Improving BiqMac

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July 2016

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- solver for Binary quadratic and Max-cut problems

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- C implementation of a branch-and-bound method

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- solver for Binary quadratic and Max-cut problems
- C implementation of a branch-and-bound method
- using a relaxation based on semidefinite optimization (SDO)
- solved by combination of bundle and interior point methods
- for several problem classes best performing solver
- available via biqmac.aau.at or NEOS-server

Overview

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Semidefinite Optimization

$$
\begin{aligned}
(\textbf{LO}) \quad \min \quad & c^\top x \\
\text{s.t.} \quad & Ax = b \\
& x \geq 0, x \in \mathbb{R}^n
\end{aligned}
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Semidefinite Optimization

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\langle C, X \rangle = \operatorname{trace}(CX) = (\operatorname{vec}(C))^\top \operatorname{vec}(X)
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$$\mathcal{A}(X) = \begin{pmatrix} \langle A_1, X \rangle \\ \langle A_2, X \rangle \\ \vdots \\ \langle A_m, X \rangle \end{pmatrix}, \text{ thus } \begin{pmatrix} \operatorname{vec}(A_1)^\top \\ \operatorname{vec}(A_2)^\top \\ \vdots \\ \operatorname{vec}(A_m)^\top \end{pmatrix} \operatorname{vec}(X) = b$$

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SDO as LO, except "$\succeq$"

$$(X \succeq 0 \Leftrightarrow y^\top X y \geq 0 \quad \forall y \in \mathbb{R}^n)$$

Semidefinite Optimization - Duality

- $S_n^+ = \{X \in \mathcal{S}_n \colon X \succeq 0\}$ is a closed convex cone in $\mathbb{R}^{\binom{n+1}{2}}$.
- Lemma: $\mathcal{S}_n^{+*} = S_n^+$,
  i.e., the cone of semidefinite matrices is self-dual.

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- Slater-constraint qualification guarantees strong duality,
- solvable in polynomial time.

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Max-Cut Problem

given: graph $G = (V, E)$, $V(G) = \{1, \ldots, n\}$, $|E(G)| = m$, w_{ij}

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i.e., find $x \in \{\pm 1\}^n$ such that $\sum w_{ij}(1 - x_i x_j) = x^t L x$ is maximized.

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Unconstrained Binary Quadratic Problem

given: symmetric matrix Q, vector c

$$\begin{aligned} \min \quad & x^t Q x + c^t x \\ \text{s.t.} \quad & x \in \{0, 1\}^n \end{aligned}$$

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Solving MC and solving UBQP is essentially the same.

SDO Relaxation

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solving the SDO relaxation: primal-dual interior-point method

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solving the SDO relaxation: primal-dual interior-point method

- based on Newton's method
- let the constraints be given as $\mathcal{A}(X) = (\vdots)$ with

$$\mathcal{A}(X) = \begin{pmatrix} \langle A_1, X \rangle \\ \langle A_2, X \rangle \\ \vdots \\ \langle A_m, X \rangle \end{pmatrix}$$, in each iteration solve $\boxed{M \Delta y = rhs}$

where

$$m_{ij} = \operatorname{trace}(X A_i Z^{-1} A_j)$$

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$$m_{ij} = \operatorname{trace}(X A_i Z^{-1} A_j)$$

- forming the final system matrix: $O(mn^3 + m^2 n^2)$

SDO Relaxation of k-QKP

for max-cut we have the constraints

$$\operatorname{diag}(X) = \begin{pmatrix} \left\langle \begin{pmatrix} 1 & 0 & \cdots \\ 0 & 0 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, X \right\rangle \\ \left\langle \begin{pmatrix} 0 & 0 & \cdots \\ 0 & 1 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, X \right\rangle \\ \vdots \\ \left\langle \begin{pmatrix} \ddots & \vdots & \vdots \\ \cdots & 0 & 0 \\ \cdots & 0 & 1 \end{pmatrix}, X \right\rangle \end{pmatrix} = e$$

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this yields the system

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$\Longrightarrow$ cheap construction of system matrix.

SDO Relaxation of k-QKP

Hence,

$$\begin{aligned} \max \quad & \langle L, X \rangle \\ \text{s.t.} \quad & \operatorname{diag}(X) = e \\ & X \succeq 0 \end{aligned}$$

can be solved efficiently by interior-point methods.

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SDO relaxation $+$ primal heuristic Goemans-Williamson rounding

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SDO relaxation + primal heuristic Goemans-Williamson rounding
$\leadsto$ branch-and-bound algorithm

next step: stronger bounds by including triangle inequalities

strengthen SDO relaxation

observation: $x_i, x_j, x_k \in \{\pm 1\}$ and $X = xx^t$ then the triangle inequalities hold, i.e.,

$$\begin{aligned}
-x_{ij} - x_{ik} - x_{jk} &\leq 1 \\
-x_{ij} + x_{ik} + x_{jk} &\leq 1 \\
x_{ij} - x_{ik} + x_{jk} &\leq 1 \\
x_{ij} + x_{ik} - x_{jk} &\leq 1
\end{aligned} \qquad 1 \leq i < j < k \leq n$$

$\ldots X \in MET$

- matrix X dimension n
- $4\binom{n}{3}$ additional constraints

Strengthen SDO Relaxation

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- number of linear constraints: $n + 4\binom{n}{3}$

- serious computational effort
- use bundle method

Bundle Method

We would like to compute

$$z^* = \max \ \{\langle L, X\rangle : \operatorname{diag}(X) = e,\ \mathcal{M}(X) \le b,\ X \succeq 0\}$$

Optimizing over $\operatorname{diag}(X) = e, X \succeq 0$ without $\mathcal{M}(X) \le b$ is "easy", but inclusion of $\mathcal{M}(X) \le b$ makes SDO difficult.

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partial Lagrangian dual ($\gamma \geq 0$ dual to $\mathcal{M}(X) \leq b$):

$$\mathcal{L}(X;\gamma) = \langle L, X\rangle + \gamma^t(b - \mathcal{M}(X))$$

dual functional:

$$f(\gamma) = \max_{\operatorname{diag}(X)=e, X\succeq 0} \mathcal{L}(X;\gamma)$$

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dual functional:

$$f(\gamma) = \max_{\operatorname{diag}(X)=e, X\succeq 0} \mathcal{L}(X;\gamma)$$

and thus

$$z^* = \min_{\gamma\in\mathbb{R}^m_{\ge 0}} f(\gamma)$$

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any $\tilde{\gamma} \in \mathbb{R}^m_{\geq 0}$ provides upper bound on z^*

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$\longrightarrow$ try to find tight upper bound (i.e., approximate minimizer of $f(\gamma)$) by using bundle methods.

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iterative procedure, main computational effort in each iteration:

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$$\max_{\operatorname{diag}(X)=e, X \succeq 0} \langle L - \mathcal{M}^t(\hat{\gamma}), X \rangle$$

Bundle Method

Experience using bundle method

- in combination with interior point methods is a good tool to approximate SDOs with a huge number of constraints

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- the number of function evaluations to reach good approximations is surprisingly small
- getting to the “real” optimum is hard

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1. Introduction
   - BiqMac
   - Semidefinite Optimization
   - Max Cut and Unconstrained Binary Quadratic Problems
2. SDO Relaxation
   - Solving the SDO Relaxation
   - Strengthening the SDO Relaxation
3. Improving BiqMac

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stronger relaxation: "exact subgraphs" [Malwina Duda, PhD Thesis, forthcoming]

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...non-convex problem

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...non-convex problem

$$\mathcal{L}_\sigma(y, V; Y) = b^t y + \langle Y, C - \mathcal{A}^t y + VV^t \rangle + \frac{\sigma}{2} \| C - \mathcal{A}^t y + VV^t \|^2$$

Augmented Lagrangian

$$\min_{y,V} \mathcal{L}_\sigma(y, V; Y)$$

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First-order optimality conditions:

$$\nabla_y \mathcal{L}_\sigma(y, V; Y) = 0$$
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$$\nabla_y \mathcal{L}_\sigma(y, V; Y) = b - \mathcal{A}Y - \sigma(\mathcal{A}(C - \mathcal{A}^t y + VVt)) = 0$$

$$\implies \quad y = (\mathcal{A}\mathcal{A}^t)^{-1} \left[\mathcal{A} \left(VV^t + C + \frac{1}{\sigma} Y \right) - \frac{1}{\sigma} b \right]$$

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$\longrightarrow$ express $\mathcal{L}_\sigma$ as a function of V only.

augmented Lagrangian

$$\begin{aligned} \min \quad & f(V) \\ \text{s.t.} \quad & h(V) = 0 \end{aligned}$$

$$\mathcal{L}_\sigma(V; Y) := f(V) + \langle Y, h(V) \rangle + \frac{\sigma}{2} \|h(V)\|^2$$

f and h are sufficiently smooth functions

augmented Lagrangian

Data: f, h
Output: V, Y

augmented Lagrangian

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Initialization: $k = 0$, select $\sigma_k > 0$, $V_k \in \mathbb{R}^{(m+1)\times r}$

augmented Lagrangian

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Initialization: $k = 0$, select $\sigma_k > 0$, $V_k \in \mathbb{R}^{(m+1)\times r}$
while $\|h(V_k)\| > \varepsilon$

augmented Lagrangian

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Initialization: $k = 0$, select $\sigma_k > 0$, $V_k \in \mathbb{R}^{(m+1)\times r}$
while $\|h(V_k)\| > \varepsilon$
  (a) Solve $\min_V \mathcal{L}_{\sigma_k}(V; Y_k)$ approximately, giving V_k

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augmented Lagrangian

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(c) Select $\sigma_{k+1} \geq \sigma_k$

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How to solve the inner minimization?
$\longrightarrow$ descent method (e.g., Fletcher-Reeves)

Computational effort: Depends on cost of function evaluation and computation of the gradient.
$\rightsquigarrow$ relatively cheap in our case.

Optimality Conditions

Optimality conditions of the SDO:

$$
\begin{aligned}
\mathcal{A}Y &= b \\
Y &\succeq 0 \\
\mathcal{A}^t y - C &= Z \\
Z &\succeq 0 \\
ZY &= 0
\end{aligned}
$$

Optimality Conditions

Optimality conditions of the SDO:

$$\begin{array}{rcll} \mathcal{A}Y & = & b & \text{by construction} \\ Y & \succeq & 0 & \\ \mathcal{A}^t y - C & = & Z & \\ Z & \succeq & 0 & \text{by construction} \\ ZY & = & 0 & \text{by construction} \end{array}$$

Optimality Conditions

Optimality conditions of the SDO:

$$
\begin{array}{rcll}
\mathcal{A}Y & = & b & \text{by construction} \\
Y & \succeq & 0 & \text{to be maintained} \\
\mathcal{A}^t y - C & = & Z & \text{stopping criterion} \\
Z & \succeq & 0 & \text{by construction} \\
ZY & = & 0 & \text{by construction}
\end{array}
$$

Summary

- Exact solution method for max cut and unconstrained binary quadratic problems

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Thank you!