Multiple Observations and Goodness of Fit in Generalized Inverse Optimization

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This paper develops a generalized inverse linear optimization framework for imputing objective function parameters given a data set containing both feasible and infeasible points. We devise assumption-free, exact solution methods to solve the inverse problem; under mild assumptions, we show that these methods can be made more efficient. We extend a goodness-of-fit metric previously introduced for the problem with a single observed decision to this new setting, proving and numerically illustrating several important properties.

**Key words:** inverse optimization; linear optimization; goodness of fit; model estimation

1. Introduction

Motivated by the growing availability of data that represents decisions, there is an increasing interest in the use of inverse optimization to gain insight into decision-generation (e.g., optimization) processes. In particular, inverse optimization finds optimization model parameters that render observed decisions minimally suboptimal for the model. Current inverse methods often minimize either the distance between the observed and optimal decisions (Faragó et al. 2003, Aswani et al. 2017) or the optimality gap associated with the observed decisions (Troutt et al. 2006, 2008, Keshavarz et al. 2011, Chan et al. 2014, Bertsimas et al. 2015).
Approaches in the first category measure error in the space of decisions, aiming to replicate the observed solution as closely as possible by finding parameters to a forward optimization problem that allow it to generate an optimal solution of minimal distance to the observed data, measured by a $p$-norm. For example, given a solution to a network optimization problem, the goal may be to find arc costs that correspond to an optimal flow that is minimally perturbed from the original flow vector (Faragó et al. 2003). Similarly, given observations of an individual’s food consumption, the practitioner may estimate a utility function that corresponds to an optimal diet of minimal deviation from the individual’s existing eating habits.

Approaches in the second category quantify error in terms of objective function value or optimality conditions. When modeling a general convex optimization problem, one approach is to minimize a function of the Karush-Kuhn-Tucker condition residuals (Keshavarz et al. 2011). For modelling linear optimization, we can characterize the error as the duality gap, or the difference in objective function values between the optimal and observed decisions with respect to the imputed parameters. Objective space inverse optimization aims to construct forward models that produce optimal values similar to the objective values of the observed decisions, even if the corresponding solutions themselves may be distant. For example, given observations of a cell’s chemical reaction rates, one may be more interested in estimating a functional form of the cell’s metabolic objective function than replicating the reactions themselves (Zhao et al. 2015). Another example comes from cancer therapy, where given a previous radiation therapy treatment plan, the goal is to find objective function weights that reproduce the dosimetric tradeoffs (i.e., objective values), rather than the physical characteristics of the radiation beams (Chan et al. 2014).

Although most papers in the literature develop models that specifically cater to one of these two categories, there exists some previous work on frameworks to encompass both decision and objective space variants (Esfahani et al. 2015, Chan et al. 2017). Esfahani et al. (2015) considered the observation of a random signal that parameterizes an unknown forward problem and a corresponding optimal decision. They leveraged the stochastic nature of the problem to propose a
distributionally robust inverse optimization methodology minimizing an arbitrary loss function. Chan et al. (2017) proposed a generalized inverse linear optimization framework and specialized it to objective and decision space variants for the case of a single, observed feasible decision, and used geometric insights to develop an analytic method for imputing model parameters. Accompanying the framework, they introduced a unitless and scale-invariant goodness-of-fit metric to measure how well the inverse solution reproduces the input data. Consequently, the goal of the current paper is to unify several key aspects of the different inverse optimization approaches in the literature within the generalized framework of Chan et al. (2017), namely (a) tractability with multiple observed decisions (Keshavarz et al. 2011, Bertsimas et al. 2015); (b) no restrictions on feasibility of the observed decisions (Aswani et al. 2017, Esfahani et al. 2015); and (c) integration with goodness of fit measurement (Chan et al. 2017). Our specific contributions are as follows:

1. We develop a generalized inverse linear optimization model that can specialize to both decision and objective space models, and is applicable to arbitrary data sets representing decisions, without restriction on cardinality or feasibility. We propose general solution methods, often leveraging the geometric properties associated with the problem. We show that some of the models admit analytical solutions under certain mild assumptions.

2. We extend the goodness-of-fit metric proposed by Chan et al. (2017), known as the coefficient of complementarity, to the more general setting considered in this paper. We prove several important properties of this metric for the general setting of multiple and potentially infeasible observed decisions. Our coefficient of complementarity helps build a unified framework for model fitting and evaluation in linear inverse optimization for an arbitrary data set.

3. We present numerical results that illustrate the different inverse optimization methods and the contrasting types of error measurement. We then provide examples on the uses of different methodologies as well as the use of the coefficient of complementarity in assessing model fitness.

2. Background on generalized linear inverse optimization

We first review the formulation and main results from Chan et al. (2017), who introduced an inverse optimization model for linear optimization problems (LPs) that generalizes both decision and
objective space models, specifically for a dataset of a single feasible observed decision. Let \( x, c \in \mathbb{R}^n \) denote the decision and cost vectors respectively, and \( A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m \) denote the constraint matrix and right-hand side vector respectively. Let \( \mathcal{I} = \{1, \ldots, m\} \) index the set of cardinality \( m \) (i.e., the rows of \( A \)) and \( \mathcal{J} = \{1, \ldots, n\} \) index the set of cardinality \( n \) (i.e., the elements of \( c \)). We refer to the following LP as the forward optimization model

\[
\text{FO}(c): \quad \text{minimize} \quad c^T x \\
\text{subject to} \quad x \in P := \{x | Ax \geq b\}.
\]

We assume that \( \text{FO}(c) \) does not have any redundant constraints. Given a feasible observed decision \( \hat{x} \in P \), the corresponding (single-point) generalized inverse linear optimization problem is

\[
\text{GIO}(\{\hat{x}\}): \quad \text{minimize} \quad \|\epsilon\| \\
\text{subject to} \quad A^T y = c, \quad y \geq 0 \\
\quad c^T \hat{x} = b^T y + c^T \epsilon \\
\quad \|c\|_N = 1 \\
\quad c \in \mathcal{C}, \epsilon \in \mathcal{E}.
\]

In formulation (1), \( y \in \mathbb{R}^m \) represents the dual vector for the constraints of the forward problem. The vector \( \epsilon \in \mathbb{R}^n \) represents a perturbation that brings \( \hat{x} \) to a point \( x^* = \hat{x} - \epsilon \) that satisfies strong duality (1c). The norm in the objective is general and can be chosen based on application-specific considerations. Constraints (1b) ensure dual feasibility. Constraint (1d) is a normalization constraint to prevent the trivial solution of \( c = 0 \), where \( \|\cdot\|_N \) denotes an arbitrary norm. Finally, constraints (1e) define application-specific perturbation and cost vectors via the sets \( \mathcal{E} \) and \( \mathcal{C} \), respectively. Thus, the tuple \((\|\cdot\|, \mathcal{C}, \mathcal{E})\) constitutes the inverse optimization hyperparameters that define a model instance. By selecting these hyperparameters appropriately, we specialize \( \text{GIO}(\{\hat{x}\}) \) into inverse optimization models that minimize error in the decision or objective space.

Previous inverse optimization work has explored different variants of the normalization constraint (1d). Chan et al. (2017) assumed \( \|\cdot\|_N = \|\cdot\|_1 \). For tractability, Esfahani et al. (2015) used
an $l_\infty$ constraint $\lVert \cdot \rVert_N = \lVert \cdot \rVert_\infty$. As we deal with general solution methods and cannot always leverage the geometric structure, we often suggest using $\lVert \cdot \rVert_N = \lVert \cdot \rVert_\infty$ when concerned with tractability.

Although formulation (1) is non-convex, it admits a closed-form solution, which can be identified by determining the projection from $\hat{x}$ to the boundary of $P$ of minimum distance as measured by $\lVert \cdot \rVert$. Specifically, let $H_i = \{x \mid a_i^T x = b_i\}$ be the hyperplane corresponding to the $i^{th}$ constraint and

$$
\pi_i(\hat{x}) = \text{arg min}_{x \in H_i} \lVert x - \hat{x} \rVert
$$

be the projection of $\hat{x}$ to $H_i$. Mangasarian (1999) showed that the arbitrary norm hyperplane projection problem has an analytic solution

$$
\pi_i(\hat{x}) = \hat{x} - \frac{a_i^T \hat{x} - b_i}{\lVert a_i \rVert_D} \nu(a_i),
$$

where $\lVert \cdot \rVert_D$ denotes the dual norm of $\lVert \cdot \rVert$ and $\nu(a_i) \in \text{arg max}_{\lVert v \rVert = 1} \{v^T a_i\}$.

As we state in Theorem 1 below, finding the projection to the closest hyperplane defined by the constraints of the forward problem leads to an optimal solution to formulation (1).

**Theorem 1 (Chan et al., 2017).** Let $\hat{x} \in P$, $i^* \in \text{arg min}_i \{a_i^T \hat{x} - b_i\}$, and let $e_i$ be the $i^{th}$ unit vector. There exists an optimal solution to $\text{GIO}(\{\hat{x}\})$ with the structure

$$
(c^*, y^*, \epsilon^*) = \left(\frac{a_i^*}{\lVert a_i^* \rVert_N}, \frac{e_i^*}{\lVert a_i^* \rVert_N}, \hat{x} - \pi_{i^*}(\hat{x})\right).
$$

Theorem 1 characterizes the geometric structure of the solution in the single-point inverse optimization problem. If $\hat{x} \in P$, then by Theorem 1 an optimal solution describes a supporting hyperplane (i.e., $\mathcal{H} = \{x \mid c^*^T x = b^T y^*\}$) that also corresponds to a constraint of the forward problem.

### 3. Generalized inverse optimization with arbitrary data sets

We extend the model and results of the previous section to the case of multiple observed decisions with no restriction on their feasibility. Let $\hat{x} = \{\hat{x}_1, \ldots, \hat{x}_Q\}$ represent a data set of $Q$ observed decisions and let $Q = \{1, \ldots, Q\}$ index this set. The goal of the inverse optimization problem is to determine a single cost vector $c^*$ that minimizes the aggregate error induced by this set of points with respect to $\text{FO}(c^*)$. To measure this, we introduce a perturbation vector $\epsilon_q$ for every $q \in Q$.

The multi-point generalized inverse optimization problem is formulated as follows:

$$
\text{GIO}(\hat{x}) : \quad \text{minimize} \quad \sum_{q=1}^Q \lVert \epsilon_q \rVert
$$

\[(4a)\]
subject to  \( A^T y = c, \ y \geq 0 \)  
\( c^T \hat{x}_q = b^T y + c^T \epsilon_q, \ \forall q \in Q \)  
\( ||c||_{\mathcal{X}} = 1 \)  
\( c \in \mathcal{C}, \epsilon_q \in \mathcal{E}_q, \ \forall q \in Q. \)

Constraints (4b) and (4d) are carried from the single-point model, while (4c) and (4e) are multi-point extensions of (1c) and (1e) respectively, ensuring that for each \( q \in Q \), the data points \( \hat{x}_q \) achieve strong duality with respect to \( c \) after valid perturbations \( \epsilon_q \). The objective now minimizes the aggregate of norms of the perturbation vectors.

Similar to formulation (1) for the single-point scenario, \( \text{GIO}(\hat{X}) \) is non-convex due to the bilinear terms in (4c) and the normalization constraint (4d). Unlike in the single-point case however, there is no general closed-form solution (cf. Theorem 1) to formulation (4). Instead, we develop tailored solution methods for each of the objective space and decision space variants of \( \text{GIO}(\hat{X}) \). We first show how to specialize formulation (4) to these two model classes.

3.1. Objective space

For linear forward optimization models, inverse optimization in the objective space is based on the premise that sub-optimal observed decisions are characterized by sub-optimal objective values. Consider the dual problem for \( \text{FO}(c) \). For each observed decision \( \hat{x} \), the corresponding duality gap is a distance measure between the objective value of \( \hat{x} \) and the optimal value of the dual problem. By choosing the norm in the objective function and the sets \( \mathcal{E}_q \) for each \( q \in Q \) appropriately, the objective function in formulation (4) can be transformed to measure a function of the duality gap.

3.1.1. Absolute duality gap. The absolute duality gap method for inverse optimization minimizes the aggregate duality gap between the primal and dual objective values for each observed decision:

\[
\text{GIO}_A(\hat{X}) : \quad \text{minimize} \quad \sum_{q=1}^{Q} ||\epsilon_q||, 
\]
subject to \( A^\top y = c, \ y \geq 0 \) \hspace{1cm} (5b)

\[ c^\top \hat{x}_q = b^\top y + \epsilon_q, \ \forall q \in Q \] \hspace{1cm} (5c)

\[ \|c\|_N = 1. \] \hspace{1cm} (5d)

The above formulation replaces the perturbation vectors from formulation $\mathbf{1}$ with scalar duality gap variables \((\epsilon_1, \ldots, \epsilon_Q)\). First, we show that $\text{GIO}_A(\hat{X})$ can be recovered from $\text{GIO}(\hat{X})$ with an appropriate choice of the model hyperparameters.

**Proposition 1.** Let \( \mu(c) \in \mathbb{R}^n \) be a parameter satisfying \( \|\mu(c)\|_\infty = 1 \) and \( \mu(c)^\top c = 1 \). A solution \((c^*, y^*, \epsilon_1^*, \ldots, \epsilon_Q^*)\) is optimal to $\text{GIO}_A(\hat{X})$ if and only if \((c^*, y^*, \epsilon_1^* \mu(c^*), \ldots, \epsilon_Q^* \mu(c^*))\) is optimal to $\text{GIO}(\hat{X})$ with the hyperparameters: \((\|\cdot\|_N, \mathcal{C}, \mathcal{E}_1, \ldots, \mathcal{E}_Q) = (\|\cdot\|_\infty, \mathbb{R}^n, \{\epsilon_1 \mu(c)\}, \ldots, \{\epsilon_Q \mu(c)\})\).

Proposition\[\mathbf{1}\] shows that the specialization of $\text{GIO}(\hat{X})$ to $\text{GIO}_A(\hat{X})$ depends on each \( \epsilon_q \) being a rescaling of a parameter \( \mu(c) \) dependent only on the cost vector. Note that \( \mu(c) \) is ultimately a vehicle to aid the specialization of $\text{GIO}(\hat{X})$, and is useful primarily to interpret the solutions of $\text{GIO}_A(\hat{X})$ in the broader context of $\text{GIO}(\hat{X})$. For all \( c \) satisfying \( \|c\|_N = 1 \), \( \mu(c) \) must satisfy \( \|\mu(c)\|_\infty = 1 \) and \( \mu(c)^\top c = 1 \). Given a specific choice of \( \|\cdot\|_N \), we can then propose a structured form for \( \mu(c) \). For example, if \( \|\cdot\|_N = \|\cdot\|_1 \), we can set \( \mu(c) = \text{sgn}(c) \) to be the sign vector of \( c \), ensuring that the two conditions on \( \mu(c) \) are satisfied for all \( c \) with \( \|c\|_1 = 1 \). Alternatively, if \( \|\cdot\|_N = \|\cdot\|_\infty \), we can set \( \mu(c) = \text{sgn}(c_j^*) e_{j^*} \) to be a signed \( j^* \)-th unit vector, where \( j^* \in \arg \max_{j \in J} \{|c_j|\} \). We remark that these structured restrictions are not necessarily unique forms for \( \mu(c) \) for their respective normalization constraints.

**General solution method.** $\text{GIO}_A(\hat{X})$ is a non-convex problem due to the normalization constraint \( \text{5d} \). We propose a general method for this problem however, by leveraging a polyhedral decomposition of the norm constraint. The following theorem shows how, when using an \( l_\infty \) constraint, the problem can be reformulated into a polynomial number of LPs. A similar approach was used by Esfahani et al. (2013) for their models.
**Theorem 2.** Let \((c^*, y^*, \epsilon^*_1, \ldots, \epsilon^*_Q)\) be optimal to GIO\(_A(\hat{X})\) under \(\|\cdot\|_N = \|\cdot\|_\infty\). There exists \(j \in J\) such that \((c^*, y^*, \epsilon^*_1, \ldots, \epsilon^*_Q)\) is also optimal to GIO\(_A(\hat{X}; j)\), defined as:

\[
\begin{align*}
\text{GIO}_A(\hat{X}; j) : \quad & \text{minimize} & & \sum_{q=1}^Q |\epsilon_q| \\
& \text{subject to} & & A^T y = c, \ y \geq 0 \\
& & & c^T \hat{x}_q = b^T y + \epsilon_q, \ \forall q \in Q \\
& & & (c_j = 1) \lor (c_j = -1) \\
& & & |c_k| \leq 1, \ \forall k \in J / \{j\}.
\end{align*}
\]

(6)

**Proof of Theorem 2.** Let \(j^* \in \arg \max_{j \in J} \{|c^*_j|\}\), implying \(|c^*_j| = 1\). Then, \((c^*, y^*, \epsilon^*_1, \ldots, \epsilon^*_Q)\) is feasible to GIO\(_A(\hat{X}; j^*)\). Conversely, for any \(j \in J\), every feasible solution to GIO\(_A(\hat{X}; j)\) is feasible to GIO\(_A(\hat{X})\), so all optimal solutions to each GIO\(_A(\hat{X}; j)\) lie in the feasible set of GIO\(_A(\hat{X})\). \(\square\)

Although formulation (6) is a disjunctive optimization problem, it can be decomposed into two LPs, one with the constraint \(c_j = 1\) and the other with \(c_j = -1\). Thus, Theorem 2 leverages the polyhedral structure of the \(l_\infty\) norm ball to propose a set of LPs that individually constrain \(c\) to lie on different facets of the ball. This approach can also be used for other polyhedral normalization constraints. For the \(l_1\) norm, however, polyhedral decomposition leads to an exponential number of LPs due to an exponential \((2^n)\) number of facets of the \(l_1\) ball.

**Non-negative cost vectors.** Certain application-specific knowledge may restrict the set of feasible cost vectors, reducing the search effort. For example, consider an application where the cost vector is known to be non-negative (i.e., \(C \subseteq \mathbb{R}_+^n\)). Here, it is advantageous to set \(\|\cdot\|_N = \|\cdot\|_1\), because the normalization constraint can then be reformulated to \(c^T 1 = 1\) and GIO\(_A(\hat{X})\) simplifies to a single LP. An analogous result was shown for the single-point scenario by Chan et al. (2017).

**Feasible observed decisions.** Another scenario that simplifies the problem significantly is when the observed points are all feasible for the forward model (i.e., \(\hat{X} \subset P\)). Most of the inverse optimization literature to date has focused on this situation. When all observed decisions are feasible, then \(\hat{X}\) can be replaced by a singleton set \(\{\bar{x}\}\), where \(\bar{x}\) is the centroid of the points in
\( \hat{X} \). A similar result was first presented in Goli (2015, Chapter 4), but for a model with a different normalization constraint that did not necessarily prevent trivial solutions. We present the analogous result in the context of our inverse formulation \((5)\), and use it to solve \( \text{GIO}_A(\{\hat{x}\}) \) analytically.

**Proposition 2.** If \( \hat{X} \subseteq P \) and \( \bar{x} \) is the centroid of \( \hat{X} \), \( \text{GIO}_A(\hat{X}) \) is equivalent to \( \text{GIO}_A(\{\bar{x}\}) \).

**Infeasible observed decisions.** Finally, we address scenarios where the observed decisions \( \hat{X} \) are all outside of the feasible set. We first consider the case where \( \hat{X} \) consists of a single, infeasible observed decision, \( \hat{x} \), in which case \( \text{GIO}_A(\{\hat{x}\}) \) possesses an analytic solution.

**Proposition 3.** Assume \( \hat{x} \notin P \).

1. When \( \hat{x} \) satisfies \( \mathbf{a}_i^T \hat{x} > b_i \) for some \( i \in I \), then there exists \( i^* \in I \) for which \( \bar{y} \) is

\[
\bar{y}_i = \frac{1}{\mathbf{a}_i^T \hat{x} - b_i}, \quad \bar{y}_j = \frac{1}{b_i - \mathbf{a}_i^T \hat{x}}, \quad \bar{y}_k = 0 \quad \forall k \in I / \{i, i^*\} \tag{7}
\]

and \( \tilde{c} = \mathbf{A}^T \bar{y} \). The corresponding normalized solution \((c^*, y^*, \epsilon^*) = (\tilde{c} / \|\tilde{c}\|_N, \bar{y} / \|\tilde{c}\|_N, 0)\) is an optimal solution to \( \text{GIO}_A(\{\hat{x}\}) \) and the optimal value is 0.

2. When \( \mathbf{a}_i^T \hat{x} \leq b_i, \forall i \in I \), there exists \( i^* \in I \) such that \( \tilde{y} \) is an optimal solution to \( \text{GIO}_A(\{\hat{x}\}) \).

Proposition 3 provides geometric insights regarding the structure of optimal solutions when \( \hat{x} \) is an infeasible point. Recall that the hyperplane \( \mathcal{H} = \{\mathbf{x} | \mathbf{c}^T \mathbf{x} = b^T \mathbf{y}^*\} \) is a supporting hyperplane of \( P \). From Proposition 3, if \( \hat{x} \) is infeasible but satisfies \( \mathbf{a}_i^T \hat{x} > b_i \) for some \( i \), then the imputed parameters induce a supporting hyperplane constructed as a strict convex combination of two constraints of \( \text{FO}(\mathbf{c}) \), as illustrated in Figure 1a. In contrast, for the situation where \( \mathbf{a}_i^T \hat{x} \leq b_i \) for all \( i \in I \), but with strict inequality holding for at least one index, we generate an alternate forward problem \( \text{FOA}(\mathbf{c}) := \min_{\mathbf{x}} \{ -\mathbf{c}^T \mathbf{x} | \mathbf{A} \mathbf{x} \leq \mathbf{b} \} \) by reversing the sign of all constraints and the cost vector, making the observed decision feasible for the new model. We then formulate an inverse optimization problem equivalent to the original one, but using the feasibility of the decision, apply Theorem 1. An example of this situation is shown in Figure 1b. Additionally, note that if any single constraint is satisfied with equality, regardless of the other constraints, we can solve \( \text{GIO}_A(\{\hat{x}\}) \) with optimal value 0.
In objective space inverse optimization, we only need to assess level sets corresponding to the imputed cost vector; all points along a level set will yield the same duality gap. Thus, any feasible point on a level set associated with zero duality gap suffices as an optimal decision of the imputed forward model. In Figure 1a, the observed decision lies on the level set with zero duality gap, and the corresponding primal optimal solution is $(0,0)$. In Figure 1b, the projection of $\hat{x}$ is infeasible. A primal feasible optimal solution of case (b) is also $(0,0)$ as it lies on the same level set. Moreover, this geometric insight can be extended to the case of multiple infeasible decisions.

**Corollary 1.** Suppose that $a^T\hat{x}_q \leq b_i$ for all $i \in \mathcal{I}$ and $q \in \mathcal{Q}$ and that $\hat{X} \not\subseteq \mathcal{P}$. Let $\bar{x}$ be the centroid of $\hat{X}$. Then, $GIO_A(\hat{X})$ is equivalent to $GIO_A(\{\bar{x}\})$ to the alternate forward problem $FOA(c)$.

### 3.1.2. Relative duality gap.

An alternative objective space model is to minimize the relative duality gap (i.e., the ratio of the duality gap of $\hat{x}$ over the optimal objective value of $FO(c)$). This problem is formulated as

\[
GIO_r(\hat{X}) : \begin{array}{cl}
\text{minimize} & \sum_{q=1}^{Q} |\epsilon_q - 1| \\
\text{subject to} & A^Ty = c, \quad y \geq 0
\end{array} \tag{8a}
\]
\[
\mathbf{c}^\top \hat{\mathbf{x}}_q = \epsilon_q \mathbf{b}^\top \mathbf{y}, \quad \forall q \in Q \tag{8c}
\]

\[
\|\mathbf{c}\|_N = 1. \tag{8d}
\]

Duality gap variables $\epsilon_q$ replace the perturbation vectors used in the general formulation (4). We assume that $\mathbf{b} \neq \mathbf{0}$ in $\text{GIO}_R(\hat{\mathbf{X}})$ to prevent the problem from being trivial, but given a feasible solution to $\text{GIO}_R(\hat{\mathbf{X}})$ satisfying $\mathbf{b}^\top \mathbf{y} = \mathbf{0}$, we define the relative duality gap as 1. First, we show $\text{GIO}_R(\hat{\mathbf{X}})$ can be recovered from formulation (4) with the appropriate hyperparameters.

**Proposition 4.** Let $\mu(\mathbf{c}) \in \mathbb{R}^n$ be a parameter satisfying $\|\mu(\mathbf{c})\|_\infty = 1$ and $\mu(\mathbf{c})^\top \mathbf{c} = 1$. A solution $(\mathbf{c}^*, \mathbf{y}^*, \epsilon_1^*, \ldots, \epsilon_Q^*)$ for which $\mathbf{b}^\top \mathbf{y}^* \neq \mathbf{0}$, is optimal to $\text{GIO}_R(\hat{\mathbf{X}})$ if and only if

\[
(\mathbf{c}^*, \mathbf{y}^*, \mathbf{b}^\top \mathbf{y}^* (\epsilon_1^* - 1) \mu(\mathbf{c}^*), \ldots, \mathbf{b}^\top \mathbf{y}^* (\epsilon_Q^* - 1) \mu(\mathbf{c}^*))
\]

is optimal to $\text{GIO}(\hat{\mathbf{X}})$ with hyperparameters:

\[
(\|\cdot\|, \mathcal{C}, \mathcal{E}_1, \ldots, \mathcal{E}_Q) = \left(\|\cdot\|_\infty / \|\mathbf{b}^\top \mathbf{y}^*\|, \mathbb{R}^n, \{\mathbf{b}^\top \mathbf{y}^* (\epsilon_1 - 1) \mu(\mathbf{c}^*)\}, \ldots, \{\mathbf{b}^\top \mathbf{y}^* (\epsilon_Q - 1) \mu(\mathbf{c}^*)\}\right).
\]

Proposition 4 addresses the case where $\mathbf{b}^\top \mathbf{y}^* \neq 0$ only. However, if $\mathbf{y}^*$ is such that $\mathbf{b}^\top \mathbf{y}^* = 0$, we can show that $\text{GIO}_R(\hat{\mathbf{X}})$ and $\text{GIO}(\hat{\mathbf{X}})$ yield the same optimal value regardless of the hyperparameters.

Suppose that an optimal solution to $\text{GIO}_R(\hat{\mathbf{X}})$ satisfies $\mathbf{b}^\top \mathbf{y}^* = 0$. Then for all $q \in Q$, $\mathbf{c}^* \mathbf{x}_q = 0$ and $\epsilon_q = 1$ is a free variable, leading to an optimal value of 0. On the other hand, we can use the same $(\mathbf{c}^*, \mathbf{y}^*, 0, \ldots, 0)$ as a feasible solution to $\text{GIO}(\hat{\mathbf{X}})$ and observe that setting $\epsilon_q = 0$ for all $q \in Q$ satisfies the strong duality constraint in the generalized problem, giving an optimal value of 0.

**General solution method.** Unlike the absolute duality gap problem, which is non-convex only because of the normalization constraint, $\text{GIO}_R(\hat{\mathbf{X}})$ possesses an additional non-convexity due to a bilinear term in the duality gap constraint (8c). First, we deal with the bilinearity by reformulating $\text{GIO}_R(\hat{\mathbf{X}})$ to three simpler optimization problems. We subsequently deal with the normalization constraint in each of the three optimization problems by using polyhedral decomposition.
Proposition 5. Consider the following three problems:

\begin{align*}
    \text{GIO}^+_R(\hat{X}; K) & : & \min & \sum_{q=1}^{Q} |\epsilon_q - 1| \\
    \text{s.t.} & & A^T y = c, & y \geq 0 \\
    & & c^T \hat{x}_q = \epsilon_q, & \forall q \in Q \\
    & & b^T y = 1 \\
    & & \|c\|_N \geq K,

    \text{GIO}^-_R(\hat{X}; K) & : & \min & \sum_{q=1}^{Q} |\epsilon_q - 1| \\
    \text{s.t.} & & A^T y = c, & y \geq 0 \\
    & & c^T \hat{x}_q = -\epsilon_q, & \forall q \in Q \\
    & & b^T y = -1 \\
    & & \|c\|_N \geq K,

    \text{GIO}^0_R(\hat{X}; K) & : & \min & 0 \\
    \text{s.t.} & & A^T y = c, & y \geq 0 \\
    & & c^T \hat{x}_q = 0, & \forall q \in Q \\
    & & b^T y = 0, & y^T 1 = 1 \\
    & & \|c\|_N \geq K.
\end{align*}

Let \( z^+ \) be the optimal value of \( \text{GIO}^+_R(\hat{X}; K) \) if it is feasible, otherwise \( z^+ = \infty \). Let \( z^- \) and \( z^0 \) be defined similarly for \( \text{GIO}^-_R(\hat{X}; K) \) and \( \text{GIO}^0_R(\hat{X}; K) \), respectively. Let \( z^* = \min \{ z^+, z^-, z^0 \} \) and let \( (c^*, y^*, \epsilon^*_1, \ldots, \epsilon^*_Q) \) be the corresponding optimal solution. We assume \( \epsilon^*_1 = \cdots = \epsilon^*_Q = 1 \) for \( \text{GIO}^0_R(\hat{X}; K) \). There exists \( K \) such that the optimal value of \( \text{GIO}^-_R(\hat{X}) \) is \( z^* \) and an optimal solution to \( \text{GIO}^-_R(\hat{X}) \) is \( (c^*/\|c^*\|_N, y^*/\|c^*\|_N , \epsilon^*_1, \ldots, \epsilon^*_Q) \).

Proof of Proposition 5. Let \( (\hat{c}, \hat{y}) \) be an optimal solution to \( \text{GIO}^-_R(\hat{X}) \) and let

\[ K = \begin{cases} 
1/\|b^T \hat{y}\| & \text{if } b^T \hat{y} \neq 0 \\
1/\|\hat{y}\|^T 1 & \text{otherwise.}
\end{cases} \]

We omit the duality gap variables (\( \epsilon_1, \ldots, \epsilon_Q \)) for conciseness. First, we show that this solution maps to a corresponding feasible solution for one of \( \text{GIO}^+_R(\hat{X}; K) \), \( \text{GIO}^-_R(\hat{X}; K) \), or \( \text{GIO}^0_R(\hat{X}; K) \) with the same objective value. We then conversely show that every feasible solution to formulations (9)–(11) has a corresponding feasible solution in \( \text{GIO}^-_R(\hat{X}) \) with the same objective value.

First, suppose (a) \( b^T \hat{y} > 0 \) and consider \( (\hat{c}, \hat{y}) = (\hat{c}/b^T \hat{y}, \hat{y}/b^T \hat{y}) \). This solution is feasible to \( \text{GIO}^+_R(\hat{X}; K) \) as \( b^T \hat{y} = 1 \) and \( \|\hat{c}\|_N = K \). Furthermore, by substituting \( \hat{c} = \hat{c}/b^T \hat{y} \), we see that the objective value of this solution for \( \text{GIO}^+_R(\hat{X}; K) \) is equal to the optimal value for \( \text{GIO}^-_R(\hat{X}) \):

\[ \sum_{q=1}^{Q} |\hat{c}^T \hat{x}_q - 1| = \sum_{q=1}^{Q} |(\hat{c}^T \hat{x}_q) / (b^T \hat{y}) - 1|. \]

Similarly, when (b) \( b^T \hat{y} < 0 \), we construct \( (\hat{c}, \hat{y}) = \)
(\hat{c}/|b^\top \hat{y}|, \hat{y}/|b^\top \hat{y}|), which is feasible to GIO^-_R(\hat{X}; K) and incurs the same objective value as the optimal value of GIO^-_R(\hat{X}). Finally, if (c) $b^\top \hat{y} = 0$, then the optimal value of GIO^-_R(\hat{X}) is 0. Let $(\hat{c}, \hat{y}) = (\hat{c}/\|\hat{c}\|_N, \hat{y}/\|\hat{c}\|_N)$. It is straightforward to show that this solution is feasible for GIO^-_R(\hat{X}; K).

Thus, an optimal solution to GIO^-_R(\hat{X}) can be scaled to construct a solution that is feasible for exactly one of the formulations (9)–(11).

The converse is proven by showing that every feasible solution of (9)–(11) can be scaled to a feasible solution of GIO^-_R(\hat{X}). Let $(\tilde{c}, \tilde{y})$ be a feasible solution to one of the formulations (9)–(11), and construct $(\hat{c}, \hat{y}) = (\tilde{c}/\|\tilde{c}\|_N, \tilde{y}/\|\tilde{c}\|_N)$. This solution is feasible for GIO^-_R(\hat{X}) and shares the same objective function value.

In terms of objective value, all feasible solutions of GIO^+_R(\hat{X}; K), GIO^-_R(\hat{X}; K), and GIO^0_R(\hat{X}; K) have a one-to-one correspondence with feasible solutions of GIO^-_R(\hat{X}) and the best optimal solution to formulations (9)–(11) can be scaled to an optimal solution for GIO^-_R(\hat{X}).

GIO^-_R(\hat{X}; K), GIO^-_R(\hat{X}; K), and GIO^0_R(\hat{X}; K) remain non-convex due to the normalization constraint $\|c\|_N \geq K$. We show that as in GIO^-_A(\hat{X}), with an appropriate choice of $\|\cdot\|_N$ in the normalization constraint, these problems can be solved via linear optimization (proof omitted).

**Corollary 2.** Let $(c^*, y^*, \varepsilon^*_1, \ldots, \varepsilon^*_Q)$ be optimal to GIO^+_R(\hat{X}; K) under $\|\cdot\|_N = \|\cdot\|_\infty$. There exists a $j \in J$ such that $(c^*, y^*, \varepsilon^*_1, \ldots, \varepsilon^*_Q)$ is also optimal to GIO^+_R(\hat{X}; K, j), defined as:

\[
\text{GIO}^+_R(\hat{X}; K, j) : \begin{align*}
&\text{minimize} \sum_{q=1}^Q |\varepsilon_q - 1| \\
&\text{subject to} \quad A^\top y = c, \quad y \geq 0 \\
& \quad c^\top \hat{x}_q = \varepsilon_q, \quad \forall q \in Q \\
& \quad b^\top y = 1 \\
& \quad (c_j \geq K) \lor (c_j \leq K).
\end{align*}
\] (13)

The disjunctive optimization problem (13) can be written as two LPs. Consequently, Corollary 2 implies that GIO^+_R(\hat{X}; K) can be decomposed into a set of LPs, each replacing the $\|c\|_\infty \geq K$ constraint with a different linear constraint. We repeat the same approach to decompose GIO^-_R(\hat{X}; K) and GIO^0_R(\hat{X}; K). Furthermore, an alternative decomposition can be performed when $\|\cdot\|_N = \|\cdot\|_1$. 
Finally, we address the determination of an appropriate $K$. The proof of Proposition 5 implies that for any $K > 0$, every feasible solution of $\text{GIO}_R^+(\hat{X}; K)$, $\text{GIO}_R^-(\hat{X}; K)$, and $\text{GIO}_R^0(\hat{X}; K)$ can be mapped to a feasible solution of $\text{GIO}_R(\hat{X})$. Moreover, the normalization constraint $\|c\|_N \geq K$ in these formulations implies that the feasible region for each problem grows as $K$ decreases. The proof then shows that for some sufficiently small $K > 0$, an optimal solution to $\text{GIO}_R(\hat{X})$ can be mapped to a feasible (and therefore, also optimal) solution of one of $(9) - (11)$.

To determine a sufficiently small $K$, note that the mapping of a solution of $\text{GIO}_R(\hat{X})$ to solutions of one of $(9) - (11)$ involves scaling the solution by $b^T y$, $-b^T y$, or $y^T 1$, respectively. Bounding these terms allow us to determine a sufficiently small $K$. Formally, consider the following problem:

$$\begin{align*}
\text{maximize}_y & \quad \max \{ |b^T y|, y^T 1 \} \\
\text{subject to} & \quad \|A^T y\|_N = 1, \ y \geq 0.
\end{align*}$$

(14)

We refer to formulation (14) as the auxiliary problem for $\text{GIO}_R(\hat{X})$. Let $K^*$ be defined as the reciprocal of the optimal value of the auxiliary problem. Note $K^*$ is well-defined, because any feasible $y$ to (14) must satisfy $y^T 1 > 0$. We use $K^*$ to reformulate $\text{GIO}_R(\hat{X})$ to $\text{GIO}_R^+(\hat{X}; K^*)$, $\text{GIO}_R^-(\hat{X}; K^*)$, and $\text{GIO}_R^0(\hat{X}; K^*)$.

**Theorem 3.** Let $z^+$ be the optimal value of $\text{GIO}_R^+(\hat{X}; K^*)$ if it is feasible, otherwise $z^+ = \infty$. Let $z^-$ and $z^0$ be defined similarly for $\text{GIO}_R^-(\hat{X}; K^*)$ and $\text{GIO}_R^0(\hat{X}; K^*)$, respectively. Let $z^* = \min \{ z^+, z^-, z^0 \}$ and let $(c^*, y^*, \epsilon^*_1, \ldots, \epsilon^*_q)$ be the corresponding optimal solution. Then, $(c^*/\|c^*\|_N, y^*/\|c^*\|_N, \epsilon^*_1, \ldots, \epsilon^*_q)$ is optimal to $\text{GIO}_R(\hat{X})$.

**Proof of Theorem** Let $(\hat{c}, \hat{y})$ be optimal to $\text{GIO}_R(\hat{X})$ and $K$ be defined as in (12). Since $\hat{y}$ is a feasible solution to the auxiliary problem (14), $1/K^* \geq \max \{ |b^T \hat{y}|, \hat{y}^T 1 \}$, implying $K^* \leq K$.

The proof of Proposition 5 showed that scaling $(\hat{c}, \hat{y})$ appropriately yielded a corresponding feasible solution to one of $\text{GIO}_R^+(\hat{X}; K)$, $\text{GIO}_R^-(\hat{X}; K)$, or $\text{GIO}_R^0(\hat{X}; K)$. Because $K^* \leq K$, the scaled solution must also be feasible for the respective $\text{GIO}_R^+(\hat{X}; K^*)$, $\text{GIO}_R^-(\hat{X}; K^*)$, or $\text{GIO}_R^0(\hat{X}; K^*)$. Moreover, every solution of $\text{GIO}_R^+(\hat{X}; K^*)$, $\text{GIO}_R^-(\hat{X}; K^*)$, or $\text{GIO}_R^0(\hat{X}; K^*)$ can be scaled to a feasible solution of $\text{GIO}_R(\hat{X})$, completing the proof. □
The auxiliary problem can be written as three optimization problems, each with the same constraints as (14) but a different objective: $b^T y$, $-b^T y$, and $y^T 1$. Since the auxiliary problem has a normalization constraint similar to the one in $\text{GIO}_A(\hat{X})$, we can use the same methods to solve it.

In the most general case, solving $\text{GIO}_R(\hat{X})$ is more computationally intensive than solving $\text{GIO}_A(\hat{X})$. We must first identify $K^*$, which we can use to reformulate $\text{GIO}_R(\hat{X})$ into three norm-constrained optimization problems. Subsequently, given an appropriate choice of $\|\cdot\|_N$, each problem is decomposed into a series of LPs. For instance, doing so leads to $2n$ LPs if $\|\cdot\|_N = \|\cdot\|_\infty$ and $2^n$ LPs if $\|\cdot\|_N = \|\cdot\|_1$. These steps coupled with the auxiliary problem (14) used to determine $K^*$ require the solution of $12n$ LPs when $\|\cdot\|_N = \|\cdot\|_\infty$, or $6(2^n)$ when $\|\cdot\|_N = \|\cdot\|_1$. In some cases, however, it may be possible to find an optimal solution to $\text{GIO}_R(\hat{X})$ by solving exactly three LPs.

**Corollary 3.** Let $\text{GIO}_{R,LP}^+(\hat{X})$, $\text{GIO}_{R,LP}^-(\hat{X})$, and $\text{GIO}_{R,LP}^0(\hat{X})$ be LP relaxations of $\text{GIO}_R^+((X;K)$, $\text{GIO}_R^-(\hat{X};K)$, and $\text{GIO}_R^0(\hat{X};K)$, respectively, obtained by removing the normalization constraint $\|c\|_N \geq K$. Let $z_{LP}^+$ be the optimal value of $\text{GIO}_{R,LP}^+(\hat{X})$ if it is feasible, otherwise $z_{LP}^+ = \infty$. Let $z_{LP}^-$ and $z_{LP}^0$ be defined similarly for $\text{GIO}_{R,LP}^-(\hat{X})$ and $\text{GIO}_{R,LP}^0(\hat{X})$, respectively. Let $z_{LP}^* = \min \{z_{LP}^+, z_{LP}^-, z_{LP}^0\}$ and let $(c^*, y^*, \epsilon_1^*, \ldots, \epsilon_Q^*)$ be an optimal solution of the corresponding problem. If $c^* \neq 0$, then $z_{LP}^*$ is equal to the optimal value of $\text{GIO}_R(\hat{X})$ and $(c^*/\|c^*\|_N, y^*/\|c^*\|_N, \epsilon_1^*, \ldots, \epsilon_Q^*)$ is an optimal solution to $\text{GIO}_R(\hat{X})$.

The key difference between Proposition 5 and Corollary 3 is the non-zero assumption (i.e., $c^* \neq 0$). By relaxing the normalization constraint, we permit potential solutions for which $c^* = A^T y^* = 0$ is a linearly dependent combination of the rows of $A$. However, if $c^* \neq 0$ is an optimal solution to the relaxed problem, it is also an optimal solution to $\text{GIO}_R(\hat{X})$. Therefore, to solve $\text{GIO}_R(\hat{X})$, we suggest first solving the three relaxed problems, which are LPs, from Corollary 3. If $c^* = 0$, then we use the more general approach. These steps are summarized in Algorithm 1.

**Feasible observed decisions.** Consider the scenario where the observed points are all feasible for the forward problem. As in the absolute duality gap case, we can show that the relative duality gap model reduces to a single-point problem, which has an analytic solution using Theorem 1.
Algorithm 1 General solution method for $\text{GIO}_R(\hat{X})$

Input: Data set $\hat{X}$

Output: Imputed model parameters $(c^*, y^*, \epsilon_1^*, ..., \epsilon_Q^*)$

1: Solve $\text{GIO}_R^{+}(\hat{X})$, $\text{GIO}_R^{-}(\hat{X})$, $\text{GIO}_R^{0}(\hat{X})$. Let $z^+_{LP}$, $z^-_{LP}$, $z^0_{LP}$ be the respective optimal values.
2: Let $z^*_{LP} \leftarrow \min \{z^+_{LP}, z^-_{LP}, z^0_{LP}\}$ and $(c^*, y^*, \epsilon_1^*, ..., \epsilon_Q^*)$ be the corresponding optimal solution.
3: if $c^* \neq 0$ then
4:     return $(c^*, y^*, \epsilon_1^*, ..., \epsilon_Q^*)$
5: else
6:     Solve the auxiliary problem (14). Let $K^*$ be the reciprocal of the optimal value.
7:     Solve $\text{GIO}_R^{+}(\hat{X}; K^*)$, $\text{GIO}_R^{-}(\hat{X}; K^*)$, $\text{GIO}_R^{0}(\hat{X}; K^*)$. Let $z^+, z^-, z^0$ be the respective optimal values.
8:     Let $z^* \leftarrow \min \{z^+, z^-, z^0\}$ and $(c^*, y^*, \epsilon_1^*, ..., \epsilon_Q^*)$ be the corresponding optimal solution.
9:     return $(c^*, y^*, \epsilon_1^*, ..., \epsilon_Q^*)$
10: end if

Proposition 6. If $\hat{X} \subset P$ and $\bar{x}$ is the centroid of $\hat{X}$, then $\text{GIO}_R(\hat{X})$ is equivalent to $\text{GIO}_R(\{\bar{x}\})$.

Infeasible observed decisions. For a single infeasible point, the solution to $\text{GIO}_R(\{\hat{x}\})$ is broken into two cases. The proofs (omitted) are similar to the absolute duality gap case.

Proposition 7. Assume $\hat{x} \notin P$.

1. When $\hat{x}$ satisfies $a^T_i \hat{x} > b_i$ for some $i \in I$, then there exists $i^* \in I$ such that (11) is an optimal solution to $\text{GIO}_R(\{\hat{x}\})$ and the optimal value is 0.

2. When $a^T_i \hat{x} \leq b_i$, $\forall i \in I$, there exists $i^* \in I$ such that (13) is an optimal solution to $\text{GIO}_R(\{\hat{x}\})$.

Proposition 7 is the relative duality gap analogue of Proposition 3, as it provides an analytic solution for $\text{GIO}_R(\{\hat{x}\})$ when $\hat{x}$ is infeasible. Thus, geometric insights similar to those of the absolute duality gap case can be derived. Furthermore, Part 2 of Proposition 7 can be extended to multiple observations. The proof (omitted) can be derived following the proof of Proposition 3.
Corollary 4. Suppose that \( a_i^T \hat{x}_q \leq b_i \) for all \( i \in I \) and \( q \in Q \) and let \( \bar{x} \) be the centroid of \( \hat{X} \). Then, \( \text{GIO}_R(\hat{X}) \) is equivalent to \( \text{GIO}_R(\{\bar{x}\}) \) over the alternate forward problem \( \text{FOA}(c) \).

3.2. Decision space

The decision space methodology measures error in the space of decision variables, rather than objective values. In particular, the goal is to identify a cost vector that induces optimal decisions for the forward problem that are of minimum aggregate distance to the corresponding observed decisions. The decision space inverse optimization problem is formulated as

\[
\text{GIO}_p(\hat{X}) : \begin{align*}
\text{minimize} & \quad \sum_{q=1}^{Q} \|e_q\|_p \\
\text{subject to} & \quad A^T y = c, \quad y \geq 0 \\
& \quad c^T \hat{x}_q = b^T y + c^T e_q, \quad \forall q \in Q \\
& \quad A (\hat{x}_q - e_q) \geq b, \quad \forall q \in Q \\
& \quad \|c\|_N = 1.
\end{align*}
\]

The above formulation closely resembles the generalized formulation (4) with the objective function being the aggregate of the \( p \)-norms \((p \geq 1)\) of the perturbation vectors. A notable addition is constraint (15d), which enforces primal feasibility of the perturbed decisions \( \hat{x}_q - e_q \). It is straightforward to show (proof omitted) that \( \text{GIO}_p(\hat{X}) \) is a variant of \( \text{GIO}(\hat{X}) \).

Proposition 8. A solution \((c^*, y^*, e_1^*, \ldots, e_Q^*)\) is optimal to \( \text{GIO}_p(\hat{X}) \) if and only if it is optimal to \( \text{GIO}(\hat{X}) \) with the following hyperparameters: \((\|\cdot\|, C, E_1, \ldots, E_Q) = \left(\|\cdot\|_p, \mathbb{R}^n, \{e_1 \mid A (\hat{x}_1 - e_1) \geq b\}, \ldots, \{e_Q \mid A (\hat{x}_Q - e_Q) \geq b\}\right)\).

Model (15) is non-convex due to the normalization constraint (15e), as well as the strong duality constraint (15c). In the case of a single, feasible \( \hat{x} \), Theorem 1 shows that the direct projection of \( \hat{x} \) to the closest hyperplane is to a point \( x^* \) that is feasible, implying that an optimal cost vector coincides with one of the constraints defining the feasible region. In the multi-point case, we
show that an optimal cost vector has the same form as in the single-point case. However, directly projecting all points \( \hat{x}_q \) to that optimal hyperplane may result in some of the projections being infeasible, requiring the explicit inclusion of primal feasibility constraints \((15d)\). Thus, rather than the hyperplane projection \( \pi_i(\hat{x}_q) \) from \((2)\), consider the following feasible projection problem:

\[
\begin{align*}
\text{minimize} & \quad \|\hat{x}_q - x\|_p \\
\text{subject to} & \quad Ax \geq b \\
& \quad a_i^T x = b_i.
\end{align*}
\]

Let \( \psi_i(\hat{x}_q) \) be an optimal solution to problem \((16)\), which identifies the closest feasible point to \( \hat{x} \) on the hyperplane \( \mathcal{H}_i = \{ x \mid a_i^T x = b_i \} \). We first show how we can derive a structured optimal solution to \( \text{GIO}_p(\hat{x}) \) by using the feasible projections of the observed decisions.

**Lemma 1.** There exists \( i \in I \) such that an optimal solution to \( \text{GIO}_p(\hat{x}) \) is given by

\[
(e^*, y^*, e_1^*, \ldots, e_Q^*) = \left( \frac{a_i}{\|a_i\|_N}, \frac{e_i}{\|a_i\|_N}, \hat{x}_q - \psi_i(\hat{x}_q) \right),
\]

**Proof of Lemma.** Without loss of generality, assume that \( \|a_i\|_N = 1 \) for all \( i \in I \). Solution \((17)\) is feasible to \( \text{GIO}_p(\hat{x}) \) for all \( i \in I \). We show that for any feasible solution that is not of the form \((17)\), there exists a feasible solution of that form whose objective value is at least as good.

Consider a feasible solution \((\tilde{e}, \tilde{y}, \tilde{e}_1, \ldots, \tilde{e}_Q)\) to \( \text{GIO}_p(\hat{x}) \), where \( \tilde{y} \neq e_i \) for any \( i \in I \). Without loss of generality, assume \( \tilde{y}_1, \ldots, \tilde{y}_k > 0 \) for some \( 1 < k \leq m \) and let \( K = \{1, \ldots, k\} \) denote the corresponding index set. Let \( \hat{x}_q = \hat{x}_q - \tilde{e}_q \) denote the perturbed decision for all \( q \in Q \). The primal feasibility constraint \((15d)\) implies that \( A\hat{x}_q \geq b \) for all \( q \in Q \). The strong duality constraint \((15c)\) implies that for all \( q \in Q \), \( 0 = c^T \hat{x}_q - b^T \tilde{y} = \sum_{i=1}^{k} \tilde{y}_i (a_i^T \hat{x}_q - b_i) \), which follows from substituting \( \tilde{c} = \sum_{i=1}^{k} \tilde{y}_i a_i \). Using the non-negativity of \( \tilde{y} \) and primal feasibility (i.e., \( a_i^T \hat{x}_q \geq b_i \) for all \( i \in I \)), we see that \( \hat{x}_q \) for all \( q \in Q \) are feasible solutions to the feasible projection problem \((16)\) for each \( i \in K \).

Let \( (\tilde{e}, \tilde{y}, \tilde{e}_1, \ldots, \tilde{e}_Q) = (a_{i^*}, e_{i^*}, \hat{x}_1 - \psi_{i^*}(\hat{x}_1), \ldots, \hat{x}_Q - \psi_{i^*}(\hat{x}_Q)) \) for an arbitrary index \( i^* \in K \). For all \( q \in Q \), \( \psi_{i^*}(\hat{x}_q) \) is, by definition, an optimal solution to \((16)\). Therefore, we have \( \sum_{q=1}^{Q} \|\hat{x}_q - \psi_{i^*}(\hat{x}_q)\|_p \leq \sum_{q=1}^{Q} \|\tilde{e}_q\|_p \), with the inequality following from the optimality of \((16)\). Thus,
given any feasible solution to \( \text{GIO}_p(\hat{X}) \) not of the form defined in (17), we can construct a feasible solution of the form (17) with the objective value at least as good as the original.

The intuition behind Lemma 1 is as follows. Given a feasible vector \((\epsilon_1, \ldots, \epsilon_Q)\), every observed decision \(\hat{x}_q\) is perturbed by \(\epsilon_q\) to a point that satisfies both strong duality and primal feasibility. Strong duality implies that \(H = \{x \mid c^* x = b^T y^*\}\) is a supporting hyperplane, and so \(\hat{x}_q - \epsilon_q\) lies on that supporting hyperplane for all \(q \in Q\). Thus, the proof of Lemma 1 elucidates that every feasible solution not of the form (17) must tightly satisfy multiple constraints, and is dominated by solutions that involve the feasible projection to just one of those constraints (i.e., of the form (17)).

This result holds regardless of the feasibility of the observed decisions and of the chosen norm. Moreover, Lemma 1 suggests an efficient method to compute an optimal solution to \( \text{GIO}_p(\hat{X}) \).

**Theorem 4.** Consider the following optimization problem:

\[
\min_{i \in \mathcal{I}} \min_{\epsilon_{1,i}, \ldots, \epsilon_{Q,i}} \sum_{q=1}^{Q} \|\epsilon_{q,i}\|_p \tag{18a}
\]

s.t. \( A(\hat{x}_q - \epsilon_{q,i}) \geq b, \quad \forall q \in Q \) \hspace{1cm} (18b)

\( a_i^T(\hat{x}_q - \epsilon_{q,i}) = b_i, \quad \forall q \in Q. \) \hspace{1cm} (18c)

For each \(i \in \mathcal{I}\), let \((\epsilon_{1,i}^*, \ldots, \epsilon_{Q,i}^*)\) denote an optimal solution to the inner optimization problem and let \(i^* \in \arg \min_{i \in \mathcal{I}} \sum_{q=1}^{Q} \|\epsilon_{q,i}^*\|\) denote an optimal index determined by the outer optimization problem. Then, \((a_{i^*}/\|a_{i^*}\|_N, \epsilon_{i^*}/\|a_{i^*}\|_N, \epsilon_{1,i^*}, \ldots, \epsilon_{Q,i^*})\) is an optimal solution to \( \text{GIO}_p(\hat{X}) \).

### 3.2.1. A lower bound on the optimal value.

While \( \text{GIO}_p(\hat{X}) \) can be solved by solving \(m\) convex problems, we can derive a simple lower bound that can be computed analytically, leveraging the geometric insight from the single-point problem.

We simply remove the primal feasibility constraint (15d), which means the relaxed problem can be solved by solving (18) without constraint (18b) for each \(i\). Without primal feasibility, the projection of points in \(\hat{X}\) to each of the hyperplanes defining the constraints can be done using \(\pi_i(\cdot)\) defined in (2) (instead of \(\psi_i(\cdot)\)), which has an analytic solution.
Proposition 9. Let $z^*$ be the optimal value to $\text{GIO}_p(\hat{X})$ and $\bar{x}$ be the centroid of $\hat{X}$. Then,

$$
    z^* \geq \min_{i \in I} \left\{ Q \left( \frac{a_i^T \bar{x} - b_i}{\|a_i\|_D} \right) \right\}.
$$

Proposition 9 suggests that the optimal value is lower bounded by the optimal value of a single-point problem $\text{GIO}_p(\{\bar{x}\})$. This relationship offers an efficient means of approximately solving $\text{GIO}_p(\hat{X})$. Instead of solving $m$ convex optimization problems, we can attain a bound by taking the minimum of $m$ ratios and imputing the corresponding cost vector. The following example illustrates the intuitive finding that the lower bound may recover an optimal solution.

Example 1: Let $\text{FO}(c) : \min_x \{ c_1 x_1 + c_2 x_2 \mid 0.71 x_1 + 0.71 x_2 \geq 0.42, \ 0.24 x_1 + 0.97 x_2 \geq 0.29, \ -0.89 x_1 + 0.45 x_2 \geq -0.67, \ x_1 \leq 1, \ x_2 \leq 1, \ x_1 \geq 0 \}$ and $\hat{X} = \{(0.3,0.45),(0.48,0.4),(0.63,0.35),(0.78,0.3)\}$. The forward problem, observed decisions and their corresponding projections from solving $\text{GIO}_2(\hat{X})$ are shown in Fig. 2a. The optimal value of $\text{GIO}_2(\hat{X})$ is 0.86 with $c^* = (0.24,0.97)$. Computing the lower bound produces an optimal value of 0.82, but actually yields the same optimal cost vector.

This lower bound also elucidates a connection between the decision space problem and the absolute duality gap problem. Under appropriate choice of the hyperparameters when the data points are feasible, the optimal value of $\text{GIO}_A(\hat{X})$ is exactly the lower bound to $\text{GIO}_p(\hat{X})$. 
Table 1  Summary of the different variants of GIO(\(\hat{X}\)).

| \(\|\cdot\|\) | \(C\) | \(E_q, \forall q \in Q\) | Solution approach |
|----------------|------|-----------------|-----------------|
| \(\|\|_\infty\) | \(\mathbb{R}^n\) | \(\{\epsilon_q \mid \epsilon_q = \epsilon_q \mu(c)\}\) | Polyhedral decomposition |
| \(\|\|_\infty/|b^T y|\) | \(\mathbb{R}^n\) | \(\{\epsilon_q \mid \epsilon_q = b^T y (\epsilon_q - 1) \mu(c)\}\) | Algorithm [1] |
| \(\|\|_p\) | \(\mathbb{R}^n\) | \(\{\epsilon_q \mid A (x_q - \epsilon_q) \geq b\}\) | Formulation [18]. |

Corollary 5. If \(\hat{X} \subset P\), then the lower bound to GIO\(_\infty(\hat{X})\) determined by Proposition 4 is equal to the optimal value of GIO\(_A(\hat{X})\).

3.3. Summary of variants

The objective space and decision space variants of GIO(\(\hat{X}\)) are summarized in Table 1. The hyperparameters (\(\|\cdot\|, C, E_1, \ldots, E_Q\)) can be viewed as a structured template; a practitioner may introduce additional constraints and expand \(C\) (e.g., modeling constraints on \(c\)) or each \(E_q\) as necessary for a specific application. An initial discussion on the differences between objective and decision space inverse optimization for the practitioner appears in Chan et al. (2017). Here, we compare the variants for data sets containing multiple (potentially infeasible) points.

First, the choice of inverse optimization variant can be based on the application and the practitioner’s preference, (i.e., whether the goal is to reconstruct optimal solutions that correspond to the observed decisions or to find a best fit objective function). In the following example, we will observe that using an inappropriate inverse optimization methodology may lead to a different imputed cost vector and corresponding forward model. As a result, the imputed model may return higher sub-optimality in the desired measure, in comparison to using the appropriate model.

Example 2  Let FO(\(c\)) : \(\min_x \{c_1 x_1 + c_2 x_2 \mid x_1 \leq 0, x_2 \geq 0\}\) and \(\hat{X} = \{(-2,4), (-2,2), (3,4)\}\). As shown in Fig. 2B, using GIO\(_2(\hat{X})\) results in \(c_2^* = (-1,0)\), the three points being projected to the plane \(x_1 = 0\), and \(\sum_{q=1}^3 \|\epsilon_q^*\|_2 = 7\), while solving GIO\(_A(\hat{X})\) leads to \(c_A^* = (-0.57,0.43)\) and all observations project to \(x_A^* = (0,0)\), an optimal solution to FO(\(c_A^*\)). The \(l_2\) error from projecting
to $x^*_A$ is $\sum_{q=1}^{3} \|\hat{x}_q - x^*_A\|_2 = 12.3$, a 75% increase from that of the decision space model. Similarly, $\sum_{q=1}^{3} |c^*_A^T \hat{x}_q - c^*_A^T 0| = 4.86$ while $\sum_{q=1}^{3} |c^*_2^T \hat{x}_q - c^*_2^T 0| = 7$, a 44% increase.

Another consideration when selecting the model variant is computational tractability. $\text{GIO}_p(\hat{X})$ grows linearly in complexity with regards to the number of constraints, as each constraint requires solving an additional convex optimization problem. Objective space models with $\|\cdot\|_N = \|\cdot\|_\infty$ can be decomposed to on the order of $2n$ LPs, while using $\|\cdot\|_N = \|\cdot\|_1$ leads to $2^n$ LPs. As noted earlier, certain application-specific constraints can significantly reduce the complexity (e.g., when $c \geq 0$). Of the two objective space models, $\text{GIO}_R(\hat{X})$ has an advantage only when solving $\text{GIO}_R(\hat{X})$ without the normalization constraint via three LPs yields a non-zero cost vector (see Corollary 3). Ultimately, from the perspective of computational tractability, a choice between decision and objective space leads the practitioner to consider the dimensionality of the forward model. If the number of constraints, $m$, is sufficiently small, it may be preferable to solve $m$ convex optimization problems of the decision space method rather than a potentially exponential number of LPs required by the objective space methods. On the other hand, in special cases, e.g., when all observed decisions are feasible, objective space models reduce to single-point models with analytic solutions (see Propositions 2 and 3), in contrast to the decision space model which does not become easier.

In this section, we constructed a unifying framework of inverse linear optimization with an arbitrary data set. However, the means of evaluating the fitness of these models is not immediately clear. Next, we present a general and context-free goodness-of-fit metric for inverse optimization with an arbitrary data set, a generalization of Chan et al.’s (2017) coefficient of complementarity.

4. Measuring goodness of fit

In this section, we present a unified view of measuring model-data fitness error by developing a metric that is easily and consistently interpretable across different inverse linear optimization methods, forward models, and applications. As shown in Example 3, simply assessing the aggregate error from the inverse optimization model may not provide a complete picture of model fitness.
Moreover, a context-free goodness of fit metric is useful when comparing different forward models for a given data set, or when faced with an unfamiliar application.

Several previously-proposed fitness measures for inverse optimization were context-specific (Troutt et al. 2006, Chow and Recker 2012). The first general goodness-of-fit metric was developed in Chan et al. (2017), but only in the context of a single feasible observed decision (i.e., $\text{GIO}({\hat{x}})$).

This metric, referred to as the coefficient of complementarity and denoted $\rho({\hat{x}})$, provides a scale-free, unitless measure of goodness of fit between model and data, analogous to the coefficient of determination $R^2$ in linear regression. It is defined as

$$\rho({\hat{x}}) = 1 - \frac{\|e^*\|}{\frac{1}{m} \sum_{i=1}^{m} \|e_i\|}.$$ 

The numerator of the ratio is the residual error in inverse optimization, or the optimal value of $\text{GIO}({\hat{x}})$). The denominator is the average of the errors corresponding to the projections of $\hat{x}$ to each of the $m$ the constraints (i.e., $e_i = \hat{x} - \pi_i(\hat{x})$ for $i \in I$). Just as $R^2$ calculates the ratio of error of a linear regression model over a baseline mean-only model, $\rho({\hat{x}})$ measures the relative improvement in error from using $\text{FO}(c^*)$ compared to a baseline corresponding to the average error induced by all $m$ candidate optimal cost vectors (cf. Theorem 1).

We extend $\rho({\hat{x}})$ to make it applicable to generalized inverse optimization problems (i.e., $\text{GIO}(\hat{X})$) without restriction on $\hat{X}$. When obvious, we omit the data set in notation. We denote the absolute duality gap, relative duality gap, and $p$-norm variants of $\rho$ as $\rho_A$, $\rho_R$, and $\rho_p$, respectively.

### 4.1. Multi-point coefficient of complementarity

We define the (multi-point) coefficient of complementarity, $\rho(\hat{X})$, as

$$\rho(\hat{X}) = 1 - \frac{\sum_{q=1}^{Q} \|e^*_q\|}{\frac{1}{m} \sum_{i=1}^{m} \left(\sum_{q=1}^{Q} \|e_{q,i}\|\right)}.$$  

(20)

The numerator is the optimal value of $\text{GIO}(\hat{X})$, i.e., the residual error from an optimal solution to the inverse optimization problem. The denominator terms $\sum_{q=1}^{Q} \|e_{q,i}\|$ represent the aggregate error induced by choosing $(c, y) = (a_i/\|a_i\|_N, e_i/\|a_i\|_N)$ (i.e., baseline feasible solutions), and are computed as follows:
• For absolute duality gap, $\text{GIO}_A(\hat{X})$,

\[ \sum_{q=1}^{Q} \| e_{q,i} \| = \sum_{q=1}^{Q} \frac{\| a_i^T \hat{x}_q - b_i \|}{\| a_i \|_1}. \tag{21} \]

• For relative duality gap, $\text{GIO}_R(\hat{X})$, under the assumption that $b_i \neq 0$ for all $i \in I$,

\[ \sum_{q=1}^{Q} \| e_{q,i} \| = \sum_{q=1}^{Q} \frac{\| a_i^T \hat{x}_q \|}{b_i} - 1. \tag{22} \]

• For decision space, $\text{GIO}_p(\hat{X})$, $\sum_{q=1}^{Q} \| e_{q,i} \|$ is the optimal value of the corresponding inner problem in formulation (18).

The denominator in $\rho(\hat{X})$ represents a baseline against which the inverse solution is measured. Our choice of baseline is a direct extension from the single-point case, where an optimal cost vector can be found by selecting amongst one of the vectors $a_i$ defining the $m$ constraints. We maintain this choice of baseline for several reasons. First, an optimal solution will be exactly one of the $a_i$ in the general decision space problem (cf. Lemma 1) and in several special cases of the objective space problem (cf. Propositions 2 and 6). Second, calculation of the denominator is straightforward either directly from the data (e.g., (21) and (22)) or via the solution of $m$ convex (possibly linear) optimization problems (18). Third, this definition provides a direct generalization of the single-point $\rho(A\{\hat{x}\})$, inheriting several attractive mathematical properties (cf. Section 4.2). In addition, for objective space models, the multi-point coefficient of complementarity is equal to an appropriate single-point $\rho$ when all data points are feasible.

**Proposition 10.** Let $\hat{x}$ be the centroid of $\hat{X} \subset \mathcal{P}$. Then, $\rho_A(\hat{X}) = \rho_A(A\{\hat{x}\})$ and $\rho_R(\hat{X}) = \rho_R(A\{\hat{x}\})$.

We omit the proof since it follows from Propositions 2 and 6 and straightforward algebraic manipulation of $\rho(\hat{X})$ with the appropriate denominator.

**4.2. Properties of $\rho$**

Chan et al. (2017) show that $\rho(A\{\hat{x}\})$ possesses several mathematical properties analogous to the properties of $R^2$ from linear regression. Here, we show that the same properties hold for the more general $\rho(\hat{X})$. For the remainder of this section, we write $\rho(\hat{X})$ as $\rho$ for convenience.
Theorem 5. The following properties hold for \( \rho \) defined in (21):

1. **Optimality:** \( \rho \) is maximized by an optimal solution to \( \text{GIO}(\hat{X}) \).

2. **Boundedness:** \( \rho \in [0, 1] \).

3. **Monotonicity:** For \( 1 \leq k < n \), let \( \text{GIO}^{(k)}(\hat{X}) \) be \( \text{GIO}(\hat{X}) \) with additional constraints \( c_i = 0 \), for \( k + 1 \leq i \leq n \). Let \( \rho^{(k)} \) be the coefficient of complementarity for \( \text{GIO}^{(k)}(\hat{X}) \). Then, \( \rho^{(k)} \leq \rho^{(k+1)} \).

The first property underlines how \( \rho \) fits into the generalized inverse optimization framework. One can select any cost vector and calculate the induced error and \( \rho \) value with respect to the data \( \hat{X} \). However, a solution obtained via \( \text{GIO}(\hat{X}) \) is guaranteed to attain the maximum value for \( \rho \).

The second property makes \( \rho \) easily interpretable as a measure of goodness of fit, with higher values indicating improved fit. Note that \( \rho = 1 \) if and only if \( \sum_{q=1}^{Q} \| \epsilon_q^* \| = 0 \) (i.e., every point in \( \hat{X} \) is an optimal solution to \( \text{FO}(c^*) \)). In this case, the model perfectly describes all of the data points, analogous to the best fit line passing through all data points in a linear regression. Conversely, \( \rho = 0 \) if and only if \( \sum_{q=1}^{Q} \| \epsilon_q^* \| = \sum_{q=1}^{Q} \| \epsilon_{q;i} \| \) for all \( i \in I \). This scenario occurs when an optimal solution to the inverse optimization problem does not reduce the model-data fit error with respect to any of the baseline solutions, akin to when a linear regression returns an intercept-only model.

The third property states that goodness of fit is nondecreasing as additional degrees of freedom are provided to the practitioner. This property is analogous to the property that \( R^2 \) is nondecreasing in the number of features in a linear regression model. Because of this similarity, \( \rho \) also shares one of the weaknesses of \( R^2 \), namely the potential of overfitting. Thus, when using \( \rho \) to compare the goodness of fit of several inverse optimization models, a user should ensure that higher values of \( \rho \) represent true improvements in fit, rather than artificial increases that lack generalizability.

### 4.3. Numerical examples

We present examples highlighting behavioral properties and usefulness of the coefficient of complementarity. Example 3 illustrates the value of using \( \rho \) instead of error when comparing different models. Intuitively, a given error within a larger feasible region indicates better fit than the same error within a smaller feasible region: \( \rho \) captures this intuition by measuring error in the context of the geometry of the feasible set of the forward model.
Example 3 Let $\text{FO}(c; u, v) : \min_{x} \{c_1 x_1 + c_2 x_2 \mid -0.71 x_1 + 0.71 x_2 \geq -2.83, x_1 \leq 7, x_2 \leq v, x_1 \geq u; x_2 \geq 1\}$ and let $\hat{X} = \{(5, 2.5), (4.75, 3.75), (5.5, 3)\}$. Solving $\text{GIO}(\hat{X})$ in both cases yields $c^* = (-0.5, 0.5)$ and $\sum_{q=1}^{3} |\epsilon_q^*| = 2.75$. However, for $\text{FO}(c; -2, 10)$, $\rho = 0.76$, while for $\text{FO}(c; 4, 4)$, $\rho = 0.34$. In Fig. 3a, the data points are closer to the facet that identifies the optimal cost vector, relative to the other facets, while in Fig. 3b, the data points are near the “center” of the polyhedron, and not substantially closer to any one facet.

Next, we present an example that demonstrates the behaviour of $\rho$ when the forward problem remains the same but the data set changes. In Example 4, case (a), the points are close together and all project to the same facet, resulting in the same optimal cost vector. In (b), the points are further apart, each with a different preferred cost vector, but the aggregate error is minimized by selecting a cost vector that is not preferred by any of them. In the latter case, the inverse solution is a compromise between the preferences of the individual data points, resulting in poorer fit.

Example 4 Let $\text{FO}(c) : \min_{x} \{c_1 x_1 + c_2 x_2 \mid x_1 \leq 7, x_2 \leq 7, x_1 \geq 1, x_2 \geq 1\}$, $\hat{X}_1 = \{(3.75, 2), (4, 2.25), (4.25, 2)\}$ and $\hat{X}_2 = \{(1.5, 2), (4, 6.25), (6.5, 2)\}$. Both $\text{GIO}(\hat{X}_1)$ and $\text{GIO}(\hat{X}_2)$ impute $c^* = (0, 1)$. In Fig. 4a, the data points are closer together and all clearly prefer the bottom
Figure 4  \( \text{GIO}_A(\hat{\mathcal{X}}_1) \) and \( \text{GIO}_A(\hat{\mathcal{X}}_2) \) for the same \( \text{FO}(c) \). Illustration of Example 4.

(a) \( \hat{\mathcal{X}}_1 = \{(3.75, 2), (4.25, 2), (4.25, 2)\} \). \( \rho = 0.64 \).

(b) \( \hat{\mathcal{X}}_2 = \{(1.5, 2), (4.625), (6.5, 2)\} \). \( \rho = 0.17 \).

facet, while in Fig. 4b, the points are further apart, with each point biased towards a different facet. We find \( \rho = 0.64 \) and \( \rho = 0.17 \) for the two problems, respectively.

As decision space and objective space models have differing interpretations and loss measures, the corresponding coefficients of complementarity yield different fitness values. In the final example, we demonstrate the difference using a heatmap of \( \rho \) values, where three points in the data set are fixed and the fourth is left variable. Due to the inclusion of primal feasibility constraints in \( \text{GIO}_p(\hat{\mathcal{X}}) \), the differences in behaviour are most apparent for infeasible points.

Example 5  Let \( \text{FO}(c) : \min_{x} \{c_1x_1 + c_2x_2 \mid 0.71x_1 + 0.71x_2 \geq 4.24, 0.71x_1 - 0.71x_2 \geq -2.83, x_1 \leq 7, x_2 \leq 7, x_2 \geq 1\} \) and consider all data sets of the form \( \hat{\mathcal{X}} = \{(2, 5), (3, 6), (5, 4), (\gamma_1, \gamma_2)\} \), where \(-2 \leq \gamma_1, \gamma_2 \leq 10\). Heatmaps of \( \rho \) for \( \text{GIO}_A(\hat{\mathcal{X}}) \) and \( \text{GIO}_2(\hat{\mathcal{X}}) \) are shown in Fig. 5. The best fitness for \( \text{GIO}_A(\hat{\mathcal{X}}) \) is achieved when the fourth point lies along \( \mathcal{H}_1 = \{(x_1, x_2) \mid 0.71x_1 - 0.71x_2 = -2.83\} \).

If we were to solve \( \text{GIO}_A(\hat{\mathcal{X}}) \) with the three fixed points, the imputed cost vector is \( c^* = (0.5, -0.5) \). Thus, any point that lies on \( \mathcal{H}_1 \) yields zero additional duality gap loss to the existing solution. We use a similar argument to describe the good fitness along \( \mathcal{H}_2 = \{(x_1, x_2) \mid 0.71x_1 + 0.71x_2 = 4.24\} \).

Fitness decreases as the fourth point moves away from these two hyperplanes.
We observe different behavior for $\rho$ in $\text{GIO}_2(\hat{X})$: the best fitness occurs when the fourth point lies along the facets of $\mathcal{P}$ defined by $\mathcal{H}_1$ and $\mathcal{H}_2$. Due to the primal feasibility requirement in the decision space problem, $\rho$ decreases as we move further away from these facets in any direction. If the fourth point is infeasible, it must project to a feasible point and thus incur some positive error.

5. Conclusion

Inverse optimization is an increasingly popular model fitting paradigm that allows one to estimate the parameters of an optimization problem that best describe observed data representing decisions. This paper unifies different inverse linear optimization methodologies by developing a generalized inverse optimization methodology that (a) specializes into objective or decision space models, (b) is applicable to data sets without restriction on size or feasibility, and (c) integrates a context- and scale-free measure of goodness of fit. We formulate the generalized inverse optimization model and develop solution methods for several key variants of the model. Building this shared theoretical framework for generalized inverse optimization with arbitrary data sets, we also unify the measurement of goodness of fit in this general setting. We prove several key properties of the general coefficient of complementarity, extending previous results in the literature that were shown in more restricted cases. Overall, the framework presented in this paper provides a unified view of the model fitting and model evaluation components of inverse linear optimization for an arbitrary data set.
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EC.1. Proofs of Statements

Proof of Proposition 1. For any $c$, setting each $\epsilon_q = \epsilon_q \mu(c)$ implies $\|\epsilon_q\|_\infty = |\epsilon_q| \|\mu(c)\|_\infty = |\epsilon_q|$. Thus, (4a) becomes (5a). Similarly, (4c) becomes (5c), since $c^T \epsilon_q = \epsilon_q c^T \mu(c) = \epsilon_q$. Then, any feasible solution to $\text{GIO}(\hat{X})$ with the suggested hyperparameters yields a feasible solution to $\text{GIO}_A(\hat{X})$ and vice versa, with the same objective value. □

Proof of Proposition 2. If all observations are feasible, then by weak duality $\epsilon_q \geq 0 \forall q \in Q$, and we can simplify the objective function $\sum_{q=1}^Q |\epsilon_q| = \sum_{q=1}^Q \epsilon_q = \sum_{q=1}^Q (c^T \tilde{x}_q - b^T y) = (c^T \bar{x} - b^T y) Q$, where the last equality follows by the definition of the centroid (i.e., $\bar{x} = \sum_{q=1}^Q \tilde{x}_q / Q$). We similarly compress constraint (5c) to a single constraint for $\bar{x}$, resulting in $\text{GIO}_A(\{\bar{x}\})$. □

Proof of Proposition 3.

1. Assume that, without loss of generality, there exist $i, j \in \mathcal{I}$ such that $a_i^T \hat{x} > b_i$ and $a_j^T \hat{x} < b_j$, respectively. The corresponding $\tilde{y}$ defined in (I) satisfies the strong duality constraint (5d) with $\epsilon = 0$. Furthermore, $(\tilde{c}, \tilde{y})$ satisfy the duality feasibility constraints (5b) by construction. We normalize the solution to satisfy constraint (5d), noting that the normalized solution still satisfies all other constraints. This solution is thus feasible to $\text{GIO}_A(\{\bar{x}\})$ with zero cost and therefore is optimal.

2. In this case, the duality gap is non-positive (i.e., $\epsilon \leq 0$). We rewrite the single-point version of (I) with $\delta = -\epsilon$, shown in model (EC.1) below. Now consider the forward problem $\min_{\bar{x}} \{-c^T \bar{x} \mid A \bar{x} \leq b\}$ with the observed solution $\hat{x}$ and the corresponding inverse optimization model being (EC.2).

\[
\begin{align*}
\text{minimize} & \quad \delta & \quad \text{minimize} & \quad |\gamma| \\
\text{subject to} & \quad A^T \bar{y} = c, \; \bar{y} \geq 0 & \quad \text{subject to} & \quad A^T \bar{y} = c, \; \bar{y} \geq 0 \\
& \quad c^T \hat{x} = b^T \bar{y} - \delta & \quad -c^T \hat{x} = -b^T \bar{y} + \gamma \\
& \quad \|c\|_N = 1. & \quad \|c\|_N = 1.
\end{align*}
\]

By assumption, $\hat{x}$ is feasible for the above-defined forward problem and therefore, $\gamma \geq 0$ in (EC.2). Consequently, formulation (EC.1) is equivalent to (EC.2) after removing the absolute value in
the objective and rearranging the duality gap constraint. We can solve formulation (EC.2) using
Theorem 1, arriving at an optimal solution for the original inverse optimization problem.

Proof of Corollary 1. Since all observations are infeasible for the initial forward problem, the
duality gap terms are all non-positive (i.e., \( \epsilon_q \leq 0 \) for all \( q \in Q \)). As such, we use the same argument
as used in Prop. 3 Part 2 to show that the formulation of \( \text{GIO}_A(\hat{\mathbf{x}}) \) is equivalent to the formulation
of an absolute duality gap inverse optimization problem over the alternative forward problem
\[
\min_{\mathbf{x}} \{-c^T \mathbf{x} \mid A \mathbf{x} \leq \mathbf{b}\}.
\]
As \( \hat{\mathbf{x}} \subset \{ \mathbf{x} \mid A \mathbf{x} \leq \mathbf{b} \} \), Proposition 2 reduces the problem to \( \text{GIO}_A(\{\bar{\mathbf{x}}\}) \).

Proof of Proposition 4. For any \( c \), setting \( \epsilon_q = b^T y (\epsilon_q - 1) \mu(c) \) forces
\[
\|\epsilon_q\|_{\infty} / |b^T y| = |\epsilon_q - 1|,
\]
giving us the objective (8a). The same substitution into (4c) gives the strong duality constraint (8c).
Thus, every feasible solution of \( \text{GIO}_R(\hat{\mathbf{x}}) \) has a corresponding feasible solution in \( \text{GIO}(\hat{\mathbf{x}}) \) (after
setting the hyperparameters), and vice versa, with the same objective value.

Proof of Corollary 3. Let \((\hat{c}, \hat{y}, \hat{\epsilon}_1, \ldots, \hat{\epsilon}_Q)\) be an optimal solution to \( \text{GIO}_R(\hat{\mathbf{x}}) \). From Propo-
sition 5, this solution can be rescaled to construct a feasible solution for one of \( \text{GIO}^+_R(\hat{\mathbf{x}}) \),
\( \text{GIO}_{R,L,P}(\hat{\mathbf{x}}) \), and \( \text{GIO}^0_{R,L,P}(\hat{\mathbf{x}}) \) with the same objective value. Conversely, for each of the relaxed
problems, let \((\tilde{c}, \tilde{y}, \tilde{\epsilon}_1, \ldots, \tilde{\epsilon}_Q)\) be a feasible solution. Assuming that \( \tilde{c} \neq 0 \), this solution can be
rescaled to construct \((\tilde{c}, \tilde{y}, \tilde{\epsilon}_1, \ldots, \tilde{\epsilon}_Q) = (\tilde{c} / \|\tilde{c}\|_N, \tilde{y} / \|\tilde{c}\|_N, \tilde{\epsilon}_1, \ldots, \tilde{\epsilon}_Q)\), which is a feasible solution
to \( \text{GIO}_R(\hat{\mathbf{x}}) \) with the same objective value. Thus, if the minimum of \( \text{GIO}^+_R(\hat{\mathbf{x}}) \), \( \text{GIO}_{R,L,P}(\hat{\mathbf{x}}) \),
and \( \text{GIO}^0_{R,L,P}(\hat{\mathbf{x}}) \) yields an optimal solution with a non-zero imputed cost vec-
tor, the two problems share the same optimal solution.

Proof of Proposition 6. When all of the observed points are feasible, \( c^T \hat{x}_q - b^T y \geq 0 \), \( \forall q \in Q \).
Thus, objective (8a) becomes \[
\sum_{q=1}^Q |\epsilon_q - 1| = \sum_{q=1}^Q \frac{c^T \hat{x}_q - b^T y}{|b^T y|} = Q \left( \frac{c^T \bar{x} - b^T y}{|b^T y|} \right).
\]
Noting that \( \bar{x} \) must also be feasible, the last term equals the objective for \( \text{GIO}_R(\{\bar{x}\}) \).

Proof of Theorem 4. For each \( i \), the inner optimization problem produces solutions with the
structure in (17). Thus, the inner optimization problems, along with the corresponding \((c, y)\)
enumerate all possible solutions to \( \text{GIO}_p(\hat{\mathbf{x}}) \) with the structure in (17). By Lemma 1 we select
the one yielding the lowest objective value.
Proof of Proposition 9. Using Theorem 4, we bound the optimal value of \( \text{GIO}_p(\hat{X}) \) as follows:

\[
\begin{align*}
\min_{i \in \mathcal{I}} \, \min_{\epsilon_{1,i}, \ldots, \epsilon_{Q,i}} \sum_{q=1}^{Q} \| \epsilon_{q,i} \| \\
\text{s.t. } A(\hat{x}_q - \epsilon_{q,i}) \geq b_i, \forall q \in Q \\
a_i^T(\hat{x}_q - \epsilon_{q,i}) = b_i, \forall q \in Q
\end{align*}
\]

\[
= \min_{i \in \mathcal{I}} \left\{ \sum_{q=1}^{Q} \psi_i(\hat{x}_q) \right\} \geq \min_{i \in \mathcal{I}} \left\{ \sum_{q=1}^{Q} \pi_i(\hat{x}_q) \right\} \quad \text{(EC.3)}
\]

\[
= \min_{i \in \mathcal{I}} \left\{ \sum_{q=1}^{Q} \left( \frac{a_i^T \hat{x}_q - b_i}{\| a_i \|_D} \right) \right\} = \min_{i \in \mathcal{I}} \left\{ \frac{Q}{\| a_i \|_D} \right\} \quad \text{(EC.4)}
\]

where the inequality comes from the fact that the projection problem (2) is a relaxation of the feasible projection problem (16), and the first equality of (EC.4) comes from Theorem 1. \( \square \)

Proof of Corollary 5. If \( \hat{X} \subset \mathcal{P} \), then by Proposition 9 solving \( \text{GIO}_A(\hat{X}) \) is equivalent to solving \( \text{GIO}_A(\{\bar{x}\}) \). By choosing \( p = \infty \) for the decision space problem, (19) has the same structure as an optimal solution to \( \text{GIO}_A(\{\bar{x}\}) \) as prescribed by Theorem 1. \( \square \)

Proof of Theorem 5.

1. Given \( \hat{X} \), \( A \), and \( b \), the denominator term in \( \rho \) is fixed. An optimal solution to \( \text{GIO}(\hat{X}) \) minimizes the numerator of \( 1 - \rho \), thus maximizing \( \rho \).

2. We prove \( 1 - \rho \in [0,1] \). It is easy to see that \( 1 - \rho \geq 0 \), because it is the ratio of sums of norms, which are nonnegative. To show \( 1 - \rho \leq 1 \), note that \( \sum_{q=1}^{Q} \| \epsilon_q^* \| \leq \sum_{q=1}^{Q} \| \epsilon_{q,i} \| \) for all \( i \), as setting \( c = a_i/\| a_i \|_N \) will yield a feasible but not necessarily optimal solution to \( \text{GIO}(\hat{X}) \).

3. An optimal solution to \( \text{GIO}^{(k)}(\hat{X}) \) is feasible for \( \text{GIO}^{(k+1)}(\hat{X}) \), since the latter problem is a relaxation of the former. Invoking the first statement in this theorem, \( \rho^{(k)} \leq \rho^{(k+1)} \). \( \square \)