Some Recent Results on Discrete and Nonconvex Quadratic Programming

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Based on works joint with H. Mittelmann, ASU X. Li and R. Yang, IESE, UI

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Introduction

New SDP Relaxations for Quadratic Assignment Problems

New Clustering-based Approaches for 0-1 Binary QP

Probabilistic Analysis of Nonconvex QP

Quadratic Optimization

min
$$x^TQx + q^Tx$$

s.t. $Ax = b$
 $x \ge 0, x \in \{0,1\}^n \text{ or } \{-1,1\}^n.$

 One of the basic optimization models widely used in many applications from experiment design and portfolio selection;

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- ▶ In general, it is NP-hard. For some special cases, even getting a good approximation is hard too.



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- Called new "LP" in this century.



Transformation from QP to SDP

SDP based approach for QP has been well-studied in both the continuous and discrete optimization communities since 1990s:

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- ► The well-known SDP based method for max-cut by Goemans and Williamson (1994), Nesterov (1998);
- ► The SDP relaxation is based on the relaxation of the gram matrix $X = xx^T$ (or lifting techniques):

$$\begin{split} X\succeq 0, \mathrm{diag}\left(X\right) &= 1 \quad \text{if } x\in\{-1,1\}^n;\\ X\succeq 0 \text{ or } &\left(\begin{array}{cc} 1 & x^T\\ x & X\end{array}\right)\succeq 0, X\geq 0 \quad \text{if } x\in\{0,1\}^n, \end{split}$$



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 - ► Recent exciting developments on compressed sensing Donoho (2006), Candés and Tao (2006)!



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 - Even computing a good lower bound for problems of size n = 30 is too expensive (the classical lifting technique leads to $\mathcal{O}(n^4)$ constraints) Hahn et'al 2007;



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- Many existing works on how to derive/solve these expensive relaxations, but only works for small-scale problems.

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- ▶ Fact 4: In many applications, the matrices A or B are associated with specific graphes, i.e., B is the Hamming distance matrix of a hypercube or the Manhattan distance matrix of a rectangular grids;
- ► Fact 5: The matrices A and B have nonnegative elements, thus dominated by its first principal component.



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 - ▶ Use the Laplacian operator: $D = \text{diag}(\sum(B)), B = D (D B);$
 - ▶ Specific splitting $B = \alpha E B^-$, where E is the all-1 matrix.



Special Splitting Examples

► The Hamming distance matrix with a binary codebook

$$C = \{c_1 = `00', c_2 = `01', c_3 = `10', c_4 = `11'\}.$$

$$B = \begin{pmatrix} 0 & 1 & 1 & 2 \\ 1 & 0 & 2 & 1 \\ 1 & 2 & 0 & 1 \\ 2 & 1 & 1 & 0 \end{pmatrix}, E - B = \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \succeq 0.$$

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Manhattan distance matrix from facility location

$$B = [b_{ij}] \in \Re^{n \times n}, \quad b_{ij} = |i - j|, \quad \frac{n - 1}{2}E - B \succeq 0. \tag{1}$$

Construction of Valid Cut

Given a matrix Y and a function f, we define a mapping

$$F(Y) = [f(Y_1); f(Y_2); \cdots; f(Y_n)].$$

Theorem: Suppose that $F(\cdot)$ is a mapping defined with a symmetric function $f(\cdot)$ and X is a permutation matrix. Then we have

$$F(XBX^T) = XF(B).$$

Constructing Cut: Choose f to be convex, and relax it to

$$F(Y) = F(XBX^T) \le XF(B).$$

A Sample Relaxation

Let (B^+, B^-) be a PSD splitting of B and $Y^+ = XB^+X^T$, $Y^- = XB^-X^T$. Using symmetric mappings max, min, \mathcal{L}_1 and \mathcal{L}_2 , we derive

min
$$\operatorname{Tr}(A(Y^{+} - Y^{-}))$$

s.t. $Y^{+} - XB^{+}X^{T} \succeq 0$, $Y^{-} - XB^{-}X^{T} \succeq 0$;
 $\operatorname{diag}(Y^{+}) = X\operatorname{diag}(B^{+})$, $Y^{+}e = XB^{+}e$;
 $\operatorname{diag}(Y^{-}) = X\operatorname{diag}(B^{-})$, $Y^{-}e = XB^{-}e$;
 $(X \min(B^{+}))_{i} \leq y_{i,j}^{+} \leq (X \max(B^{+}))_{i}$, $\forall i \neq j$;
 $(X \min(B^{-}))_{i} \leq y_{i,j}^{-} \leq (X \max(B^{-}))_{i}$, $\forall i \neq j$;
 $\mathcal{L}_{2}(Y^{+}) \leq X\mathcal{L}_{2}(B^{+})$, $\mathcal{L}_{2}(Y^{-}) \leq X\mathcal{L}_{2}(B^{-})$;
 $X \geq 0$, $Xe = X^{T}e = e$.

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 - Develop new solving techniques for these new relaxation models.

0-1 Binary QP

We consider the following binary QP

(StQP) max
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s.t. $\sum_{i=1}^{n} x_i = k, \quad x \in \{0,1\}^n.$

 Applications: the densest k-subgraph, feature selection in learning;

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- Extra constraints can be added;
- NP-hard, even a good approximation is hard unless P=NP.
 PTAS have been ruled out recently(S. Khot, SIAM J.
 Computing, 2006, Best paper award in SIAM).



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s.t. $Xe = k * \operatorname{diag}(X)$
 $\sum_{i=1}^{n} x_{ii} = k$
 $X \succeq 0, \quad X \geq 0.$

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- Question: What's wrong?

Convex QP: Relaxation or Geometric Embedding: I

We rewrite the problem as QAP:

$$\max \quad x^{T}(Q - \lambda_{\min}(Q)I)x$$

$$s.t \quad \sum_{i=1}^{n} x_{i} = k, x_{i} \in \{0, 1\}.$$
(2)

 $\lambda_{\min}(Q)$ denotes the minimal eigenvalue of Q.

Relaxation for a cheap bound?

Convex QP: Relaxation or Geometric Embedding:II

▶ Let $\bar{Q} = (Q - \lambda_{\min}(Q)I) \succeq 0$. We can interpret each element of \bar{Q} as the inner product of two data points in a data set on the surface of a unit sphere in a certain dimensional space;

$$\mathcal{V} = \{v_i : ||v_i||^2 = -\lambda_{\min}(Q), \ i = 1, \dots, v_n\}, \bar{Q}_{ij} = v_i^T v_j.$$

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$$\mathcal{V} = \{v_i : \|v_i\|^2 = -\lambda_{\min}(Q), \ i = 1, \cdots, v_n\}, \, \bar{Q}_{ij} = v_i^T v_j.$$

► Geometric Embedding: Consider a specific clustering problem of finding a single cluster of fixed size whose within cluster sum of squared distances is minimal:

$$\min_{|\mathcal{V}_1|=k} \sum_{v \in \mathcal{V}_1} \|v - \frac{\sum_{v \in \mathcal{V}_1} v}{k} \|^2.$$
 (3)

Here $|\mathcal{V}_1|$ denotes the cardinality of the subset \mathcal{V}_1 .



Approximation to A Simple Clustering Problem

Theorem: Problem (StQP) and the clustering problem (3) share the same optimal solution set.

Problem (3) is equivalent to

$$\min_{c} \min_{|\mathcal{V}_1| = k} \sum_{v \in \mathcal{V}_1} \|v - c\|^2.$$
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Some simple and effective approximation algorithms/heuristics:

▶ Use an iterative scheme as in the classical K-means clustering that subsequently update *c* and cluster;

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- ▶ Use an iterative scheme as in the classical K-means clustering that subsequently update *c* and cluster;
- Try different starting points and select the best one as final output (provable 2-approximation);
- Use the first eigenvector of Q to find the cluster...



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- ▶ Perform a local search $(O(n^2))$;
- In total $O(n^3 + n^2 k \log n + n^2)$.

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- ▶ Future direction: Extensions to other binary QPs such as $x^TQx + q^Tx$; and faster approximation algorithms based on the spectrum of Q.

Sparse Solutions to Linear Equation System

min
$$||x||_0$$

s.t. $Ax = b, x \ge 0$.

Replacing the objective in the above model by $||x||_1$, we end up with an LP problem. As proved by Candés and Tao (2006), Donoho (2006):

Theorem: If the input data matrix A follows certain distribution and there exists a sparse solution, then the solution from the LP problem is also optimal for the original L_0 optimization problem with a high probability.

From Linear Equation to QP

The LP problem can be equivalently stated as

min
$$||Ax - b||^2$$

s.t. $\sum_{i=1}^{n} x_i = 1, x \ge 0.$

Let us consider a generalized case:

$$\min \quad x^T Q x + q^T x \tag{5}$$

s.t.
$$\sum_{i=1}^{n} x_i = 1, x \ge 0.$$
 (6)

Question: Under what conditions, the above problem admits sparse solutions?

Checking the Co-positivity of Matrices

Question: Given a matrix Q, is there a nonnegative vector x such that $x^TQx < 0$?

Mathematically, we can address the above problem by solving the following problem:

min
$$x^T Qx$$
 (7)
s.t.
$$\sum_{i=1}^{n} x_i = 1, x \ge 0.$$

Such a model arise also from learning and feature selection. The problem has been proved to be NP-hard (Murty and Kabadi, 1987). It is also called standard quadratic programming problem in the literature.

A Simple SDP Relaxation

min
$$\operatorname{Tr}(QX)$$
 (8)
s.t. $\sum_{i,i=1}^{n} x_{ij} = 1, X \succeq 0, X \geq 0.$

Observation: My simple matlab code always gives me rank-one solution, which implies the SDP relaxation solved the original problem precisely!

Checking the Co-positivity of Random Matrices

We have proved the following result.

Theorem: If the matrix Q is random following certain distributions, then with a high probability that the optimal solution of problem (7) is sparse and it can be found in polynomial time.

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 - ► For SDP, under what conditions, the SDP problem has rank 1 solution? How can we use this information to develop more effective resolution techniques?

Questions

For reference, please refer to my personal web site https://netfiles.uiuc.edu/pengj/www/ or contact pengj@illinois.edu