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Approximating the cone of copositive kernels to estimate the stability number of infinite graphs

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Abstract

It has been shown that the stable set problem in an infinite compact graph, and particularly the kissing number problem, reduces to an optimization problem over the cone of copositive kernels. We propose two converging hierarchies approximating this cone. Both are extensions of existing inner hierarchies for the finite dimensional copositive cone. We implement the first two levels of the new hierarchies for the kissing number problem.

Keywords: copositive programming, semidefinite approximations, lifting, kissing number

1 Introduction

Consider the stable set problem in an infinite dimensional undirected graph $G = (V, E)$. This problem is motivated by fundamental combinatorial optimization arrangements, such as sphere packings, convex body packings, binary codes and spherical codes [5]. The *kissing number* problem, for which

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we implement our hierarchies, is an instance of the spherical codes problem. Following de Laat and Vallentin [6], we work with *compact topological packing graphs*, graphs whose vertex set is compact and every finite clique is contained in an open clique. The stability number of these graphs is finite.

Let $V \subset \mathbb{R}^n$ be a compact set. Denote the space of real-valued continuous functions on V by $C(V)$. We call *kernels* the following subset of continuous functions: $\mathcal{K}(V) = \{K \in C(V \times V) : K(x,y) = K(y,x),\ \forall\, x, y \in V\}$. A kernel K is said to be *copositive* if any finite principal submatrix of K is copositive [4]. We denote copositive kernels on V by $\mathcal{COP}(V)$. The stability number of $G = (V, E)$ is the optimal solution to the following problem [4]:

$$\begin{aligned} \alpha(G) = \inf_{K \in \mathcal{K}(V),\ \lambda \in \mathbb{R}} \quad & \lambda \\ \text{s.t.} \quad & K \in \mathcal{COP}(V) \\ & K(v,v) = \lambda - 1 && \text{for all } v \in V \\ & K(u,v) = -1 && \text{for all } (u,v) \notin E. \end{aligned} \tag{1}$$

Optimization over $\mathcal{COP}(V)$ is NP-hard even for finite V, so the goal is to replace $\mathcal{COP}(V)$ by simpler convex objects and obtain some bounds on $\alpha(G)$.

In this paper we propose *inner* approximations for $\mathcal{COP}(V)$. Let $\mathbb{S}^n$ be the space of $n \times n$ symmetric matrices over $\mathbb{R}$, and denote the set $\{1, ..., n\}$ by $[n]$. Kernels generalize the notion of symmetric matrices since $\mathbb{S}^n \cong \mathcal{K}([n])$. The following inner hierarchies were introduced for $\mathcal{COP}([n])$ by Parrilo [8], Peña et al. [9] and De Klerk and Pasechnik [2] respectively:

$$\mathcal{K}_r^n = \Big\{M \in \mathbb{S}^n : \Big(\sum_{i=1}^n x_i^2\Big)^r \sum_{i=1}^n \sum_{j=1}^n M_{ij} x_i^2 x_j^2 \text{ is a sum of squares}\Big\}. \tag{2}$$

$$\begin{aligned} Q_r^n = \Big\{M \in \mathbb{S}^n : (e^\top x)^r (x^\top M x) = \sum_{|\beta|=r} x^\beta x^\top N_\beta x + \sum_{|\beta|=r} x^\beta x^\top S_\beta x, \\ N_\beta, S_\beta \in \mathbb{S}^n,\ N_\beta \geq 0 \text{ and } S_\beta \succeq 0 \text{ for all } \beta \in \mathbb{N}^n, |\beta| = r\Big\}, \end{aligned} \tag{3}$$

$$\mathcal{C}_r^n = \big\{M \in \mathbb{S}^n : (e^\top x)^r (x^\top M x) \text{ has nonnegative coefficients}\big\}, \tag{4}$$

where $e = (1, ..., 1)$, $|\beta| := \beta_1 + ... + \beta_n$ and $x^\beta := x_1^{\beta_1} \cdots x_n^{\beta_n}$.

We have the inclusions $\mathcal{C}_r^n \subseteq Q_r^n \subseteq \mathcal{K}_r^n \subseteq \mathcal{COP}([n])$ for any r [9], and all hierarchies converge to $\mathcal{COP}([n])$ as r grows to infinity. We generalize the sets (4) and (3) to the case of copositive kernels on any compact $V \subset \mathbb{R}^n$ and show convergence of the obtained hierarchies.

Some approximations for the cone of copositive kernels on general V already exist. The first one comes from replacing copositivity in the definition of $\mathcal{COP}(V)$ by positive semidefiniteness. For the spherical codes problem, where V is the unit sphere S^{n-1} in $\mathbb{R}^n$, this procedure results in the Delsarte, Goethals and Seidel LP upper bound [3]. Further, De Laat and Vallentin [6] propose a hierarchy las_r^* which can be viewed as an extension of $\mathcal{K}_r^n$ (2) tailored to the stable set problem in infinite graphs. In the case of spherical codes, the bound for las_0^* corresponds to the Delsarte, Goethals and Seidel bound, and las_1^* coincides with a variation of the Bachoc and Vallentin SDP bound [1]. Additional research is needed to understand the precise relation between our hierarchies and las_r^*.

In order to approximate the kissing number, we use $V = S^{n-1}$ and extend the definitions of $\mathcal{C}_r^n$ and Q_r^n to $\mathcal{C}_r^{S^{n-1}}$ and $Q_r^{S^{n-1}}$, respectively. The result for $Q_0^{S^{n-1}}$ is the Delsarte, Goethals and Seidel bound, and for $Q_1^{S^{n-1}}$, it is similar to the Bachoc and Vallentin bound. $Q_r^{S^{n-1}}$ could be implemented for small $r \geq 2$, which may improve the existing upper bounds on the kissing number.

2 Generalizing inner approximations

Let $\mathcal{N}_d^V = \{F \in C(V^d) : F(v) \geq 0,\ \forall\ v \in V^d\}$ be the set of the non-negative continuous functions on V^d. For $F \in C(V^{d+2})$ and $v = (v_1, \ldots, v_d) \in V^d$, let $F^v = F(:, :, v_1, \ldots, v_d)$ be the 2-slice of F obtained by fixing all but the first two variables. A function $F \in C(V^{d+2})$ is called *2-slice psd (2-psd)* if F^v is positive definite for all $v \in V^d$.

We further need two operators. Denote by $Sym(d)$ the group of permutations on d elements. Then for any $d \in \mathbb{N}$, define $\sigma : C(V^d) \to C(V^d)$ as the symmetrization (Reynolds) operator:

$$\sigma(F)(v) := \frac{1}{d!} \sum_{\pi \in Sym(d)} F(\pi v), \text{ for all } v \in V^d. \tag{5}$$

If $d \in \mathbb{N}$, we define the lifting operator $\cdot^{\oplus r} : C(V^d) \to C(V^{d+r})$ for any $r \in \mathbb{N},\ v \in V^d$ as

$$F^{\oplus r}(v, u_1, ..., u_r) := F(v), \text{ for all } u_1, ..., u_r \in V. \tag{6}$$

We introduce the following sets:

$$\mathcal{C}_r^V = \{K \in \mathcal{K}(V) :\ \sigma(K^{\oplus r}) = \sigma(N),\ N \in \mathcal{N}_{r+2}^V\}, \tag{7}$$

$$\begin{aligned} Q_r^V = \{K \in \mathcal{K}(V) : \sigma(K^{\oplus r}) = \sigma(N) + \sigma(S), \\ N, S \in \mathcal{C}(V^{r+2}),\ N \in \mathcal{N}_{r+2}^V,\ S \text{ is 2-psd}\}. \end{aligned} \tag{8}$$

Proposition 2.1 *If $V = [n]$, then $\mathcal{C}_r^V = \mathcal{C}_r^n$ and $Q_r^V = Q_r^n$ for any r.*

3 Convergence of approximations

We will need a notion of *strictly copositive* kernels. Let Δ^n be the standard simplex in $\mathbb{R}^n$, $\Delta^n = \{x \in \mathbb{R}^n : \; e^\top x = 1, \; x \geq 0\}$. We call a kernel K strictly copositive if there exists $\varepsilon > 0$ such that for any choice of $v_1, ..., v_n \in V$, $\min_{x \in \Delta^n} \sum_{i=1}^n \sum_{j=1}^n K(v_i, v_j) x_i x_j \geq \epsilon$. This implies, in particular, that any finite submatrix of K if strictly copositive.

Denote the set of strictly copositive kernels by $\mathcal{COP}^+(V)$. We have a result similar to the ones obtained for $\mathcal{C}_r^n$ and Q_r^n in [2] and [9] respectively:

Theorem 3.1 *For a compact $V \subset \mathbb{R}^n$,*

$$\mathcal{C}_0^V \subseteq \mathcal{C}_1^V \subseteq \cdots \subseteq \mathcal{COP}(V), \quad Q_0^V \subseteq Q_1^V \subseteq \cdots \subseteq \mathcal{COP}(V)$$

$$\text{and } \mathcal{COP}^+(V) \subseteq \bigcup_r \mathcal{C}_r^V \subseteq \bigcup_r Q_r^V.$$

Proof sketch. To prove that the sets grow when r grows, we use properties of operators σ (5) and $.^{\oplus}$ (6). Inclusions in $\mathcal{COP}(V)$ hold since if $K \in \mathcal{K}(V)$ is nonnegative or positive definite, then for any $v_1, ..., v_n \in V$, $\sum_{i=1}^n \sum_{j=1}^n K(v_i, v_j) \geq 0$, and all kernels with this property are copositive [4]. The second line holds as any strictly copositive matrix belongs to $\mathcal{C}_r^n$ for sufficiently large r by Pólya theorem. We use the convergence results for Pólya theorem from Powers and Reznick [10] and De Klerk and Pasechnik [2]. □

Now apply Theorem 3.1 to approximate the stability number $\alpha(G)$ of a compact topological packing graph $G = (V, E)$. Let $\gamma_r(G)$ and $\nu_r(G)$ be the upper bounds on $\alpha(G)$ obtained by replacing $\mathcal{COP}(V)$ in Problem (1) with $\mathcal{C}_r^V$ (7) and Q_r^V (8) respectively.

Theorem 3.2 *Assume that there exists a $K \in \mathcal{COP}^+(V)$ that is feasible for Problem (1). Then $\gamma_r(G) \downarrow \alpha(G)$ and $\nu_r(G) \downarrow \alpha(G)$.*

Proof sketch. The existence of a feasible $K \in \mathcal{COP}^+(V)$ implies that $\alpha(G)$ is the optimal solution to Problem (1) where $\mathcal{COP}(V)$ is replaced with $\mathcal{COP}^+(V)$. Then Theorem 3.2 holds by Theorem 3.1. □

4 Application to the kissing number problem

The *kissing number* κ_n is the maximum number of non-overlapping unit spheres S^{n-1} in $\mathbb{R}^n$ that can simultaneously touch a given unit sphere. Let $G^{S^{n-1}} = (S^{n-1}, E)$ be the graph where $(u, v) \in E$ if $u^\top v \in (\frac{1}{2}, 1)$. Then κ_n is equal to the stability number $\alpha(G^{S^{n-1}})$.

Corollary 4.1 *If $G = G^{S^{n-1}}$, then $\gamma_r(G) \downarrow \kappa_n$ and $\nu_r(G) \downarrow \kappa_n$.*

Proof sketch. By Theorem 3.2, it is enough to show that there exists $K \in \mathcal{COP}^+(S^{n-1})$ feasible for Problem (1) when $G = G^{S^{n-1}}$. For this purpose, we modify the optimal solution of Problem (1) using the reformulation of the stability number problem in finite graphs by Motzkin and Straus [7]. □

For any r, $\gamma_r(G)$ is easier to build, but weaker than $\nu_r(G)$ since $\gamma_r(G) = \infty$ for $r < \kappa_n - 1$ [2]. Thus we concentrate on $\nu_r(G)$. We exploit the convexity of Problem (1) and the invariance of $G^{S^{n-1}}$ under the orthogonal group O_n. Hence, we only need to consider the functions invariant under O_n and characterize $(Q_r^{S^{n-1}})^{O_n}$. In order to implement the bound, we approximate continuous functions by polynomials, whose degree we restrict to d.

Constructing $(Q_r^{S^{n-1}})^{O_n}$ involves the non-negativity condition and the 2-psd condition. The former can be approximated with one of the existing sufficient polynomial non-negativity conditions, e.g., via Putinar's Positivstellensatz. The 2-psd condition deserves separate attention. When $r = 0$, 2-psd polynomials in $C(S^{n-1} \times S^{n-1})$ are positive definite polynomials, and we use the following result of Schoenberg [11]:

Proposition 4.2 *A polynomial $p : (S^{n-1})^2 \to \mathbb{R}$ invariant under O_n is 2-psd iff*

$$p(x, y) = \sum_{i \in \mathbb{N}} c_i P_i^{\frac{n-3}{2}, \frac{n-3}{2}}(x^\top y), \text{ for some } c_i \geq 0.$$

Here $P_i^{\frac{n-3}{2}, \frac{n-3}{2}}$ are Jacobi polynomials of order $(\frac{n-3}{2}, \frac{n-3}{2})$ and degree i.

When $r = 1$, 2-psd polynomials in $C((S^{n-1})^3)$ are positive definite when the last point is fixed. Then the following characterization applies. It is based on the results of Bachoc and Vallentin [1].

Proposition 4.3 *For $x, y, z \in S^{n-1}$, let $t = x^\top y$, $u = x^\top z$, $v = y^\top z$. A polynomial $p : (S^{n-1})^3 \to \mathbb{R}$ of degree d invariant under O_n is 2-psd iff:*

$$p(x, y, z) = \sum_{i=0}^{d} c_i(u, v) \big((1 - u^2)(1 - v^2)\big)^{\frac{i}{2}} P_i^{\frac{n-4}{2}, \frac{n-4}{2}} \left(\frac{t - uv}{\sqrt{(1 - u^2)(1 - v^2)}} \right),$$

where $c_i(u,v) = [\,1\ u\ \dots\ u^{d-i}\,]C_i[\,1\ v\ \dots\ v^{d-i}\,]^\top$, $C_i \in \mathbb{S}^{d-i+1}$, *and* $C_i \succeq 0$.

We exploit the results of Propositions 4.2 and 4.3, use the definitions of operators σ (5) and $.^{\oplus}$ (6) and obtain a linear program for $(Q_0^{S^{n-1}})^{O_n}$ and an SDP for $(Q_1^{S^{n-1}})^{O_n}$. Our approximation for r=0 incorporates the one by Delsarte, Goethals and Seidel [3]. For r=1, our bound resembles the bound of Bachoc and Vallentin [1]. The precise connection between our approximations and the existing ones is to be established. Another goal of further research is to characterize general 2-psd functions and compute $\nu_r(G^{S^{n-1}})$ for $r \geq 2$.

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