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## Reformulation of 0-1 Quadratic Programs

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$$
E=k \frac{1}{2} \sum_{i}^{N} \sum_{j \neq i}^{N} \frac{x_{i} x_{j}}{r_{i j}}+\sum_{i}^{N} \epsilon_{i} x_{i}
$$

where $r_{i j}$ is the distance between impurities $i$ and $j, \epsilon_{i}$ is the energy for impurity $i$ och $x_{i}$ is a binary variable stating if impurity $i$ is occupied or not. If $n$ impurities are occupied then $\sum_{i}^{N} x_{i}=n$.

$$
E=\frac{1}{2} \mathbf{x}^{\top} \mathbf{Q} \mathbf{x}+\mathbf{c}^{\top} \mathbf{x}
$$

where element $M_{i j}=\frac{1}{r_{i j}}$ and $c_{i}=\epsilon_{i}$.

# $\min x^{\top} Q x+c^{\top} x$ 

subject to

$$
\begin{aligned}
& \sum_{i=1}^{n} x_{i}=\frac{n}{2} \\
& x_{i} \in\{0,1\}
\end{aligned}
$$



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$$
\begin{aligned}
& T_{r s t u}= \max _{v, w \in\{-1,0,1\}} \frac{1}{(r-t+n v)^{2}+(s-u+n w)^{2}} \\
& f_{i j}= \begin{cases}1 & \text { if } i \leq m \text { and } j \leq m \\
0 & \text { otherwise }\end{cases} \\
& d_{i j}=d_{n(r-1)+\operatorname{sn}(t-1)+u}=T_{r s t u}
\end{aligned}
$$

where $(r, s)$ are the coordinates for $i$ and $(t, u)$ are the coordinates for $j$

# $\min x^{\top} Q x+c^{\top} x$ 

subject to
$\sum_{i=1}^{n} x_{i}=m$

$$
x_{i} \in\{0,1\}
$$

$$
\min \|A x-b\|^{2}
$$

$$
\min x^{\top} \mathbf{Q} x+\mathbf{c}^{\top} x+k
$$

where $Q$ is $A^{T} A$ and $A$ is a random matrix of size $n \times n, c$ is $-2 A^{T} b$ where $b$ is noice and $k$ is $b^{T} b$.

$$
\begin{gathered}
\min x^{\top} Q x+c^{\top} \mathbf{x} \\
\text { subject to } \\
x_{i} \in\{0,1\}
\end{gathered}
$$

minimize $\operatorname{tr}(Q X)+c^{\top} x$
subject to $A x=a$
$\operatorname{diag}(X)=x$
$\left[\begin{array}{cc}1 & x^{T} \\ x & X\end{array}\right] \geq 0$

$$
\begin{array}{lll}
\operatorname{minimize} & \operatorname{tr}(Q X)+c^{\top} x & \\
\text { subject to } & A x=a & \\
& \operatorname{diag}(X)=x & \\
& {\left[\begin{array}{cc}
1 & x^{\top} \\
x & x
\end{array}\right] \geq 0} & \\
& x_{i} x_{j} \geq 0 & \forall i, j \\
& x_{i} x_{j} \geq x_{i}+x_{j}-1 & \forall i, j \\
& x_{i} x_{j} \leq x_{i} & \forall i, j \\
& x_{i} x_{j} \leq x_{j} & \forall i, j
\end{array}
$$

Results: CG—12|21

| Problem | UB | LB | Gap | Time | SDP LB | SDP gap | SDP time |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 50 | 117.29 | 116.54 | $0.62 \%$ | 2895.8 | 114.72 | $2.18 \%$ | 0.5 |
| 100 | 367.75 | 367.45 | $0.08 \%$ | 9468.3 | 363.21 | $1.23 \%$ | 1.0 |
| 150 | 698.90 | 694.00 | $0.70 \%$ | 14400.6 | 692.35 | $0.94 \%$ | 2.0 |
| 200 | 1097.12 | 1087.62 | $0.87 \%$ | 14400.9 | 1087.39 | $0.89 \%$ | 3.1 |

Table: Average results for CG problems without strengthened SDP

| Problem | UB | LB | Gap | Time | SDP LB | SDP gap | SDP time |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 50 | 117.29 | 116.54 | $0.62 \%$ | 2895.8 | 114.72 | $2.18 \%$ | 0.5 |
| 100 | 367.75 | 367.45 | $0.08 \%$ | 9468.3 | 363.21 | $1.23 \%$ | 1.0 |
| 150 | 698.90 | 694.00 | $0.70 \%$ | 14400.6 | 692.35 | $0.94 \%$ | 2.0 |
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Table: Average results for CG problems without strengthened SDP

| Problem | UB | LB | Gap | Time | SDP LB | SDP gap | SDP time |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 50 | 117.29 | 117.29 | $0.00 \%$ | 2.9 | 117.27 | $0.02 \%$ | 8.1 |
| 100 | 367.75 | 367.75 | $0.00 \%$ | 26.5 | 367.69 | $0.02 \%$ | 8.5 |
| 150 | 698.66 | 698.66 | $0.00 \%$ | 170.8 | 698.53 | $0.02 \%$ | 10.0 |
| 200 | 1096.68 | 1096.68 | $0.00 \%$ | 4621.8 | 1096.44 | $0.02 \%$ | 14.2 |

Table : Average results for CG problems with strengthened SDP

## CG problems SDP gap



Figure : CG gap

Problem number vs. time


Figure: Solution times for tai36c

Problem number vs. gap


Figure: Gap for tai36c

CPLEX and SDP time for some BLS problems of size 40


CPLEX and SDP time for some BLS problems of size 60


## CPLEX and SDP time for some BLS problems of size 80



## CPLEX and SDP time for some BLS problems of size 100



## Some references

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# Thank you for listening! 

## Questions?

