An $(n-2)$-dimensional Quadratic Surface Determining All Cliques and a Least Square Formulation for the Maximum Clique Problem *

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Abstract

Arranging an n-vertex graph as the standard simplex in $\mathbf{R}^n$, we identify graph cliques with simplex faces formed by clique vertices. An unstrict quadratic inequality holds for all points of the simplex; it turns to equality if and only if the point is on a face corresponding to a clique. This way this equality determines a quadratic surface in $\mathbf{R}^n$ characterizing all graph cliques. Since the standard simplex is a polyhedron located within the hyperplane $e^T x = 1$, we may decrease the dimensionality by 1 considering the intersection of this surface with the hyperplane. Therefore, we obtain a quadratic surface of dimensionality $(n-2)$ determining all graph cliques. We call it the *clique wrapper*.

The higher the dimensionality of a standard simplex face, the less the distance from it to the geometric center of the simplex. Therefore, the maximum clique problem is equivalent to finding a point of the clique wrapper closest to the geometric center of the simplex and lying not outside the simplex. When the latter is relaxed, all stationary points of such a least square program can be found via roots of one univariate rational equation. If the adjacency matrix of the graph does not have multiple eigenvalues, the number of the stationary points is not above $2(n-1)$. If a clique is such that any vertex outside it has the same number of adjacent vertices in the clique, the geometric center of the clique face is such a stationary point.

1 Introduction

Let $G(V, E)$ be a simple undirected graph, $V = \{1, 2, \ldots, n\}$. The *adjacency matrix* of G is a matrix $A_G = (a_{ij})_{n \times n}$, where $a_{ij} = 1$ if $(i, j) \in E$, and $a_{ij} = 0$ if $(i, j) \notin E$. A *clique* Q is a subset of V such that any two vertices of Q is connected by an edge. The *maximum clique problem* asks for a clique of maximum cardinality. We denote this cardinality by $\omega(G)$.

This problem is NP-hard [1]. So, it is considered unlikely that an exact polynomial time algorithm for it exists. Moreover, it was shown in [2] that unless $NP = ZPP$ no polynomial time algorithm can approximate maximum clique within a factor of $n^{1-\epsilon}$ for any $\epsilon > 0$.

The *standard simplex* in $\mathbf{R}^n$ is the polyhedron

$$\Delta = \{x \in \mathbf{R}^n : \ x \geq 0, \ e^T x = 1\}, \tag{1}$$

where e is all-one vector of length n. That is, $e^T x = \sum_{i \in V} x_i$. Vertices of the standard simplex are the basis vectors e_i (with the single i-th unit entry and all the other zero entries.) As usually, we denote the $n \times n$ identity matrix by I_n writing simply I when the appropriate size is understood. The all-one $n \times n$ matrix will be denoted by O_n with the similar index omission when the size is understood.

2 The Quadratic Clique Wrapper

Let the i-th vertex of the graph $G(V, E)$ be located at e_i. Then the graph is drawn on the standard simplex. Each vertex subset $S \subseteq V$ forms to an $(|S| - 1)$-dimensional face of the simplex. Hence we may identify S with its simplex face.

Theorem 1

$$\forall x \in \Delta : \quad x^T(A_G + I)x \leq 1. \tag{2}$$

The equality occurs if and only if x is on a face formed by a clique $Q \subseteq V$.

Proof. Since $x \geq 0$, $x^T(A_G + I)x \leq x^T O x = (e^T x)^2$. Since $e^T x = 1$, this value is 1, so $x^T(A_G + I)x \leq 1$.

Let x be on a face formed by a clique $Q \subseteq V$. Then the nonzero entries of x correspond to the vertices forming Q. Since a clique forms an all-one submatrix of $(A_G + I)$, we have

$$x^T(A_G + I)x = \sum_{i \in Q} \sum_{j \in Q} x_i x_j = \left(\sum_{i \in Q} x_i \right)^2 = 1.$$

In the other case, the nonzero entry subset of x correspond to a vertex subset $S \subseteq V$ not forming a clique. Thus,

$$x^T(A_G + I)x < \sum_{i \in S} \sum_{j \in S} x_i x_j = 1.$$

QED.

Therefore, the equality $x^T(A_G + I)x = 1$ determines a quadratic surface coinciding with all simplex faces corresponding to graph cliques and going over all the other simplex faces. Since simplex vertices are one-vertex cliques, they lay on the surface. Next, since Δ is located within the hyperplane $e^T x = 1$, we can decrease the surface dimensionality considering its intersection with the hyperplane only. This way we come to the notion of the *clique wrapper*.

Definition 1 *The* clique wrapper *for a graph $G(V, E)$ is the quadratic surface*

$$\mathcal{W}(G) = \{x \in \mathbf{R}^n : x^T(A_G + I)x = 1, \ e^T x = 1\}. \tag{3}$$

Thus, we have defined a quadratic surface in an $(n-1)$-dimensional space designating all graph cliques. The dimesionality of the surface itself is $(n-2)$.

Obviously, the higher the dimensionality of a simplex face, the less the distance from it to the origin. Namely, the distance from any $(k-1)$-dimensional face to the origin is $\sqrt{k(1/k)^2} = 1/\sqrt{k}$. Hence, the maximum clique problem is equivalent to the following least square problem

$$\min x^T x, \tag{4}$$

$$\text{s.t. } x^T(A_G + I)x = 1, \ e^T x = 1, \ x \geq 0, \ x \in \mathbf{R}^n.$$

We will also consider the relaxed version of this least square program, where the nonnegativity constraint $x \geq 0$ is omitted. We can prove that the relaxed program is enough to recognize a special type of maximal cliques.

Theorem 2 *Let Q be a maximal clique of the graph $G(V,E)$ of size k. If each vertex $v \in V \setminus Q$ has the same number of adjacent vertices in Q, then the geometric center x of the face determined by Q*

$$x_i = \begin{cases} 1/k, & i \in Q \\ 0, & i \in V \setminus Q \end{cases}$$

is a stationary point of the relaxed least square program

$$\min x^T x, \tag{5}$$

$$s.t.\ x^T(A_G + I)x = 1,\ e^T x = 1,\ x \in \mathbf{R}^n.$$

Proof. Consider the Lagrangian of the program (5)

$$L(x, \mu, \eta) = x^T x + \mu(x^T(A_G + I)x - 1) + \eta(e^T x - 1).$$

The program stationary points are those obeying the equation system

$$\frac{1}{2}\frac{\partial L}{\partial x_i} = x_i + \mu(x_i + \sum_{j:(i,j)\in E} x_j) + \frac{\eta}{2} = 0.$$

Let each vertex $v \in V \setminus Q$ has exactly c neighbors in Q. Since Q is maximal, $c < k$. Assigning $x_i = 1/k$ for each $i \in Q$ and $x_i = 0$ for each $i \in V \setminus Q$, we obtain the equality

$$\frac{1}{k} + \mu + \frac{\eta}{2} = 0$$

from all equations corresponding to the clique vertices, and

$$\mu\frac{c}{k} + \frac{\eta}{2} = 0$$

from all equations corresponding to the other vertices. This system always has a solution $\mu = -\frac{1}{k-c}$, $\eta = \frac{2c}{k(k-c)}$. QED.

In the next section we show how all stationary points of the relaxed program may be found solving one univariate equation.

3 Deriving the Stationary Points

Thus, we will derive stationary points of the program (4) with the nonnegativity constraint relaxed assuming they provide significant information on location of the maximum clique optima.

First of all, we get rid of the equality constraint $e^T x = 1$ using the orthogonal projection onto the hyperplane determined by the equality. We move the origin into the geometric center of the standard simplex $x^0 = (1/n, 1/n, \ldots, 1/n)^T$. That is, we introduce new variables

$$\hat{x}_i = x_i - \frac{1}{n},\ i \in V.$$

This way we obtain an equivalent least square problem

$$\min \hat{x}^T \hat{x}, \tag{6}$$

$$\text{s.t. } \hat{x}^T(A_G + I)\hat{x} + 2(x^0)^T A_G \hat{x} = 1 - \frac{1}{n} - (x^0)^T A_G x^0,\ e^T \hat{x} = 0,\ \hat{x} \in \mathbf{R}^n.$$

Now the equality constraint determines a linear subspace. The orthogonal projector onto it is matrix $P = (p_{ij})_{n\times n}$, where

$$p_{ij} = \begin{cases} 1 - 1/n, & \text{if } i = j \\ -1/n, & \text{if } i \neq j. \end{cases}$$

Thus, the program (6) may be reformulated as

$$\min \hat{x}^T \hat{x}, \tag{7}$$

$$\text{s.t. } \hat{x}^T P(A_G + I)P\hat{x} + 2(x^0)^T A_G P\hat{x} = 1 - \frac{1}{n} - (x^0)^T A_G x^0,\ \hat{x} \in \mathbf{R}^n.$$

Diagonalize the quadratic form performing the eigendecomposition:

$$P(A_G + I)P = Q\text{diag}(\lambda_1, \ldots, \lambda_k)Q^T.$$

Here we take only eigenvectors corresponding to nonzero eigenvalues. Its number $k \leq n-1$ because the matrix is projected onto an $(n-1)$-dimensional subspace. So, Q is the $n \times k$ matrix of eigenvectors (stored as columns.) This way we formulate the problem (7) in the eigenvector space

$$\min y^T y, \tag{8}$$

$$\text{s.t. } y^T \text{diag}(\lambda_1, \ldots, \lambda_k)y + 2c^T y = s,\ y \in \mathbf{R}^k,$$

where

$$\hat{x} = Qy,\ y = Q^T\hat{x},\ c = Q^T\left((x^0)^T A_G P\right)^T,\ s = 1 - \frac{1}{n} - (x^0)^T A_G x^0.$$

The Lagrangian of (8) is

$$L(y, \mu) = y^T y - \frac{1}{\mu}(y^T \text{diag}(\lambda_1, \ldots, \lambda_k)y + 2c^T y - s).$$

We take the Lagrangian multiplier as $-\frac{1}{\mu}$ for the sake of simplicity of further expressions. The stationary criterion

$$\frac{1}{2}\frac{\partial L}{\partial y_i} = y_i - \frac{1}{\mu}(\lambda_i y_i + c_i) = 0$$

gives

$$y_i = \frac{c_i}{\mu - \lambda_i}. \tag{9}$$

Substituting these expressions into the constraint, we obtain an univariate equation

$$\sum_{i=1}^{k} \frac{c_i^2(2\mu - \lambda_i)}{(\mu - \lambda_i)^2} = s. \tag{10}$$

Unless there is a degenerative case of multiple eigenvalues with zero c_i values corresponding to them, this equation encodes all stationary points of the program (8). It is equivalent to a polynomial of degree $2k$, so there are not more than $2k$ stationary points to consider.

References

[1] Garey, M., and Johnson, D. (1979). Computers and Intractability: A Guide to the Theory of NP-Completeness. *Freeman & Co.*

[2] Håstad, J. (1996). Clique is hard to approximate within $n^{1-\epsilon}$. In: *Proc. 37th Annual IEEE Symposium on the Foundations of Computer Science (FOCS)*, 627–636.