Mixed-Integer SOCP in optimal contribution selection of tree breeding

Makoto Yamashita (Tokyo Institute of Technology) Sena Safarina (Tokyo Institute of Technology) Tim J. Mullin (Forestry Research Institute of Sweden)

2016/08/12

This research is supported by JSPS KAKENHI (Grant 15K00032)



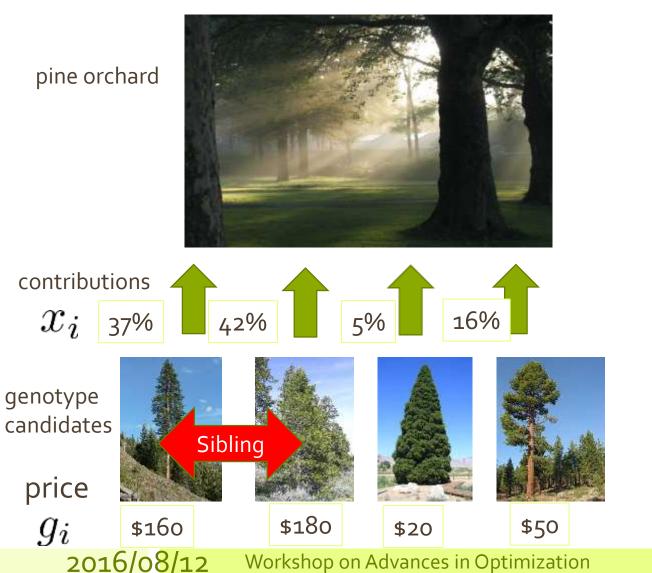
The Workshop on Advances in Optimization August 12-13, 2016 at the TKP Shinagawa Conference Center, Tokyo

Agenda

- 1. Optimal Contribution Problem
- 2. Equally Contribution Problem
- 3. Conic (LP, SOCP, SDP) Relaxations
- 4. Steep-Ascent Method
- 5. Numerical Results

 $\begin{array}{lll} \max &: \quad \boldsymbol{g}^T \boldsymbol{x} \\ \text{s.t.} &: \quad \boldsymbol{e}^T \boldsymbol{x} = 1 \\ & \quad ||\boldsymbol{B}\boldsymbol{x}|| \leq \sqrt{2\theta} \quad \text{SOCP} \\ & \quad \boldsymbol{l} \leq \boldsymbol{x} \leq \boldsymbol{u} \\ & \quad \boldsymbol{x}_1, \dots, \boldsymbol{x}_Z \in \left\{ 0, \frac{1}{N} \right\} \\ & \quad \text{Integer} \end{array}$

Optimal Contribution Problem



$\max_{oldsymbol{x} \in \mathbb{R}^Z}$:	$oldsymbol{g}^Toldsymbol{x}$	best performance
s.t.	:	$e^T x = 1$	unity
		$oldsymbol{l} \leq oldsymbol{x} \leq oldsymbol{u}$	bounds
		$\frac{\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}}{2} \leq \theta$	genetic diversity

QCP (quadratic-constrained problem)

Existing methods for Optimal Contribution Problems

Meuwissen (1997) : Lagrangian multiplier method implemented in GENCONT (www.genebankdata.cgn.wur.nl/gencont/gencont.html)

Pong-Wong and Wooliams (2007) : SDP approach implemented in TREEPLAN \max $x_{\in \mathbb{R}^Z}$ s.t. :

Yamashita et al. (2015) : SOCP Approach

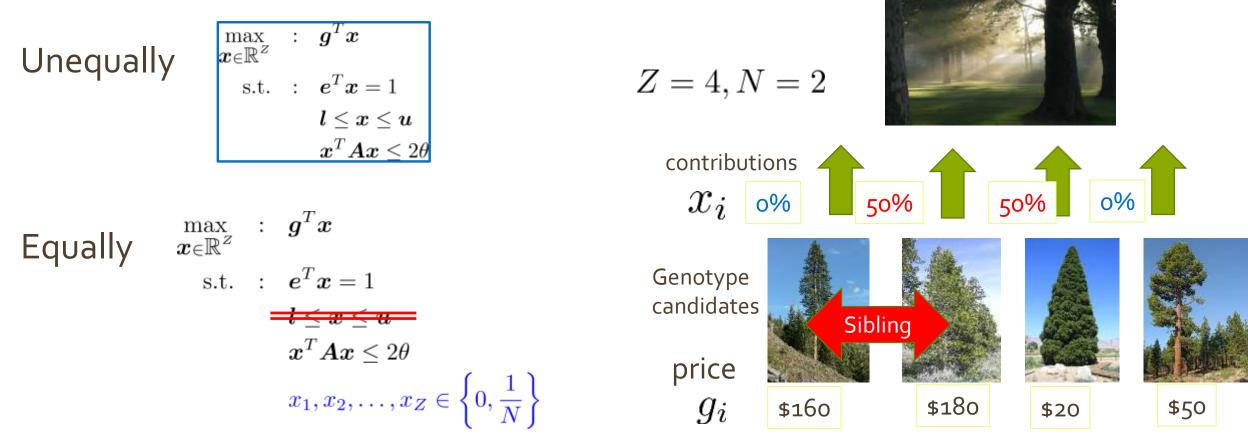
 $\max_{oldsymbol{x}\in\mathbb{R}^Z}$: $oldsymbol{g}^Toldsymbol{x}$ s.t. : $e^T x = 1$ $l \leq x \leq u$ $||\boldsymbol{B}\boldsymbol{x}|| \leq \sqrt{2\theta}$ $\boldsymbol{A} = \boldsymbol{B}^T \boldsymbol{B} \ (\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \le 2\theta \Leftrightarrow ||\boldsymbol{B} \boldsymbol{x}|| \le \sqrt{2\theta})$ A^{-1} is sparse and has special structure

Computation time (in second)

T I										
$g^{\scriptscriptstyle \perp} x$		Z	GENCONT	SDP	SOCP					
$e^T x = 1$ A is positive of	definite	2,045	67.43	70.21	0.09					
$l \leq x \leq u$		15,100	OOM	21994.87	2.92					
$\frac{\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}}{2} \leq \theta \blacksquare \left(\begin{array}{cc} 2\theta & \boldsymbol{x}^T \\ \boldsymbol{x} & \boldsymbol{A}^- \end{array} \right)$	$\left(egin{array}{cc} 2 heta & m{x}^T \ m{x} & m{A}^{-1} \end{array} ight)$ is positive semide	100,100	OOM	OOM	17.92					

OOM is out of memory

Unequally Contribution Problems and Equally Contribution Problems



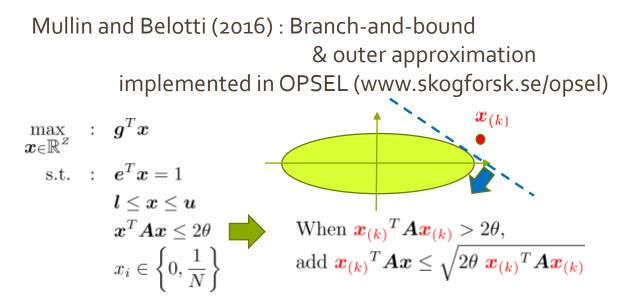
Choose exactly N genotypes from Z candidates.

Existing methods for *Equally* Contribution Problems

Meuwissen (1997) : Lagrangian multiplier method implemented in GENCONT

(www.genebankdata.cgn.wur.nl/gencont/gencont.html)

 $\begin{array}{rcl} \max_{\boldsymbol{x} \in \mathbb{R}^Z} & : & \boldsymbol{g}^T \boldsymbol{x} \\ \text{s.t.} & : & \boldsymbol{e}^T \boldsymbol{x} = 1 \\ \hline & & & \\ & & & \\ \hline & & & \\ & &$



CPLEX can handle mixed-integer SOCP

$$egin{array}{lll} \max & : & oldsymbol{g}^T oldsymbol{x} \ \mathbf{x} \in \mathbb{R}^z & : & oldsymbol{e}^T oldsymbol{x} = 1 \ & oldsymbol{l} \leq oldsymbol{x} \leq oldsymbol{u} \ & oldsymbol{x}^T oldsymbol{A} oldsymbol{x} \leq oldsymbol{u} \ & oldsymbol{x}^T oldsymbol{A} oldsymbol{x} \leq oldsymbol{2} oldsymbol{ heta} \ & oldsymbol{x}_i \in oldsymbol{\left\{0, rac{1}{N}
ight\}} \end{array}$$

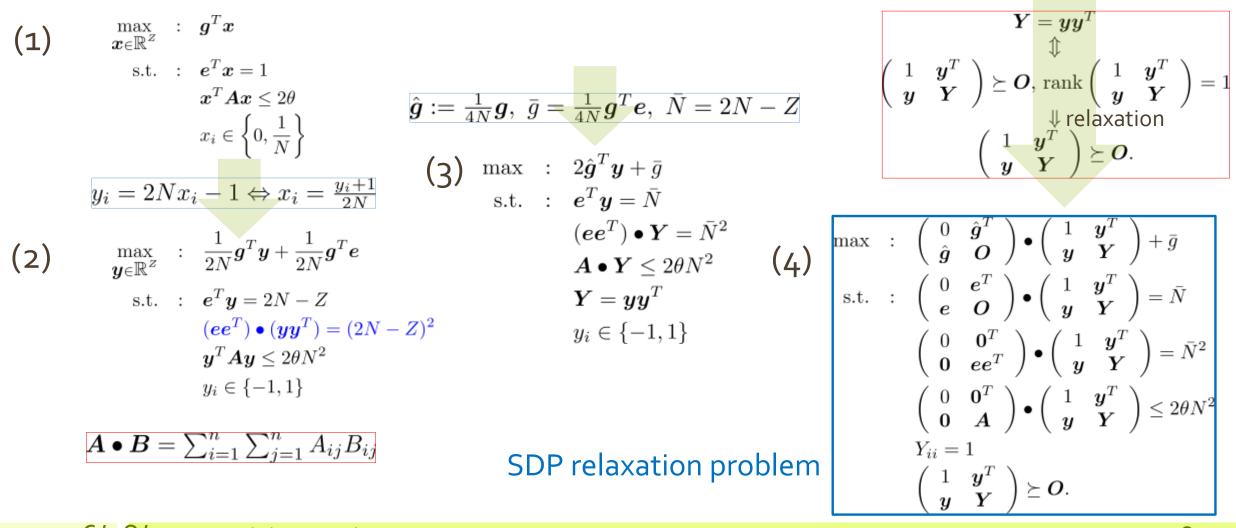
Z = 200, N = 50 (Choose 50 genotypes from 200 candidates)

Solver	time	duality gap
OPSEL	12 hours	0.5%
CPLEX	ıday	11.45%
CPLEX	1 month	11.43%

Finding feasible solutions is very hard.

We should seek an approximate solution in a practical time.

SDP relaxation for Equally Contribution Problem

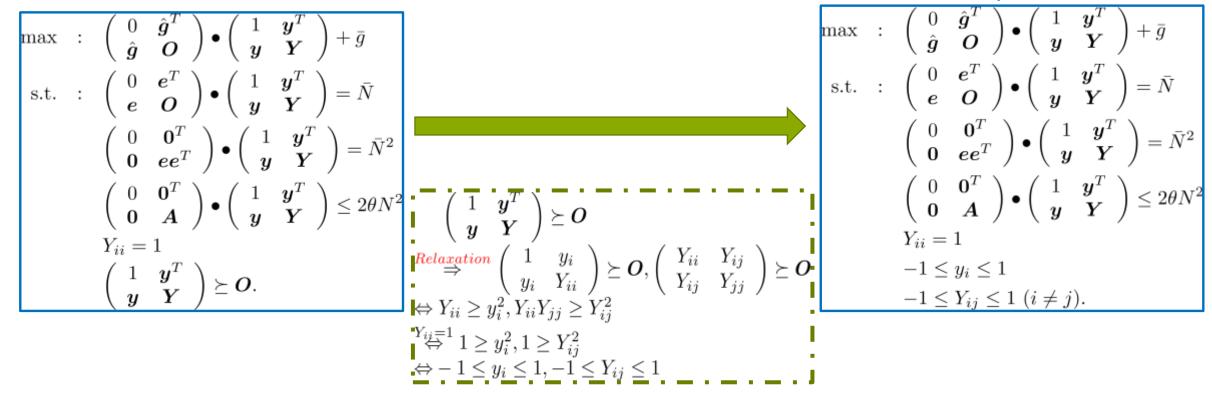


2016/08/12 Workshop on Advances in Optimization

LP relaxation for Equally Contribution Problem

SDP relaxation problem

LP relaxation problem



SOCP relaxation for Equally Contribution ProblemEqually Contribution ProblemSOCP relaxation

$$\begin{array}{ll} \max & : & \boldsymbol{g}^T \boldsymbol{x} \\ \mathbf{x} \in \mathbb{R}^Z & & \\ \text{s.t.} & : & \boldsymbol{e}^T \boldsymbol{x} = 1 \\ & & || \boldsymbol{B} \boldsymbol{x} || \leq \sqrt{2\theta} \\ & & x_i \in \left\{ 0, \frac{1}{N} \right\} \end{array}$$

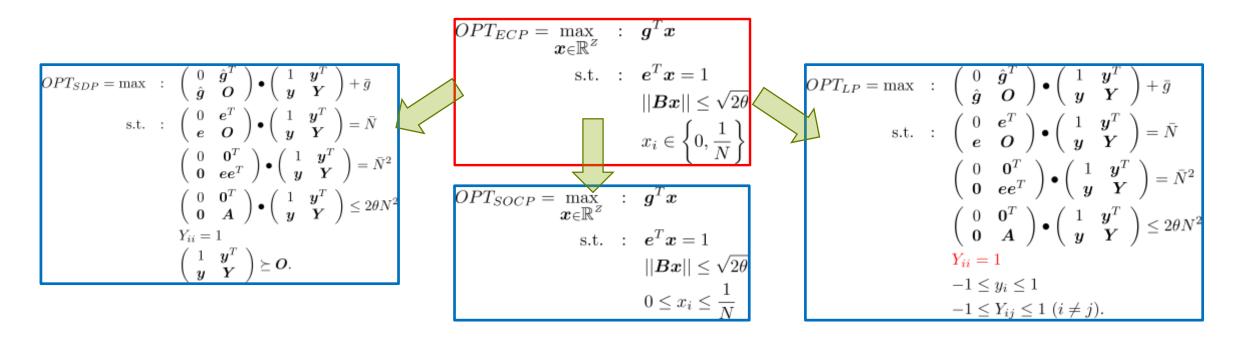
$$egin{array}{lll} \max &: & oldsymbol{g}^T oldsymbol{x} \ \mathbf{x} \in \mathbb{R}^Z &: & \mathbf{g}^T oldsymbol{x} \ ext{s.t.} &: & oldsymbol{e}^T oldsymbol{x} = 1 \ & || oldsymbol{B} oldsymbol{x} || \leq \sqrt{2 heta} \ & 0 \leq x_i \leq rac{1}{N} \end{array}$$

 $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \leq 2\theta \Leftrightarrow ||\boldsymbol{B} \boldsymbol{x}|| \leq \sqrt{2\theta} \text{ (by } \boldsymbol{A} = \boldsymbol{B}^T \boldsymbol{B})$

This problem is a piece of cake, due to the structure of B.



The relation between three conic relaxations



1: 2: Some steps are necessary to prove $OPT_{ECP} \leq OPT_{SDP} \leq OPT_{SOCP}$ 3: Some assumptions on input data are necessary for

Easy to show $OPT_{ECP} \leq OPT_{SDP} \leq OPT_{LP}$ $OPT_{ECP} \leq OPT_{SDP} \leq OPT_{SOCP} \leq OPT_{LP}$ due to the constraint $Y_{ii} = 1$

An SDP-based randomized algorithm for QCQP and its theoretical analysis

$$OPT_{QCQP} = \max_{\boldsymbol{y} \in \mathbb{R}^{n}} : \boldsymbol{y}^{T} \boldsymbol{A}^{0} \boldsymbol{y} + (\boldsymbol{b}^{0})^{T} \boldsymbol{y} + c^{0}$$

s.t. : $\boldsymbol{y}^{T} \boldsymbol{A}^{k} \boldsymbol{y} + (\boldsymbol{b}^{k})^{T} \boldsymbol{y} + c^{k} \leq 0 (k = 1, \dots, m)$
$$OPT_{SDP} = \max : \boldsymbol{B}^{0} \bullet \boldsymbol{Y}$$

s.t. : $\boldsymbol{B}^{k} \bullet \boldsymbol{Y} \leq 0 (k = 1, \dots, m)$
 $\boldsymbol{B}^{m+1} \bullet \boldsymbol{Y} = 1$
 $\boldsymbol{Y} \succeq \boldsymbol{O}$
$$\boldsymbol{B}^{k} = \begin{pmatrix} c^{k} & (\boldsymbol{b}^{k})^{T} \\ \boldsymbol{b}^{k} & \boldsymbol{A}^{k} \end{pmatrix} (k = 0, 1, \dots, m), \boldsymbol{B}^{m+1} = \begin{pmatrix} 1 & \boldsymbol{0}^{T} \\ \boldsymbol{0} & \boldsymbol{O} \end{pmatrix}$$

Cholesky factorization of SDP solution

 $\boldsymbol{Y}^* = \boldsymbol{V}^T \boldsymbol{V}, \qquad \boldsymbol{V} = [\boldsymbol{v}_0, \boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n]$

Randomly-generated solution

$$\hat{\boldsymbol{y}} \in \mathbb{R}^n : \hat{y}_i = \sqrt{Y_{ii}^*} \operatorname{sign}(\boldsymbol{v}^T \boldsymbol{v}_0) \operatorname{sign}(\boldsymbol{v}^T \boldsymbol{v}_i) \ (i = 1, \dots, n)$$
$$\boldsymbol{v} \text{ is randomly chosen from } \{\boldsymbol{v} \in \mathbb{R}^n : ||\boldsymbol{v}|| = 1\}.$$

Tseng (2003) analyzed the expected objective value $E[\hat{y}^T A^0 \hat{y} + (b^0)^T \hat{y}] \geq \frac{2}{\pi} OPT_{SDP} + (1 - \frac{2}{\pi}) \rho_{SDP}$

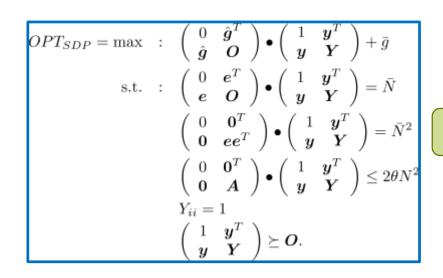
$$\rho_{SDP} = \min : B^{0} \bullet Y$$

s.t. : $B^{k} \bullet Y = B^{k} \bullet Y^{*} (k \in \mathcal{I})$
 $B^{m+1} \bullet Y = 1$
 $Y \succeq O$

$$\mathcal{I} = \left\{ k \in \{1, 2, \dots, m\} : \boldsymbol{B}^k \text{ is diagonal} \right\}$$

2016/08/12 Workshop on Advances in Optimization

A theoretical analysis of SDP relaxation for equally contribution problems



Generate \hat{y} by the randomized algorithm Check the objective value $2\hat{g}^T\hat{y} + \bar{g}$

 $\begin{pmatrix} 0 & \boldsymbol{0}^{T} \\ \boldsymbol{0} & \boldsymbol{e}\boldsymbol{e}^{T} \end{pmatrix} \bullet \begin{pmatrix} 1 & \boldsymbol{y}^{T} \\ \boldsymbol{y} & \boldsymbol{Y} \end{pmatrix} = \bar{N}^{2} \begin{bmatrix} \frac{2}{\pi} OPT_{SDP} + \left(1 - \frac{2}{\pi}\right) \left(-2\hat{\boldsymbol{g}}^{T}\boldsymbol{e} + \bar{\boldsymbol{g}}\right) \leq E[2\hat{\boldsymbol{g}}^{T}\hat{\boldsymbol{y}} + \bar{\boldsymbol{g}}] \leq \alpha OPT_{SDP} + \left(1 - \alpha\right) \left(2\hat{\boldsymbol{g}}^{T}\boldsymbol{e} + \bar{\boldsymbol{g}}\right) \\ \begin{pmatrix} 0 & \boldsymbol{0}^{T} \\ \boldsymbol{\eta} \end{pmatrix} = \left(1 - \frac{\boldsymbol{y}^{T}}{2}\right) \left(-2\hat{\boldsymbol{g}}^{T}\boldsymbol{e} + \bar{\boldsymbol{g}}\right) \leq E[2\hat{\boldsymbol{g}}^{T}\hat{\boldsymbol{y}} + \bar{\boldsymbol{g}}] \leq \alpha OPT_{SDP} + \left(1 - \alpha\right) \left(2\hat{\boldsymbol{g}}^{T}\boldsymbol{e} + \bar{\boldsymbol{g}}\right) \end{bmatrix}$

$$\alpha = \min\left\{\frac{2}{\pi} \frac{\theta}{1 - \cos\theta} : 0 \le \theta \le \pi\right\} \sim 0.878$$

	Ζ	2θ	lower bound	(Average of 1000 trials)	upper bound	OPT_{SDP}
	200	0.0334	16.161	25.812	30.340	25.386
	1050	0.0627	5.075	32.305	112.600	24.938
	2045	0.0711	279.259	446.089	2007.212	438.659
_	5050	0.1081	5.775	284.965	806.205	42.786

Unfortunately, the bounds are not very sharp.

Most of the generated solutions are not feasible for the equally contribution problems.

$$\hat{\boldsymbol{x}}^T \boldsymbol{A} \hat{\boldsymbol{x}} > 2\theta$$

A maximization problem with a penalty term

- We need a method to obtain an approximate solution in a practical time
- We move the quadratic constraints into the objective function

$$OPT_{ECP} = \max_{\boldsymbol{x} \in \mathbb{R}^{Z}} : \boldsymbol{g}^{T}\boldsymbol{x}$$
s.t. $: \boldsymbol{e}^{T}\boldsymbol{x} = 1$
 $x^{T}\boldsymbol{A}\boldsymbol{x} \leq 2\theta$
 $x_{i} \in \left\{0, \frac{1}{N}\right\}$

$$OPT_{PNL} = \max_{\boldsymbol{x} \in \mathbb{R}^{Z}} : \boldsymbol{g}^{T}\boldsymbol{x} - \lambda \max\{\boldsymbol{x}^{T}\boldsymbol{A}\boldsymbol{x} - 2\theta, 0\}$$
s.t. $: \boldsymbol{e}^{T}\boldsymbol{x} = 1$
 $x_{i} \in \left\{0, \frac{1}{N}\right\}$

We can prove $OPT_{ECP} = OPT_{PEL}$ for sufficiently large λ .

For the weight λ , we use the Lagrange multiplier corresponding to $\mathbf{x}^T \mathbf{A} \mathbf{x} = 2\theta$.

$$egin{array}{rl} \max & : & oldsymbol{g}^Toldsymbol{x} \ oldsymbol{x} \in \mathbb{R}^Z & & \ ext{s.t.} & : & oldsymbol{e}^Toldsymbol{x} = 1 \ oldsymbol{x}^Toldsymbol{A}oldsymbol{x} = 2 heta \end{array}$$

Steep-ascent method

$$DPT_{PNL} = \max_{\boldsymbol{x} \in \mathbb{R}^Z} : f_{\lambda}(\boldsymbol{x}) := \boldsymbol{g}^T \boldsymbol{x} - \lambda \max\{\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} - 2\theta, 0\}$$

s.t. : $\boldsymbol{e}^T \boldsymbol{x} = 1$
 $x_i \in \left\{0, \frac{1}{N}\right\}$

Idea: Search a better point by swapping $x_i = 0$ and $x_j = \frac{1}{N}$

- 1. Set $\mathbf{x}^+ \in \mathbb{R}^Z$ as an solution of a conic relaxation problem. Sort \mathbf{x}^+ and get the descending order s such that $x_{s(1)}^+ \ge x_{s(2)}^+ \ge x_{s(3)}^+ \ge \ldots \ge x_{s(Z)}^+$. Set $\mathbf{x}^0 \in \{0, 1/N\}^Z$ such that $x_{s(i)}^0 = 1/N$ for $i = 1, \ldots, N$ and $x_{s(i)}^0 = 0$ for $i = N + 1, \ldots, Z$. Set $V_0 = \{i \in \{1, \ldots, Z\} : \mathbf{x}_i^0 = 0\}$ and $V_{1/N} = \{i \in \{1, \ldots, Z\} : \mathbf{x}_i^0 = 1/N\}$. Set the iteration counter h = 0.
- 2. Find $(i^h, j^h) = \operatorname{argmax} \left\{ f_{\lambda} (\boldsymbol{x}^h + \frac{1}{N} \boldsymbol{e}_i \frac{1}{N} \boldsymbol{e}_j) \mid (i, j) \in V_0 \times V_{1/N} \right\}.$

3. If
$$f_{\lambda}(\boldsymbol{x}^h + \frac{1}{N}\boldsymbol{e}_{i^h} - \frac{1}{N}\boldsymbol{e}_{j^h}) \leq f_{\lambda}(\boldsymbol{x}^h)$$
, output \boldsymbol{x}^h as the solution

4. Set
$$\mathbf{x}^{h+1} = \mathbf{x}^h + \frac{1}{N}\mathbf{e}_{i^h} - \frac{1}{N}\mathbf{e}_{j^h}, V_0 = V_0 \cup \{j_h\} \setminus \{i_h\}, V_{1/N} = V_{1/N} \cup \{i_h\} \setminus \{j_h\}, h \leftarrow h + 1 \text{ and return to Step 2.}$$

Steep-ascent and discrete convex functions

- Our steep-ascent method is a modification of the steep-descent method for M-convex functions that was implemented in ODICON. <u>http://www.misojiro.t.u-tokyo.ac.jp/~tutimura/odicon/</u>
- Unfortunately, our objective function is not an M-convex function. However, *the steep-ascent method finds at least a local optimizer*.

$$OPT_{PNL} = \max_{\boldsymbol{x} \in \mathbb{R}^Z} : \boldsymbol{f}_{\lambda}(\boldsymbol{x}) := \boldsymbol{g}^T \boldsymbol{x} - \lambda \max\{\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} - 2\theta, 0\}$$

s.t. : $\boldsymbol{e}^T \boldsymbol{x} = 1$
 $x_i \in \left\{0, \frac{1}{N}\right\}$

• By specializing the algorithm of ODICON in this specific problem, our implementation is 20 times faster than ODICON.

Core i7 3770K, 32GB LP by CPLEX, SOCP by ECOS, SDP by SDPT3

Comparison of three conic relaxations

Algorithm	Z	2θ	$oldsymbol{g}^Toldsymbol{x}$	$x^T A x$	iter	time (s)
CR (LP)			28.068	0.0574	0	0.07
SA (LP)			25.029	0.0334	21	0.10
CR (SOCP)	200	0.0334	26.156	0.0334	0	0.02
SA $(SOCP)$	200	0.0554	25.090	0.0334	13	0.06
CR (SDP)			25.386	0.0321	0	1.29
SA (SDP)			25.207	0.0334	4	1.30
CR (LP)			57.630	0.3672	0	10.17
SA (LP)		0.1081	38.696	0.1080	23	11.17
CR (SOCP)	5050		43.036	0.1081	0	0.21
SA (SOCP)	5050		42.691	0.1080	3	0.37
CR (SDP)			42.786	0.0980	0	2221.22
SA (SDP)			42.431	0.1080	3	2221.40
CR (LP)			603.783	0.4568	0	129.55
SA (LP)	15222	0.0388	438.791	0.0388	42	139.03
CR (SOCP)			468.367	0.0388	0	0.99
SA (SOCP)			460.769	0.0388	9	2.56
CR (SDP)			288.739	0.0195	0	17433.38^{\dagger}
SA (SDP)			460.409	0.0388	43	17441.93^{\dagger}

- SDP attains the best approximation
- However, numerically instable (due to lack of interior-point)
- SOCP is much fast
- When combining with the steep-ascent, SOCP is competitive with SDP

N = 50

CR: convex relaxation (the solution may not be feasible for equally contribution problem) SA: the steep-ascent method starting from the conic relaxation

Comparison with other existing methods

Algorithm	Z	2θ	$g^T x$	$x^T A x$	$f_{\lambda}(oldsymbol{x})$	#chosen	time (s)
GENCONT	200	0.0334	25.290	0.0342	20.087	50	0.06
OPSEL			25.191	0.0334	25.191	50	1779.13
CPLEX	200		25.190	0.0334	25.190	50	4270.77
SA (SOCP)			25.090	0.0334	25.090	50	0.06
GENCONT			24.983	0.0627	24.983	48	7.91
OPSEL	1050	0.0627	24.858	0.0627	24.858	50	> 10800
CPLEX	1050		Cannot obtain a feasible solution in 3 hours				> 10800
SA (SOCP)			24.831	0.0627	24.831	50	0.09
GENCONT			42.780	0.1089	-306.701	50	1769.72
OPSEL	5050	0.1081	42.702	0.1081	42.702	50	> 10800
CPLEX	5050	0.1081	42.456	0.1066	42.456	50	2.02
SA (SOCP)			42.691	0.1080	42.691	50	0.37
GENCONT		10100 0.0701	Out of memory				
OPSEL	10100		46.252	0.0700	46.252	50	> 10800
CPLEX			Cannot	obtain a	feasible sol	ution in 3 hours	> 10800
SA (SOCP)			46.568	0.0701	46.568	50	0.87

N = 50

The steep ascent method with SOCP outputs favorable solutions in very short time.

We stopped OPSEL and CPLEX when [gap < 1%] or [time > 3 hours].

2016/08/12 Workshop on Advances in Optimization

Conclusion

- Optimal contribution problems in tree breeding
- Conic (LP, SOCP, SDP) relaxation problems
- Steep ascent method
- SOCP relaxation with the steep ascent method outputs a favorable solution in a practical time.

- Can we tighten the SDP relaxation with a shorter time?
- Other optimization problems?

• Thank you very much for your attention!!