1 Introduction

This file explains an SDP relaxation problem generated from an optimal contribution problem in tree breeding.

The problem we want to solve can be described as an mixed-integer SOCP problem below.

$$
\begin{array}{rclcl}
OPT_{OCP} & := & \max & : & \boldsymbol{g}^T \boldsymbol{x} \\
 & & \text{subject to} & : & \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \le 2\theta \\
 & & & & \boldsymbol{e}^T \boldsymbol{x} = 1 \\
 & & & & \boldsymbol{l} \le \boldsymbol{x} \le \boldsymbol{u} \\
 & & & & x_1, \ldots, x_n \in \left\{0, \frac{1}{N}\right\}.
\end{array} \tag{1}
$$

Here, Z is the number of genotypes and the variables are $x_1, x_2, \ldots, x_n$. The vectors $\boldsymbol{g}, \boldsymbol{l}, \boldsymbol{u} \in \mathbb{R}^Z$ and the matrix $\boldsymbol{A}$ are given. In particular, $\boldsymbol{A}$ is a symmetric positive definite matrix. For the details of $\boldsymbol{A}$, please refer to Yamashita et al. [1] We use $\boldsymbol{e} \in \mathbb{R}^Z$ is the vector of all ones. The parameter is $\theta \in \mathbb{R}$ and this is also given. Since each variable should be 0 or $\frac{1}{N}$, this problem is not a convex problem. In the above problem, we have to choose exactly N genotypes from Z candidates.

In the material below, we use $|S|$ to denote the cardinality of a set S. The vectors $\boldsymbol{e}_S$ is the vector of all ones of the lengths $|S|$.

2 Steps to derive an SDP relaxation

To derive an SDP relaxation, w first remove the variables that can be fixed by the constraint $\boldsymbol{l} \le \boldsymbol{x} \le \boldsymbol{u}$. For example, if $u_i < \frac{1}{N}$, then we fix $x_i = 0$. We use two sets F and V so that $\boldsymbol{F} \cup V \subset \{1, \ldots, Z\}$ and if $i \in F$, x_i can be fixed to 0 or $\frac{1}{N}$. The elements x_i with $i \in V$ remain as variables.

We sort $\boldsymbol{x}$ so that $V = \{1, 2, \ldots, |V|\}$ and $F = \{|V|+1, \ldots, Z\}$. Then we divide the vector $\boldsymbol{x}$ into $\boldsymbol{x}_V$ and $\boldsymbol{x}_F$. In particular, $\boldsymbol{x}_F$ is a constant vector due to $\boldsymbol{l} \le \boldsymbol{x} \le \boldsymbol{u}$, we denote it as $\boldsymbol{c}_F$. Therefore, the vector $\boldsymbol{x}$ can be expressed as $\begin{pmatrix} \boldsymbol{x}_V \\ \boldsymbol{c}_F \end{pmatrix}$. In addition, we divide the given vectors and matrices in the corresponding dimensions. Therefore, we now have

$$
\begin{array}{rclcl}
OPT_{OCP} & = & \max & : & \boldsymbol{g}_V^T \boldsymbol{x}_V + \boldsymbol{g}_F^T \boldsymbol{c}_F \\
 & & \text{subject to} & : & \boldsymbol{x}_V^T \boldsymbol{A}_{VV} \boldsymbol{x}_V + 2\boldsymbol{c}_F^T \boldsymbol{A}_{FV} \boldsymbol{x}_V + \boldsymbol{c}_F^T \boldsymbol{A}_{FF} \boldsymbol{c}_F \le 2\theta \\
 & & & & \boldsymbol{e}_V^T \boldsymbol{x}_V + \boldsymbol{e}_F^T \boldsymbol{c}_F = 1 \\
 & & & & x_i \in \left\{0, \frac{1}{N}\right\} \text{ for } i \in V.
\end{array}
$$

We introduce the binary variables $y_1, \ldots, y_{|V|} \in \{-1, 1\}$ through the relation $\boldsymbol{y}_V := 2N\boldsymbol{x}_V - \boldsymbol{e}_V \in \mathbb{R}^{|V|}$. We also define

$$
\begin{array}{rcl}
g_{\min} & := & \min\{g_i : i = 1, \ldots, Z\} \\
\bar{\boldsymbol{g}}_V & := & \dfrac{1}{4N}(\boldsymbol{g}_V - g_{\min}\boldsymbol{e}_V) \ge 0 \\
\bar{g} & := & \dfrac{1}{2N}(\boldsymbol{g}_V - g_{\min}\boldsymbol{e}_V)^T \boldsymbol{e}_V + (\boldsymbol{g}_F - g_{\min}\boldsymbol{e}_F)^T \boldsymbol{c}_F + g_{\min} \\
\bar{\boldsymbol{c}}_F & := & \boldsymbol{A}_{VV}\boldsymbol{e}_V + 2N\boldsymbol{A}_{VF}\boldsymbol{c}_F \\
\bar{\theta} & := & 2N^2(2\theta - \boldsymbol{c}_F^T \boldsymbol{A}_{FF} \boldsymbol{c}_F) - \dfrac{1}{2}\boldsymbol{e}_V^T \boldsymbol{A}_{VV} \boldsymbol{e}_V - 2N\boldsymbol{c}_F^T \boldsymbol{A}_{FV} \boldsymbol{e}_V \\
\bar{N} & := & 2N(1 - \boldsymbol{e}_F^T \boldsymbol{c}_F) - |V|.
\end{array}
$$

Note that $\boldsymbol{g}^T\boldsymbol{x} = 2\bar{\boldsymbol{g}}_V^T\boldsymbol{y}_V + \bar{g}$ by $\boldsymbol{e}^T\boldsymbol{x} = 1$. Therefore, we can describe the problem in another form.

$$\begin{array}{rcll} OPT_{OCP} & = & \max & : \ 2\bar{\boldsymbol{g}}_V^T\boldsymbol{y}_V + \bar{g} \\ & & \text{subject to} & : \ \boldsymbol{y}_V^T\boldsymbol{A}_{VV}\boldsymbol{y}_V + 2\bar{\boldsymbol{c}}_F^T\boldsymbol{y}_V \le 2\bar{\theta} \\ & & & \ \ \boldsymbol{e}_V^T\boldsymbol{y}_V = \bar{N} \\ & & & \ \ (\boldsymbol{e}_V\boldsymbol{e}_V^T) \bullet (\boldsymbol{y}_V\boldsymbol{y}_V^T) = \bar{N}^2 \\ & & & \ \ y_i \in \{-1, 1\} \ \text{ for } i \in V. \end{array}$$

We add a redundant equation $(\boldsymbol{e}_V\boldsymbol{e}_V^T) \bullet (\boldsymbol{y}_V\boldsymbol{y}_V^T) = \bar{N}^2$ to make the relaxation tighter.

We introduce a variable matrix $\boldsymbol{Y}_{VV} \in \mathbb{S}^{|V|}$ and derive an SDP relaxation.

$$\begin{array}{rcll} OPT_{SDP} & = & \max & : \begin{pmatrix} 0 & \bar{\boldsymbol{g}}_V^T \\ \bar{\boldsymbol{g}}_V & \boldsymbol{O} \end{pmatrix} \bullet \begin{pmatrix} 1 & \boldsymbol{y}_V^T \\ \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} + \bar{g} \\ & & \text{subject to} & : \begin{pmatrix} -2\bar{\theta} & \bar{\boldsymbol{c}}_F^T \\ \bar{\boldsymbol{c}}_F & \boldsymbol{A}_{VV} \end{pmatrix} \bullet \begin{pmatrix} 1 & \boldsymbol{y}_V^T \\ \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} \le 0 \\ & & & \ \begin{pmatrix} -2\bar{N} & \boldsymbol{e}_V^T \\ \boldsymbol{e}_V & \boldsymbol{O} \end{pmatrix} \bullet \begin{pmatrix} 1 & \boldsymbol{y}_V^T \\ \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} = 0 \\ & & & \ \begin{pmatrix} -\bar{N}^2 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{e}_V\boldsymbol{e}_V^T \end{pmatrix} \bullet \begin{pmatrix} 1 & \boldsymbol{y}_V^T \\ \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} = 0 \\ & & & \ \begin{pmatrix} -1 & \boldsymbol{0}^T \\ \boldsymbol{0} & e_i\boldsymbol{e}_i^T \end{pmatrix} \bullet \begin{pmatrix} 1 & \boldsymbol{y}_V^T \\ \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} = 0 \text{ for } i \in V \\ & & & \ \begin{pmatrix} 1 & \boldsymbol{y}_V^T \\ \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} \succeq \boldsymbol{O} \end{array}$$

Finally, we employ an slack variable t and a variable y_{00} to derive a standard SDP form.

$$\begin{array}{rcll} -OPT_{SDP} & = & \min & : \begin{pmatrix} 0 & 0 & \boldsymbol{0}^T \\ 0 & 0 & -\bar{\boldsymbol{g}}_V^T \\ \boldsymbol{0} & -\bar{\boldsymbol{g}}_V & \boldsymbol{O} \end{pmatrix} \bullet \begin{pmatrix} t & 0 & \boldsymbol{0}^T \\ 0 & y_{00} & \boldsymbol{y}_V^T \\ \boldsymbol{0} & \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} - \bar{g} \\ & & \text{subject to} & : \begin{pmatrix} 1 & 0 & \boldsymbol{0}^T \\ 0 & -2\bar{\theta} & \bar{\boldsymbol{c}}_F^T \\ \boldsymbol{0} & \bar{\boldsymbol{c}}_F & \boldsymbol{A}_{VV} \end{pmatrix} \bullet \begin{pmatrix} t & 0 & \boldsymbol{0}^T \\ 0 & y_{00} & \boldsymbol{y}_V^T \\ \boldsymbol{0} & \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} = 0 \\ & & & \ \begin{pmatrix} 0 & 0 & \boldsymbol{0}^T \\ 0 & -2\bar{N} & \boldsymbol{e}_V^T \\ \boldsymbol{0} & \boldsymbol{e}_V & \boldsymbol{O} \end{pmatrix} \bullet \begin{pmatrix} t & 0 & \boldsymbol{0}^T \\ 0 & y_{00} & \boldsymbol{y}_V^T \\ \boldsymbol{0} & \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} = 0 \\ & & & \ \begin{pmatrix} 0 & 0 & \boldsymbol{0}^T \\ \boldsymbol{0} & -\bar{N}^2 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{e}_V\boldsymbol{e}_V^T \end{pmatrix} \bullet \begin{pmatrix} t & 0 & \boldsymbol{0}^T \\ 0 & y_{00} & \boldsymbol{y}_V^T \\ \boldsymbol{0} & \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} = 0 \\ & & & \ \begin{pmatrix} 0 & 0 & \boldsymbol{0}^T \\ 0 & -1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{0} & e_i\boldsymbol{e}_i^T \end{pmatrix} \bullet \begin{pmatrix} t & 0 & \boldsymbol{0}^T \\ 0 & y_{00} & \boldsymbol{y}_V^T \\ \boldsymbol{0} & \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} = 0 \text{ for } i \in V \\ & & & \ \begin{pmatrix} 0 & 0 & \boldsymbol{0}^T \\ 0 & 1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{O} \end{pmatrix} \bullet \begin{pmatrix} t & 0 & \boldsymbol{0}^T \\ 0 & y_{00} & \boldsymbol{y}_V^T \\ \boldsymbol{0} & \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} = 1 \\ & & & \ \begin{pmatrix} t & 0 & \boldsymbol{0}^T \\ 0 & y_{00} & \boldsymbol{y}_V^T \\ \boldsymbol{0} & \boldsymbol{y}_V & \boldsymbol{Y}_{VV} \end{pmatrix} \succeq \boldsymbol{O} \end{array}$$

Note that this SDP problem does not have interior-points and this fact causes numerical difficulty.

References

[1] Makoto Yamashita, Tim J Mullin, and Sena Safarina. An efficient second-order cone programming approach for optimal selection in tree breeding. *arXiv preprint arXiv:1506.04487*, 2015.