Inverse Learning: A Data-driven Framework to Infer Optimizations Models

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We consider the problem of inferring optimal solutions and unknown parameters of a partially-known constrained problem using a set of observations or past decisions. We assume that the constraints of the original optimization problem are known while optimal decisions and the objective are to be inferred. The observations are assumed to be solutions (feasible or infeasible) to this partially-known problem. Many real-world decision-making problems can be interpreted in this setting. In such situations, the quality of the optimal solution is evaluated in relation to the existing observations and the known parameters of the constrained problem. Due to the nature of such problems and the presence of many constraints in the decision-making process, a method previously used is inverse optimization. This method can be used to infer the utility functions of a decision-maker and to find the optimal solutions based on these inferred parameters indirectly. However, little effort has been made to generalize the inverse optimization methodology to data-driven settings. Additionally, minor attention has been given to the quality of the inferred optimal solutions based on the results of such methods. In this work, We present a data-driven inverse linear optimization framework (Inverse Learning) that aims to infer the optimal solution to an optimization problem directly based on the observed data and the existing known parameters of the problem alongside with inferring the unknown parameters of the problem. We utilize a series of simplified linearly-constrained models and show that our model provides optimal solutions that retain the characteristics of the observed data. We validate our model on a dataset in the diet recommendation problem setting to find personalized diets for prediabetic patients with hypertension. Our results show that our model obtains optimal personalized daily food intakes that preserve the original data trends while providing a range of options to patients and providers. The results show that our proposed model is able to both capture optimal solutions with minimal perturbation from the given observations and, at the same time, achieve the inherent objectives of the original problem. We show an inherent trade-off in the quality of the inferred solutions with different metrics and provide insights into how a range of optimal solutions can be inferred in constrained environments.

Key words: data-driven decision making, inverse optimization, diet recommendation problem, linear optimization, learning

1. Introduction

Optimization models are used in solving many real-world problems. The parameters and criteria surrounding the models are often derived from expert opinions or known facts, resulting in models that often adhere to a one-size-fits-all format. Such general models exist in many applied settings,
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from diet recommendations to radiation therapy planning to energy and service industry models. While some tailoring and personalization may exist in such settings, often, optimization problems are written generally and not individually for each user interested in employing the model. Therefore, the results of such models are not satisfactory in specific settings, and expert opinion still drives the actual decisions. In this work, we introduce a data-driven approach (referred to as Inverse Learning) that uses such existing decisions made by experts to infer the utility functions along with optimal decisions in a constrained setting, hence, personalizing the resulting obtained optimization problem to every user based on their existing data and implicit goals and criteria.

While there have been tremendous advances in data-driven inference models in general, many such models mainly apply to settings where the problem is not constrained. In such settings, practical machine learning and statistical models are readily available that can be used to infer meaningful results. Such methods are generally powerful in inference settings that contain only points of observations and possibly their respective labels. However, the same cannot be said about the application of machine learning models in constrained settings. These models often fail to grasp the important role of constraints and known parameters of the original problem in the inference process.

One inference method that is capable of considering high constraint environments in the learning process is Inverse Optimization. Inverse optimization is used to infer the parameters of a (forward) optimization problem based on observed data points (solutions) and has been studied in different settings. The use of this method can be traced back to the work of Burton and Toint (1992) who considered the inverse shortest path problem and discussed inverse combinatorial problems. Inverse settings of combinatorial and general linear optimization problems have since gained more attention (Yang and Zhang 1999, Zhang and Liu 1996, 1999, Zhang and Ma 1999). Heuberger (2004) provided a survey on inverse combinatorial problems and the existing methods when approaching such problems. Ahuja and Orlin (2001) were the first to use the term “Inverse Optimization” and pose it as a general problem in linear programming. A common setting in inverse optimization is to infer the utility function and implicit preferences of a decision-maker in a highly constrained environment by recovering the cost vector of a forward optimization problem (Aswani et al. 2018, Esfahani et al. 2018) and using the inferred parameters to find optimal solutions to the original problem. The majority of the literature on inverse optimization methods considers a single optimal (Ahuja and Orlin 2001, Iyengar and Kang 2005) or near-optimal observation as the sole observed data point (Chan et al. 2018, Zhang and Xu 2010, Schaefer 2009, Wang 2009, Keshavarz et al. 2011, Ghate 2020, Lasserre 2013, Naghavi et al. 2019, Roland et al. 2013, Bertsimas et al. 2015). In such cases, the prevalent approach is to infer the unknown parameters according to some predefined metric (such as distance to the observed data point). In practice, however, a collection of
past decisions can be observed either from similar but differently constrained problems (Černý and Hladík 2016) or from one constrained forward optimization problem (Shahmoradi and Lee 2019, Babier et al. 2018b).

In general, inverse Optimization methodologies have received increasing attention in applied settings. Some applied settings of inverse optimization methodologies include finance (Bertsimas et al. 2012), network and telecommunication problems (Faragó et al. 2003), supply chain planning (Pibernik et al. 2011), transportation problems (Chow and Recker 2012) and auction mechanisms (Beil and Wein 2003). Bärmann et al. (2018) consider a setting where the decision-maker decides on the variables in different application domains and provide an online-learning framework for inverse optimization. Konstantakopoulos et al. (2017) combine inverse optimization and game theory methods to learn the utility of agents in a non-cooperative game. There has also been a growing interest in the applications of inverse optimization methods in healthcare settings like cancer treatment (Corletto et al. 2003, Chan et al. 2014), patient care delivery systems (Chan et al. 2019) and the diet recommendation problem (Ghobadi et al. 2018, Shahmoradi and Lee 2019, Aswani et al. 2019). Applications in healthcare settings stem from inverse optimization’s unique ability to infer unknown parameters in multi-objective and highly constrained settings (Babier et al. 2018a, Chan and Lee 2018, Gorissen et al. 2013).

Because of their potential applicability in real-world problems, multi-observation settings in inverse optimization have received some attention over recent years (Babier et al. 2018b, Esfahani et al. 2018, Aswani et al. 2018, Tan et al. 2019, Hewitt and Frejinger 2020). For instance, in the case of a decision-maker’s utility function, multiple instances of the final choices might be available through past behavior and historical data. Ghobadi and Mahmoudzadeh (2020), Chan and Kaw (2020), Schede et al. (2019) consider the problem of recovering the feasibility set parameters (constraints) as opposed to utility parameters. Recently, studies have also considered the settings where there exists a stream of observations as input of the inverse optimization model, as opposed to an existing batch of observations. Dong et al. (2018), Tan et al. (2019) consider a new approach to formulating the inverse optimization problem in data-driven settings as a form of deep learning model. Aswani et al. (2018) characterized the existing models for data-driven inverse optimization and pointed out that the existing heuristics methods fail to produce reasonable solutions. They provide other heuristics in the general inverse optimization setting that they show are “statically consistent”. Statistical approaches in noisy settings for inferring parameters of an optimization problem are also explored (Aswani 2019, Shahmoradi and Lee 2019).

Additionally, due to the diverse applications of optimization problems, some studies have considered methods to either learn the parameters or objectives of optimization problems (Lombardi et al. 2017, Hewitt and Frejinger 2020, Pawlak and Krawiec 2017, Kolb et al. 2018) or completely
replace them using statistical learning or machine learning methods (Jabbari et al. 2016). For instance, Hewitt and Frejinger (2020) provide a supervised learning method to map the optimal solutions of optimization models to observed decisions and add constraints using the results of the mapping to the original optimization problem in order to provide better optimal solutions. However, such approaches are not able to balance the effects of the observations and the parameters of the problem in the inference process and tend to infer solution solely or mainly based on the existing observations (as is the usual practice in machine learning approaches).

In a more specific domain, some studies have concentrated on the inverse linear optimization setting rather than the general literature of the inverse optimization problem because of the potential applicability of such models (Ahuja and Orlin 2001, Chan et al. 2018, Shahmoradi and Lee 2019). As pointed out in the existing literature, inverse problems aim to “find a cost vector that can generate an optimal solution that is closest to the observations” (Shahmoradi and Lee 2019). Distance as a metric in inferring optimal solutions to the forward problem has been considered in many of the existing models in inverse optimization literature. However, the prevalent approach in inverse linear programming is to infer the unknown cost vector based on the distance metric first and then introduce it to the original optimization problem and solve it to find optimal solutions without considering the initial observations in the optimization process. In this scenario, a usual result is that the inferred cost vectors of the models are usually orthogonal to one of the constraints and the optimal forward solution space has a dimension greater than or equal to one. In this case, solving the forward optimization problem with the inferred cost vector is not guaranteed to find the closest point to the observations, even if such a point exists in the optimal solution set corresponding to the inferred cost vector. In these cases, the existing models fail to provide an optimal solution that preserves the characteristics of the observations.

In this study, we develop a modified methodology that is flexible in its ability to infer optimal solutions to constrained linear optimization problems based on a given set of solutions and problem parameters. To the best of our knowledge, no previous study has considered non-extreme points as potential optimal solutions in the inverse linear setting. Additionally, unlike many works in the literature, we do not assume any previous knowledge of the characteristics of the given observations. We provide a modified inverse linear optimization methodology that finds the closest point to all the observation contained in the space of all potential optimal solutions. We show that such a point can be found by solving a series of linearly-constrained problems. We also provide insights into an important inherent trade-off in the inference of solutions in constrained settings regarding the observations and the known parameters of the original problem.

In order to test the model in an applied setting, we consider the dietary behavior of individuals diagnosed with hypertension who are at risk of developing type II diabetes. It is known that diet plays
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a vital role for these patients to control their condition. A typical diet that clinicians recommend for such patients is the Dietary Approaches to Stop Hypertension (DASH) diet (Sacks et al. 2001, Liese et al. 2009), which aims to control sodium intake and lower blood pressure (a known risk factor of diabetes). These patients are typically given guidelines about the DASH diet; however, these guidelines are rarely personalized or tailored to individual patients’ tastes and lifestyles. Therefore, many patients find long-term adherence to these diets challenging. To increase the likelihood of adherence, we utilize our framework to personalize the DASH diet for hypertension patients by considering their past food choices. We first formulate a forward optimization problem with the DASH diet’s nutritional constraints that maximize palatability of the recommended diet. Next, we utilize the inverse learning framework to infer the palatability cost function based on multiple observations of a patient’s daily food intake and provide optimal daily food intakes.

The main contributions of this paper can be summarized as follows:

1. We propose a new data-driven framework for inverse optimization of utility functions and learning optimal solutions based on the existing knowledge of past observations and parameters of the original problem.

2. We indicate an inherent trade-off in the quality of inferred optimal solutions in constrained environments with relation to the observations and the known parameters of the original problem and provide a decision support tool to address this trade-off.

3. We introduce a new model that provides a greater degree of flexibility by inferring a range of solutions from the observations to the preferred optimal solutions.

4. We provide a real-world application to the framework with the diet recommendation setting and demonstrate that our model can provide multiple daily meals, each with particular desirable attributes that prolong adherence to the diets.

The rest of the paper is organized as follows. In Section 2, we motivate the problem via the diet recommendation problem. In section 3, we formulate a new linear programming problem with two sets of constraints and introduce a new framework for optimizing the unknown utility parameters and optimal solution of the linear programming together. Section 5 illustrates comparisons of the new framework with existing data-driven inverse linear optimization models. In Section 6, we test our framework in the diet recommendation problem. Concluding remarks are provided in Section 7.

2. Motivation: The Diet Recommendation Problem

Inverse optimization methodologies have been applied to many application areas, ranging from healthcare (Ayer 2015) to finance (Bertsimas et al. 2012) and diet (Gobadi et al. 2018). In this work, we consider one of the widely studied applied problems in optimization and motivate how the proposed methodology of this paper can be used in this problem. Specifically, we consider the
diet behavior of individuals with hypertension who are at the risk of developing type II diabetes. Roughly one out of every two adults in the United States have hypertension or high blood pressure. Hypertension has adverse health effects and can be a cause of heart disease and strokes. For such patients, diet plays a vital role in delaying or avoiding diabetes. Many clinicians recommend the Dietary Approaches to Stop Hypertension (DASH) [Sacks et al., 2001] that aims to decrease sodium intake and control blood pressure. DASH has been shown to lower both systolic and diastolic blood pressure in individuals [Sacks et al., 2001]. DASH aims to reduce and control the amount of daily sodium intake of individuals diagnosed or at risk of hypertension. With that said, patients typically perceive diet as a short-term commitment or aim for high goals that may not be maintainable in the long-term. To increase the likelihood of adherence to the diet, in this work, we consider the palatability of each dish for the patient. To this end, we assume an optimization model that maximizes palatability (or adherence) for given diets while ensuring the DASH diet constraints are satisfied. We observe the patient’s dish choices while on the diet for days. Based on these observations, we infer the preferences of the patients using inverse optimization.

In the optimization community, the diet recommendation problem was first posed by Stigler (1945) as finding an optimal set of intakes of different foods with minimum cost while satisfying minimum nutrient conditions for an average person [Stigler, 1945, Garille and Gass, 2001]. Since then, many studies have focused on finding optimal diets for individuals and communities based on the models provided by Stigler (1945), Sacks et al. (2001), Bas (2014). Much of the previous literature has focused on providing more realistic constraints and relaxing previous simplifying assumptions (linear relationship between the nutrients and foods and varying effects of different combinations of foods [Bas, 2014]) of the original diet problem. In many of the approaches in the literature, as much as there has been attention to achieving palatable diets for the individual, there is little success in providing general methods that are both flexible and result in diets with high preferences. When optimizing for diets, palatability, and similarity of the diet to the individual’s original eating habits are essential in ensuring prolonged adherence to the diet. Many of the existing methods in the literature rely on defining realistic constraints in hopes of achieving more palatable diets [Ferguson et al., 2006, Xu et al., 2018]. Without direct considerations of the original diets, many inferred diets, while rich in target nutrients, are not similar to the original preferences of the individual, which results in difficulty in prolonged adherence to the proposed diet. Therefore, direct consideration of the actual diet of the individual or the trend diet of the community is of substantial importance when considering the diet problem.

As it will be shown in the results of this paper, there is no single optimal diet for any given set of actual diets. As Gedrich et al. (1999) pointed out, “an ‘optimal diet’ does not necessarily meet all the nutrient requirements of a person.” This indicates the delicate role of the parameters and
constraints of the diet problem as well as the objective of the problem in determining the optimal diet along with the patient’s original diet behaviors. As Stigler (1945) pointed out, considering the monetary costs of the foods as the objective function and minimizing the cost will probably result in diets that, even if they satisfy the nutrient needs of the individual, will be very basic and probably not palatable. Ghobadi et al. (2018) considered the costs of foods as equivalent notions of personalized preferences of the individual to each food. In this sense, by maximization, it can be argued that the preferences of the individual are being maximized. Providing an approach that can efficiently and accurately give a notion of such a cost vector is a challenge that can be tackled using inverse optimization methodologies.

3. Inverse Optimization Methodology

In this section, we provide a modified inverse optimization framework concentrated on inferring the unknown parameters of an optimization problem. We first establish a general forward linear optimization problem in Section 3.1 and then introduce models for single- and multi-observation inverse optimization problems aimed to infer unknown parameters and the optimal solution of the defined forward linear optimization problem in Sections 3.2 and 3.3. Next, we present a solution algorithm to the inverse optimization models in Section 3.4. We discuss how such an algorithm provides important characteristics of inverse solutions that we will use to develop the inverse learning models in later sections. We also highlight the differences between our the proposed model and algorithm with the literature.

3.1. Preliminaries

We first define the forward optimization problem and its dual form and provide necessary notations in developing subsequent models. Contrary to the conventional literature, we consider two distinct sets of constraints in developing the forward optimization (FO) formulation; (i) A non-empty set of constraints which are considered important and desired by the decision-maker referred to as relevant constraints and (ii) a set of constraints (if any) which although are needed for the construction of the forward problem, the decision-maker is indifferent about whether these constraints are tight at optimality. These constraints can include constraints that ensure the problems are well defined. We denote such constraints as trivial constraints. The distinction between relevant and trivial constraints is motivated by applied settings in which not all constraints have the same significance in the inference of optimal solutions. The distinction ensures that meaningful forward optimal solutions are later inferred. Also, if all constraints are equally important or there is no knowledge on the significance of the constraints, they can all be assumed as relevant constraints, and the set of trivial constraints is then assumed to be empty. Therefore, this distinction provides a more general model
of the optimization problem. Let $c \in \mathbb{R}^n$, $A \in \mathbb{R}^{m_1 \times n}$, $b \in \mathbb{R}^{m_1}$, $(m_1 \geq 1)$, $W \in \mathbb{R}^{m_2 \times n}$, and $q \in \mathbb{R}^{m_2}$. We define the forward linear optimization problem (FO) as follows:

$$\text{FO}(c) : \begin{array}{ll}
\text{maximize} & c'x \\
\text{subject to} & Ax \geq b, \\
& Wx \geq q, \\
& x \in \mathbb{R}^n.
\end{array} \tag{1a-1d}$$

The inequality (1b) represents the set of relevant constraints that the decision-maker is interested in and (1c) is the set of other constraints that we previously defined as trivial constraints. The objective function (1a) is the unknown cost function that is to be inferred. We assume that a set of observations of FO solutions, $x^k \in \mathbb{R}^n$, $k \in \{0, \ldots, K\}$ is given for FO. If only a single observation is given, we denote it by $x^0$. We also assume that the feasible region of FO, denoted by $\chi$, is nonempty, full dimensional, and free of redundant constraints. Given that the objective parameter $c$ is the only unknown parameter of FO, we denote $\chi^{opt}(c)$ as the set of optimal solutions to FO for cost vector $c$, and $\chi^{opt} := \bigcup_{c \neq 0} \chi^{opt}(c)$ assumed to be non-empty. Any feasible solution $x$ for FO is denoted as a feasible learning solution if it is contained in $\chi^{opt}$. For ease of notation, let $J_1 = \{1, \ldots, m_1\}$, $J_2 = \{1, \ldots, m_2\}$, $K = \{1, \ldots, K\}$ be the set of indices of relevant constraints, trivial constraints, and the observations, respectively. Since the inverse optimization models will be defined based on optimality conditions of the forward problem using duality theorems, we also formulate the dual problem of FO here as follows:

$$\text{DFO} : \begin{array}{ll}
\text{minimize} & y'b + u'q, \\
\text{subject to} & A'y + W'u = c, \\
& y \geq 0, u \geq 0.
\end{array} \tag{2a-2c}$$

In the above formulation, $y$ is the vector of dual variables associated with the relevant constraints, and $u$ is the vector of dual variables associated with the trivial constraints. The following remark connects the optimality conditions of a proposed solution of FO to the notion of a feasible learning point.

**Remark 1.** A feasible solution for $\text{FO}(c)$ is contained in $\chi^{opt}$ if and only if there exists a primal-dual feasible pair $(x, (y, u))$ for $\text{FO}(c)$ and $\text{DFO}$ such that $c'x = y'b + u'q$ and $c \neq 0$.

In the next sections, upon formulating the inverse optimization models, we concentrate on inferring FO and its unknown parameters along with optimal solutions for FO considering the above
discussions on the characteristics of the forward solutions. In what follows, a single-observation inverse optimization model to recover $c$ in $FO$, as is common in the inverse optimization literature, will be developed based on the given definitions for the forward optimization problem. We distinguish our single observations inverse optimization model from the literature by pointing out how the distinction of constraints can be incorporated into an inverse optimization scheme. We then extend this formulation to a multi-observation setting, which is more prevalent in practice, where multiple solutions of $FO$ are observed. We define the multi observation inverse optimization model in a way that can infer an optimal solution to $FO$ intelligently and simultaneously with the unknown utility parameter. Since the inverse optimization models are nonlinear and, in some contexts, non-convex (similar to other models in the inverse optimization literature), we next introduce an equivalent simplified linearly-constrained reformulation, which can be employed to solve the original nonlinear non-convex inverse optimization problems.

3.2. Single-Observation Inverse Optimization

In this section, we formulate a single observation inverse optimization model based on the forward optimization problem introduced in Section 3.1. We point out that the aim of an inverse optimization model should be to infer unknown parameters of $FO$ such that they result in an optimal solution to $FO$ that is a feasible learning point, which is minimally perturbed from the observations. Let $x^0 \in \mathbb{R}^n$ be a single observation, which is assumed to be a $FO$ solution. This observation can be feasible or infeasible to the given (known) feasible region of the $FO$. We define the following single-observation optimization ($SIO$) model by minimally perturbing $x^0$ so that it becomes optimal for $c$.

$$
\text{SIO}(x^0) : \text{minimize } \mathcal{D}(\epsilon, A) \quad (3a)
$$

subject to

$$
A(x^0 - \epsilon) \geq b, \quad (3b)
$$

$$
W(x^0 - \epsilon) \geq q, \quad (3c)
$$

$$
c'(x^0 - \epsilon) = b'y, \quad (3d)
$$

$$
A'y = c, \quad (3e)
$$

$$
\|c\|_L = 1, \quad (3f)
$$

$$
y \geq 0 \quad u = 0, \quad (3g)
$$

$$
c, \epsilon \in \mathbb{R}^n, y \in \mathbb{R}^{m_1}, u \in \mathbb{R}^{m_2}, \quad (3h)
$$

where constraints (3b) and (3c) enforce primal feasibility of the perturbed point $x^0 - \epsilon$. Constraints (3e) and (3g) are dual feasibility constraints and constraint (3d) is the strong duality constraint.
which makes the perturbed point an optimal forward solution for $\text{FO}(\mathbf{c})$. The vector $\mathbf{y} \in \mathbb{R}^{m_1}$ are dual variables corresponding to constraints $[3b]$ and $\epsilon \in \mathbb{R}^n$ is the vector of perturbation of the observed solution. Constraint $[3f]$ is a normalization constraint on the unknown parameter which avoids trivial and undesired solutions such as $\mathbf{c} = \mathbf{0}$. We point out that this non-convex constraint can be replaced by the linear constraint $\sum_{j \in J_1} y_j = 1$ if there is no any redundant constraints and/or equality constraints in the feasible set of $\text{FO}$. However, in order to keep the formulations more general, we keep constraint $[3f]$ in the model. The objective function, $D \geq 0$, is a distance measure of choice on the perturbation vector $\epsilon$ and the relevant constraint matrix $\mathbf{A}$. The following proposition establishes that the $\text{SIO}$ formulation is well-defined, and its feasible region is nonempty.

**Proposition 1.** $\text{Formulation SIO is feasible.}$

**Proof of Proposition 1.** To show the feasibility of $\text{SIO}$, we show that it has at least one feasible solution. Since the constraints of $\text{FO}$ are all non-redundant, we know that for each constraint of $\text{FO}$ there exists an $\text{FO}$ feasible point for which the constraint is tight. Let $\mathbf{a}_j$ be the $j^{\text{th}}$ row of $\mathbf{A}$ (such $j$ certainly exists since the set of acceptable constraints is nonempty), and $\mathbf{e}_j$ be the $j^{\text{th}}$ unit vector; By above, there exists an $\text{FO}$ feasible point $\hat{\mathbf{x}}$ for which the equality $\mathbf{a}_j \hat{\mathbf{x}} = b_j$ holds. Defining $\mathbf{c}_0 = \frac{\mathbf{a}_j}{||\mathbf{a}_j||_L}$, $\mathbf{y}_0 = \frac{\mathbf{e}_j}{||\mathbf{a}_j||_L}$ and $\epsilon_0 = \mathbf{x}^0 - \hat{\mathbf{x}}$, the solution $(\mathbf{c}_0, \mathbf{y}_0, \epsilon_0)$ is feasible for $\text{SIO}$ since all constraints $[3b]$–$[3h]$ are satisfied; $[3b]$ and $[3c]$ hold by the feasibility of $\hat{\mathbf{x}}$, $[3d]$ is satisfied by the assumption $\mathbf{a}_j \hat{\mathbf{x}} = b_j$ holding and the definition of $\mathbf{c}_0$ and $\mathbf{y}_0$, and $[3e]$ to $[3h]$ are directly the results of the definition of the parameters. \(\square\)

The $\text{SIO}$ model is similar to some models from the literature of inverse linear optimization in inferring the $\text{FO}$ formulation by finding the optimal cost vector $\mathbf{c}^*$; however, it has a number of additional benefits. First, dual variables are only introduced in the inverse problem for relevant constraints, and therefore, the inferred utility parameter is a conic combination of the rows of the left-hand side matrix of forward problem constraints corresponding to the relevant constraints. By making this adjustment, we make sure that trivial constraints, which are generally of little interest to the decision-maker, do not influence the inferred parameters. Second, the $\text{SIO}$ formulation is capable of inferring the optimal solution of $\text{FO}$ too. In particular, if $(\mathbf{c}^*, \mathbf{y}^*, \mathbf{u}^*, \epsilon^*)$ is an optimal set of solutions for $\text{SIO}$, then the point $\mathbf{x}^* = (\mathbf{x}^0 - \epsilon^*)$ is an optimal solution to $\text{FO}(\mathbf{c}^*)$ and is contained in $\chi_{opt}(\mathbf{c}^*)$. Additionally, the optimal solution $\mathbf{x}^*$ found by $\text{SIO}$ is (by the design of $\text{SIO}$) the closest point contained in $\chi_{opt}(\mathbf{c}^*)$ to $\mathbf{x}^0$ based on the objective metric. This is important since solving the $\text{FO}$ problem does not always find the closest optimal point to the observed solution due to the possible existence of multiple optimal solutions, a prevalent phenomenon in inverse optimization.

As stated in Proposition 1, the $\text{SIO}$ formulation is well-defined and finds the unknown utility parameter $\mathbf{c}$. However, inferring the utility function based on only a single observation is not ideal
and in practice, often several solutions to \( \text{FO} \) are available, e.g., based on expert decision-making or observing user’s behavior. Additionally, considering each point individually and solving \( \text{SIO} \) for each point requires immense additional computation time and usually results in conflicting results since the trends in the observations, if any, are not captured in this way. Hence, we extend our formulation to a multi-observation setting. Unlike existing models in the literature, our multi-observation inverse optimization not only recovers the unknown utility function \( c \) but it readily provides an optimal solution to the \( \text{FO} \) model as well, without requiring to solve \( \text{FO} \) separately. In what follows, we discuss the multi-observation inverse optimization model and its properties.

3.3. Multi-Observation Inverse Optimization

Let \( X = \{x^k \in \mathbb{R}^n : k \in K\} \) be a set of given observations. These observations (solutions to the \( \text{FO} \) model) may be feasible or infeasible for the given feasible region of \( \text{FO} \). We assume the observations are not random but solutions and/or previous decisions provided by an expert or user where they were trying to optimize based on some unknown or partially known utility function. Hence, an underlying assumption is that the observations carry implicit information about the optimal utility function. This assumption is not necessary for the formulation but provides more meaningful answers when it holds. We formulate the multi-observation inverse optimization (\( \text{IO} \)) as follows:

\[
\text{IO}(X) : \begin{align*}
\text{minimize} & \quad D(E, A) \\
\text{subject to} & \quad Az \geq b, \\
& \quad Wz \geq q, \\
& \quad c'z = b'y, \\
& \quad z = (x^k - \epsilon^k), \quad \forall k \in K \\
& \quad c, z \in \mathbb{R}^n, \quad y \in \mathbb{R}^{m_1}, \quad E \in \mathbb{R}^{n \times K}.
\end{align*}
\]

The constraint (4e) projects all the observations to a single point \( z \) contained in \( \chi^{opt} \). The constraints (4b), (4c), and (4d) ensure forward feasibility and strong duality holds for this projected point, respectively. The dual feasibility constraints and the normalization constraints are the same as the \( \text{SIO} \) model. The objective function, \( D \geq 0 \), is again a distance measure of choice on the perturbation matrix \( E \) and the relevant constraint matrix \( A \), where the \( k^{th} \) column of \( E \) is defined as \( \epsilon^k \). Examples of such distance measures include the sum of distances to all the observations \( D(E, A) = \sum_{k=1}^{K} \| \epsilon^k \|_1 \) which finds the projected point by minimizing the total perturbation of all the observations or the maximum distance to the observations \( D(E, A) = \max \{ \| \epsilon^k \|_1 : k \in K \} \) to make the resulting point more homogeneously distanced from the observations. Similar to \( \text{SIO} \), in Proposition 2 we show that our \( \text{IO} \) formulation is well-defined and has a non-empty feasible region.
Proposition 2. The IO model is feasible.

Proof of Proposition 2. Let $a_j$ be the $j$th row of $A$ and $e_j$ be the $j$th unit vector (the set of acceptable constraints is nonempty). By above, there exists an FO feasible point $\hat{x}$ for which the equality $a_j\hat{x} = b_j$ holds. Defining $c_0 = \frac{a_j}{\|a_j\|_L}$, $y_0 = \frac{e_j}{\|a_j\|_L}$, $z_0 = \hat{x}$ and $e^k = x^k - \hat{x}$, for all $k \in K$, the solution $(c_0, y_0, z_0, \{e_0^1, \ldots, e_0^K\})$ is feasible for IO since: (4b) and (4c) hold by the feasibility of $\hat{x}$, (4d) holds by the assumption $a_j\hat{x} = b_j$ and the definition of $c_0$ and $y_0$, and (4e) to (4f) are directly the results of the definition of the parameters. □

The IO model finds a single point $z$ contained in $\chi^{\text{opt}}$ which has the minimum sum of perturbations from all the observations based on the user-defined distance measure $D$. Since IO ensures forward feasibility and also strong duality conditions for all $z$ based on relevant constraints, for any feasible solution $z$ for IO, at least one of the relevant constraints will be binding. Therefore, for any feasible point $z$ of IO, there exists a vector orthogonal to one of the constraints which makes that point optimal for FO if that vector is used as the cost vector of FO. We formalize this property in Remark

Remark 2. Let $\chi$ be the feasible region of FO, then for any IO solution $(c, y, E, z)$, there exists a face of $\chi$, $F = \{x \in \chi: a_jx = b_j, j \in J\}$ for some $J \subseteq J_1$ such that $z \in F$.

Remark 2 points out that each feasible solution to IO corresponds to a point on a specifically defined face of $\chi$. This characterization motivates Proposition 3 which provides an structured optimal solution for IO.

Proposition 3. There is an optimal solution $(c, y, E, z)$ for IO where $c$ is orthogonal to at least one of the relevant constraints of FO.

Proof of Proposition 3. Since the objective of IO is the minimization of a non-negative distance function, the feasibility of IO asserts the existence of an optimal solution. Let $(c^*, y^*, E^*, z^*)$ be an optimal solution to IO. From constraint (3i), we have $y^* \neq 0$. Constraints (3e) and (4d) yield complementary slackness conditions for $z^*$. Let $j$ be such that $y_j > 0$, then we should have $a_jz^* = b_j$. Therefore, $z^*$ is contained on the boundary of $j$th relevant constraint. Let $c^0 = \frac{a_j}{\|a_j\|_L}$, $y^0 = \frac{e_j}{\|a_j\|_L}$, $E^0 = E^*$, $z^0 = z^*$. This solution is also a feasible solution for IO and since it has the same objective value, it is an optimal solution for IO. □

The IO formulation can be solved to optimality to infer the $c$ vector. However, the non-linearity and non-convexity exist in constraints (4d) and (3i) makes the problem hard to solve. We point out that if the relevant constraints are all non-redundant and there is no equality constraints among them, then the normalization constraint (3i) can be replaced by the linear constraint $\sum_{j \in J_1} y_j = 1$. Nevertheless, in the most general form, IO is a non-convex quadratic optimization problem.
However, Proposition 3 provides a way of finding feasible solutions to IO by choosing a cost vector orthogonal to each of the relevant constraints and solving the FO with that vector replaced for \( c \); the resulting optimal point of FO along with the cost vector are feasible solutions for IO. This orthogonality of the objective function and constraints often leads to the FO having multiple optimal solutions and hence, randomly returning one of the extreme points on the constraint (or any other point on this constraint if an interior-point like method is used). Therefore, the returned solution of FO might be far from the observations which is the case of some of the existing models in the literature. However, as mentioned earlier, we have formulated IO in a way that finds an inverse optimal utility parameter and the best forward optimal point for that utility parameter together. Therefore, we can combine the two alternatives mentioned above to find inverse and forward optimal solutions. In the next section, we present a new framework as an alternative to solving the inverse optimization.

3.4. Algorithmic Solution of IO

The IO model introduced above has the unique capability that it finds a forward optimal solution which binds at least one of the relevant constraints initially introduced in the original FO. Based on Proposition 3, there is always an optimal solution to IO with a cost vector \( c \) orthogonal to one of the relevant constraints. As a result, it is possible to find an optimal solution using such vectors as input to the problem. Consider the following formulation which is a linearly constrained version of IO by letting \( c = \frac{a_j}{\|a_j\|_L} \) and \( y = \frac{e_j}{\|a_j\|_L} \) for some \( j \in J_1 \):

\[
\text{BIL}_j(X) : \begin{align*}
\text{minimize} & \quad D(E, A) \\
\text{subject to} & \quad a_j z_j = b_j, \\
& \quad A z_j \geq b, \\
& \quad W z_j \geq q, \\
& \quad z_j = (x^k - e^k_j). \quad \forall k \in K
\end{align*}
\]

Formulation \( \text{BIL}_j \) finds the closest forward feasible point on the boundary of the \( j \)th relevant constraint and is denoted as the Base Inverse Learning formulation or \( \text{BIL}_j \) as it will be used in the next section to develop the main Inverse Learning model. Note that Constraints (3e), (3f) and (3g) are already satisfied with this choice and are no longer needed in this formulation. In other words, by this choice of variables, we can eliminate the non-linear and non-convex constraints and make the problem linearly constrained as opposed to IO. The optimal solution of this problem is a projected point onto the feasible section of the hyperplane \( a_j x = b_j \) with the minimum sum of distances to all the observations. We can solve the above linearly constrained problem for all the non-redundant
relevant constraints of the forward problem. This will result in at most \( m_1 \) different projected points contained in \( \chi^{opt} \). Each such projected point will have the interesting characteristic of binding at least one of the relevant constraints. Since the minimum of the general \( D(E, A) \) metric is desirable in the context of the problem, Algorithm 1 can be used to find the projection on at least one of the relevant constraints with the minimum value with respect to the metric defined in the objective of BIL to all the observations. Obviously, under the 1-norm or \( \infty \)-norm, the above problem can be reduced to a linear programming.

**Algorithm 1** Finding the closest Point on \( \chi^{opt} \) to all the observations with metric \( D \)

```plaintext
for \( j \in \{1, \ldots, m_1\} \) do
  Solve BIL\(_j\)
  if \( j = 1 \) then
    \( D^{opt}_{\text{opt}} = D_{\text{opt}}^{j} \)
    \( j_{\text{opt}} = j \)
  else if \( D_{\text{opt}}^{j} < D^{opt}_{\text{opt}} \) then
    \( D^{opt}_{\text{opt}} = D_{\text{opt}}^{j} \)
    \( j_{\text{opt}} = j \)
  end if
end for
```

**Theorem 1.** Let \((c^*, y^*, E^*, z^*)\) be an optimal solution to IO with the objective value of \( D^* \) and \( D^{opt}_{\text{opt}} \) and \( j_{\text{opt}} = j \) and \( z_{\text{opt}} \) be the results of Algorithm 1. Then, \( D^* = D^{opt}_{\text{opt}} \).

**Proof of Theorem 1.** From previous results, at least one relevant constraint is tight at \( z^* \). We denote this constraint as constraint \( j \). As a result, we have \( a_j z^* = b_j \) which is exactly (5b). (5e) is also easily seen to hold for \( z^* \). Therefore, \( z^* \) is feasible for BIL\(_j\). Now, assume to the contrary that Algorithm 1 returns an optimal solution \( D_{\text{opt}}^{\text{opt}}, j_{\text{opt}} \) and \( z_{\text{opt}} \) with \( D_{\text{opt}}^{\text{opt}} < D^* \). Let \( y^0 = \frac{\epsilon_{\text{opt}}}{\| a_{\text{opt}} \|_L} \) and \( c^0 = \frac{a_{\text{opt}}}{\| a_{\text{opt}} \|_L} \). It can be easily checked that \((c^0, y^0, E_{\text{opt}}, z_{\text{opt}})\) is also feasible for IO. This is a contradiction to \((c^*, y^*, E^*, z^*)\) being optimal for IO. \( \square \)

As discussed above, Algorithm 1 finds the closest point contained on \( \chi^{opt} \) to a set of given observation points with respect to a defined metric. However, inference in the setting of constrained environments includes a trade-off between the observed decision and the constraints of the forward problem. The resulting forward optimal solution of 1, although being the closest possible to all the observations (if the metric is the distance to the observations), usually does not make a large number of the forward problem’s relevant constraints active. While this might be desirable in some settings,
in some decision making environments, it might be more desirable to bind more constrains at optimality. For instance, in the diet recommendation problem, which is discussed in the application section, it might be more desirable to take into account and bind more than one nutritional constraint at optimality to provide diets that are rich in a higher number of nutrients. In other words, the true cost vector might not be contained in the cone of all the active relevant constraints at $z_{opt}$. If this is the case, then by arguments similar to the steps of the simplex algorithm, it is possible to improve $z_{opt}$ based on such a cost vector. However, this can be achieved at the cost of moving further away from the observations. This trade-off calls for a method that is flexible in providing a range of potential forward optimal solutions that represent different characteristics in terms of the number of binding relevant constraints and their objective value. In the next section, we introduce a general Inverse Learning model that is flexible with regard to this important trade-off in constrained problems. Then, we show how the inverse learning methodology can be used to improve the solution found above with regard to the relevant constraints.

4. Inverse Learning Methodology

In the previous sections, we developed a modified inverse optimization model that is capable of inferring the forward optimization problem with its optimal solution in the presence of a set of observations. In this section, we generalize the models and introduce the inverse learning model which provides added flexibility and more control over pre-known information regarding both the observations and parameters of the forward linear optimization problem. We further discuss how the results of our methodology can be employed to interpret the underlying preferences of the decision-maker and infer the unknown utility parameters of the forward problem in Section 4.3.

As discussed in the previous sections, IO and Algorithm 1 find a point contained in $\chi_{opt}$ with at least one tight relevant constraint with the minimum objective metric with respect to all the observations. However, this inferred solution usually binds only a few relevant constraints, which indicates that the resulting forward optimal solution can be possibly improved in the direction of some of the relevant constrains. Additionally, binding a few relevant constrains might not be preferable depending on the application context. In order to address these issues, we provide a model that is flexible in choosing the number of binding relevant constraints in the inferred optimal solution and which provides a projection point with minimum objective value with respect to the observations which binds more relevant constraints. Here, we develop a model based on the assumption that the decision-maker is interested in binding a certain number of relevant constraints. Obviously, depending on the specific application setting, the user can consider the maximum or minimum number of binding relevant constraints to arrive at the appropriate decision. We propose
the following mixed integer linear programming formulation to find the decision point contained in $\chi^{opt}$ that binds a certain number of relevant constraints with minimum objective value:

\[
\text{IL}(X, p) : \text{minimize} \quad D(E, A) \quad (6a)
\]

subject to

\[
b \leq A z \leq b + M (1 - v) \quad (6b)
\]

\[
W z \geq q, \quad (6c)
\]

\[
z = (x^k - \epsilon^k), \quad \forall k \in \mathcal{K} \quad (6d)
\]

\[
\sum_{j \in \mathcal{J}_1} v_j = p, \quad \forall j \in \mathcal{J}_1 \quad (6e)
\]

\[
v_j \in \{0, 1\}. \quad \forall j \in \mathcal{J}_1 \quad (6f)
\]

In the above formulation, $p$ can range from 1 to $N$, the dimension of $\text{FO}$. $\text{IL}$ finds the closest point $z$ to the set of observations with respect to the metric in the objective such that it is contained in a face of $\chi$ binding $n$ relevant constraints. Note that in developing the $\text{IL}$ model, the big-M method is used to make the model flexible in selecting a certain number of relevant constraints. Also, note that setting $p = 1$ reduces $\text{IL}$ to a model that finds the same decision resulting from $\text{I}$. Remark 3 formalizes this statement.

**Remark 3.** $\text{IO}$ is a special case of $\text{IL}$. Setting $p = 1$ in $\text{IL}$ results in the same decision that Algorithm 1 finds.

Remark 3 emphasizes on the inherent flexibility of $\text{IL}$ in its ability to infer forward optimal solutions that bind a certain number of relevant constraints. In what follows, we discuss the feasibility of $\text{IL}$ and how different choices of $p$ affect the inferred optimal solutions.

**Proposition 4.** If $\chi$ has at least one feasible extreme point among relevant constraints, then $\text{IL}$ is feasible for all $p \in \{1, ..., N\}$.

**Proof of Proposition 4.** Let $x^0$ be a corner point of the feasible region of $\text{FO}$ which binds exactly $N$ relevant constraints. Let $B \subseteq \mathcal{J}_1$ be the set of indices of relevant constraints that are tight at $x^0$. For $p_0 \in \{1, ..., N\}$, let $B_{p_0} \subseteq B$ be a set of indices of $p_0$ tight constraints at $x^0$ and let $v_{p_0}$ be a vector such that $v_j = 1 \quad \forall j \in B_{p_0}$ and $v_j = 0$ otherwise for $j \in \mathcal{J}_1$. Also, let $E_0$ be the matrix of distances from $x^0$ to all the observations. Then, $(v_{p_0}, E_0, x^0)$ is feasible for $\text{IL}$ with $p = p_0$. $\square$

**Proposition 5.** If $\text{IL}$ is feasible for $p_1, p_2 \in \mathcal{J}_1$ such that $p_1 \leq p_2$ and $\text{IL}^*_{p_1}$ and $\text{IL}^*_{p_2}$ are equal to the objective values of $\text{IL}$ for $p_1, p_2$ at optimality, then $D^*_{p_1} \leq D^*_{p_2}$.

**Proof of Proposition 5.** Let $z^*_{p_1}$ and $z^*_{p_2}$ be the optimal solutions of $\text{IL}$ for $p_1, p_2 \in \mathcal{J}_1$ respectively. We show that $z^*_{p_2}$ is a feasible solution for $\text{IL}$ with $p = p_1$. This can be easily seen by choosing $p_1$...
number of binding relevant constraints of $z^*_{p_2}$. Let $B$ be a subset of indices of tight constraints at $z^*_{p_2}$ with $|B| = p_1$ and let $v$ be a vector such that $v_j = 1 \forall j \in B$ and $v_j = 0$ otherwise for $j \in J_1$. Also, let $E_{p_2}$ be the matrix of the distances of $z^*_{p_2}$ to the observations. It can be seen that $(v, E_{p_2}, z^*_{p_2})$ is feasible for $\text{IL}$ with $p = p_1$. Therefore, $D^*_{p_1} \leq D^*_{p_2}$. \hfill □

Proposition 5 shows how the $\text{IL}$ model is capable of balancing the trade-off between being closer to the observed decisions and binding more relevant constraints at optimality. As we increase the value of $p$, we go farther from the observations but find optimal decisions with better characteristics. The next theorem characterizes the set of all inverse feasible cost vectors for the optimal decision point that $\text{IL}$ finds.

**Theorem 2.** Let $(v^*, E^*, z^*)$ be an optimal solution for $\text{IL}$ with $p = p_0$ and let $T \subseteq J_1$ be the set of indices of the relevant constraints that are tight at $z^*$. Then, $z^*$ is optimal for $\text{FO}(c)$ for any $c \in \text{cone}(a_t : t \in T)$.

**Proof of Theorem 3** Let $c \in \text{cone}(a_t : t \in T)$ be such a cost vector; $c = \sum_{t \in T} \lambda_t a_t$ with $\lambda_t \geq 0$. It suffices to show that the dual feasibility and strong duality conditions hold for $z^*$ in $\text{FO}$. We have $c^t z^* = (\sum_{t \in T} \lambda_t a_t^t) z^* = \lambda_t b_t$ with $\lambda_t \geq 0 \forall t \in T$. Let $y$ be such that $y_j = \lambda_t \forall t \in T$ and $y_j = 0$ otherwise. We have $A' y = c$ and $y$ and $c^t z^* = b' y$. \hfill □

**Corollary 1.** If $(v^*, E^*, z^*)$ is an optimal solution for $\text{IL}$ with $p = 1$, and $T \subseteq J_1$ is the set of indices of the relevant constraints that are tight at $z^*$, then for any $\bar{c} = \sum_{t \in T} \lambda_t a_t$ with $\bar{y}$ such that $y_j = \lambda_t \forall t \in T$ and $y_j = 0$ otherwise, $(\bar{c}, \bar{y}, E^*, z^*)$ is an optimal solution for $\text{IO}$.

It is noteworthy to emphasize that the results of $\text{IL}$ with increased values for $p$ explicitly indicate the trade-off in inference of optimal solutions based on given observations and constraints. $\text{IL}$ with $p = 1$ solves for the closest point to all the given observations (given a distance metric) and therefore, puts more attention on the given observations when inferring a forward optimal solution while $\text{IL}$ with $p = N$ solves for the closest extreme point of $\text{FO}$ among relevant constraints (if $\text{IL}$ is feasible for $p = N$) from all the observations and therefore maximizes the attention to the relevant constraints of the forward problem. Also, note that by increasing the value of $p$, as shown in Proposition 5, the inferred decision constantly moves away from the observations and at the same time, binds more constraints. This is important in constructing transitional optimal solutions towards preferences of the user. In what follows, we modify $\text{IL}$ in a way that can progressively increase the quality of the inferred decision, while constantly moving away from the observations by increasing $p$.

### 4.1. Dependent Sequencing of Inferred Optimal Solutions

As mentioned earlier, in order to capture the effects of the inherent trade-off in constrained inference using inverse optimization regarding observations and constraints, when implementing the $\text{IL}$
methodology, a range of solutions can be obtained. However, such decisions with increasing value of $p$ are not usually comparable since the solutions might jump between different faces of $\chi_{opt}$ with little to no shared binding constraints. An alternative way to provide a range of more comparable solutions based on the number of binding relevant constrains is to use the resulting inferred decision resulting from IL with some value of $p$ and introduce the binding relevant constraints of that decision to a modified inverse learning model which binds the same relevant constraints and attempts to bind an additional relevant constraint to arrive at a new decision. Let $z_{opt}$ be the inferred point from from IL with $p = p_0$ and let $B_{z_{opt}}$ be the set of indices of binding relevant constraints at $z_{opt}$ such that $|B_{z_{opt}}| = p_0$. Then, the following formulation moves $z_{opt}$ in a direction that binds at least one more relevant constraint with minimal perturbation from the observations, if such a constraint exists:

\[
\begin{align*}
\text{minimize}_{v, E, z} & \quad D(E, A) \\
\text{subject to} \quad b \leq Az \leq b + M(1 - v) \\
Wz \geq q, \\
z = (x^k - e^k), \quad \forall k \in K \\
\sum_{j \in J_1} v_j = p_0 + 1, \\
v_j = 1, \quad \forall j \in B_{z_{opt}}, \\
v_j \in \{0, 1\}, \quad \forall j \in J_1
\end{align*}
\]  

If the above formulation is feasible for a given $z_{opt}$, then a new point contained in $\chi_{opt}$ is inferred that binds more relevant constraints but moves farther from the original observations. Based on the above model, the following Propositions will be stated without proof.

**Proposition 6.** If formulation 7 is feasible for $p_1, p_2 \in J_1$ such that $p_1 \leq p_2$, the following hold:

1. if $D_{p_1}^*$ and $D_{p_2}^*$ are equal to the objective values for $p_1, p_2$ at optimality, then $D_{p_1}^* \leq D_{p_2}^*$.
2. if $z_{p_1}^*$ and $z_{p_2}^*$ are equal to the inferred decisions at optimality, then $z_{p_1}^*$ and $z_{p_2}^*$ are both contained on a face of $\chi$.

**Proof of Proposition 6.** The proof of the first part of the proposition can be outlined with similar arguments as the proof of Proposition 5. Therefore, we just provide the proof of the second statement in the proposition by simply pointing out that if maximal faces containing $z_{p_1}^*$ and $z_{p_2}^*$ share at some binding constraints and therefore, there exists a face of $\chi$ that contains both $z_{p_1}^*$ and $z_{p_2}^*$.

The results of the above proposition show that all the inferred solutions from formulation 7 are contained in a face of $\chi$. This supports the idea of dependent sequencing of optimal solutions in order to improve and provide a larger number of options to the user or the decision maker.
4.2. Inclusion of Additional Optional Constraints’ Knowledge

Finally, in order to further extend the flexibility of the methodology developed in this section to also account for explicit information on constraints provided by the user or the decision maker, we consider a setting where, in addition to the existing knowledge which distinguished between relevant and trivial constraints, extra information about the inherent preferences of the decision maker are also at hand with regard to the constraints. This setting arises from the fact that although IL is capable of finding the closest decision given any number of binding constraints, there is limited guarantee over the quality of the inferred decision even in cases where the original observations have the required qualities, mainly due to the fact that in such inference, the model favours the knowledge on the constraints rather than the observations. In this setting, it is possible that decision maker prefers to be even farther from the original observed decisions at the expense of binding other (more proffered) constraints at optimality. This calls for a model that can consider such preferred constraints if there are any. we model such a setting by extending using a multi-objective formulation that can be used to find the closest point to all the observations that has the maximum number of tight such preferred constraints. We denote the set of indices of preferred constraints as $S \subseteq J_1$.

\[
\text{MIL}(X, p) : \min_{v, E, z} \omega_1 \frac{1}{K} \mathcal{D}(E, A) - \omega_2 \frac{|S|}{|S|} \sum_{s \in S} v_s
\]

subject to

1. $b \leq Az \leq b + M(1 - v)$
2. $Wz \geq q$
3. $z = (x^k - \epsilon^k)$, $\forall k \in K$
4. $\sum_{j \in J_1} v_j = p$
5. $v_j \in \{0, 1\}$, $\forall j \in J_1$

Using competing terms in the objective, MIL explicitly demonstrates the trade-off between how close the inferred decision can be to the observations and how many of the preferred constraints are tight at optimality. Note that, in general, the utopia point of the above multi-objective formulation cannot be achieved and depending on the weights, MIL is capable of erring on the side of the preferred constraints or the distance from the original given observations. Also, note that we can also remove the hard constraints on the number of tight relevant constraints in this multi-objective model and include an additional objective term maximizing the number of such constraints. Figure demonstrates how MIL is capable of considering explicit additional knowledge on preferred constraints in inferring optimal solutions. The following proposition shows how the inferred optimal point by MIL performs against IL.
Proposition 7. Let \((v_{GIL}, E_{GIL}, z_{GIL})\) be an optimal solution for IL with \(n = n_0\) and let \((v_{MGIL}, E_{MGIL}, z_{MGIL})\) be an optimal solution for MIL with \(n = n_0\) for a given set of observations and forward constraints. Then, \(\sum_{k=1}^{K} \| \epsilon^k_{GIL} \|_l \leq \sum_{k=1}^{K} \| \epsilon^k_{MGIL} \|_l\).

Proof of Proposition 7. Let \(B_{GIL}\) be the set of indices of binding relevant constraints for \(z_{GIL}\) and let \(S^*_{MGIL}\) be the set of indices of binding preferred constraints for MIL. We consider two cases and:

- **Case 1**: (If \(S^*_{MGIL} \subseteq B_{GIL}\)) In this case, we can conclude that \(z_{MGIL} = z_{GIL}\) and therefore \(\sum_{k=1}^{K} \| \epsilon^k_{GIL} \|_l = \sum_{k=1}^{K} \| \epsilon^k_{MGIL} \|_l\).
- **Case 2**: (If \(S^*_{MGIL} \not\subseteq B_{GIL}\)). In this case, \(\exists s \in S^*_{MGIL}\) such that \(s \notin B_{GIL}\). This means that while \(z_{MGIL}\) does bind \(n_0\) relevant constraint but is not equal to the optimal solution of IL. Therefore, we have \(\sum_{k=1}^{K} \| \epsilon^k_{GIL} \|_l \leq \sum_{k=1}^{K} \| \epsilon^k_{MGIL} \|_l\). \(\square\)

In this section, we provided detailed modeling techniques for the Inverse Learning methodology and showed how this model is capable of incorporating existing knowledge about the problem to achieve more flexible optimal solutions. In what follows, we apply the models developed in this section to a simple two dimensional problem and then, in the application section, we demonstrate how these formulations are used to find different and flexible forward optimal solutions and also, in the setting of the diet problem, maximize preferred nutritional requirements and provide diets that are richer in preferred nutrients and are also low in the undesirable ones.
4.3. Utility Function Inference from IL

The inverse learning methodology introduced in this work is capable of learning forward optimal solutions based on given observations and sets of constraints of the original problems. In this section, we provide a method that can be used to infer the inverse optimal cost vector using the results of IL. Based on the work of Tavasli\'oglu et al. (2018), if $z^*$ is the resulting forward optimal solution from IL, then the set of feasible cost vectors which make $z^*$ optimal can be characterized as follows:

$$Q(z^*) = \left\{ (c, y) \in \mathbb{R}^n \times \mathbb{R}^m \mid A'y = c, c'z^* = b'y, \|c\|_L = 1 \right\}$$ (9)

As mentioned earlier, existing methods in inverse linear optimization usually limit the inferred utility function to a vector orthogonal to one of the constraints of the original forward problem. Here, we aim to distinguish a utility parameter contained in $Q$ such that the forward objective value for all the original observations is maximized. Since we have characterized the forward optimal solution, an optimization model can be developed to directly input all the observations and choose from the elements of $Q$ a cost vector with the maximum sum of forward objective value:

$$\begin{align*}
\text{maximize} & \quad \sum_{k=1}^{K} c'x^k \\
\text{subject to} & \quad c \in Q(z^*)
\end{align*}$$ (10a)

Using the above formulation, the resulting utility parameter has the best performance for all the initial observations with regard to the objective value of FO. It is worth noting that the resulting inverse optimal utility parameter from Model 10 depends on the choice of the distance norm used to define $Q$. For instance, for $L = 1$, the inferred cost vector will tend to be orthogonal to a constraint depending on the distribution of the observations and if $L = 2$, the inferred cost vector will use the second order distances to provide a unique cost vector in the cone of the binding relevant constraints. In Section 5, we show how inference of the utility parameter using formulation 10 can be compared with other models in the literature.

5. Numerical Example

In this section, we provide a two-dimensional example to visually illustrate the results of our inverse learning framework. The example considers a forward problem with seven constraints and some feasible or infeasible observations as shown in Figure 2. This illustrative example demonstrates the differences between our inverse learning models. We additionally compare our models with the existing models in the literature as baseline comparison models that are most relevant to our work, namely the absolute duality gap (ADG) formulation (Babier et al. 2018b) and the mixed-integer inverse optimization (MIIO) method (Shahmoradi and Lee 2019). All the models are compared...
based on their inferred inverse optimal cost vectors and their inferred forward optimal solutions. More specifically, in the case of ADG formulation, the inferred cost vector is used to find the optimal forward solution by directly solving the forward problem using the inferred parameters. In the case of the MIIO formulation, since two of the parameters, $\theta$ and $E$, need to be pre-defined, we let $\theta = 1$, as suggested by the authors for data without outliers and also considered $\theta = 0.75$ for the first example. To find the best value for $E$, we wrote a bisection algorithm that finds the minimum $E$ in such a way that it maximizes the objective of the MIIO formulation, i.e., such that it finds a corner point ($\sum_j v_j = N$). For all the models and whenever appropriate, we used the 1-norm as the distance measure to infer forward optimal solutions and 2-norm to infer the cost vectors.

**Example 1.** Let $\text{FO}(c) = \max_{x \in \mathbb{R}^2} \{c'x \mid \Gamma_1 : -x_1 + x_2 \leq 10, \quad \Gamma_2 : -0.5x_1 + x_2 \leq 11, \quad \Gamma_3 : 0.5x_1 + x_2 \leq 16, \quad \Gamma_4 : x_1 + x_2 \leq 20, \quad \Gamma_5 : x_1 \leq 10, \quad \Gamma_6 : x_1 \geq 0, \quad \Gamma_7 : x_2 \geq 0\}$. In this example, assume that $\Gamma_1$ to $\Gamma_5$ are relevant constraints and $\Gamma_3$ is a preferred constraint.

![Figure 2](image.png) An illustrative 2D example: (a) comparing Inverse Learning models with the existing models in the literature. (b) comparing inferred inverse optimal cost vectors from different models.

Figure 2(a) shows the results of the methodologies developed in this work in comparison with baseline models from existing literature of multi-observation inverse optimization. As shown in the figure, in the presence of mostly feasible observations with some infeasible (yet close to the boundary) observations, the ADG model infers a forward problem solution with $x_2 = 0$, which is in contrast with the behavior of all the original observations. Also, since MIIO is developed with the notion of minimizing the perturbation of all the observations, usually, the farthest observation
to a potential inferred point influences the results heavily. In such case, even by reducing the $\theta$ parameter, the inferred forward solution is not able to capture the trend in the observations. In summary, this figure demonstrates how other models do not capture the behavior of the observations when inferring forward optimal solutions; Given the 20 observation points in Figure 2 which show a progressive trend towards the upper right corners of the forward feasible set, the existing models fail to infer the corner points close to this trend; this is while all the Inverse Learning models are pointing towards forward optimal solutions that reflect the trend in the data. $\text{IL}_{(p=1)}$ finds the closest point on the boundary to the set of observations. $\text{IL}_{(p=2)}$ infers the closest forward feasible corner point of the relevant constraints to the observations, finally MIL is taking the inferred point to a corner point which binds as many preferred constraints possible (in this case, only one preferred constraint exists). Figure 2(b) shows the inferred cost vectors of each model. As seen in the figure, using 2-norm allows for the inverse learning model to find a cost vector that is more informed from the observations and does not only depend on the knowledge of the forward feasible set. Table 1 compares the results of different models shown in Figure 2.

| Model         | Average Distance to Observations | Set of Optimal Cost Functions | Inferred Cost Function | Number of Binding Relevant Constraints | Average Objective Value* |
|---------------|----------------------------------|------------------------------|------------------------|----------------------------------------|--------------------------|
| $\text{IL}_{(p=1)}$ | 6.08                             | $C((1,0))$                   | $(1,0)$                  | 1                                      | 5.90                     |
| $\text{IL}_{(p=2)}$ | 7.00                             | $C((1,0),(1,1))$             | $(0.72,0.69)$           | 2                                      | 9.30                     |
| MIL           | 7.42                             | $C((1,1),(0.5,1))$           | $(0.71,0.71)$           | 2                                      | 9.32                     |
| $\text{MIIO}_{(\theta=1)}$ | 8.75                             | $C((-1,0),(-1,1))$          | -                      | 1                                      | -                        |
| $\text{MIIO}_{(\theta=0.75)}$ | 8.66                             | $C((-1,1),(-0.5,1))$        | -                      | 2                                      | -                        |
| ADG           | 11.44                            | $(1,0)$                      | $(1,0)$                 | 1                                      | 5.90                     |

*Average forward objective values for all the observations using the inferred cost vector in the forward problem.

As shown in Table 1 all applicable variants of the Inverse Learning methodology outperform existing models in the literature in terms of inferring optimal solutions with minimum perturbation of observations. Additionally, the inferred inverse optimal utility parameter is also more aligned with the trends that the observations are showing. Finally, as a metric for the performance of the inferred cost vector, it is shown how the Inverse Learning methodologies can provide better results in terms of the original objective function of the forward problem based on the inferred inverse optimal cost vector. In the next section, we implement the Inverse Learning methodology to an applied example of the diet recommendation problem.

6. Application: Personalized Diet Recommendations

The Inverse Learning framework is a general inference methodology in linear-constrained settings that can be applied to domains which require finding utility functions and/or optimal solutions of a linear forward optimization problem based on a set of expert- or user-driven observations. The
embedded flexibility in the Inverse Learning methodology enables it to tailor to the application domain and incorporate additional data that would be otherwise challenging to consider in inverse optimization models. This flexibility improves the alignment of the inferred solutions with the underlying utility function of the decision-makers.

In this section, we provide an example application for the Inverse Learning framework, namely, the personalized diet recommendations problem. The diet recommendation problem is among the most well-studied problems in operations research [Stigler 1945, Bassi 1976]. This problem aims to find the optimal food intake of a patient or a set of patients based on some given cost function and subject to a given set of nutritional constraints. In the inverse optimization literature, the diet recommendation problem has been studied to recover the appropriate cost function (or equivalently, the utility function) (Ghobadi et al. 2018, Shahmoradi and Lee 2019) or constraint parameters (Ghobadi and Mahmoudzadeh 2020) based on a given set of observations. In this study, we concentrate mainly on the quality of the inferred optimal solutions based on a given set of observations. Similar to Ghobadi et al. (2018), in the definition of the diet recommendation problem, we assume that the cost function is associated with the inverse preferences of the individual, meaning that the more palatable a particular food item for the individual, the less its cost.

In this work, we consider specific groups of patients diagnosed with hypertension who are at the risk of developing type-2 diabetes and explore the effects of specialized diets on their ability to control their blood pressure and their illness progression. The recommendations are provided based on a set of given observations from the food choices of the patients. The observations may be feasible or infeasible for the forward optimization problem constructed on nutritional constraints for the specific demographics of the patients, which is a common occurrence in a diet application. The goal is to recommend diets to these patients that not only are rich in nutrients but are also palatable to their individual taste as much as possible and hence, encourage long-term adherence. We emphasize that, depending on the original observations, richness of diets and their palatability to the individual’s taste may be competing objectives, as such, we show how the Inverse Learning methodology can provide reasonable ranges of potentially optimal solutions to handle such a setting.

Long-term adherence is one of the main challenges in dieting as healthy diets are often far from the dieter’s daily habits and it often proves challenging to change life-style. This challenge is especially costly for chronic patients who may be able to control their condition through dieting, e.g., type II diabetes, prediabetes, and hypertension patients. Providing a diet that is healthy and that considers the life-style, individual preferences, and needs will increase the chances of adherence.

Using the Inverse Learning models, we provide a range of diet recommendations for hypertension and prediabetic patients. The recommendations allow for choosing the closest healthy diet to the patient’s observations or providing a progression plan for the patient to work towards a healthier diet.
Utilizing the flexibility of the Inverse Learning framework, we are also able to identify constraints that are more beneficial or preferred for the patient to be binding at optimality. These preferences may reflect the provider’s recommendation or the patient’s preferences and lifestyle. In the rest of this section, we first provide a summary of the data used in this section and how the data was prepared for this application. Next, we solve provide the results of employing the inverse learning models to a set of observations and provide a range of diets based on the patient’s or provider’s preferences.

6.1. Data

We model the diet recommendation problem as a linear optimization problem. The input to inverse learning models include a set of constraints and a set of observations, assuming that the cost function is unknown. For the specific application of the diet recommendation problem, databases from the United States Department of Agriculture (USDA) and the National Health and Nutrition Examination Survey (NHANES) were used to generate constraints and observations. NHANES database includes self-reported information on daily intakes of 9954 patients for two days. Such daily intakes serve as observations for our models. In our diet recommendation application, we focus on hypertension and prediabetes which are often considered as adverse effects of bad dietary habits. Targeted diets are considered to reduce the risk of these diseases and the patients typically need to follow these diets for long periods. One such target diet is the Dietary Approaches to Stop Hypertension (DASH) and is frequently recommended to these patients to control their sodium intakes and blood pressure levels. We consider the DASH diet as the recommended diet for our FO problem and build lower-bound and upper-bound nutritional constraints based on this diet for each age and gender group. (Liese et al. 2009, Sacks et al. 2001). We also use nutrients per serving data for each food group from USDA in order to construct the feasibility set of the diet recommendation forward problem. It is worth mentioning that for this application, we grouped certain similar food types and ultimately considered 38 total food groups (reducing the original 5085 food types for simplicity and tractability of the dimension of the problem) and consider 22 nutrient constraints on the main nutrients and 76 box constraints on the food types limiting the intake of each food item to be below eight servings per day. Bounds on nutrients for the target diet for a patient group including women of ages higher than 51, relevant constraints ans select feasible set coefficients for a select subset of the food items are presented in Table 2. More details about the constraints, food items, the observations, and any other relevant information are available in an electronic companion where the data can be downloaded as well (Ahmadi et al. 2020).

We close this section by providing some points of consideration regarding the data gathered for this study. Since the DASH diet recommendations are based on weekly amounts for some groups of
foods and the observed diets of the patients were on a daily basis, the recommendations of the DASH diet were broken down to daily bounds instead of original weekly bounds. These modifications, in turn, results in constraints on the lower bounds on the nutrients being, in some cases, too restrictive for data gathered over daily intakes. However, we opt to use such daily bounds in order to adapt to daily intakes in the observations. It is worth noting that these limitations on the data part do not hinder the capacity of the models outlined in this paper to infer optimal diets.

6.2. Recommending Diets with Inverse Learning

Motivated by the search for optimal decisions in linear optimization settings, in the methodology section, we introduced the \( \text{IL} \) formulation which showed a trade-off between the distance of a potentially optimal decision from the given set of observations and the number of relevant constraints that are active at optimality. For the specific application of the diet recommendation problem, in this section, we use the dependent sequencing model provided in formulation \( \text{IL} \) in order to arrive at optimal decisions. We showcase how the inverse learning methodology developed in this work can be used to infer optimal diets. We demonstrate different outcomes of the models and point out the transition from concentration on the given observations (IL\((p=1)\)) when inferring optimal solutions to concentration on the number of active relevant constraints (IL with increased values of \( p \) depending on the problem). We also show how the decision maker can inform the models of their preferred constraints and find optimal solutions that balance between the distance metric and binding the preferred constraints that the decision maker selects. Figure \ref{fig:recommending_diets} shows the results of inferring recommended diets for a set of 230 patients with 460 daily intake data of women with the group age of 51+ who are diagnosed with hypertension and are at risk of diabetes. We solve \( \text{IL} \) with dependent sequencing for \( p = 1 \) to \( p = 4 \). Additionally, in this example, we consider the lower-bounds of sodium, saturated fat and cholesterol and the upper-bound of dietary fiber to be the proffered
relevant constraints of the decision maker and solve the MIL models for \( p = 1 \) to \( p = 4 \) in order to address the effect of considering proffered relevant constraints on recommended diets. As shown in Figure 3, as the value of \( p \) increases, the inferred optimal solution tends to move towards healthier diets, for both IL and MIL at the cost of deviating more from the observations (for visualization purposes, ranges of intake for each food group are shown as box plots of the observations and 10, 25, 50, 75 and 90 percentiles are shown). Specifically, diets recommended by MIL show a more aggressive trend towards food groups richer in dietary fiber (such as citrus fruits) and food groups containing less sodium in order to adhere to the choices of the decision maker regarding the preferred relevant constraints. The same trend is also seen in the nutrients. Figure 4 compares the amounts of nutrients contained in each of the diets recommended using different values of \( p \). As the value of \( p \) increases, the inverse learning models will provide healthier diets (reduced amounts of fats for IL and reduces amounts of carbohydrates, fats, cholesterol and sodium for MIL).

Table 3 summarizes the average distances of all the inferred diets to the observations and lists the number of binding nutritional relevant, preferred relevant and trivial nutritional constraints in each of the recommended diets. As indicated in this table, at each value of \( p \), the average distance of the inferred diet increases from the observations increases and in general, as expected, IL recommends diets that are closer to the observations in comparison to MIL in all values of \( p \), however, in the case of this particular example, it can be seen that the price of providing healthier diets with MIL is not heavily larger the IL in terms of being close to the observations. Additionally, as shown in the table, the number of binding relevant constraints in both models increase with the value of \( p \) with MIL binding more relevant and preferred relevant constraints for each value of \( p \) and the number of binding trivial constraints decrease (as a result of binding more relevant constraints and navigating other faces of the forward feasible set) with again MIL binding less trivial constraints for each value of \( p \). In summary, it rests with the user/decision maker to indicate which of the two competing parameters of being close to original diets and having healthier diets with more binding relevant constraints are more important for their specific purpose.

### Table 3: Nutrient bounds and inferred amounts compared in recommended diets

| Value of \( p \) | Average Distance to Observations | Number of Binding Relevant Constraints | Number of Binding Trivial Constraints | Number of Preferred Relevant Constraints |
|------------------|----------------------------------|----------------------------------------|--------------------------------------|------------------------------------------|
|                  | IL  | MIL | IL  | MIL | IL  | MIL | IL  | MIL |
| 1                | 18.1| 18.4| 2   | 3   | 6   | 4   | 0   | 1   |
| 2                | 18.1| 18.5| 2   | 4   | 6   | 3   | 0   | 2   |
| 3                | 18.3| 18.8| 3   | 4   | 4   | 3   | 1   | 3   |
| 4                | 18.4| 19.2| 4   | 6   | 4   | 3   | 2   | 4   |

6.3. Discussion

In this section, we showed how different models developed in this work are capable of recommending diets with different desirable characteristics. The results show the inverse learning methodology
Figure 3  Comparison of recommended diets by IL and MIL with different values for $p$ and a set of 460 observations.

is capable of recommending optimal diets for sets of given dietary behaviors of individuals. The different approaches employed show the degree of flexibility of the inverse learning methodologies. It should be noted that although inverse learning is a data-driven inference methodology and as such, the quality of the inferred solutions depend on the input observations, the results show that the methodology is capable of navigating the optimal decision space of the optimization problem and finding the best possible solutions given the observations. We also note that the inverse learning models are faster in practice for (as investigated for the diet recommendation problem) than the existing models in the literature. Additionally, the results were provided such that little pre-analysis was performed in the input data. Therefore, future directions include providing more extensive pre-analysis tools for the data and streaming the data into the inference model in order to obtain more interpretable results.

7. Conclusions

We introduce the inverse learning framework as an application-driven inverse optimization method that can be used in a wide range of applied settings. This new framework provides greater flexibility
in inferring optimal solutions to a highly constrained linear optimization problem. We show that in the setting of the diet recommendation problem, this framework can be used to infer optimal diets based on initial dietary behaviors of the individual that are more aligned with their preferences and are healthy at the same time. We showed how the pre-known preferences and habits of the individual can be inserted directly into the models to ensure the palatability of the inferred diets.

We applied our method to the diet recommendation problem with a given set of observations on the daily diets of individuals prone to hypertension and diabetes in order to infer the best daily diets with considerations on specific nutrient constraints based on the DASH diet. We compared the results with existing methods in the literature and the results showed that our method is more successful in inferring closer optimal solutions to the original observations. We also demonstrated flexible features of our approach in considering specific constraints when inferring solutions and showed that there is a trade-off between retaining the characteristics of the original observations or binding specific relevant constraints. In all cases, the method is able to provide appropriate diets for the given set of observations.

Figure 4  Comparison of nutrients of recommended diets by IL and MIL for different values of $p$. The lower-bounds on carbohydrate, saturated fat, cholesterol and sodium are preferred relevant constraints.
Using the novel Inverse Learning methodologies in the diet recommendation problem shows that these models are capable of finding forward optimal solutions that preserve the characteristics of the observations to a higher extent compared to the existing models in the literature, while being more flexible in incorporating features of the problem domain by categorizing the constraints, resulting in more meaningful optimal solutions. We show that the inverse learning methodologies can be used to provide multiple forward optimal solutions with different characteristics and we can provide a range of optimal solutions for an inferred utility parameter.

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