau(i)$$

if and only if $d_\tau(r) < d_\tau(i)$ which entails $a_{ir} = 0$ for at least one $i \in \tau$. Hence $d_{\tau\cup\{m\}}(i) = d_\tau(i) = d_\tau(j)$ for all $j \in \tau$. Now if $\tau \cup \{m\}$ were regular, too, then this would entail also $d_{d\cup\{m\}}(j) = d_\tau(j)$ for all $j \in \tau$, and hence $a_{jr} = 0$ which means $0 = d_\tau(r) = d_{\tau\cup\{m\}}(r) = d_{\tau\cup\{m\}}(i) = d_\tau(i) \geq 1$, which is absurd.

(c) is a consequence of Lemma 4 and the result 19. in [2, p. 86]. □

Evidently, Theorem 10 yields together with the preceding remark on internal stability the assertion of Theorem 9. Let us now shortly discuss the disturbance bound $\sqrt{\varepsilon/\rho(A_\sigma)}$ from Lemma 2 used in step 3 of the above algorithm if $A = \widehat{A_\mathcal{G}}$ and $z = b_\sigma$. Then of course $\mathcal{G}_\sigma$ is a regular graph and $P_\sigma = (\frac{1}{2} + d_\sigma)^{-1} A_\sigma$ is a (doubly) stochastic and symmetric matrix with Perron eigenvector b_σ. Since both z and $\tilde{x}$ belong to S_σ, the difference is perpendicular to this eigenvector (indeed, $b_\sigma'(\tilde{x} - z) = \frac{1}{k} - \frac{1}{k} = 0$), and hence the estimate for the quadratic form in the proof of Lemma 2 could be improved to

$$|(\tilde{x} - z)' A_\sigma (\tilde{x} - z)| \leq |\lambda_2(P_\sigma)| (\tfrac{1}{2} + d_\sigma) \|\tilde{x} - z\|^2,$$

where $\lambda_2(P_\sigma)$ denotes the eigenvalue of P_σ with largest modulus smaller than one, i.e.

$$|\lambda_i(P_\sigma)| \leq |\lambda_2(P_\sigma)| < 1 \quad \text{for all eigenvalues } \lambda_i(P_\sigma) \neq 1.$$

Since P_σ is the transition matrix of a ergodic reversible Markov chain, several estimates for $|\lambda_2(P_\sigma)|$ can be obtained, see, e.g. [29], [30, pp. 46f.], and references

[⋆] If both $\mathcal{G}_\tau$ and $\mathcal{G}_{\tau\cup\{r\}}$ are regular, both τ and $\tau \cup \{r\}$ are cliques.

therein. Now suppose that we have arrived at a maximal clique σ of size k. At first we remove all nodes of degree less than k. If less than $k+1$ nodes have at least degree k, stop: σ is the maximum clique. Else one has to apply one of the escape procedures. For instance, we can make use of both auxiliary problems (1.1) and (1.4) to arrive at the following application of Theorem 7 to the maximum clique problem:

THEOREM 11. *Let σ be a maximal clique of size k. Then the following assertions are equivalent:*

(a) σ is a maximum clique;

(b) $Q_k = (2k-1)ee' - 2kA_{\mathcal{G}}$ is $\mathbb{R}^n_+$-copositive;

(c) $R_k = (k-1)ee' - kA_{\mathcal{G}}$ is $\mathbb{R}^n_+$-copositive.

Proof. For $M = S^n$ we have $h = e$; $\gamma = 1$; and $D = I_n$ as well as $\Gamma = \mathbb{R}^n$, in the notation of Theorem 7. Now observe that with $f(x) = x'\widehat{A_{\mathcal{G}}}x$, we have for $\bar{x} = b_\sigma$ the objective value $f(\bar{x}) = (1 - \frac{1}{2k})$ and hence

$$Q_{\bar{x}} = \left(1 - \frac{1}{2k}\right) ee' - \widehat{A_{\mathcal{G}}} = \left(\frac{1}{2} - \frac{1}{2k}\right) ee' - A_{\mathcal{G}} = \frac{1}{2k} Q_k,$$

while for $f(x) = x'A_{\mathcal{G}}x$ we get similarly $Q_{\bar{x}} = \frac{1}{k}R_k$. □

Checking copositivity is NP-hard. Of course, one can apply the full arsenal of shortcut methods as described in [5, section 4] to obtain an improvement efficiently, or else to establish global optimality. Unfortunately, neither Q_k nor R_k have any negative definite principal submatrices, so one cannot hope for essential reduction of the number of emerging subproblems if one follows a block pivoting strategy as in [5].

This, however is possible in choosing the criterion of Theorem 6, exploiting the special structure of (1.3) in an efficient way. Interestingly enough, this approach is in some sense counter-greedy: indeed, it rests on the use of *independent sets*, i.e. cliques of the complementary graph $\overline{\mathcal{G}}$ with regularized adjacency matrix $\widehat{A_{\overline{\mathcal{G}}}} = ee' - \widehat{A_{\mathcal{G}}}$. The reason for this phenomenon is that any principal submatrix of $\widehat{A_{\mathcal{G}}}$ is indefinite unless it belongs to an independent set when it coincides with $\frac{1}{2}I_m$ where m is the size of the independent set.

Hence, given a maximal clique σ of size k, search for a maximal independent set $\tau \subset \mathcal{V}\backslash\sigma$, by applying the previous procedure to the corresponding submatrix of $ee' - \widehat{A_{\mathcal{G}}}$. (If τ is a singleton, then the complement of σ is also a clique, and we may replace σ with its complement if the latter has more members; in these cases the block pivoting algorithm reduces to an ordinary pivoting step.)

We will now show that, unlike the general case treated in [5], block pivoting by means of a maximal independent set yields only a moderate number (namely $m+1$) of generated subproblems detecting copositivity of considerably smaller

matrices. To this end, we need some more notation. Partition the matrices Q_i from (2.5) with $A = \widehat{A_{\mathcal{G}}}$ and $x = b_\sigma$ according to the sets τ and $\mathcal{V}\backslash\tau$ as follows:

$$Q_i = \begin{bmatrix} A_i^{(\tau)} & B_i^{(\tau)} \\ [B_i^{(\tau)}]' & C_i^{(\tau)} \end{bmatrix}.$$

For $j \in \tau$ denote by r_j' the j-th row of $B_i^{(\tau)}$. We also introduce the square matrices of order $n - m$

$$Q_{i,j}^{(\tau)} = \begin{cases} C_i^{(\tau)}, & \text{if } j = 0; \\ C_i^{(\tau)} - e r_j' - r_j e' - \frac{1}{2m} e e', & \text{if } j \in \tau. \end{cases}$$

Finally, put

$$\Gamma_i^{(\tau)} = \{z \in \mathbb{R}^{\mathcal{V}\backslash\tau} : e'z \le 0, z_\ell \ge 0 \text{ if } \ell \notin \sigma, z_i \le z_j \text{ if } j \in \sigma\},$$

as well as

$$\Gamma_{i,j}^{(\tau)} = \begin{cases} \{z \in \Gamma_i^{(\tau)} : e'z = 0 \text{ and } B_i^{(\tau)} z \ge 0\}, & \text{if } j = 0, \\ \{z \in \Gamma_i^{(\tau)} : r_s' z \ge r_j' z + \frac{1}{2m} e'z \text{ for all } s \in \tau\}, & \text{if } j \in \tau. \end{cases}$$

THEOREM 12. *Suppose that σ is a maximal clique of size k and that every node has at least degree k. Pick a (disjoint) maximal independent set τ of size $m \le n-k$. Then Q_i is copositive w.r.t. the cone Γ_i (2.6) if and only if the following $m+1$ copositivity conditions on square matrices of order $n-m$ are satisfied:*

$$Q_{i,j}^{(\tau)} \quad \textit{is} \quad \Gamma_{i,j}^{(\tau)}\textit{-copositive for all } j \in \tau \cup \{0\}.$$

Moreover, in the negative case we obtain the following improving feasible direction (cf. Theorem 6):

(a) If $z \in \Gamma_{i,0}^{(\tau)}$ satisfies $z' Q_{i,0}^{(\tau)} z < 0$, then $v = \begin{bmatrix} o \\ z \end{bmatrix} \in \Gamma_i$ satisfies $v' Q_i v < 0$;

(b) If $z \in \Gamma_{i,j}^{(\tau)}$ satisfies $z' Q_{i,j}^{(\tau)} z < 0$ for some $j \in \tau$, then $v \in \mathbb{R}^n$ with coordinates

$$v_s = \begin{cases} -e'z, & \text{if } s = j, \\ 0, & \text{if } s \in \tau\backslash\{j\}, \\ z_s, & \text{if } s \in \mathcal{V}\backslash\tau. \end{cases}$$

satisfies $v \in \Gamma_i$ and $v' Q_i v < 0$.

Proof. First note that under the assumptions of the theorem, (2.5) entails that $A_i^{(\tau)} = -\frac{1}{2k} I_m$ is negative definite, so that Theorem 6 and Remark 6 in [5] apply to Q_i instead of Q, and Γ_i instead of Γ. So without loss of generality, let us assume for the moment that $\tau = \{1, \ldots, m\}$; that $i = n$ and that $\sigma = \{n-k+1, \ldots, n\}$. Then (2.6) with $x = b_\sigma$ tells us that $\Gamma_i = \{v \in \mathbb{R}^n : D_i v \ge o\}$ with

$$D_i = \left[\begin{array}{c|c} e' & e' \\ -e' & -e' \\ I_m & O \\ O & R \end{array}\right] = [E|F]$$

where O denote zero matrices of suitable size, and R is the $(n-m-1)\times(n-m)$-matrix

$$R = \left[\begin{array}{c|c|c} I_{n-m-k} & O & o \\ O & I_{k-1} & -e \end{array}\right].$$

Recall that e here is generic notation for vectors, consisting of unit entries, of (possibly) different length. The partition of D_i into the $(n+1)\times m$-matrix E and the $(n+1)\times(n-m)$-matrix F corresponds to the indices belonging to τ, or $\mathcal{V}\backslash\tau$, respectively. First note that $Ew \geq o$ trivially implies $w = o$, so that the cone Γ_0 in Theorem 6 of [5] is trivial. Hence we can concentrate on condition (b) of that theorem. Now for any list I of row indices and its complement $J = \{1,\ldots,n+1\}\backslash I$ partition E and F accordingly:

$$E = \begin{bmatrix} E_I \\ E_J \end{bmatrix} \quad \text{and} \quad F = \begin{bmatrix} F_I \\ F_J \end{bmatrix}.$$

Next we have to identify the system

$$\mathcal{I}^{\square} = \{I \subset \{1,\ldots,n+1\} : E_I \text{ is square and nonsingular}\}.$$

Suppose $I \in \mathcal{I}^{\square}$. Obviously, I contains no index exceeding $m+2$. Furthermore, either $I = \{3,\ldots,m\}$ (this is Case (0) below); or I contains exactly one of the indices $\{1,2\}$ corresponding to $\pm e'$. We distinguish Case $(+)$ where $1 \in I$, and Case $(-)$ where $2 \in I$. In either of the Cases $(\pm)$, there is exactly one $j \in \tau\backslash I$. For all cases, we now calculate $\Gamma_I^{\square}$ and $Q_I^{\square}$.

Case (0). Here $E_I = I_m$, $F_I = O$ while $E_J = [e|-e|O]'$ and $F_J = [e|-e|R']'$. Hence $Q_I^{\square} = C_i^{(\tau)} = Q_{i,0}^{(\tau)}$ and

$$\Gamma_I^{\square} = \{z \in \mathbb{R}^{\mathcal{V}\backslash\tau} : B_i^{(\tau)} z \geq 0 \text{ and } F_J z \geq o\}.$$

But since $F_J z \geq o$ is equivalent to $e'z = 0$ and $Rz \geq o$ we by definition of R arrive at $\Gamma_I^{\square} = \Gamma_{i,0}^{(\tau)}$.

Case $(+)$. Denote by $j \in \tau$ the index of the row not occurring in E_I, and by P_j the (symmetric, involutive) $m \times m$ permutation matrix which interchanges the first and the j-th column of a matrix if postmultiplied. Of course premultiplication does the same with rows so that, e.g., $r_j' = e_1' P_j B_i^{(\tau)}$ if $e_1' = [1,0,\ldots,0]$. Then we have

$$E_I = \left[\begin{array}{c|c} 1 & e' \\ o & I_{m-1} \end{array}\right] P_j \quad \text{and} \quad F_I = \begin{bmatrix} e' \\ O \end{bmatrix}$$

while

$$E_J = \begin{bmatrix} -e' \\ e_1' \\ O \end{bmatrix} P_j \quad \text{and} \quad F_J = \begin{bmatrix} -e' \\ o' \\ R \end{bmatrix}.$$

Straightforward calculations then yield $E_I^{-1}F_I = P_j[\begin{smallmatrix} e' \\ O \end{smallmatrix}]$ so that

$$Q_I^{\square} = C_i^{(\tau)} - [e|O]P_jB_i^{(\tau)} - [B_i^{(\tau)}]'P_j \begin{bmatrix} e' \\ O \end{bmatrix} - \frac{1}{2k}[e|O] \begin{bmatrix} e' \\ O \end{bmatrix} = Q_{i,j}^{(\tau)}$$

and $\Gamma_I^{\square} = \{z \in \mathbb{R}^{\mathcal{V}\setminus\tau} : G_I z \geq o \text{ and } H_I z \geq o\}$ with

$$\begin{aligned} G_I &= (E_I')^{-1}\left[B_i^{(\tau)} + \frac{1}{2k}E_I^{-1}F_I\right] \\ &= \left[\begin{array}{c|c} 1 & o' \\ -e & I_{k-1} \end{array}\right] P_jB_i^{(\tau)} + \frac{1}{2k}\left[\begin{array}{c|c} 1 & o' \\ -e & I_{k-1} \end{array}\right]\begin{bmatrix} e' \\ O \end{bmatrix} \\ &= \left[\begin{array}{c|c} 1 & o' \\ -e & I_{m-1} \end{array}\right] P_jB_i^{(\tau)} + \frac{1}{2k}\begin{bmatrix} e' \\ -ee' \end{bmatrix} \end{aligned}$$

and

$$H_I = F_J - E_JE_I^{-1}F_I = \begin{bmatrix} -e' \\ o' \\ R \end{bmatrix} - \begin{bmatrix} -e' \\ e_1' \\ O \end{bmatrix}\begin{bmatrix} e' \\ O \end{bmatrix} = \begin{bmatrix} o' \\ -e' \\ R \end{bmatrix}$$

wherefrom one can easily deduce that

$$\Gamma_I^{\square} = \left\{z \in \Gamma_{i,j}^{(\tau)} : r_j'z + \frac{1}{2k}e'z \geq 0\right\}.$$

Case $(-)$. Now

$$E_I = \left[\begin{array}{c|c} -1 & -e' \\ o & I_{m-1} \end{array}\right] P_j \quad \text{and} \quad F_I = \begin{bmatrix} -e' \\ O \end{bmatrix}, \quad \text{hence again}$$
$$E_I^{-1}F_I = P_j \begin{bmatrix} e' \\ O \end{bmatrix}$$

while

$$E_J = \begin{bmatrix} e' \\ e_1' \\ O \end{bmatrix} P_j \quad \text{and} \quad F_J = \begin{bmatrix} e' \\ o' \\ R \end{bmatrix}.$$

As in Case $(+)$ one obtains also in this case $Q_I^{\square} = Q_{i,j}^{(\tau)}$ but now

$$\Gamma_I^{\square} = \left\{z \in \Gamma_{i,j}^{(\tau)} : r_j'z + \frac{1}{2k}e'z \leq 0\right\}.$$

For fixed $j \in \tau \not\in I$, one thus can merge both cases into one copositivity condition, namely that $Q_{i,j}^{(\tau)}$ be $\Gamma_{i,j}^{(\tau)}$-copositive. Therefore Theorem 6 of [5] yields the claimed characterization of Γ_i-copositivity of Q_i. Also assertions (a) and (b) follow from (b2) of that theorem. □

Table I. Comparison of replicator dynamics based on Comtet versus Motzkin and Straus.

Result/density	0.1	0.75	0.5	0.75	0.9	total
Comtet better	74	71	64	54	67	330
same clique size	40	25	36	29	26	156
Motzkin–Straus better	26	44	40	57	46	213
Comtet fails	0	0	1	1	3*	5
Motzkin–Straus fails	55	61	50	29	16*	211

*: one case where both fail is not included. See text.

Note that unlike the general case treated in [5], block pivoting by means of a maximal independent set yields only a moderate number (namely $m + 1$) of generated subproblems detecting copositivity of considerably smaller matrices. These observations seem to justify the hope that the proposed procedure has indeed some merits, which is supported also by first, very encouraging empirical evidence. This is the subject of the next section.

4. Empirical Findings

Recently, Pelillo [26] has performed extensive simulation to assess the quality of a very similar approach, namely to employ replicator dynamics (2.3) with $A = A_{\mathcal{G}}$ instead of $A = \widehat{A_{\mathcal{G}}}$. Interestingly enough, this optimization model emerged as a special relaxation labeling network, a parallel distributed computational model extremely popular in computer vision and pattern recognition. In the first part of [26], 3100 randomly generated graphs with up to $n = 500$ nodes were considered and the performance of local optimization of (1.1) by following the paths of (2.3) was compared to well-known exact clique finding algorithms, the backtracking procedure by Bron and Kerbosch [9], and the partially enumerative algorithm by Callaghan and Pardalos [11]. With the exception of dense graphs of order exceeding $n = 100$ where the latter methods have been excessively slow, Pelillo reported quite satisfying results both on quality and speed of his algorithm (see Tables I through III in [26]), although he stresses again the problem of spurious solutions to the Motzkin–Straus program.

Hence in a first attempt to assess the properties of the Comtet-based algorithm proposed here we investigated the behaviour of this and Pelillo's path-following methods on a total of 700 randomly generated graphs of order $n = 10$ up to $n = 500$ with varying expected density $\delta = 0.1$; 0.25; 0.5; 0.75; and 0.9. Both dynamical systems have been iterated equally long, and the results are shown in Table I. The resulting points were used to extract subsets of vertices in the same way as in Section 3 above, and if this is not a clique, a failure is reported. Superiority is measured by sizes of the cliques found.

Summarizing Table I, one finds that replicator dynamics based on Comtet is beaten by that based on Motzkin and Straus in only 30% of the cases, but is more reliable by far, since it cannot produce spurious solutions. This may be seen as an indication that the positive features of the Motzkin–Straus program as reported in [26] *a fortiori* carry over to the Comtet program. Interestingly, only in very small (and sparse) graphs and very rarely, identical cliques have been produced by both algorithms (a total of 26), as opposed to the number of cases (156) where both clique sizes are the same. As this is the only feature where the order matters, it is more transparent to show the figures aggregated over the orders $(n = 10, 20, \ldots, 100, 200, \ldots, 500)$ in Table I.

Increasing the number of iterations in case of $n = 75$, as a moderate order example, seems to have no effect to remove the occurrence of spurious solutions to the Motzkin–Straus program while reliability of Comtet-based replicator approach is increased. This observation backs the conjecture expressed as the end of [26], and it seems that while this study has been performed in ignorance of that article, the Comtet regularization indeed provides the proper penalty term addressed in [26] to remove the nuisance of spurious solutions. For each density as in Table I, ten randomly drawn graphs of order $n = 75$ were investigated. The asymptotic maximum clique size in a graph with n nodes and expected density δ is determined by Matula's formula

$$M(n, \delta) = 2 \log_{1/\delta} n - 2 \log_{1/\delta} \log_{1/\delta} n + 2 \log_{1/\delta} \frac{e}{2} + 1.$$

As n gets large, the probability that maximum clique size takes the two nearest integer neighbours of $M(n, \delta)$ tends to one [18], [2]. However, one has to be aware of the caveats expressed by [18] with regard to high density graphs. Both algorithms have been iterated 500 times, a number far beyond the median number of iterations required as reported in [26]. The results are contained in Table II. Still 10% failures occurred with the Motzkin–Straus program as opposed to none with the Comtet approach, indicating that not only numerical reasons are responsible for this behaviour. As a rough quality measure, the sizes of cliques found were divided by the number of cases where no failure occurred, and still these averages do not differ too much from each other.

To obtain an absolute picture, a larger simulation study has been performed. A total of 4000 randomly drawn graphs were investigated by the package `Mathematica` [33], using the built-in routine `MaximumClique` [31], a straight forward enumerative procedure which becomes prohibitively slow for dense graphs with order exceeding $n = 17$. Thus we generated 100 graphs of each order from $n = 10$ to $n = 17$, with the same expected densities as in Table I. The results are reported in Table III, where *ineff* counts the cases where a clique is returned which does not have maximal size (note that the proposed algorithm never failed to produce a clique!); *ave.clique size* refers to the average size of the maximum clique; and *time* is a discretized indicator of relative CPU time effort compared to `Mathematica`'s routine `MaximumClique`, which is obtained in the following way: let q denote the

Table II. Average clique sizes relative to the number of cliques found: Comtet versus Motzkin and Straus. See text.

Result/density	0.1	0.25	0.5	0.75	0.9
Comtet better	1	3	3	3	6
same clique size	7	5	4	4	1
Motzkin/Straus better	2	2	3	3	3
Ave.clique size (Comtet)	3.00	4.20	6.60	11.5	21.0
Ave.cl.size (Motzkin/Straus)	3.11	4.37	6.86	11.6	15.1
Asympt.max.clique size	4.47	6.03	9.07	14.3	18.3

Table III. Performance of replicator dynamics based on Comtet. Format of main entries: *ineff/ave.clique size/time*. See text.

nodes/density	0.1	0.25	0.5	0.75	0.9	tot.escape steps
10	0/2.06/−3	1/2.74/−1	1/3.83/−1	2/5.62/−0	0/7.26/−1	24
11	0/2.20/−3	3/2.95/−1	0/4.19/+0	1/5.81/+0	1/8.02/−0	39
12	0/2.17/−2	2/2.98/−1	0/4.32/+0	1/6.21/+1	1/8.58/+0	37
13	0/2.18/−2	2/3.11/−2	0/4.40/+1	1/6.58/+1	0/8.87/+1	47
14	1/2.28/−2	3/3.16/−0	1/4.83/+1	1/6.89/+1	2/9.49/+1	68
15	1/2.37/−1	1/3.23/−0	3/4.85/+1	1/7.14/+2	2/9.75/+1	78
16	2/2.36/−1	4/3.30/+0	3/4.80/+2	5/7.38/+3	1/10.6/+2	100
17	4/2.47/−1	2/3.36/+1	6/5.01/+3	4/7.66/+3	2/10.8/+3	115
tot.escape steps	64	111	140	135	58	508

ratio of the average time consumed when running our algorithm (150 iterations) in the way described above, with the escape step replaced by simply removing one element from a non-maximum clique after another from the graph and restarting the procedure, divided by the average time used by `MaximumClique`. Then the values of $+3; +2; +1; +0; -0; -1; -2; -3$ are returned whenever q falls into the ranges with the following boundaries: 0; 0.05; 0.1; 0.5; 1; 2; 10; 20; ∞.

Apart from the obvious advantage as far as time is concerned, Table III suggests that the problematic densities where no global minimum is encountered during the first local search, are indeed 0.5 and 0.75, in which cases the comparison between Comtet and Motzkin–Straus-based algorithm is not so clear in Tables I and II. So there is even more hope to increase efficiency with the implementation of the copositivity checking devices described in the previous section. Note that a maximum clique has not been detected in mere 1.6% of the cases. Of course, a large simulation study and detailed comparisons are necessary to establish the algorithm for practical purposes, especially in view of recent DIMACS challenges (cf. [14]). First experiences with this project (without an escape step) are reported in [8].

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Appendix: Lemma 13

If B is a positive symmetric $(n \times n)$ matrix and p is a non-negative vector with $\|p\|^2 = \sum_i p_i^2 = 1$, then for any positive integer m we have

$$[p'Bp]^m \leq p'B^m p.$$

Equality obtains if and only if p is the (unique) eigenvector of B belonging to the dominating eigenvalue.

Proof. We proceed by induction on n, the order of B. Denote by $\lambda_1, \ldots, \lambda_n$ the eigenvalues of B. Due to Perron's theorem [1, p. 278], there is a positive, dominating eigenvalue with multiplicity one, λ_1 say, with a positive eigenvector w_1. Let $u = [u_1, \ldots, u_n]'$ denote the coordinates of p in the orthonormal basis $w_1, \ldots, w_n$ of eigenvectors of B, put $v_i = u_i^2$, and define $T(v) = \sum_{i=1}^n \sqrt{v_i} w_i$. Then T maps the standard simplex S^n continuously in the unit sphere in $\mathbb{R}^n$, and the region $R = \{v \in S^n : T(v) \geq o\}$ is contained in the polytope $P = \{v \in S^n : a_1'v \geq 0\}$, where $a_k = [\lambda_1^k, \ldots, \lambda_n^k]' \in \mathbb{R}^n$ for any positive integer k. Indeed, for any such k we have $a_k'v = \sum_i \lambda_i^k u_i^2 = p'B^k p > 0$ if $T(v) = p \geq o$ and $u_i^2 = v_i$. Now denote by

$$f(v) = a_m'v - [a_1'v]^m = p'B^m p - [p'B_p]^m,$$

and consider the problem to minimize f over R. Since $D_v^2 f(v) = -m(m-1)[a_1'v]^{m-2} a_1 a_1'$, f is concave on the polytope P, thus it is also concave on the region R. Now consider any p in the image of R under T, i.e. $T(v) = p \geq o$, which does not coincide with the strictly positive eigenvector w_1 corresponding to the Perron eigenvalue λ_1. Then necessarily $v \neq z = [1, 0, \ldots, 0]'$. The ray through v emanating from z hits the boundary of S^n in a point $\tilde{v}$ which satisfies $\tilde{v}_1 = 0$ and hence $\tilde{p} = T(\tilde{v}) = \sum_{i=2}^n \sqrt{\tilde{v}_i} w_i$ is perpendicular to w_1. Hence $\tilde{p}$ must have a negative coordinate and thus does not belong to the non-negative orthant, i.e. $\tilde{v} \notin R$. For continuity reasons, there has to be a point $\bar{v} \in R$ on the ray such that v is a convex combination of z and $\bar{v}$; and that $\bar{p} = T(\bar{v})$ is on the boundary of the non-negative orthant, i.e. $\bar{p}_j \geq 0$ and (w.l.o.g.) $\bar{p}_1 = 0$. From concavity of f on R we conclude $f(v) \geq \max\{f(z), f(\bar{v})\} = \max\{0, f(\bar{v})\}$. Partitioning

$$B = \begin{bmatrix} \alpha & | & q' \\ q & | & C \end{bmatrix} \quad \text{and} \quad B^m = \begin{bmatrix} \alpha_m & | & q_m' \\ q_m & | & C_m \end{bmatrix},$$

where C and C_m are square matrices of order $n-1$, we immediately see from strict positivity of B that all entries of C_m exceed those of the power matrix C^m, so that putting $y = [\bar{p}_2, \ldots, \bar{p}_n] \in \mathbb{R}^{n-1}$ we arrive at

$$f(\bar{v}) = \bar{v}'B^m\bar{v} - [\bar{v}'B\bar{v}]^m = y'C_m y - [y'Cy]^m > y'C^m y - [y'Cy]^m \geq 0$$

by induction hypothesis. Hence any such $p = T(v) \in T(R)$ satisfies $f(v) > 0$. Of course one cannot be sure that T maps R onto S_+, the intersection of the unit ball with the non-negative orthant, but the same reasoning applies to any map T_s of the form $T_s(v) = \sum_{i=1}^{n} s_i \sqrt{v_i} w_i$ where $s = [s_1, \ldots, s_n]'$ is an arbitrary sequence of signs. The assertion of the lemma then follows from the fact that $p' B^k p = a_k' v$ if $T_s(v) = p$ and $S_+ \subseteq \bigcup_{s \in \{-1,1\}^n} T_s(P)$. □

The above method of proof differs from that in [22]. for instance, here it is immediately evident that the sign restriction on p can be dispensed with if m is even, or if B is a positive semidefinite matrix with entries of arbitrary sign. Indeed, in these cases f is concave on the whole of S^n, and therefore attains its minimal value at the vertices, where it has value zero, so that the inequality of Lemma 13 holds for *all* p with $p'p = 1$. Note further that for establishing the inequality of Lemma 13, symmetry of B is not required, since only quadratic forms are involved. The uniqueness result then refers to p being the Perron eigenvector of $B + B'$. Hence Lemma 13 bears some similarity with the result of Loewy and London [20, p. 179] which in the above terminology would read $f(\frac{1}{n}e) \geq 0$.

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