Multi-point Inverse Optimization of Constraint Parameters

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Abstract

Consider a problem where a set of feasible observations are provided by an expert and a cost function is defined that characterizes which of the observations dominate the others and are hence, preferred. Our goal is to find a set of linear constraints that would render all the given observations feasible while making the preferred ones optimal for the cost (objective) function. Providing such feasible regions (i) builds a baseline for categorizing future observations as feasible or infeasible, and (ii) allows for using sensitivity analysis to discern changes in optimal solutions if the objective function changes in the future.

To this end, we propose a multi-point inverse optimization framework to recover the constraint set of a forward optimization problem. We focus on linear models in which the objective function is known but the constraint matrix is partially or fully unknown. We propose a general multi-point inverse optimization methodology that recovers the complete constraint matrix. We then introduce a tractable equivalent reformulation that can be solved more efficiently. Furthermore, we provide and discuss several generalized measure functions to inform the desirable properties of the feasible region based on user preference and historical data. Our numerical case studies verify the validity of our approach, emphasize the differences between the proposed measures, and provide intuition for large-scale implementations.

Keywords: Inverse optimization, constraint parameters, multiple observations, measure function, duality theorems, linear programming

1. Introduction

Conventional (forward) optimization problems find an optimal solution for a given set of parameters. Inverse optimization, on the other hand, infers the parameters of a forward optimization problem given a set of observed solutions (typically a single point). In the
literature, inverse optimization is often employed to derive the parameters of the cost vector of an optimization problem while the constraint parameters are assumed to be fully known. In this paper, we focus on the opposite case. We impute the constraint parameters (as opposed to the objective function) of a linear forward problem given a cost vector and a set of observations.

When imputing the cost vector, it is usually assumed that the observed solution is a candidate optimal solution (Ahuja and Orlin, 2001; Iyengar and Kang, 2005). More recently, a number of studies also consider the case where the observed solution is not necessarily a candidate for optimality. They propose inverse models to minimize error-metrics that capture the optimality gap of the observed solution (Keshavarz et al., 2011; Chan et al., 2014, 2018; Bertsimas et al., 2015; Aswani et al., 2018; Naghavi et al., 2019). More recently, multiple or uncertain observations are considered, where the cost vector is imputed based on a given set or an uncertainty set of feasible observations (Keshavarz et al., 2011; Troutt et al., 2006, 2008; Chow and Recker, 2012; Aswani et al., 2018; Bertsimas et al., 2015; Ghabadi et al., 2018; Esfahani et al., 2018). Finally, Tavashoglu et al. (2018) find a set of inverse-feasible cost vectors, instead of a single cost vector, that makes feasible observations optimal.

Extending from only imputing the cost vector, some studies consider the case where both the objective function and the right hand side (RHS) of the constraints are imputed simultaneously for specific types of problems (Dempe and Lohse, 2006; Chow and Recker, 2012; Černý and Hladík, 2016). Note that when the feasible region is being imputed, a given observation can always become optimal since the constraints can be adjusted to position the given observation on the boundary of the feasible region. A number of studies focus on imputing only the constraint parameters of the forward problem. Given a single observation, Černý and Hladík (2016) find RHS of the constraints from a pre-specified set of possible parameters. In other studies, the RHS is imputed in such a way that the observed solution becomes optimal (Chow and Recker, 2012; Birge et al., 2017) or near optimal according to a pre-specified distance metric (Dempe and Lohse, 2006; Güler and Hamacher, 2010; Saez-Gallego and Morales, 2018). Most related to our work is Chan and Kaw (2019) who propose a single-point inverse optimization method for finding constraint parameters that make the given observation optimal for some unknown cost vector. They use specific distance metrics that are based on a prior belief on the constraint parameters and discuss possibility of trivial solutions. Although the forward problem we consider is similar to that of Chan and Kaw (2019), we propose a multi-point inverse optimization method that makes the preferred solutions optimal for a specific cost vector. We introduce generalized distance metrics that do not necessarily rely on a prior belief on constraint parameters and generate non-trivial solutions by design.
While inverse optimization problems for imputing the cost vector often retain the complexity of their corresponding forward problems (e.g., linear programming), imputing the constraint parameters often constitutes a non-convex problem due to the presence of multiple bilinear terms which are more complex to solve, and global optimality of the solutions is not guaranteed. To address these concerns, a few studies in the literature focus on specific problem instances and find certain criteria or assumptions to reduce the complexity (Birge et al., 2017; Brucker and Shakhlevich, 2009). Others propose a solution methodology that solves a sequence of convex optimization problems under a specific distance metric (Chan and Kaw, 2019). In this paper, instead of attempting to solve a nonlinear non-convex problem, we use the problem’s theoretical properties and propose a simplifying equivalent reformulation that does not include any bilinear terms and hence, can be solved more efficiently. We also further simplify the problem by providing closed-form solutions or suggesting decomposition approaches for specific cases.

To the best of our knowledge, this paper is the first in the literature to propose a multi-point inverse optimization framework for inferring the full constraint matrix of a linear programming model based on several observations. We propose tractable reformulations of the nonlinear problems and suggest several measures that allow the models to infer the constraint parameters without requiring any prior expert-opinion on the properties of the parameters. Our numerical case studies verify the validity of our approach, emphasize the differences between the proposed measures, and provide intuition for large-scale implementation. The contributions of this paper are as follows:

- We propose a modified single-point inverse optimization methodology that infers a set of partially-unknown constraint parameters of the forward problem so as to make a given observation optimal for a specific cost vector.
- We extend this model to a multi-point inverse optimization methodology that inputs any number of observations and finds the constraint parameters so as to make all the observations feasible and the preferred observation(s) optimal for a specific cost vector.
- We develop an equivalent tractable reformulation of the multi-point inverse optimization model that eliminates the bilinearity of the original model and hence, can be solved more efficiently.
- We introduce a set of generalized measure functions that can be used to induce the desirable properties of the feasible region of the forward problem and do not necessarily rely on a prior belief on the constraint parameters.
We test and validate our proposed methodology on numerical case studies and demonstrate the characteristics of each of the measure functions introduced.

The rest of this paper is organized as follows: In Section 2, we provide motivation for the proposed methodology by providing examples of application areas. Section 3 introduces our generalized methodology for inverse optimization of constraint parameters, its theoretical properties, and an equivalent reformulation. In Section 4, we introduce a number of specific measure functions that can be used as the objective function of the inverse optimization problem and discuss the theoretical properties of each. We illustrate the results of our methodology using two numerical case studies in Section 5. Finally, conclusions and future research directions are provided in Section 6.

2. Motivation

Inverse optimization has been applied to a number of different application areas, from healthcare (Erkin et al., 2010; Ayer, 2015) and nutrition (Ghobadi et al., 2018) applications to finance (Bertsimas et al., 2012) and electricity markets (Birge et al., 2017). In this section, we provide two example applications where imputing the feasible region based on a set of collected observations is of practical importance. These applications serve to motivate the development of our proposed methodology.

A. Cancer Treatment Planning: Consider the radiation therapy treatment planning problem for cancer patients. The input of the problem is a medical image (e.g., CT, MRI) which includes contours that delineate the cancerous region (i.e., tumor) and the surrounding healthy organs. The goal of a treatment planner is to find the direction, shape, and intensity of radiation beams such that a set of clinical metrics on the tumor and the surrounding healthy organs are satisfied. In current practice, there are clinical guidelines on the upper/lower limits for different clinical metrics. Planners often try to find an ‘acceptable’ treatment plan based on these guidelines to forward to an oncologist who will inspect it and either approve or return the plan to the planner. If the plan is not approved, the planner receives a set of instructions on which metrics to adjust. It often happens that the final approved plan may not meet all the clinical limits simultaneously as there are trade-offs between different metrics.

Suppose we have a set of approved treatment plans from previous patients. Even though there are clinical guidelines on acceptability thresholds for different metrics, in reality, there may exist approved treatment plans that do not meet these limits. There may also exist plans that do meet the the guidelines but are not approved by the oncologists since she/he
believed a better plan is achievable. Hence, the true feasible region of the forward problem in treatment planning is unknown. Considering the historically-approved plans as “feasible points”, we can employ our inverse optimization approach to find the constraints parameters, based on which we can understand the implicit logic of the oncologists in approving a treatment plan. In doing so, we would help both the oncologists and the planners by (i) generating more realistic lower/upper bounds on the clinical metrics based on past observations, (ii) improving the quality of plans given the clear guidelines and hence, reducing the number of preliminary plans passed back and forth between the planner and oncologists, and (iii) improving the quality of plans by preventing low-quality solutions that otherwise satisfy the acceptability metrics, especially for inverse treatment planning methods that heavily rely on provided metrics.

**B. Diet Problem:** Consider a diet recommendation system that suggests a variety of food items based on a user’s dietary needs and/or personal preferences. Each meal can be characterized by a set of features and/or metrics such as meat content or daily value of each nutrient. Assume the objective function of the underlying (forward) optimization problem is known. Examples of such objective functions would be minimizing total calories in a weight loss program, minimizing sugar intake in a diabetic diet, or minimizing monetary cost. In addition to dietary requirements, each person has a set of implicit constraints that would result in them finding a certain suggestion “palatable” or not. It is clear that different users would have different such constraints, and it is not explicitly possible to list what these constraints are. In such cases, our inverse optimization model can use historical data to ensure the next suggested meal in the diet recommendation system is palatable.

For example, consider a user who is mostly vegetarian and is implicitly limiting the amount of meat servings during the week, or another user who prefers to limit the amount of diary intake when consuming certain vegetables. If we observe the user’s diet choices (feasible observations) for a certain time horizon, the inverse optimization model would find the set of constraints (feasible region) that captures this behaviour by making diets that are too far off from the past observations infeasible while ensuring that the required amount of nutrients are met, the diet is palatable (feasible), and a given objective (e.g., cost, calories) is minimized.

**3. Methodology**

In this section, we first set up the forward optimization problem where, contrary to conventional inverse optimization, the cost vector is known and the unknown parameters are,
instead, the constraint parameters. We allow for the case that some of the constraint parameters might be known in advance. Let \( x, c \in \mathbb{R}^n, A \in \mathbb{R}^{m_1 \times n}, b \in \mathbb{R}^{m_1}, G \in \mathbb{R}^{m_2 \times n} \) and \( h \in \mathbb{R}^{m_2} \). We define our linear forward optimization (FO) problem as

\[
\begin{align*}
\text{FO} : \quad & \text{minimize} & \quad c'x \\
\text{subject to} & \quad Ax \geq b, \quad (1a) \\
& \quad Gx \geq h. \quad (1c)
\end{align*}
\]

We assume the constraint parameters \( A \) and \( b \) are the unknown constraint parameters that the inverse optimization aims to infer. The known constraint parameters are denoted by \( G \) and \( h \). Throughout this paper, the sets of unknown and known constraints are denoted by \( I = \{1, \ldots, m_1\} \) and \( I' = \{1, \ldots, m_2\} \), respectively. The \( i \)th row of the constraint matrices \( A \) and \( G \) is referred to as \( a_i \) and \( g_i \), respectively. Similarly, the \( i \)th elements of the \( b \) and \( h \) vectors are denoted by \( b_i \) and \( h_i \), respectively. The set \( J = \{1, \ldots, n\} \) denotes the columns in the constraint matrices (i.e., the indices of the \( x \) variable). We use bold numbers \( \mathbf{1} \) and \( \mathbf{0} \) to denote the all-ones and the all-zeros vectors, respectively.

In what follows, we first propose a single-point inverse optimization model and then extend it to multi-point inverse optimization to infer the unknown constraint parameters. Next, using the properties of the problem, we introduce an equivalent simplified reformulation which can be employed to solve the original nonlinear non-convex inverse optimization problems more efficiently.

### 3.1. Single-point Inverse Optimization

Given a single observation \( x^0 \), a cost vector \( c \), and known constraint parameters \( G \) and \( h \) (if any), we would like to formulate an inverse optimization model that finds the unknown constraint parameters \( A \) and \( b \) such that the observation \( x^0 \) is optimal for the forward problem \( \text{FO} \). Without loss of generality, we assume that the observation \( x^0 \) is feasible for the known constraints \( Gx \geq h \) since, otherwise, the forward problem will be ill-defined and the inverse problem will have no solution.

Let \( y \) and \( w \) be dual vectors for constraints (1b) and (1c) of \( \text{FO} \), respectively. The
single-point inverse optimization model (IO) can be written as follows:

\[
\begin{align*}
\text{IO} : \text{minimize} & \quad \mathcal{F}(A, b; \mathcal{D}), \\
\text{subject to} & \quad A x^0 \geq b, \quad \quad (2a) \\
& \quad c' x^0 = b' y + h' w, \quad \quad (2b) \\
& \quad A' y + G' w = c, \quad \quad (2c) \\
& \quad ||a_i|| = 1, \quad \forall i \in I, \quad (2d) \\
& \quad y, w \geq 0. \quad \quad (2e)
\end{align*}
\]

where the objective \( \mathcal{F}(A, b; \mathcal{D}) \) is a measure that drives the desired properties of the feasible region based on some given input parameter \( \mathcal{D} \). More details and examples of the measure function \( \mathcal{F}(A, b; \mathcal{D}) \) are discussed in Section 4. Constraint (2b) enforces primal feasibility of \( x^0 \). Constraints (2d) and (2f) are the dual feasibility constraints. Constraint (2c) is the strong duality constraint that ensures \( x^0 \) is the optimal solution of \( \text{FO} \). Finally, without loss of generality, constraint (2e) normalizes the left-hand-side of each unknown constraint based on some norm \( || \cdot || \) to avoid finding multiple scalars of the same constraint parameters.

Our proposed single-point IO model differs from those in the literature in several ways: (i) we consider both \( A \) and \( b \) to be unknown, (ii) we assume that the \( c \) vector is known, which means that \( x^0 \) should be optimal for a specific \( c \) vector (as opposed to \( \text{any} \ c \) vector), and (iii) we do not necessarily require any prior knowledge or conditions on the unknown parameters \( A, b \) in order to generate non-trivial solutions. We note that while prior conditions on the unknown parameters are not required in our formulation, if such knowledge exists, it can be easily incorporated as additional constraints or as part of the known constraints. We make the following assumption to ensure that the forward problem is not simply a feasibility problem.

**Assumption 1.** \( c \neq 0 \).

We note that without Assumption 1, the IO problem will be simplified since it will have many trivial solutions including \( w = y = b = A = 0 \) and \( A = -G, y = -w \). For the rest of this paper, we assume Assumption 1 holds. We next show that the IO formulation is valid and has non-trivial feasible solutions.

**Proposition 1.** The IO formulation is feasible.

*Proof.* Let \( w = 0, y = ||c|| \cdot 1, \quad b = (c' x^0)/||c||, \) and \( a_i = c/||c||, \forall i \in I, \) given \( c \neq 0 \). Then \((A, b, y, w)\) is a feasible solution to IO. \( \square \)
In general, any feasible region that makes the point \( x^0 \) optimal for FO is a feasible solution to the single-point IO problem. Therefore, the solutions to single-point IO can be trivial and its applicability can be limited since in practice, often more than one observation is available for the forward problem. If more than one observation is available, the IO formulation does not apply since the strong duality does not necessarily hold for multiple observations. Theoretically, the characteristics of the solution to the inverse optimization problem also changes. Hence, in the next section, we extend the IO formulation for the case of multiple observations and discuss its properties.

### 3.2. Multi-point Inverse Optimization

Consider a finite number of observations \( x^k, k \in \mathcal{K} = \{1, ..., K\} \) to the forward problem. One of the first goals of a multi-point inverse optimization is to find the constraint parameters in such a way that all observations, \( x^k, k \in \mathcal{K} \), become feasible. We define this property as follows.

**Definition 1.** A polyhedron \( \mathcal{X} = \{x \in \mathbb{R}^n | Dx \geq d\} \) is a valid feasible set for the forward problem if \( x^k \in \mathcal{X}, \forall k \in \mathcal{K} \).

**Remark 1.** If \( \mathcal{X} \subseteq \mathbb{R}^n \) is a valid feasible set then any set \( S \subseteq \mathbb{R}^n \) such that \( \mathcal{X} \subseteq S \) is also a valid feasible set.

Remark 1 states that if a set \( \mathcal{X} \) is a valid feasible set then any set that contains \( \mathcal{X} \) is also valid since all observations remain feasible for any superset of \( \mathcal{X} \) as well. Any set that is not valid, *i.e.*, does not contain some observation \( x^k, k \in \mathcal{K} \), cannot be a feasible set to the forward optimization by definition. Hence, all feasible regions that are imputed from the solutions of a multi-point inverse optimization must be valid feasible sets. In particular, to ensure that the feasible region of the forward problem is well-defined, we assume that the set defined by the known constraints is also a valid feasible set.

**Assumption 2.** The set \( \mathcal{G} = \{x \in \mathbb{R}^n | Gx \geq h\} \) is a valid feasible set.

The feasibility of the observations for the known constraints is similar to the assumption in the single-point IO, except that all observations (as opposed to one observation) are assumed to be feasible for the known constraints \( Gx \geq h \). Otherwise, the inverse optimization will not have a solution. Although we have \( K \) observations in the multi-point inverse optimization, we can identify the observation(s) that result in the best objective function value for the forward problem, because the \( c \) vector is given. We define the observation with the best value as the preferred observation for which strong duality must hold.
**Definition 2.** The preferred solution in a set of observations, \( \{x^k\}_{k \in \mathcal{K}} \), is defined as

\[
x^0 \in \arg \min_{x^k, k \in \mathcal{K}} \{ c'x^k \}.
\]

By this definition, \( x^0 \) is the observation that has the best objective function value in the forward problem \( \text{FO} \). If there exist multiple observations that satisfy Definition 2, without loss of generality, we arbitrarily select one of them as \( x^0 \). The multi-point inverse optimization problem aims to find a constraint set for the forward problem such that all observations are feasible and the preferred solution \( x^0 \) becomes optimal.

The following multi-point inverse optimization (MIO) formulation finds a feasible region that minimizes some distance function of the inverse optimal solution (desired properties of feasible region) from a set of input parameters \( \mathcal{D} \).

\[
\begin{align*}
\text{MIO} : \quad & \text{minimize} & \quad & \mathcal{F}(A, b; \mathcal{D}), \\
& \text{subject to} & & Ax^k \geq b, \quad \forall k \in \mathcal{K} \quad (3a) \\
& & & c'x^0 = b'y + h'w, \quad (3c) \\
& & & A'y + G'w = c, \quad (3d) \\
& & & ||a_i|| = 1, \quad \forall i \in \mathcal{I} \quad (3e) \\
& & & y, w \geq 0. \quad (3f)
\end{align*}
\]

The constraints in MIO include strong duality (3c), dual feasibility ((3d) and (3f)), and the normalization constraint (3e). In contrast to the single-point IO formulation, the primal feasibility constraint (3b) is now a set of \( \mathcal{K} \) constraints that ensures the feasibility of all observations for \( \text{FO} \). The formulation of MIO, similar to that of IO, is bilinear and hence, in general is non-convex. Analogous to IO, we first show that the MIO formulation is feasible with non-trivial solutions.

**Proposition 2.** The MIO formulation is feasible.

*Proof.* Similar to Proposition 1, let \( w = 0, y = ||c||1, b = \frac{1}{||c||} c'x^0 \), and \( a_i = \frac{1}{||c||} c \) \( \forall i \in \mathcal{I} \). The resulting solution \((A, b, y, w)\) satisfies constraints (3c)–(3f). To show that the primal feasibility constraints (3b) also hold, note that if \( \exists k \in \mathcal{K} \) such that \( Ax^k < b \), then by substituting the values of \( A \) and \( b \), we have \( \frac{1}{||c||} c'x^k < \frac{1}{||c||} c'x^0 \), or equivalently, \( c'x^k < c'x^0 \), which is a contradiction to the definition of \( x^0 \) (Definition 2). Therefore, the solution \((A, b, y, w)\) is feasible for MIO. \( \square \)

The \( A, b \) described in Proposition 2 represent the half-space \( \mathcal{C} = \{ x \in \mathbb{R}^n | c'x \geq c'x^0 \} \) whose identifying hyperplane is orthogonal to the cost vector \( c \) and passes through the
preferred solution \(x^0\). Therefore, all observations \(x^k, k \in \mathcal{K}\) are in the set \(C\) \((i.e., C\) is a valid feasible set), and it makes \(x^0\) optimal for the forward problem. Hence, \(C\) is a feasible set for the FO problem that is \textit{imputed} from a solution of MIO. In Definition 3, we generalize this concept for all valid feasible sets that are derived from MIO solutions.

**Definition 3.** A polyhedron \(\mathcal{X} = \{x \in \mathbb{R}^n \mid Dx \geq d\}\) is called an \textit{imputed feasible set} if there exists a feasible solution \((A, b, y, w)\) of MIO such that \(\mathcal{X} = \{x \in \mathbb{R}^n \mid Ax \geq b, Gx \geq h\}\).

An imputed feasible set \(\mathcal{X} = \{x \in \mathbb{R}^n \mid Dx \geq d\}\) may be represented by infinitely many constraint sets. For example, any scalar multiplication of the inequality or any other (perhaps linearly-dependent) reformulation will represent the same set \(\mathcal{X}\). The MIO formulation finds one such constraint set to characterize \(\mathcal{X}\) while satisfying the normalization constraint \((3e)\). When referring to an imputed feasible set, we consider the set \(\mathcal{X}\) and not the exact constraint parameters that define it. Note that any imputed feasible set is always a feasible region for FO that makes \(x^0\) optimal because it is inferred by a solution of MIO, and conversely, any feasible region of FO that satisfies the known constraints and makes \(x^0\) optimal is an imputed feasible set of MIO. We formalize this property in Proposition 3.

**Proposition 3.** The system \((A, b, y, w)\) is feasible for MIO if and only if the polyhedron \(\mathcal{X} = \{x \in \mathbb{R}^n \mid Ax \geq b, Gx \geq h\}\) is a valid feasible set that makes \(x^0\) optimal for the forward problem.

**Proof.** Assume that \((A, b, y, w)\) is a solution to MIO. By constraint \((3b)\), \(Ax^k \geq b, \forall k \in \mathcal{K}\), and by Definition 2, we have \(Gx^k \geq h, \forall k \in \mathcal{K}\). Hence, \(\mathcal{X}\) is a valid feasible set. Constraint \((3c)\) ensures that strong duality holds for \(x^0\), and hence, \(x^0\) must be optimal for FO.

Now let \(\mathcal{X} = \{x \in \mathbb{R}^n \mid Ax \geq b, Gx \geq h\}\) be a valid feasible set that makes \(x^0\) optimal for FO. Without loss of generality, we can assume constraint \((3e)\) holds since we can always normalize \(A\) and \(b\) so that \(\|a_i\| = 1\). The primal feasibility constraint \((3b)\) is always met by definition of \(\mathcal{X}\). Since \(x^0\) is optimal for FO, we have \(\min_{x \in \mathcal{X}} \{c'x\} > -\infty\), and therefore, the dual of FO exists and is feasible, and strong duality holds. Hence, all constraints \((3b-3f)\) are satisfied, which implies that there must exist \(y\) and \(w\) such that \((A, b, y, w)\) is feasible for MIO.

Proposition 3 characterizes the properties of all solutions to MIO and ensures that \(x^0\) is optimal for FO. Although Proposition 3 and the MIO formulation explicitly consider the optimality of \(x^0\) only, we show in Remark 2 that any other observation with the same objective function value as \(x^0\) is also optimal for the forward problem using the imputed feasible set of MIO.
Remark 2. If $\mathcal{X}$ is an imputed feasible set, any $\bar{x} \in \mathcal{X}$ such that $\bar{x} \in \arg\min_{x^{k}, \forall k \in K} \{c^{'}x^{k}\}$ is an optimal solution of FO.

Proof. Let $x^{0}$ be the preferred solution. Assume $\exists \bar{x} \in \mathcal{X}$ such that $\bar{x} \in \arg\min_{x^{k}, \forall k \in K} \{c^{'}x^{k}\}$ and $\bar{x} \neq x^{0}$. By constraint (3b), we know that $\bar{x}$ is feasible for FO. If $\bar{x}$ is not optimal for FO, then $c^{'}x^{0} < c^{'}\bar{x}$ which is a contradiction to $\bar{x} \in \arg\min_{x^{k}, \forall k \in K} \{c^{'}x^{k}\}$. Hence, $\bar{x}$ must be an optimal solution to FO.

Based on Proposition 3, an imputed feasible set $\mathcal{X}$ of MIO is a valid feasible set. Therefore, any superset of $\mathcal{X}$ will also be a valid feasible set, by Remark 1. In particular, $\mathcal{X}$ is a subset of the half-space $C = \{x \in \mathbb{R}^{n} | c^{'}x \geq c^{'}x^{0}\}$ and a superset of the convex hull of the observations, denoted by $H$. This property is shown in Lemma 1 and plays a fundamental role in simplifying the MIO formulation later in Theorem 1. For brevity of notations, we use the definitions $H$ and $C$, as defined above, throughout the rest of this paper.

Lemma 1. If $\mathcal{X}$ is an imputed feasible set of MIO, then $H \subseteq \mathcal{X} \subseteq C$.

Proof. $(H \subseteq \mathcal{X})$: Assume $H \not\subseteq \mathcal{X}$ and $\exists \bar{x} \in H, \bar{x} \not\in \mathcal{X}$. By definition of $H$, $\exists \lambda_{k} \geq 0, \forall k \in K$ such that $\bar{x} = \sum_{k \in K} \lambda_{k}x^{k}$ and $\sum_{k \in K} \lambda_{k} = 1$. This is a contradiction because $\mathcal{X}$ is a polyhedron that is a valid feasible set. Therefore, it contains all observations $x^{k}$ and any convex combination of them, including $\bar{x}$. Hence, $H \subseteq \mathcal{X}$.

$(\mathcal{X} \subseteq C)$: Similarly, assume $\mathcal{X} \not\subseteq C$ and $\exists \tilde{x} \in \mathcal{X}, \tilde{x} \not\in C$. Since $\tilde{x} \not\in C$ then $c^{'}\tilde{x} < c^{'}x^{0}$ (by definition). Therefore, $\tilde{x}$ has a better objective value than $x^{0}$, which is a contradiction to $\mathcal{X}$ being an imputed feasible set because $\mathcal{X}$ must make $x^{0}$ optimal for FO. Therefore, $\mathcal{X} \subseteq C$.

Remark 3. For a feasible set $\mathcal{X}$ imputed by MIO, $\mathcal{X} \cap C = \mathcal{X} \cup H = \mathcal{X}$.

As Lemma 1 illustrates, any imputed feasible set must be a subset of the half-space $C$. Using this property, we can reduce the solution space of MIO from $\mathbb{R}^{n}$ to the half-space $C$. Any set that lies outside of $C$ cannot be an imputed MIO solution. We can further restrict the solution space of MIO by noting that the set of known constraint, $G$, also has to be met for any MIO solution. Therefore, the solution space of MIO is always a subset of $G' = C \cap G$. As Proposition 4 implies, this solution space is the largest imputed feasible set of MIO.

Proposition 4. The set $G' = C \cap G$ is an imputed feasible set of MIO, and $\mathcal{X} \subseteq G'$ for any $\mathcal{X}$ that is an imputed feasible set of MIO.

Proof. The set $G'$ is a valid feasible set since both $C$ and $G$ are valid feasible sets as shown in the proof of Proposition 2. $G'$ also makes $x^{0}$ optimal for FO, by design. Hence, by Proposition 3, $G'$ is an imputed feasible set of MIO. For any imputed feasible set $\mathcal{X}$, it is obvious that $\mathcal{X} \subseteq C$ (by Lemma 1) and $\mathcal{X} \subseteq G$ (by definition), and hence $\mathcal{X} \subseteq G'$.
Remark 4. Let $\mathcal{X}$ be an imputed feasible set of MIO and $\mathcal{U}$ be any valid feasible set. The set $\mathcal{X} \cap \mathcal{U}$ is an imputed feasible set of MIO.

Proof. Since $\mathcal{X}$ is an imputed feasible set, by Proposition 3 we know that $\mathcal{X} = \{x \in \mathbb{R}^n | Ax \geq b, Gx \geq h\}$ is a valid feasible set that makes $x^0$ optimal for FO. The intersection $\mathcal{X} \cap \mathcal{U}$ is also valid feasible set that will make $x^0$ optimal for FO since $x^0 \in \mathcal{X} \cap \mathcal{U}$ and $x^0$ is optimal in $\mathcal{X}$ and hence on its boundary or extreme point. □

Proposition 5. For any valid feasible set $\mathcal{U}$, $\mathcal{C} \cap \mathcal{U}$ is a valid feasible set and $\mathcal{G}' \cap \mathcal{U}$ is an imputed feasible set of MIO, where $\mathcal{G}' = \mathcal{G} \cap \mathcal{C}$.

Proof. Since both $\mathcal{C}$ and $\mathcal{U}$ are valid feasible sets, so is $\mathcal{C} \cap \mathcal{U}$. The set $\mathcal{G}'$ is an imputed feasible set of MIO as shown in Proposition 4. Therefore, by Remark 4, $\mathcal{G}' \cap \mathcal{U}$ is an imputed feasible set of MIO. □

The MIO formulation includes a set of bilinear constraints which makes the formulation non-linear (i.e., constraints (3d), (3c)). Therefore, we utilize the property outlined in Proposition 4 to reduce the solution space of MIO and derive a simplified version of the formulation. That is, considering the fact that for any imputed feasible set $\mathcal{X}$ imputed by MIO, we have $\mathcal{X} \subseteq \mathcal{G}'$, where $\mathcal{G}' = \mathcal{G} \cap \mathcal{C}$, then without loss of generality, we can limit the solutions space of MIO by adding $\mathcal{C}$ to the set of known constraint of the forward problem, $\mathcal{G}$. We refer to this new set of known constraints as $\mathcal{G}'$ in the rest of the paper.

Considering the new set of known constraint that includes $\mathcal{C}$, Theorem 1 shows that MIO can be simplified to an equivalent inverse optimization model that does not include any bilinear terms. Without loss of generality, assume that $\mathcal{C} = \{x \in \mathbb{R}^n | c'x \geq c'x^0\}$ is the first unknown constraint in the formulation, that is, $g_1 = c$, $h_1 = c'x^0$.

Theorem 1. Solving MIO is equivalent to solving the following problem, with $\mathcal{C}$ being a known constraint of FO.

$$\text{e-MIO : } \begin{array}{ll}
\text{minimize} & \mathcal{F}(A, b; \mathcal{D}) \\
& a_i'x^k \geq b_i, \quad \forall i \in I, \quad k \in K \\
& ||a_i|| = 1.
\end{array}$$

Proof. (i) If $(A, b, y, w)$ is a solution of MIO, then $(A, b)$ is a solution to the e-MIO formulation since (4b) and (4c) are also constraints of MIO. (ii) Conversely, if the pair $(A, b)$ is a solution to e-MIO, let $w = (1, 0, \ldots, 0)$, $y = (0, \ldots, 0)$. The half-space $\mathcal{C}$ is the first known constraint in $Gx \geq h$ and feasible for MIO (Proposition 4), and the solution
(A, b, y, w) is feasible for MIO. Therefore, by (i) and (ii), solving e-MIO is equivalent to solving MIO.

Theorem 1 shows that by considering the half-space as one of the known constraints, instead of solving the bilinear MIO problem, we can solve a simpler problem that does not include any bilinear terms and is, therefore, easier to solve. Note that there are multiple ways to re-write constraint (4c) based on the particular application and the desired properties of the resulting model. Depending on the type of normalization constraint used in (4c), e-MIO can be a linearly- or quadratically-constrained problem, for instance.

**Corollary 1.** Any solution (A, b) to e-MIO identifies an imputed feasible set of MIO that is defined by \( \{ x \in \mathbb{R}^n \mid Ax \geq b, x \in G' \} \).

**Remark 5.** Any valid feasible set \( X \) of FO is an imputed feasible set to e-MIO.

**Proof.** The set \( X \) is a valid feasible, and the set of known constraints in e-MIO is \( G' \). Therefore, by Proposition 5 the set \( X \cap G' \) is an imputed feasible set.

As Remark 5 shows, the feasible region of e-MIO reduces to valid feasible sets of FO. By Corollary 1, we know that any solution to e-MIO corresponds to an imputed feasible set of MIO, when the set of known constraints is \( G' \). Therefore, by adding \( C \) to the set of known constraint, the complexity of the problem reduces to only finding valid feasible sets of FO through the e-MIO formulation.

4. Measure Functions

The MIO formulation minimizes a general objective function \( \mathcal{F}(A, b, D) \) which affects the optimal solution \( (A, b, y, w) \) and hence, drives the desirable properties of the imputed feasible set of FO. This imputed feasible set for the forward problem may take various shapes and forms based on the given parameter set \( D \) and the objective function \( \mathcal{F} \). In this chapter, we introduce several measure functions that can be used based on the available information on the constraints and the desired properties of the imputed feasible set. The statements in this section hold for the MIO formulation (and similarly, for the IO formulation since it is a special case of MIO). For simplicity and based on Theorem 1, we assume, without loss of generality, that the half-space \( C \) is a known constraint of the FO problem. Therefore, we use the e-MIO formulation in this section, and as Corollary 1 states, the solutions of e-MIO identify a unique imputed feasible set for FO.

In principle, three different levels of information can be considered for a given constraint of the forward problem: the constraint is (i) fully known, (ii) unknown but a prior belief on
it is known, or (iii) fully unknown. In case (i), the known constraint can be directly added to the FO formulation as a known constraint that shape the set $\mathcal{G} = \{ \mathbf{x} \in \mathbb{R}^n | \mathbf{Gx} \geq \mathbf{h} \}$. Case (ii), in which the constraint is unknown but a prior belief on the constraint parameter is available, has been considered in the literature of inverse optimization. We also consider and discuss a measure function that minimally perturbs these prior beliefs on constraint parameters. In case (iii), where no information on the constraint is assumed, it is possible to find a large variety of imputed feasible sets for MIO. We introduce four different measure functions that aim to find the appropriate constraints when no prior belief on the constraints is available.

In this section, we consider and discuss cases (ii) and (iii), where little or no information on the unknown constraints is available. To this end, we first discuss the theoretical properties of imputed feasible sets of MIO when a prior belief on the constraint set is available in Section 4.1. Next, we present and discuss four different measure functions that can be employed in the absence of a prior belief in Section 4.2.

4.1. Prior Belief on Constraints Available

A convention in the literature of inverse optimization is to consider availability of a prior belief on the optimal solution of the inverse problem (i.e., a prior belief on the constraint parameters of FO). The objective of the inverse problem is to minimize some measure of distance (e.g., norm) of the imputed constraint parameters from that prior belief. In this section, we study the use of prior belief as the objective of our e-MIO model. We refer to this measure function as the Adherence Measure.

Let the assumed prior belief on the constraint parameters, denoted as $\hat{\mathbf{A}}$ and $\hat{\mathbf{b}}$, be given as the input parameter $\mathcal{D}$. For ease of notations, let $\Delta = [\mathbf{A} \ \mathbf{b}]$ be the matrix that appends the column $\mathbf{b}$ to the $\mathbf{A}$ matrix and $\hat{\Delta} = [\hat{\mathbf{A}} \ \hat{\mathbf{b}}]$ be the prior belief. We define the Adherence Measure as the measure function that captures the distance of $\Delta$ from the prior belief $\hat{\Delta}$ according to a norm distance metric $\| \cdot \|$. 

$$\mathcal{F}(\mathbf{A}, \mathbf{b}; \mathcal{D}) = \mathcal{F}(\mathbf{A}, \mathbf{b}, \hat{\Delta}) = \sum_{i \in \mathcal{I}} \omega_i \| \Delta_i - \hat{\Delta}_i \|, \quad \text{(Adherence Measure)}$$

where parameter $\omega_i$ is the objective weight capturing the relative importance of constraint $i$, and $\Delta_i$ and $\hat{\Delta}_i$ are the $i^{th}$ rows of matrices $\Delta$ and $\hat{\Delta}$, respectively.

**Proposition 6.** If $\mathcal{X} = \{ \mathbf{x} \in \mathbb{R}^n | \mathbf{x} \in \hat{\Delta} \}$ is a valid feasible set, then $\mathbf{A} = \hat{\mathbf{A}}$ and $\mathbf{b} = \hat{\mathbf{b}}$ is an optimal solution to e-MIO under the Adherence Measure.

**Proof.** By assumption, $\mathcal{X}$ is a valid feasible set and hence by Remark 5, an imputed feasible
set to e-MIO. Therefore, $\Delta = \hat{\Delta}$ is a feasible solution to e-MIO with $F(A, b; \mathcal{D}) = 0$ under the Adherence Measure. Hence, $A = \hat{A}$, $b = \hat{b}$ is an optimal solution to e-MIO.

Proposition 6 shows that if the set identified by the prior belief $\hat{\Delta}$ is a valid feasible set, i.e., $\hat{A}x^k \geq \hat{b}$, $\forall k \in \mathcal{K}$, then there is a closed-form solution to e-MIO. If it is not a valid feasible set, then at least one of the observations $x^k$, $k \in \mathcal{K}$ is positioned outside of the prior belief. Therefore, $\hat{\Delta}$ needs to be minimally perturbed in order to generate a valid feasible set. This is a prevalent occurrence in practice since although a set of a priori constraints might be available, in reality, these constraints might be too tight to hold for all observations. Proposition 7 shows that for such cases, the e-MIO problem can decomposed into solving a series of smaller problems for each of the $m_1$ unknown constraints.

**Proposition 7.** The optimal solution of e-MIO with the Adherence Measure can be found by solving the following problem $m_1$ times. For $i \in \mathcal{I}$ consider

\[
\min_{a_i, b_i} ||\Delta_i - \hat{\Delta}_i||
\]

\[
a_i'x^k \geq b_i, \quad \forall k \in \mathcal{K}
\]

\[
||a_i|| = 1.
\]

**Proof.** The e-MIO problem with the Adherence Measure is separable for each constraint $i$, which means problem (5b) can be solved $m_1$ times to recover each $a_i$ and $b_i$ independently.

The Adherence Measure, which is often used in the literature, heavily relies on (i) the availability and (ii) the quality of the prior belief. In particular, if the quality of the available prior belief is poor, it would result in forcing the inverse optimization to fit the imputed feasible set to an undesirable prior belief. In what follows, we propose and discuss other measure functions that can be employed if no prior belief is available for the constraint parameters.

### 4.2. No Prior Belief on Constraints

In this section, instead of relying on a prior belief, we propose different measure functions that rely on the data (observations) to find the solution of e-MIO. We start with a simple constraint satisfaction model which is sometimes used in the literature of inverse optimization and then propose three new measure functions that each result in a different properties for the imputed feasible set of e-MIO. We also consider combining the measure functions to further define the shape of the imputed feasible region.
4.2.1. Indifference Measure

If no preference and no information about the feasible region is given, \(i.e.,\) there is no data provided to be used to derive the shape of the imputed feasible set \(\mathcal{D} = []\), then the e-MIO can be simplified to a feasibility problem by setting the objective function as zero by setting

\[
\mathcal{F}(\mathbf{A}, \mathbf{b}; \mathcal{D}) = 0.
\]

(Indifference Measure)

We refer to this measure function as the Indifference Measure.

**Proposition 8.** A closed-form optimal solution for e-MIO with Indifference Measure is

\[
a_i = \frac{c_i}{||c||}, \quad b_i = \frac{c'x^0}{||c||}, \quad \forall i \in \mathcal{I}.
\]

(6)

**Proof.** The Indifference Measure reduces e-MIO to a feasibility problem, and as shown in Section 3, the solution above is feasible for e-MIO. \(\square\)

**Remark 6.** The e-MIO formulation with the Indifference Measure has an infinite number of optimal solutions.

**Proof.** The convex hull \(\mathcal{H}\) of the observations is by definition a valid feasible set and hence, optimal for e-MIO under Indifference Measure. By Remark 1, any set \(\mathcal{X}\) that \(\mathcal{H} \subseteq \mathcal{X}\) is also a valid feasible set and subsequently, an optimal solution to e-MIO under Indifference Measure. \(\square\)

In practice, the Indifference Measure may not be the measure function of choice if there are characteristics or properties that are preferred for the feasible set of FO. In the rest of this section, we introduce three measure functions that can inform the shape of the imputed feasible set and discuss their properties.

4.2.2. Adjacency Measure

The Adjacency Measure finds a feasible region that has the smallest total distance from all of the observations. Here, the given parameter \(\mathcal{D}\) is the matrix that includes all observations, \(\mathcal{D} = [x^1, \ldots, x^K]\). This measure function minimizes the sum of the distances of each observation from all constraints. Let \(d_{ik}\) denote the distance of each observation \(x^k, k \in \mathcal{K}\) from the identifying hyperplane of the \(i^{th}\) constraint. The Adjacency Measure is defined as

\[
\mathcal{F}(\mathbf{A}, \mathbf{b}, \mathcal{D}) = \mathcal{F}(\mathbf{A}, \mathbf{b}, [x^1, \ldots, x^K]) = \sum_{k=1}^{K} \sum_{i=1}^{m_1} d_{ik},
\]

(Adjacency Measure)
where the distance \( d_{ik} \) can be calculated using any distance metric, for example, the Euclidean distance, or the slack distance defined as \( d_{ik} = a_i x^k - b_i \). Similar to the Adherence Measure, this measure function is separable for each constraint, and hence, the resulting e-MIO can be decomposed and solved for each constraint independently.

**Proposition 9.** The optimal solution of e-MIO with the Adjacency Measure can be found by solving the following problem \( m_1 \) times. For \( i \in \mathcal{I} \) write

\[
\begin{align*}
\text{minimize} & \quad \sum_{k=1}^{K} d_{ik} \\
\text{subject to} & \quad a'_i x^k \geq b_i, \quad \forall k \in \mathcal{K} \\
& \quad ||a_i|| = 1.
\end{align*}
\]

**Proof.** The Adjacency Measure is separable per \( i \), and the proof is similar to Proposition 7. \( \square \)

### 4.2.3. Fairness Measure

This measure function aims to find a feasible set such that all of its constraints are equally close to all observations and hence, is “fair”. Using the same notations as those in the Adherence Measure, we calculate the \( d_{ik} \) distance of each observation \( k \) from the identifying hyperplane of each constraint \( i \). We then calculate the average total distance for all observations, \( d_k = \sum_{i=1}^{m_1} d_{ik} \). The Fairness Measure is

\[
\mathcal{F}(A, b, \mathcal{D}) = \mathcal{F}(A, b; [x^1, \ldots, x^K]) = \sum_{k \in \mathcal{K}} (d_k - \sum_{k \in \mathcal{K}} d_k / K).
\]

This measure minimizes the deviation of the total distances for all observations and ensures that all observations have roughly the same total distance from all constraints. The Fairness Measure avoids cases were the constraints are all on one side of the observations and far away from others, and hence, it typically results in imputed feasible sets that are more confined compared to the Adjacency Measure.

### 4.2.4. Compactness Measure

The **Compactness Measure** tries to find the constraint parameters such that the minimum distance of each observation from all of the constraints is minimized. In other words, it tries to ensure that each observation is close to at least one constraint, if possible (i.e., if the observation is not an interior point). Again, let \( d_{ik} \) be the distance of observation \( k \) from
the identifying hyperplane of constraint $i$. The Compactness Measure is defined as

$$F(A, b, D) = F(A, b; [x^1, \ldots, x^k]) = \sum_{k \in \mathcal{K}} \min_{i \in \mathcal{I}} d_{ik}. \quad \text{(Compactness Measure)}$$

Minimizing the Compactness Measure can be done using the following mixed-integer reformulation.

$$\text{minimize } \sum_{k \in \mathcal{K}} \min_{i \in \mathcal{I}} d_{ik} = \text{minimize } \sum_{k \in \mathcal{K}} m_k \quad \text{(8a)}$$

subject to

$$d_{ik} = \sum_{j \in \mathcal{J}} a_{ij} x^k_j - b_i \quad \forall i \in \mathcal{I}, k \in \mathcal{K} \quad \text{(8b)}$$

$$m_k \geq d_{ik} - M \gamma_{ik}, \quad \forall i \in \mathcal{I}, k \in \mathcal{K} \quad \text{(8c)}$$

$$\sum_{i} \gamma_{ik} = |\mathcal{I}| - 1, \quad \forall k \in \mathcal{K} \quad \text{(8d)}$$

$$\gamma_{ik} \in \{0, 1\}, \quad \forall i \in \mathcal{I}, k \in \mathcal{K} \quad \text{(8e)}$$

$$m_k \geq 0. \quad \forall k \in \mathcal{K} \quad \text{(8f)}$$

To solve e-MIO with the Compactness Measure, the term (8a) is employed as the objective function and Constraints (8b)–(8f) are added to Constraints (4b) and (4c). Note that the resulting model would be a mixed-integer linear program if a linear norm is used as constraint (4c) of e-MIO.

5. Numerical Example

In this section, we test our methodology on two numerical example cases. For the ease of visualization, we use two-dimensional datasets ($n = 2$). We consider several (known and unknown) constraints in the FO formulation and multiple observations to impute the forward feasible region. The first numerical example considers $K = 5$ observations in a symmetrical form. This simple example serves the purpose of visualizing the results and understanding the intuition behind the solutions generated under each of the measure functions $F(A, b, D)$. It also provides a basis for comparison of the MIO and e-MIO formulations. The second numerical example considers a relatively larger set of observations (with $K = 19$) that is asymmetric and the inverse optimization solutions are not trivial to find by visual inspection. This example further elaborates on the insights from each of the introduced measure functions under non-trivial cases.

In our numerical results, we use the $L_2$-norm in the Adherence Measure. For all other measure functions, we use the slack distance (i.e., $d_{ik} = a_i^T x^k - b_i$) to calculate the distance
of a given point $x^k$ to the identifying hyperplane of the $i^{th}$ constraint (i.e., $a'_i x = b_i$). The slack distance may provide different results than one would expect to intuitively observe by visual inspection. We chose to use the slack distance for our illustrations because it is linear, as opposed to the nonlinear Euclidean distance. We note that there are other linear distance metrics (e.g., infinity norm) that can be used, but we find the slack distance to be more illustrative in a two-dimensional setting.

For the normalization constraint (3e), we use $|\sum_{j \in \mathcal{J}} a_{ij}| = 1$ as a proxy for the $L_1$-norm (i.e., $\sum_{j \in \mathcal{J}} |a_{ij}| = 1$). We chose this normalization method instead of the $L_1$-norm to reduce the number of binary variables to only $2n$ (as oppose to $2n(m_1 + m_2)$) in the linear mixed integer reformulation of the normalization constraint (3e), as follows:

$$\sum_{j \in \mathcal{J}} a_{ij} = \delta_{1i} - \delta_{2i}, \quad \forall i \in \mathcal{I},$$
$$\delta_{1i} + \delta_{2i} = 1,$$
$$\delta_{1i}, \delta_{2i} \in \{0, 1\}. \quad (9)$$

The only limitation of this method is that it disallows constraints in the form of $\sum_{j \in \mathcal{J}} a_{ij} = 0$, but it allows any slightest deviation from zero, which, for the purpose of our numerical results, does not have any impact on the solutions.

### 5.1. Numerical Case I

In the first numerical case, we have 5 observations, as listed in Table 1. There are two known constraints with the first one being the half-space $\mathcal{C}$, as discussed in Section 3. For this numerical case, we solved both the nonlinear MIO model and the e-MIO model to confirm that they both find the same solutions. In both models, we used the mixed-integer normalization constraint (9). The MIO model was solved using the nonlinear solver MINOS (2003) version 5.51 and the e-MIO model with CPLEX (2019) version 12.9. Both models were formulated using AMPL (1993) modeling language version 20190529. While MINOS and other nonlinear solvers are sometimes capable of solving small-scale instances to optimality, they often fail to provide a global optimal solution in larger cases. Since the first numerical case is small, MINOS was able to solve the MIO model to optimality, and the MIO and e-MIO solutions confirmed the same solutions in all instances.

In all the figures in the rest of this section, black dots denote the given observations $x^1, \ldots, x^k$, and the preferred observation ($x^0$) is highlighted in red. The blue solid lines are the hyperplanes corresponding to the given prior belief parameters ($\hat{\Delta}$), the dotted red lines represent the known constraints ($\mathcal{G}$), and the dashed black lines demonstrate the constraints
found by the inverse optimization model (Δ). The resulting imputed feasible set of MIO (including the known constraints) is marked as a shaded area.

| Data          | Value                  |
|---------------|------------------------|
| Cost vector (c) | (−1, −1)              |
| Observations (x^k) | (1, 1), (1, 2), (2, 1), (2, 2), (1.5, 1.5) |
| Known Constraints | 0.5x_1 + 0.5x_2 ≤ 2   |
|               | x_1 + x_2 ≥ 1         |
| Goal          | 4 unknown constraints  |

Table 1: Numerical Case I

Figure 1 shows the results with the Adherence Measure for three different cases of prior belief ˆΔ. For this case, the goal of inverse optimization is to perturb ˆΔ minimally to ensure the observations are feasible and x^0 is optimal. In Figure 1(a), the given prior belief ˆΔ is a valid feasible set, and as shown in Proposition 7, the optimal solution Δ is the same as the prior belief ˆΔ. In Figures 1(b) and 1(c), the given prior beliefs are not valid feasible sets but ˆΔ ⊆ G in Figure 1(b). In Figure 1(c), however, a part of the prior belief is infeasible for the known constraints and hence, ˆΔ ⊄ G. In both cases, the solution Δ is a minimally perturbed ˆΔ that makes all the observations feasible. The imputed feasible set (i.e., the shaded area) is derived from Δ and is feasible for G.

Figure 1: Results for Numerical Case I with Adherence Measure. The subfigures illustrate different scenarios for the prior belief: (a) it is a valid feasible set, (b) it is not a valid feasible set but a subset of known constraints G, and (c) it neither is a valid feasible set nor a subset of G.

Next, we use the same dataset and derive imputed feasible sets when no prior belief is available by employing the measure functions defined in Section 4. Figure 2(a) shows the results for the Indifference Measure which is used if no preference for the properties of the imputed feasible set is given. In this case, any feasible solution of MIO is also optimal. In our results, the four inferred constraints happen to be the same and equal to the hyperplane of C.
Hence the imputed feasible set is $G'$. Figure 2(b) illustrates the results with the Adjacency Measure function which minimizes the total distance between the inferred constraints and the observations. Due the symmetry of this numerical case, the obtained constraints are four identical lines that pass through observations $(1,1)$ and $(2,1)$. Figure 2(c), however, shows that employing the Fairness Measure in the objective function results in a more symmetrical imputed feasible region. As discussed before, generally, this measure is more likely to provide bounded feasible sets for the FO problem. Finally, Figure 2(d) illustrates the results for the Compactness Measure. Again, due to the symmetrical nature of Numerical Case I, two of the constraints are identical.

Lastly, we also tested a case where two of the measure functions are used sequentially to provide additional control over the properties of the imputed feasible set. In this case, first a measure function is employed as the primary objective and then another one as the secondary objective to search among the optimal solutions of the primary objective. In Figure 3, we first used the Fairness Measure to encourage similar distances between the inferred constraints and the observations. We then imposed the Adjacency Measure as a secondary objective to find a feasible set, among those with the best Fairness Measure value, that also has the minimum total distance between constraints and observations. As the figure illustrates, the imputed feasible set in this case is the same as the convex hull $H$, which is the smallest possible imputed feasible set for FO (Lemma 1).
5.2. Numerical Case II

In this section, we test our approach on a relatively larger numerical case. This example has 19 observations with \( \mathbf{x}^0 = (1, 1) \), and two known constraint with the first one being the half-space \( C \). There are 6 unknown constraints to be imputed. The details of this numerical case are summarized in Table 2. Given the larger size of this example, MINOS was not able to always find the global optimal solutions for the nonlinear MIO formulation. Hence, we only solved this example using the e-MIO formulation with the same normalization constraint (9) as that of Numerical Case I. This example further illustrates the importance and advantage of the proposed e-MIO formulation as it helps solving much larger instances of the problem to optimality, especially when the normalization constraint is linear and the problem becomes a linearly-constrained optimization model.

Figure 4 illustrates our obtained results for the case that a prior belief \( \hat{\Delta} \) is available. In Figure 4(a), the prior belief is a valid feasible set, and again as demonstrated by Proposition 7, the optimal solution \( \Delta \) is the same as the given prior belief \( \hat{\Delta} \). Note that in this example, although \( \hat{\Delta} \) is a valid feasible set, but it does not satisfy the known constraints (i.e., \( \hat{\Delta} \not\subset \mathcal{G} \)).

![Figure 3: Result for Numerical Case I with Fairness Measure as the primary objective and the Adjacency Measure as the secondary objective. The imputed feasible set is the convex hull of the observations.](image)

| Data          | Value                                                                 |
|---------------|------------------------------------------------------------------------|
| Cost vector (c) | (1, 1)                                                               |
| Observations (\( \mathbf{x}^k \)) | (2, 1), (4, 2), (4, 5), (3, 6), (2, 4), (3, 4), (3, 2), (4, 3), (1, 3), (2, 2.5), (1, 5), (5, 2.5), (5, 4), (2.7, 3.2), (2.3, 4.7), (1.4, 4.8), (3.8, 4.3), (4.8, 3.3), (1, 1) |
| Known Constraints | 0.5x_1 + 0.5x_2 \geq 1  
\-x_1 \geq -5                                                                 |
| Goal          | 6 unknown constraints                                                  |

Table 2: Numerical Case II
Conversely, Figure 4(b) illustrates the case that $\hat{\Delta}$ meets the known constraints but is not a valid feasible set. In this case, the prior belief is perturbed (expanded) in order to include all observations.

![Figure 4: Results for Numerical Case II with Adherence Measure. (a) The prior belief is a valid feasible set but not a subset of the known constraints $G$. (b) The prior belief is not valid but is a subset of $G$.](image)

We illustrate the results for the Numerical Case II with different measure functions that do not require a prior belief in Figure 5. Analogous to Numerical Case I, Figure 5(a) shows the results for Indifference Measure where any feasible solution to $MIO$ will also be an optimal solution. In our results, all six constraints equate to the a hyperplane that passes through $x^0$. Figure 5(b) illustrates the results for the Adjacency Measure which, in this case, induces an unbounded imputed feasible set. Figure 5(c) depicts the imputed feasible set that is obtained from the Fairness Measure function, and Figure 5(d) shows the results for the Compactness Measure as the objective function. In both cases, the imputed feasible sets are bounded and $x^0$ is an extreme point. This behaviour was expected and elaborated on in Section 4, since these measures would enforce each observation to be close to some constraint, as opposed to the Adjacency Measure which only minimizes the overall distance to all observations.

Finally, in Figure 6, we use a secondary objective function to combine to measure functions together. Similar to the Numerical Case I, we first solve the inverse optimization problem with the Fairness Measure and then apply the Adjacency Measure to search among
(a) Indifference Measure

(b) Adjacency Measure

(c) Fairness Measure

(d) Compactness Measure

Figure 5: Results for Numerical Case II with different measure functions.
the optimal solutions of the Fairness Measure and find a constraint set that also has the minimum total distance from all the observations. It can be observed that by using secondary objectives, we can derive different constraint parameters that are minimizing total distance and are also fair with respect to all observation, i.e., have an equally minimal distance to all observations.

Figure 6: Result for Numerical Case II with Fairness Measure as the primary objective and the Adjacency Measure as the secondary objective.

6. Conclusions

This paper provides an inverse optimization approach for imputing partially-unknown constraint parameters of a forward optimization problem. We consider the case where several observations are available. The goal is to find a feasible set for the forward problem such that all given observations become feasible and the preferred observations become optimal. We demonstrate the theoretical properties of the proposed methodology and propose a new simplified reformulation for the nonlinear non-convex inverse model. We also present and discuss several measure functions that can be used to derive imputed feasible sets that have certain desired properties. Our numerical case studies demonstrate the differences between these measure functions and serve as a basic guideline for users to choose the appropriate
measure function to find imputed sets with desired properties, depending on the available data and the relevant application.

A common concern observed in many inverse optimization studies is over-fitting, which can also potentially be present in our proposed methodology. To address this concern, an area of future work consists of extending the proposed methodology to incorporate margins of errors around each observation so that the imputed feasible sets are not over-fitted to the data. The use of robust optimization techniques can also be explored to address uncertainty in the data used in our proposed inverse optimization methodology. Another important future direction is in applying this methodology to a real-world large-scale dataset so as to demonstrate the computational benefits of the proposed simplified reformulation methodology that allows for a more efficient solution of the originally nonlinear non-convex inverse optimization problems.

References

Ahuja, R. K., Orlin, J. B., 2001. Inverse optimization. Operations Research 49 (5), 771–783.

Aswani, A., Shen, Z.-J. M., Siddiq, A., 2018. Inverse optimization with noisy data. Operations ResearchForthcoming.

Ayer, T., 2015. Inverse optimization for assessing emerging technologies in breast cancer screening. Annals of Operations Research 230, 57–85.

Bertsimas, D., Gupta, V., Paschalidis, I. C., 2012. Inverse optimization: A new perspective on the Black-Litterman model. Operations Research 60 (6), 1389–1403.

Bertsimas, D., Gupta, V., Paschalidis, I. C., 2015. Data-driven estimation in equilibrium using inverse optimization. Mathematical Programming 153 (2), 595–633.

Birge, J. R., Hortaçsu, A., Pavlin, J. M., 2017. Inverse optimization for the recovery of market structure from market outcomes: An application to the miso electricity market. Operations Research 65 (4), 837–855.

Brucker, P., Shakhlevich, N. V., 2009. Inverse scheduling with maximum lateness objective. Journal of Scheduling 12 (5), 475–488.

Černỳ, M., Hladík, M., 2016. Inverse optimization: towards the optimal parameter set of inverse lp with interval coefficients. Central European Journal of Operations Research 24 (3), 747–762.
Chan, T. C., Kaw, N., 2019. Inverse optimization for the recovery of constraint parameters. European Journal of Operational Research.

Chan, T. C. Y., Craig, T., Lee, T., Sharpe, M. B., 2014. Generalized inverse multi-objective optimization with application to cancer therapy. Operations Research 62 (3), 680–695.

Chan, T. C. Y., Lee, T., Terekhov, D., 2018. Inverse optimization: Closed-form solutions, geometry and goodness of fit. Management Science Forthcoming.

Chow, J. Y. J., Recker, W. W., 2012. Inverse optimization with endogenous arrival time constraints to calibrate the household activity pattern problem. Transportation Research Part B: Methodological 46 (3), 463–479.

Dempe, S., Lohse, S., 2006. Inverse linear programming. In: Recent Advances in Optimization. Springer, pp. 19–28.

Erkin, Z., Bailey, M. D., Maillart, L. M., Schaefer, A. J., Roberts, M. S., 2010. Eliciting patients’ revealed preferences: An inverse Markov decision process approach. Decision Analysis 7 (4), 358–365.

Esfahani, P. M., Shafieezadeh-Abadeh, S., Hanasusanto, G. A., Kuhn, D., 2018. Data-driven inverse optimization with incomplete information. Mathematical Programming 167 (1), 191–234.

Fourer, R., Gay, D., Kernighan, B., 1993. AMPL. Boyd and Fraser.

Ghobadi, K., Lee, T., Mahmoudzadeh, H., Terekhov, D., 2018. Robust inverse optimization. Operations Research Letters 46 (3), 339–344.

Güler, Ç., Hamacher, H. W., 2010. Capacity inverse minimum cost flow problem. Journal of Combinatorial Optimization 19 (1), 43–59.

Iyengar, G., Kang, W., 2005. Inverse conic programming with applications. Operations Research Letters 33 (3), 319–330.

Keshavarz, A., Wang, Y., Boyd, S., 2011. Imputing a convex objective function. In: 2011 IEEE International Symposium on Intelligent Control (ISIC). IEEE, pp. 613–619.

Naghavi, M., Foroughi, A. A., Zarepisheh, M., 2019. Inverse optimization for multi-objective linear programming. Optimization Letters 13 (2), 281–294.

Petit, T., Trapp, A. C., 2019. Enriching solutions to combinatorial problems via solution engineering. INFORMS Journal on Computing.
Saez-Gallego, J., Morales, J. M., 2018. Short-term forecasting of price-responsive loads using inverse optimization. IEEE Transactions on Smart Grid 9 (5), 4805–4814.

Saunders, M. A., Murtagh, B. A., 2003. MINOS 5.51 user’s guide.

Tavashoğlu, O., Lee, T., Valeva, S., Schaefer, A. J., 2018. On the structure of the inverse-feasible region of a linear program. Operations Research Letters 46 (1), 147–152.

Troutt, M. D., Brandyberry, A. A., Sohn, C., Tadisina, S. K., 2008. Linear programming system identification: The general nonnegative parameters case. European Journal of Operational Research 185 (1), 63–75.

Troutt, M. D., Pang, W.-K., Hou, S.-H., 2006. Behavioral estimation of mathematical programming objective function coefficients. Management Science 52 (3), 422–434.