

Separation, Inverse Optimization, and Decomposition: Some Observations

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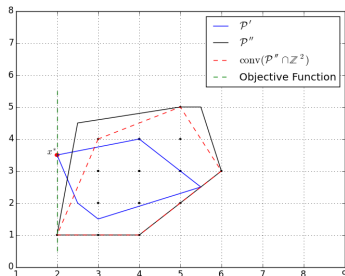
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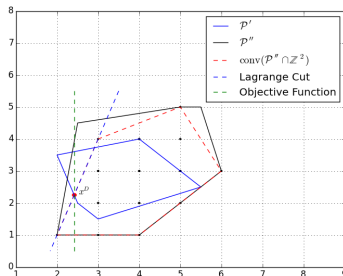


What Is This Talk About?

- Duality in integer programming (and more generally)
- Connecting some concepts.
 - Separation problem
 - Inverse optimization
 - Decomposition methods
 - Primal cutting plane algorithms for MILP



(a)



(b)

Setting

- We focus on the case of the *mixed integer linear optimization problem* (MILP), but many of the concepts are more general.

$$z_{IP} = \max_{x \in \mathcal{S}} c^\top x, \quad (\text{MILP})$$

where, $c \in \mathbb{R}^n$, $\mathcal{S} = \{x \in \mathbb{Z}^r \times \mathbb{R}^{n-r} \mid Ax \leq b\}$ with $A \in \mathbb{Q}^{m \times n}$, $b \in \mathbb{Q}^m$.

- For most of the talk, we consider the case $r = n$ and \mathcal{P} bounded for simplicity.

Duality in Mathematical Optimization

- It is difficult to define precisely what is meant by “duality” in general mathematics, though the literature is replete with various “dualities.”
 - Set Theory and Logic (De Morgan Laws)
 - Geometry (Pascal’s Theorem & Brianchon’s Theorem)
 - Combinatorics (Graph Coloring)
- In optimization, duality is *the* central concept from which much theory and computational practice emerges.

Forms of Duality in Optimization

- NP versus co-NP (computational complexity)
- Separation versus optimization (polarity)
- Inverse optimization versus forward optimization
- Weyl-Minkowski duality (representation theorem)
- Economic duality (pricing and sensitivity)
- Primal/dual functions/problems

What is Duality Used For?

- One way of viewing duality is as a tool for *transformation*.
 - Primal \Rightarrow Dual
 - H-representation \Rightarrow V-representation
 - Membership \Rightarrow Separation
 - Upper bound \Rightarrow Lower bound
 - Primal solutions \Rightarrow Valid inequalities
- Optimization methodologies exploit these dualities in various ways.
 - Solution methods based on primal/dual bounding
 - Generation of valid inequalities
 - Inverse optimization
 - Sensitivity analysis, pricing, warm-starting

Duality in Integer Programming

- The following generalized *dual* can be associated with the base instance (MILP) (see Güzelsoy and Ralphs [2007])

$$\min \{F(b) \mid F(\beta) \geq \phi_D(\beta), \beta \in \mathbb{R}^m, F \in \Upsilon^m\} \quad (\text{D})$$

where $\Upsilon^m \subseteq \{f \mid f : \mathbb{R}^m \rightarrow \mathbb{R}\}$ and ϕ_D is the (*dual*) *value function* associated with the base instance (MILP), defined as

$$\phi_D(\beta) = \max_{x \in \mathcal{S}(\beta)} c^\top x \quad (\text{DVF})$$

for $\beta \in \mathbb{R}^m$, where $\mathcal{S}(\beta) = \{x \in \mathbb{Z}^r \times \mathbb{R}^{n-r} \mid Ax \leq \beta\}$.

- We call F^* *strong* for this instance if F^* is a *feasible* dual function and $F^*(b) = \phi_D(b)$.

The Membership Problem

Membership Problem

Given $x^* \in \mathbb{R}^n$ and polyhedron \mathcal{P} , determine whether $x^* \in \mathcal{P}$.

For $\mathcal{P} = \text{conv}(\mathcal{S})$, the membership problem can be formulated as the following LP.

$$\min_{\lambda \in \mathbb{R}_+^{\mathcal{E}}} \left\{ 0^\top \lambda \mid E\lambda = x^*, 1^\top \lambda = 1 \right\} \quad (\text{MEM})$$

where \mathcal{E} is the set of extreme points of \mathcal{P} and E is a matrix whose columns are the members of \mathcal{E} .

- When (MEM) is feasible, then we have a proof that $x^* \in \mathcal{P}$.
- When (MEM) is infeasible, we obtain a separating hyperplane.
- It is perhaps not too surprising that the dual of (MEM) is a variant of the *separation problem*.

The Separation Problem

Separation Problem

Given a polyhedron \mathcal{P} and $x^* \in \mathbb{R}^n$, either certify $x^* \in \mathcal{P}$ or determine (π, π_0) , a valid inequality for \mathcal{P} , such that $\pi x^* > \pi_0$.

For \mathcal{P} , the separation problem can be formulated as the dual of (MEM).

$$\max \left\{ \pi x^* - \pi_0 \mid \pi^\top x \leq \pi_0 \ \forall x \in \mathcal{E}, (\pi, \pi_0) \in \mathbb{R}^{n+1} \right\} \quad (\text{SEP})$$

where \mathcal{E} is the set of extreme points of \mathcal{P} .

- Note that we need some appropriate normalization.

The Separation Problem

- Assuming 0 is in the interior of \mathcal{P} , we can normalize by taking $\pi_0 = 1$.
- In this case, we are optimizing over the *l-polar* of \mathcal{P} .
- This is equivalent to changing the objective of (MEM) to $\min \mathbf{1}^\top \lambda$.
- We can interpret this essentially as how much we need to expand \mathcal{P} in order to include x^* .
- If the result is more than one, x^* is not in \mathcal{P} , otherwise it is.

The 1-Polar

Assuming $\mathbf{0}$ is in the interior of \mathcal{P} , the set of all inequalities valid for \mathcal{P} is

$$\mathcal{P}^* = \left\{ \pi \in \mathbb{R}^n \mid \pi^\top x \leq 1 \ \forall x \in \mathcal{P} \right\} \quad (1)$$

and is called its *1-polar*.

Properties of the 1-Polar

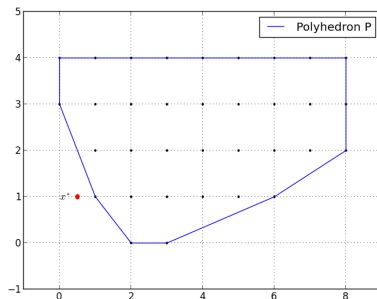
- \mathcal{P}^* is a polyhedron;
- $\mathcal{P}^{**} = \mathcal{P}$;
- $x \in \mathcal{P}$ if and only if $\pi^\top x \leq 1 \ \forall \pi \in \mathcal{P}^*$;
- If \mathcal{E} and \mathcal{R} are the extreme points and extreme rays of \mathcal{P} , respectively, then

$$\mathcal{P}^* = \left\{ \pi \in \mathbb{R}^n \mid \pi^\top x \leq 1 \ \forall x \in \mathcal{E}, \pi^\top r \leq 0 \ \forall r \in \mathcal{R} \right\}.$$

- A converse of the last result also holds.
- Separation can be interpreted as optimization over the polar.

Separation Using an Optimization Oracle

- We can solve (SEP) using a cutting plane algorithm that separates intermediate solutions from the 1-polar.
- The separation problem for the 1-polar of \mathcal{P} is precisely a linear optimization problem over \mathcal{P} .
- We can visualize this in the dual space as column generation wrt (MEM).
- Example



Separation Example: Iteration 1

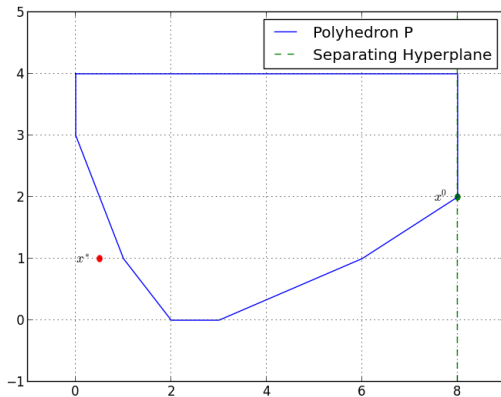


Figure: Separating x^* from \mathcal{P} (Iteration 1)

Separation Example: Iteration 2

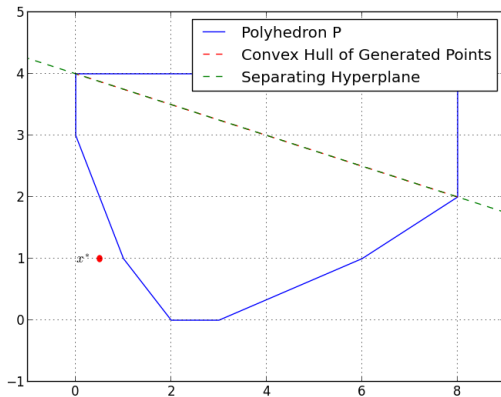


Figure: Separating x^* from \mathcal{P} (Iteration 2)

Separation Example: Iteration 3

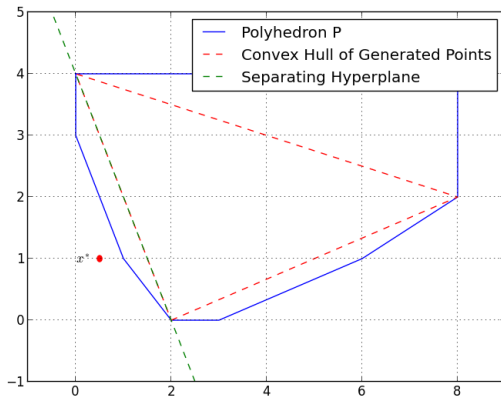


Figure: Separating x^* from \mathcal{P} (Iteration 3)

Separation Example: Iteration 4

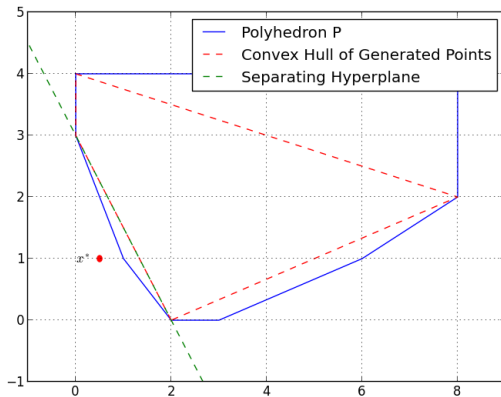


Figure: Separating x^* from \mathcal{P} (Iteration 4)

Separation Example: Iteration 5

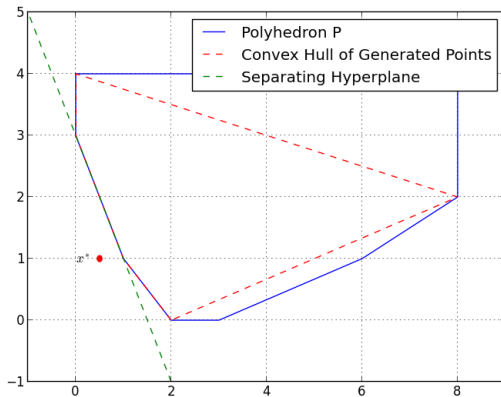


Figure: Separating x^* from \mathcal{P} (Iteration 5)

Inverse Problems

What is an inverse problem?

Given a function, an inverse problem is that of determining *input* that would produce a given *output*.

- The input may be partially specified.
 - We may want an answer as close as possible to a given *target*.
-
- This is precisely the mathematical notion of the inverse of a function.
 - A *value function* is a function whose value is the optimal solution of an optimization problem defined by the given input.
 - The inverse problem with respect to an optimization problem is to evaluate the inverse of a given *value function*.

Why is Inverse Optimization Useful?

Inverse optimization is useful when we can observe the result of solving an optimization problem and we want to know what the input was.

Example: Consumer preferences

- Let's assume consumers are rational and are making decisions by solving an underlying optimization problem.
- By observing their choices, we try ascertain their utility function.

Example: Analyzing seismic waves

- We know that the path of seismic waves travels along paths that are optimal with respect to some physical model of the earth.
- By observing how these waves travel during an earthquake, we can infer things about the composition of the earth.

Formal Setting

We consider the inverse of the (*primal*) *value function* ϕ_P , defined as

$$\phi_P(d) = \max_{x \in \mathcal{S}} d^\top x = \min_{x \in \text{conv}(\mathcal{S})} d^\top x \quad \forall d \in \mathbb{R}^n. \quad (\text{PVF})$$

With respect to a given $x^0 \in \mathcal{S}$, the inverse problem is defined as

$$\min \left\{ f(d) \mid d^\top x^0 = \phi_P(d) \right\}, \quad (\text{INV})$$

The classical objective function is taken to be $f(d) = \|c - d\|$, where $c \in \mathbb{R}^n$ is a given target.

A Small Example

- The feasible set of the inverse problem is the set of objective vectors that make x^0 optimal.
- This is precisely the dual of $\text{cone}(\mathcal{S} - \{x^0\})$, which is, roughly, a translation of the polyhedron described by the inequalities binding at x^0 .

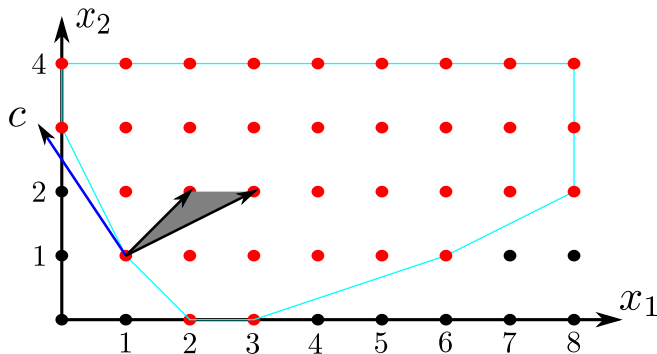


Figure: $\text{conv}(\mathcal{S})$ and cone \mathcal{D} of feasible objectives

Inverse Optimization as a Mathematical Program

- To formulate as a mathematical program, we need to represent the implicit constraints of (INV) explicitly.
- The cone of feasible objective vectors can be described as

$$\mathcal{D} = \left\{ d \in \mathbb{R}^n \mid d^\top x \leq d^\top x^0 \ \forall x \in \mathcal{S} \right\} \quad (\text{IFS})$$

- Since \mathcal{P} is bounded, we need only the inequalities corresponding to extreme points of $\text{conv}(\mathcal{S})$.
- This set of constraints is exponential in size, but we can generate them dynamically, as we will see.
- Note that this corresponds to the set of inequalities valid for \mathcal{S} that are binding at x^0 .
- Alternatively, it is the set of all inequalities valid for the so-called *corner relaxation* with respect to x^0 .

Formulating the Inverse Problem

General Formulation

$$\begin{array}{llll} \min & f(d) & & \\ \text{s.t.} & d^\top x \leq d^\top x^0 & \forall x \in \mathcal{E} & (\text{INVMP}) \end{array}$$

- With $f(d) = \|c - d\|$, this can be linearized for ℓ_1 and ℓ_∞ norms.
- The separation problem for the feasible region is again optimization over $\text{conv}(\mathcal{S})$.

Separation and Inverse Optimization

- It should be clear that inverse optimization and separation are very closely related.
- First, note that the inequality

$$\pi^\top x \leq \pi_0 \quad (\text{PI})$$

is valid for \mathcal{P} if and only if $\pi_0 \geq \phi_P(\pi)$.

- We refer to inequalities of the form (PI) for which $\pi_0 = \phi_P(\pi)$ as *primal inequalities*.
- This is as opposed to *dual inequalities* for which $\pi_0 = \phi^\pi(b)$, where ϕ^π is a *dual function* for (MILP) when the objective function is taken as π .
- The feasible set of (INV) can be seen as the set of all valid primal inequalities that are tight at x^0 .

Primal Separation

- Suppose we take $f(d) = d^\top x^0 - d^\top x^*$ for given $x^* \in \mathbb{R}^n$.
- Then this problem is something like the classical separation problem.
- This variant is what Padberg and Grötschel [1985] called the *primal separation problem* (see also Lodi and Letchford [2003]).
- Their original idea was to separate x^* with an inequality binding at the current incumbent.
- Taking x^0 to be the current incumbent, this is exactly what we're doing.
- With this objective, we need a normalization to ensure boundedness, as before.
- A straightforward option is to take $d^\top x^0 = 1$ (Note: For this normalization, 0 must be in the interior of $\text{conv}(\mathcal{S})$)
- (INVMP) is then precisely the separation problem for the corner relaxation with respect to x^0 (alternatively, the conic hull of $\mathcal{S} - \{x^0\}$).

Dual of the Inverse Problem

- Roughly speaking, the dual of (INVMP) is the membership problem for $\text{cone}(\mathcal{S} - \{x^0\})$.

$$\min_{\lambda \in \mathbb{R}_+^{\mathcal{E}}} \left\{ 0^\top \lambda \mid \bar{E} \lambda = x^* - x^0 \right\} \quad (\text{CMEM})$$

where \bar{E} is the set of extreme rays of $\text{cone}(\mathcal{S} - \{x^0\})$

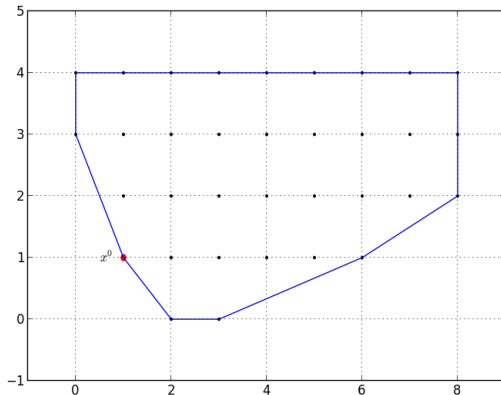
- With the normalization, this becomes

$$\min_{\lambda \in \mathbb{R}_+^{\mathcal{E}}} \left\{ \alpha \mid \bar{E} \lambda = x^* - \alpha x^0 \right\}, \quad (\text{CMEMN})$$

- We can interpret the value of α as the amount by which we need to shift x^* along the direction x^0 in order for it to be inside $\text{cone}(\mathcal{S} - \{x^0\})$.
- If the optimal value is greater than one, then $x^* - x^0$ is not in the cone, otherwise it is.

Inverse Optimization with Forward Optimization Oracle

- We can use an algorithm almost identical to the one from earlier.
- We now generate inequalities valid for the corner relaxation associated with x^0 .



Inverse Example: Iteration 1

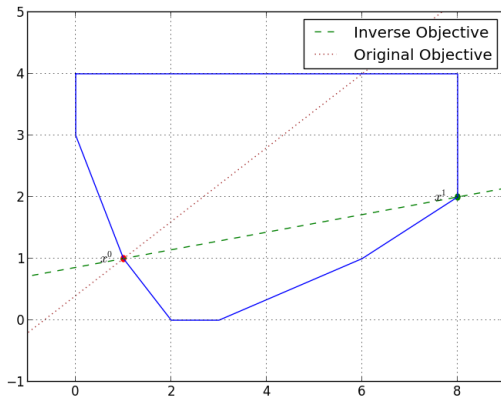


Figure: Solving the inverse problem for \mathcal{P} (Iteration 1)

Inverse Example: Iteration 2

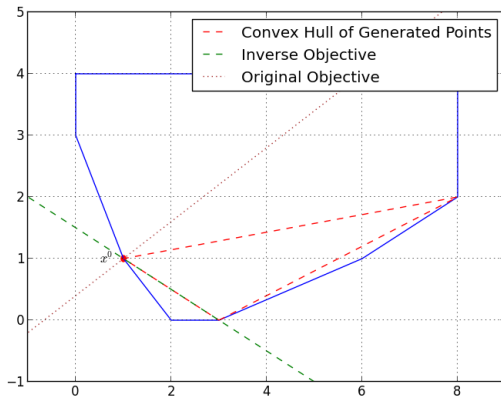


Figure: Solving the inverse problem for \mathcal{P} (Iteration 3)

Inverse Example: Iteration 3

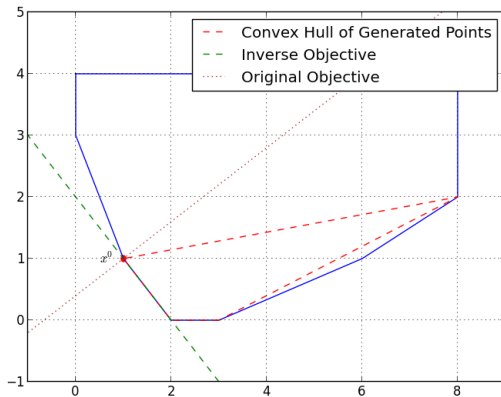


Figure: Solving the inverse problem for \mathcal{P} (Iteration 3)

Tractability of Inverse MILP

Theorem 1 *Bulut and Ralphs [2015] Inverse MILP optimization problem under ℓ_∞/ℓ_1 norm is solvable in time polynomial in the size of the problem input, given an oracle for the MILP decision problem.*

- This is a direct result of the well-known result of Grötschel et al. [1993].

Complexity of Inverse MILP

Sets

$$\mathcal{K}(\gamma) = \{d \in \mathbb{R}^n \mid \|c - d\| \leq \gamma\}$$

$$\mathcal{X}(\gamma) = \{x \in \mathcal{S} \mid \exists d \in \mathcal{K}(\gamma) \text{ s.t. } d^\top (x^0 - x) > 0\},$$

$$\mathcal{K}^*(\gamma) = \{x \in \mathbb{R}^n \mid d^\top (x^0 - x) \geq 0 \ \forall d \in \mathcal{K}(\gamma)\}.$$

Inverse MILP Decision Problem (INVD)

Inputs: $\gamma, c, x^0 \in \mathcal{S}$ and MILP feasible set \mathcal{S} .

Problem: Decide whether $\mathcal{K}(\gamma) \cap \mathcal{D}$ is non-empty.

Theorem 2 *Bulut and Ralphs [2015] INVD is coNP-complete.*

Theorem 3 *Bulut and Ralphs [2015] Both (MILP) and (INV) optimal value problems are D^p -complete.*

Connections to Constraint Decomposition

As usual, we divide the constraints into two sets.

$$\begin{aligned} \max \quad & c^\top x \\ \text{s.t.} \quad & A'x \leq b' \text{ (the “nice” constraints)} \\ & A''x \leq b'' \text{ (the “complicating” constraints)} \\ & x \in \mathbb{Z}^n \end{aligned}$$

$$\begin{aligned} \mathcal{P}' &= \{x \in \mathbb{R}^n \mid A'x \leq b'\}, \\ \mathcal{P}'' &= \{x \in \mathbb{R}^n \mid A''x \leq b''\}, \\ \mathcal{P} &= \mathcal{P}' \cap \mathcal{P}'', \\ \mathcal{S} &= \mathcal{P} \cap \mathbb{Z}^n, \text{ and} \\ \mathcal{S}_R &= \mathcal{P}' \cap \mathbb{Z}^n. \end{aligned}$$

Reformulation

- We replace the H-representation of the polyhedron \mathcal{P}' with a V-representation of $\text{conv}(\mathcal{S}_R)$.

$$\max \quad c^\top x \quad (2)$$

$$\text{s.t.} \quad \sum_{s \in \mathcal{E}} \lambda_s s = x \quad (3)$$

$$A''x \leq b'' \quad (4)$$

$$\sum_{s \in \mathcal{E}} \lambda_s = 1 \quad (5)$$

$$\lambda \in \mathbb{R}_+^{\mathcal{E}} \quad (6)$$

$$x \in \mathbb{Z}^n \quad (7)$$

where \mathcal{E} is the set of extreme points of $\text{conv}(\mathcal{S}_R)$.

- If we relax the integrality constraints (7), then we can also drop (3) and we obtain a relaxation which is tractable.
- This relaxation may yield a bound better than that of the LP relaxation.

The Decomposition Bound

Using the aforementioned relaxation, we obtain a formulation for the so-called *decomposition bound*.

$$z_{\text{IP}} = \max_{x \in \mathbb{Z}^n} \left\{ c^\top x \mid A'x \leq b', A''x \leq b'' \right\}$$

$$z_{\text{LP}} = \max_{x \in \mathbb{R}^n} \left\{ c^\top x \mid A'x \leq b', A''x \leq b'' \right\}$$

$$z_{\text{D}} = \max_{x \in \text{conv}(\mathcal{S}_R)} \left\{ c^\top x \mid A''x \leq b'' \right\}$$

$$z_{\text{IP}} \leq z_{\text{D}} \leq z_{\text{LP}}$$

It is well-known that this bound can be computed using various decomposition-based algorithms:

- Lagrangian relaxation
- Dantzig-Wolfe decomposition
- Cutting plane method

Shameless plug: Try out DIP/DipPy!

A framework for switching between various decomp-based algorithms.

Example

$$\max \quad -x_1$$

$$-x_1 - x_2 \geq -8, \quad (8)$$

$$-0.4x_1 + x_2 \geq 0.3, \quad (9)$$

$$x_1 + x_2 \geq 4.5, \quad (10)$$

$$3x_1 + x_2 \geq 9.5, \quad (11)$$

$$0.25x_1 - x_2 \geq -3, \quad (12)$$

$$7x_1 - x_2 \geq 13, \quad (13)$$

$$x_2 \geq 1, \quad (14)$$

$$-x_1 + x_2 \geq -3, \quad (15)$$

$$-4x_1 - x_2 \geq -27, \quad (16)$$

$$-x_2 \geq -5, \quad (17)$$

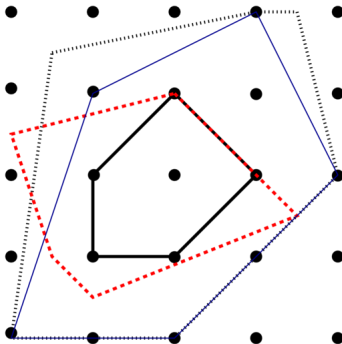
$$0.2x_1 - x_2 \geq -4, \quad (18)$$





$$x \in \mathbb{Z}''. \quad (19)$$

Example (cont)

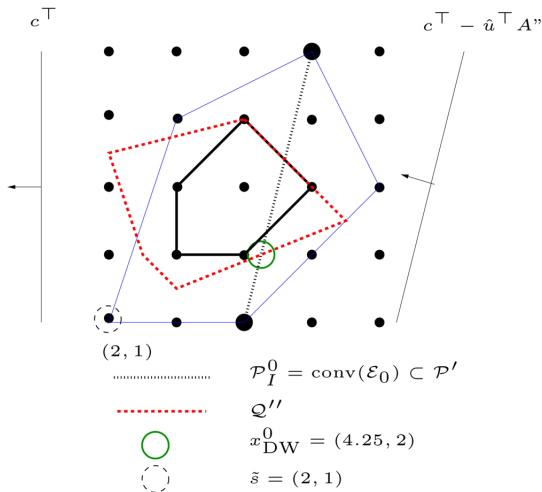
$$\begin{aligned}\mathcal{Q}' &= \{x \in \mathbb{R}^2 \mid x \text{ satisfies (8) -- (12)}\}, \\ \mathcal{Q}'' &= \{x \in \mathbb{R}^2 \mid x \text{ satisfies (13) -- (18)}\}, \\ \mathcal{Q} &= \mathcal{Q}' \cap \mathcal{Q}'', \\ \mathcal{S} &= \mathcal{Q} \cap \mathbb{Z}^n, \text{ and} \\ \mathcal{S}_R &= \mathcal{Q}' \cap \mathbb{Z}^n.\end{aligned}$$

Constraint Decomposition in Integer Programming

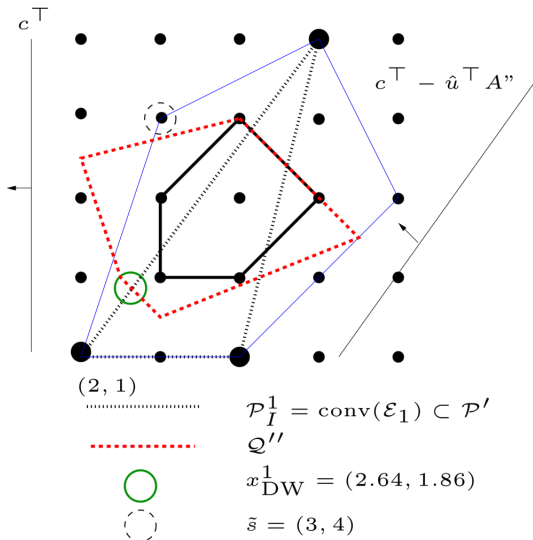


	$\text{conv}(S) = \text{conv}\{x \in \mathbb{Z}^n \mid A'x \geq b', A''x \geq b''\}$
	$\text{conv}(S_R) = \text{conv}\{x \in \mathbb{Z}^n \mid A'x \geq b'\}$
	$Q' = \{x \in \mathbb{R}^n \mid A'x \geq b'\}$
	$Q'' = \{x \in \mathbb{R}^n \mid A''x \geq b''\}$

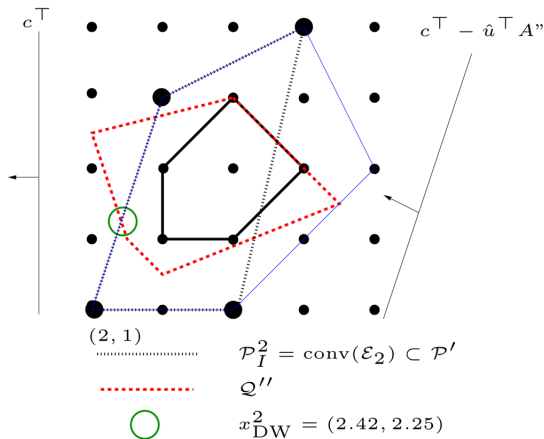
Geometry of Dantzig-Wolfe Decomposition



Geometry of Dantzig-Wolfe Decomposition



Geometry of Dantzig-Wolfe Decomposition



Lagrange Cuts

- Boyd [1990] observed that for $u \in \mathbb{R}_+^m$, a *Lagrange cut* of the form

$$(c - uA'')^\top x \leq LR(u) - ub'' \quad (\text{LC})$$

is valid for \mathcal{P} .

- If we take u^* to be the optimal solution to the Lagrangian dual, then this inequality reduces to

$$(c - u^*A'')^\top x \leq z_D - ub'' \quad (\text{OLC})$$

- If we now take

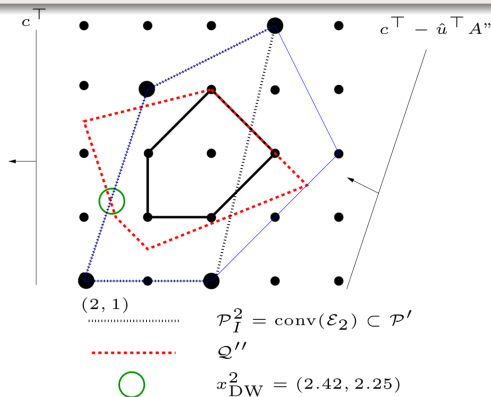
$$x^D \in \operatorname{argmax} \left\{ c^\top x \mid A''x \leq b'', (c - u^*A'')^\top x \leq z_D - ub'' \right\},$$

then we have $c^\top x^D = z_D$.

Connecting the Dots

Results

- The inequality (OLC) is a primal inequality for $\text{conv}(\mathcal{S}_R)$ wrt x^D .
- $c - uA''$ is a solution to the inverse problem wrt $\text{conv}(\mathcal{S}_R)$ and x^D .
- These properties also hold for $e \in \mathcal{E}$ such that $\lambda_e^* > 0$ in the RMP.



Conclusions and Future Work

- We gave a brief overview of connections between a number of different problems and methodologies.
- Exploring these connections may be useful to improving intuition and understanding.
- The connection to primal cutting plane algorithms is still largely unexplored, but may lead to new algorithms for inverse problems.
- Much of that is discussed here can be further generalized to general computation via Turing machines (useful?).

Thank You!



References I

- A. Boyd. The lagrangian and other primal cutting planes for linear integer programming. Technical Report TR90-03, Rice University, Department of Computational and Applied Mathematics, 1990.
- A. Bulut and T.K. Ralphs. On the complexity of inverse mixed integer linear optimization. Technical report, COR@L Laboratory Report 15T-001-R3, Lehigh University, 2015. URL <http://coral.ie.lehigh.edu/~ted/files/papers/InverseMILP15.pdf>.
- M. Grötschel, L. Lovász, and A. Schrijver. *Geometric Algorithms and Combinatorial Optimization*, volume 2 of *Algorithms and Combinatorics*. Springer, second corrected edition edition, 1993.
- M. Güzelsoy and T.K. Ralphs. Duality for mixed-integer linear programs. *International Journal of Operations Research*, 4:118–137, 2007. URL <http://coral.ie.lehigh.edu/~ted/files/papers/MILPD06.pdf>.

References II

- A. Lodi and A.N. Letchford. Primal separation algorithms. *4OR*, 1:209–224, 2003.
- M.W. Padberg and M. Grötschel. Polyhedral computations. In E. L. Lawler, Jan Karel Lenstra, A. H. G. Rinnooy Kan, and D. B. Shmoys, editors, *The Traveling Salesman Problem. A Guided Tour of Combinatorial Optimization*, chapter 9, pages 307–360. Wiley, 1985.