Convex relaxation of the binary quadratic knapsack problem

Daniela Lubke
University of Waterloo
Dept. of Combinatorics and Optimization

Joint work with: Marcia Fampa, Fei Wang, Henry Wolkowicz

CAIMS: Canadian Applied and Industrial Mathematics Society
UBC Okanagan from June 13-16, 2022

UNIVERSITY OF WATERLOO | FACULTY OF MATHEMATICS
Department of Combinatorics and Optimization

Outline

The Quadratic Knapsack Problem

$$
\begin{array}{llll}
(\textbf{QKP}) & \text{maximize} & \sum_{i\in N}\sum_{j\in N} q_{ij}x_ix_j & (= x^TQx) \\
& \text{subject to} & \sum_{j\in N} w_jx_j \le c, & \\
& & x_j \in \{0,1\}, & j \in N.
\end{array}
$$

where $0 < w_j \le c$ for all $j \in N$

- Application in capital budget investments, where c represents the capital budget to invest in n possible investments. The quadratic formulation model the case where the return of the investments considers the dependence between pair of investments.
- Subproblem on some solutions approaches for more general binary quadratic problems.
- We are interested here in finding tight upper bounds for (**QKP**).

Convexification: seeking good upper bounds

Standard approach to obtain upper bounds:
Lift the problem to the matrix space defined by $X := xx^T$

$$
(QKP_{lifted}) \quad \begin{array}{ll} \text{maximize} & \langle Q, X \rangle \\ \text{subject to} & \sum_{j \in N} w_j x_j \leq c, \\ & x_j \in \{0,1\}, \quad j \in N. \\ & X = xx^T \end{array}
$$

Convexification: seeking good upper bounds

Standard approach to obtain upper bounds:
Lift the problem to the matrix space defined by $X := xx^T$

$$
\begin{array}{lll}
(QKP_{lifted}) & \text{maximize} & \langle Q, X \rangle \\
& \text{subject to} & \sum_{j \in N} w_j x_j \leq c, \\
& & x_j \in \{0,1\}, \quad j \in N. \\
& & X = xx^T \quad \longleftarrow \text{nonconvex}.
\end{array}
$$

Relax the nonconvex constraints $X = xx^T, x_j \in \{0,1\}, j \in N$.

$$
(\mathbf{LPR}) \qquad \begin{array}{ll} \max & \langle Q, X \rangle \\ \text{s.t.} & (x, X) \in \mathcal{P}, \end{array}
$$

where $\mathcal{P}$ is a compact convex subset of $[0,1]^n \times \mathbb{S}^n$ such that

$$\{(x, X) \; : \; w^T x \leq c, \; X = xx^T, \; x \in \{0,1\}^n\} \subset \mathcal{P}.$$

Convexification: seeking good upper bounds

As $x^T Q x = x^T(Q - Q_p)x + x^T Q_p x$, consider also the relaxation

$$(\mathbf{CQP}_{Q_p}) \quad \begin{array}{rl} p^*_{\mathrm{CQP}}(Q_p) := \max & x^T(Q - Q_p)x + \langle Q_p, X\rangle \\ \text{s.t.} & (x, X) \in \mathcal{P}, \end{array}$$

where $\mathcal{P}$ is a compact subset of $[0,1]^n \times \mathbb{S}^n$, such that

$$\{(x, X) \; : \; w^T x \le c, \; X = xx^T, \; x \in \{0,1\}^n\} \subset \mathcal{P}.$$

and where

$$Q - Q_p \preceq 0,$$

Searching for:

- a matrix Q_p that leads to a good decomposition of the objective function.
- a tight relaxation $\mathcal{P}$ of the feasible set, that leads to a relaxation of **QKP** that can be efficiently solved.

Convexification: seeking good upper bounds

As $x^T Qx = x^T(Q - Q_p)x + x^T Q_p x$, consider also the relaxation

$$(\mathbf{CQP}_{Q_p}) \qquad p^*_{\mathrm{CQP}}(Q_p) := \max \quad x^T(Q - Q_p)x + \langle Q_p, X\rangle \quad \text{s.t.} \quad (x, X) \in \mathcal{P},$$

where $\mathcal{P}$ is a compact subset of $[0,1]^n \times \mathbb{S}^n$, such that

$$\{(x, X) \ : \ w^T x \le c, \ X = xx^T, \ x \in \{0,1\}^n\} \subset \mathcal{P}.$$

and where

$$Q - Q_p \preceq 0,$$

Searching for:

- a matrix Q_p that leads to a good decomposition of the objective function.
- a tight relaxation $\mathcal{P}$ of the feasible set, that leads to a relaxation of **QKP** that can be efficiently solved. $\longleftarrow$ new valid inequalities!

How to optimize the selection of Q_p?

- Search for the decomposition that minimizes the upper bound of (**QKP**) given by our convex quadratic relaxation:

$$(\mathbf{CQP}_{\,Q_p}) \quad \begin{array}{rl} p^*_{\text{CQP}}(Q_p) := \max & x^T(Q - Q_p)x + \langle Q_p, X\rangle \\ \text{s.t.} & (x, X) \in \mathcal{P}, \end{array}$$

where $Q - Q_p \preceq 0$

- To minimize the upper bound, consider the parametric problem

$$param^*_{\text{QKP}} := \min_{Q - Q_p \preceq 0} p^*_{\text{CQP}}(Q_p).$$

A primal-dual IPM to solve the parametric problem

- Minimize a log-barrier function $B_\mu(Q_p, Z)$

$$\begin{array}{lll} \min & B_\mu(Q_p, Z) := p^*_{\mathrm{CQP}}(Q_p) - \mu \log\det Z & \\ \text{s.t.} & Q - Q_p + Z = 0 & (:\Lambda) \\ & Z \succ 0, & \end{array}$$

  where Z, Λ are the slack and dual symmetric matrix variables, and $p^*_{\mathrm{CQP}}(Q_p) := max\{x^T(Q - Q_p)x + \langle Q_p, X\rangle | (x, X) \in P\}$
- Consider the Lagrangian function:

$$L_\mu(Q_p, Z, \Lambda) := p^*_{\mathrm{CQP}}(Q_p) - \mu \log\det Z + \langle Q - Q_p + Z, \Lambda\rangle.$$

- At each iteration of the **IPM**, we need to differentiate the Lagrangian function.

UNIVERSITY OF WATERLOO | FACULTY OF MATHEMATICS Department of Combinatorics and Optimization

A primal-dual IPM to solve the parametric problem

- Minimize a log-barrier function $B_\mu(Q_p, Z)$

$$\begin{array}{lll} \min & B_\mu(Q_p, Z) := p^*_{\mathrm{CQP}}(Q_p) - \mu \log\det Z & \\ \text{s.t.} & Q - Q_p + Z = 0 & (: \Lambda) \\ & Z \succ 0, & \end{array}$$

  where Z, Λ are the slack and dual symmetric matrix variables, and $p^*_{\mathrm{CQP}}(Q_p) := max\{x^T(Q - Q_p)x + \langle Q_p, X\rangle | (x, X) \in P\}$
- Consider the Lagrangian function:

$$L_\mu(Q_p, Z, \Lambda) := p^*_{\mathrm{CQP}}(Q_p) - \mu \log\det Z + \langle Q - Q_p + Z, \Lambda\rangle.$$

- At each iteration of the **IPM**, we need to differentiate the Lagrangian function.

UNIVERSITY OF WATERLOO | FACULTY OF MATHEMATICS Department of Combinatorics and Optimization

Important observations for the **IPM**

$$(\mathbf{CQP}_{Q_p}) \quad p^*_{\text{CQP}}(Q_p) := \max \; x^T(Q - Q_p)x + \langle Q_p, X\rangle \quad \text{s.t.} \; (x, X) \in \mathcal{P},$$

or

$$(\mathbf{CQP}_{Q_p}) \quad p^*_{\text{CQP}}(Q_p) := \max \; \langle Q_p, X - xx^T\rangle + x^T Q x \quad \text{s.t.} \; (x, X) \in \mathcal{P},$$

- $p^*_{\text{CQP}}(Q_p)$ is differentiable at all Q_p surch that $Q - Q_p \preceq 0$ and,

$$\nabla p^*_{\text{CQP}}(Q_p) = X - xx^T.$$

- We use a quasi-Newton direction at each iteration of our IPM. To compute the direction, we need the optimal solution of $\mathbf{CQP}_{Q_p}$.
- The relaxation $\mathbf{CQP}_{Q_p}$ is solved at each iteration of the IPM method, each time for a new perturbation Q_p, such that $Q - Q_p \preceq 0$.
- Each time the relaxation is solved, valid cuts are added to strength the relaxation.

Valid linear inequalities in the lifted matrix space

- The identity derived from $x_i \in \{0,1\}$:

$$X_{ii} = x_i$$

- McCormick inequalities derived from $x_i \geq 0$ and $1 - x_i \geq 0$

$$\begin{aligned} &X_{ij} \geq 0 \\ &X_{ii} - X_{ij} \geq 0 \\ &1 - X_{ii} - X_{jj} + X_{ij} \geq 0, \end{aligned}$$

- Inequalities derived from the product of the knapsack constraint $\sum_{j \in N} w_j x_j \leq c$, by x_i and $(1 - x_i)$:

$$\sum_{j \in N} w_j \overbrace{X_{ij}}^{x_i x_j} \leq c \overbrace{X_{ii}}^{x_i}.$$

$$\sum_{j \in N} w_j (X_{jj} - X_{ij}) \leq c(1 - X_{ii}).$$

Cover Inequalities

The subset $C \subseteq N$ is a cover if it satisfies

$$\sum_{j \in C} w_j > c$$

The *cover inequalities* **CI** is defined as

$$\sum_{j \in C} x_j \leq |C| - 1.$$

More valid inequalities in the lifted matrix space

Let us consider the cover inequality

$$\sum_{j \in C} x_j \leq \beta. \tag{1}$$

where $\beta = |C| - 1$.

Definition: (*Generalized cover inequality* **GCI**)

Define

$$\sum_{j \in C} X_{ij} \leq \beta X_{ii}.$$

$$\sum_{j \in C} X_{ij} - X_{ii} \leq \beta(1 - X_{ii}).$$

for all $i \in N$, as the derived from (1)

New valid inequalities in the lifted space

Let us consider the cover inequality

$$\sum_{j \in C} x_j \leq \beta \quad \text{where} \quad \beta = |C| - 1 \tag{1}$$

If no more than β items in C can be in the solution, then if we consider all 2-combinations of items in C, then the sum of the elements of X corresponding to there combinations cannot be greater than β choose 2.

New valid inequalities in the lifted space

Definition: (*Cover inequality in the lifted space* **CILS**)

Define

$$\sum_{i,j \in C, i<j} X_{ij} \leq \binom{\beta}{2}. \tag{2}$$

as the **CILS** derived from (16)

Proposition:

If inequality (1) is valid for **QKP** , then the **CILS** (2) is a valid inequality for QKP_{lifted}

Illustrating a **CILS**

Let

$$C := \{1, 2, 3\}$$

be a cover. So

$$\{1, 2\}, \{1, 3\}, \{2, 3\}$$

are the 2-combinations of C.
The inequality

$$x_1 + x_2 + x_3 \leq 2$$

is a cover inequality, and

$$X_{12} + X_{13} + X_{23} \leq 1$$

is a **CILS**.

More valid inequalities in the lifted space

Let us consider the cover inequality

$$\sum_{j \in C} x_j \leq \beta \quad \text{where} \quad \beta = |C| - 1 \tag{1}$$

Definition: (*Set of cover inequalities in the lifted space* **SCILS**)

Let $\bar{C} := \{(i_1, j_1), \ldots, (i_p, j_p)\}$ be a partition of C, if $|C|$ is even, or a partition of $C \setminus \{i_0\}$ for each $i_0 \in C$, if $|C|$ is odd.
Let $C_s := \bar{C}$ if $|C|$ is even and $C_s := \{(i_0, j_0) \cup \bar{C}$, if $|C|$ is odd.
Define the inequalities in **SCILS** derived from (1) as

$$\sum_{(i,j) \in C_s} X_{ij} \leq \left\lfloor \frac{\beta}{2} \right\rfloor, \quad \text{for all partitions } C_s. \tag{3}$$

Proposition

If inequality (1) is valid for QKP, then the inequalities in the **SCILS** (3) are valid for QKP_{lifted}.

Illustrating a **SCILS**

Let

$$C := \{1, 2, 3\}$$

be a cover.
Consider the partition of C

$$\{\{1\}, \{2, 3\}\}, \quad \{\{2\}, \{1, 3\}\}, \quad \{\{3\}, \{1, 2\}\}$$

The inequality

$$x_1 + x_2 + x_3 \leq 2$$

is a cover inequality, and

$$X_{11} + X_{23} \leq 1$$

$$X_{22} + X_{13} \leq 1$$

$$X_{33} + X_{12} \leq 1$$

is a **SCILS** .

An algorithmic framework (QKP)

We propose an algorithm for **QKP**, that computes upper bounds for the problem by alternating between optimizing Q_p in the convex quadratic relaxation

$$(\mathbf{CQP}_{Q_p}) \quad p^*_{\mathrm{CQP}}(Q_p) := \max \ x^T(Q - Q_p)x + \langle Q_p, X \rangle \quad \text{s.t.} \ (x, X) \in \mathcal{P},$$

and applying cutting planes generated by the valid inequalities proposed.

The algorithmic framework for QKP

- Consists of an **IPM** to improve the matrix parameter Q_p on a convex quadratic relaxation for (QKP).
- At every 10 iterations of the **IPM**, separation problems are solved to generate cuts (n **GCI**, 5 **CILS** and 5 **SCILS** are added to the relaxation of (QKP)).
- When cuts are added to the relaxation, the computation of the search direction of the **IPM** changes accordingly.
- At very iteration of the **IPM** an upper bound is computed by solving the convex quadratic relaxation for the current matrix Q_p

Results

Inst	OptGap (%)	Time (seconds)	Iter	TimeSep (seconds)
I1	0.23	1013.50	100	641.98
I2	**0.00**	632.5	64	411.67
I3	**0.00**	392.55	44	205.70
I4	**0.00**	289.97	31	160.37
I5	0.21	1093.60	10	698.04

Table: Results for $n = 50$

Results

Inst	OptGap (%)	Time (seconds)	Iter	TimeSep (seconds)
I1	**0.00**	2035.30	20	737.86
I2	0.25	2177.30	20	919.41
I3	**0.00**	2007.10	20	773.00
I4	0.12	1885.90	20	828.98
I5	0.04	2309.50	20	970.49

Table: Results for $n = 100$

Conclusions

- We presented a cutting plane algorithm (CPA) to iteratively improve the upper bound for the quadratic knapsack problem (**QKP**).
- We presented a **IPM** , which update the perturbation Q_p at each iteration of the CPA aiming at reducing the upper bound given by the relaxation.
- We also presented new classes of cuts that are added during the execution of the CPA.
  - The cuts generated are effective in improving the upper bound for the **QKP** .
  - These procedures could be applied to more general binary indefinite quadratic problems.

UNIVERSITY OF WATERLOO | FACULTY OF MATHEMATICS Department of Combinatorics and Optimization

Thank you!

daniela.lubke@uwaterloo.ca
http://danielalubke.github.io/

UNIVERSITY OF WATERLOO | FACULTY OF MATHEMATICS Department of Combinatorics and Optimization

Convex relaxation of the binary quadratic knapsack problem

Daniela Lubke
University of Waterloo
Dept. of Combinatorics and Optimization

Joint work with: Marcia Fampa, Fei Wang, Henry Wolkowicz

CAIMS: Canadian Applied and Industrial Mathematics Society
UBC Okanagan from June 13-16, 2022

UNIVERSITY OF WATERLOO
FACULTY OF MATHEMATICS
Department of Combinatorics and Optimization