Optimal solutions to the isotonic regression problem

Alexander I. Jordan, Anja Mühlemann, and Johanna F. Ziegel

University of Bern

April 10, 2019

Abstract

In general, the solution to a regression problem is the minimizer of a given loss criterion, and as such depends on the specified loss function. The non-parametric isotonic regression problem is special, in that optimal solutions can be found by solely specifying a functional. These solutions will then be minimizers under all loss functions simultaneously as long as the loss functions have the requested functional as the Bayes act. The functional may be set-valued. The only requirement is that it can be defined via an identification function, with examples including the expectation, quantile, and expectile functionals.

Generalizing classical results, we characterize the optimal solutions to the isotonic regression problem for such functionals in the case of totally and partially ordered explanatory variables. For total orders, we show that any solution resulting from the pool-adjacent-violators (PAV) algorithm is optimal. It is noteworthy, that simultaneous optimality is unattainable in the unimodal regression problem, despite its close connection.

Keywords: Order-restricted optimization problem, Partial order, Simultaneous optimality
MSC Classifications: 62G08

1 Introduction

Suppose that we have pairs of observations \((z_1, y_1), \ldots, (z_n, y_n)\) where we assume that \(y_i, i = 1, \ldots, n\) are real-valued. The aim of isotonic regression is to fit an increasing function \(\hat{g}: \{z_1, \ldots, z_n\} \rightarrow \mathbb{R}\) to these observations. The covariates \(z_1, \ldots, z_n\) can take values in any set as long as they are equipped with a partial order which we denote by \(\preceq\). Then, a function \(g: \{z_1, \ldots, z_n\} \rightarrow \mathbb{R}\) is increasing if \(z_i \preceq z_j\) implies that \(g(z_i) \leq g(z_j)\).
As it is common in regression analysis, we aim to find an estimate \( \hat{g} \) that minimizes the expected loss for some loss function \( L: \mathbb{R} \times \mathbb{R} \rightarrow [0, \infty) \). If the function \( \hat{g} \) is interpreted as an estimator of the conditional expectation of a random variable \( Y \) given \( Z \), then a natural choice for \( L \) is the squared error loss \( L(x, y) = (x - y)^2 \).

For \( i \leq j \), let \( E_{i:j} \) denote the expectation with respect to the empirical distribution of \((z_i, y_i), \ldots, (z_j, y_j)\). Assuming that \( z_1 < z_2 < \cdots < z_n \), the minimizer of the quadratic loss criterion

\[
E_{1:n}(g(Z) - Y)^2
\]

over all increasing functions \( g \) is given by

\[
\hat{g}(z_\ell) = \min_{j \geq \ell} \max_{i \leq j} E_{i:j} Y = \max_{j \geq \ell} \min_{i \leq j} E_{i:j} Y, \quad \ell = 1, \ldots, n,
\]

see Barlow et al. (1972, eq. (1.9)–(1.13)). The solution \( \hat{g} \) can be computed efficiently using the so-called pool-adjacent-violators (PAV) algorithm. These results were developed in the 1950s by several parties independently; see Brunk (1955), Ayer et al. (1955), van Eeden (1958), Bartholomew (1959a,b) and Miles (1959).

It turns out that the solution given at (2) is also the unique minimizer of the Bregman loss criterion

\[
E_{1:n} L(g(Z), Y),
\]

where the squared error loss in (1) has been replaced by a Bregman loss function \( L = L_\phi \) (Barlow et al., 1972, Theorem 1.10). That is,

\[
L_\phi(x, y) = \phi(y) - \phi(x) - \phi'(x)(y - x),
\]

where \( \phi \) is a convex function with subgradient \( \phi' \). Savage (1971) found that the Bregman class comprises all loss functions \( L \) where the expectation functional minimizes the expected loss, i.e.,

\[
\mathbb{E}_P Y = \arg \min_x \mathbb{E}_P L(x, Y),
\]

where \( Y \) is a random variable with distribution \( P \). Due to this property, any loss function in the Bregman class is also referred to as a consistent loss function for the expectation functional (Gneiting, 2011). In summary, the increasing regression function at (2) is simultaneously optimal with respect to all consistent loss functions for the expectation.

This remarkable result is in stark contrast to optimal fits of parametric models for increasing regression functions. Suppose that \( \{g_\theta : \theta \in \Theta\} \), \( \Theta \subseteq \mathbb{R}^d \) is a parametric model of increasing functions \( g_\theta \). Then, the optimal parameters with respect to the Bregman-loss criterion generally vary (substantially) depending on the chosen loss function (Patton, 2019). Consistency of the loss function merely ensures that the true parameter value of a correctly specified model minimizes the Bregman-loss criterion. Interestingly, simultaneous optimality with respect to all consistent loss functions generally also breaks down if one weakens the isotonicity constraint of the regression function to a unimodality constraint; see Section 5.
In this paper, we generalize the result of Barlow et al. (1972, Theorem 1.10) in several directions. First, instead of the expectation functional, we consider general (possibly set-valued) functionals $T$ that are given by an identification function $V(x, y)$ as defined in Definition 2.1. Second, in the case of set-valued functionals, we give a complete characterization of all possible solutions for totally ordered covariates. Third, we demonstrate that a suitably modified version of min-max or max-min solutions as in (2) continues to hold for general partial orders on the covariates.

An identification function is an increasing function that weighs negative values in the case of underestimation against positive values in the case of overestimation, with an optimal expected value of zero. The corresponding functional $T$ then maps to the optimizing argument (or set of optimizing arguments). Prime examples of such functionals are (possibly set-valued) quantiles, expectiles (Newey and Powell, 1987), or ratios of expectations. Quantiles, including the median, have previously also been treated in Robertson and Wright (1973, 1980), but not in the interpretation as set-valued functionals. Predefining a global scheme for reducing the median interval to a single point (e.g., some weighted average of lower and upper functional value) inevitably restricts the possible solutions to the isotonic regression problem. Expectiles and ratios of expectations, on the other hand, have been fully treated in Robertson and Wright (1980). These functionals map to single values and satisfy the Cauchy mean value property which is implied by identifiability.

In contrast to previous work, we treat all functionals as set-valued. In Section 3, we give explicit solutions for the lower and upper bound of the isotonic regression problem in the context of total orders. The method of proof for these results is fundamentally different from the approach of Barlow et al. (1972, Theorem 1.10) or Robertson and Wright (1980), and in contrast to the latter comes with an immediate construction principle for loss functions. Our method relies on the mixture or Choquet representations of consistent loss functions, introduced by Ehm et al. (2016) for the quantile and expectile functionals. Given the identification function $V(x, y)$ for the functional $T$, a one-parameter family of elementary loss functions that are consistent for the functional $T$ can be readily defined,

$$
S_\eta(x, y) = (\mathbb{1}\{\eta \leq x\} - \mathbb{1}\{\eta \leq y\}) V(\eta, y),
$$

where $\eta \in \mathbb{R}$. For all consistent loss functions $L$ in the class

$$
\mathcal{S} = \left\{ \int \mathbb{R} S_\eta(x, y) \, dH(\eta) : H \text{ is a nonnegative measure on } \mathbb{R} \right\},
$$

the optimal isotonic solution to the criterion (3) is bounded below by a min-max formula and bounded above by a max-min formula as in (2) with the expectation replaced by the lower and upper functional values under $T$, respectively. We show that the min-max or max-min solution is simultaneously optimal with respect to all elementary loss functions for $T$, and hence with respect to the entire class $\mathcal{S}$. In fact,
optimality of an isotonic solution with respect to the criterion (3) for \( L = S_\eta \) for some \( \eta \in \mathbb{R} \) corresponds to finding a solution with optimal superlevel set \( \{ g \geq \eta \} \). Considering an isotonicity constraint as a constraint on admissible superlevel sets of the regression function relates to the work of Polonik (1998) in the context of density estimation.

If \( T \) is a quantile, an expectile, or a ratio of expectations, then \( S \) comprises all consistent loss functions for \( T \), and if \( V(x, y) = x - y \) is the identification function of the expectation, then the class \( S \) is the class of Bregman loss functions; see Gneiting (2011) and Ehm et al. (2016). We also give results that can be directly translated to a simple algorithm that recovers the full range of optimal solutions from the lower and upper bounds and the full data set. While the bounds alone do not contain sufficient information, only few additional computations on the entire data set are necessary. Our method of proof also leads to a transparent proof of the validity of the PAV algorithm; see Section 3.2.

Recently, Moesching and Dümbgen (2019) derived a similar result of min-max and max-min formulas as lower and upper bounds for optimal isotonic solutions in the context of set-valued minimizers of convex and coercive loss functions. Brümmel and Du Preez (2013) rediscover that the PAV algorithm leads to a simultaneously optimal solution for all proper scoring rules in the context of binary events—a special class of loss functions that are consistent for the expectation functional.

In Section 4, we treat general partial orders on the covariates and demonstrate that a suitably modified version of min-max or max-min solutions continues to hold. Again, the optimal isotonic fit is simultaneously optimal with respect to all loss functions in \( S \) defined at (4). With our method of proof this extension is straightforward but for reasons of transparency, we first present the case of a total order in Section 3, and only then treat partial orders. The results by Robertson and Wright (1980) not only hold for a large class of functionals, but also for partial orders on the covariates. However, the generality of their results is limited by treating potentially set-valued functionals as maps to single values. To the best of our knowledge, the literature following Robertson and Wright (1980) is void of further results that characterize the solutions to the isotonic regression problem, or investigations into the effect of the choice of loss function among options sharing the same Bayes act.

A comprehensive overview on isotonic regression is given in the monograph by Groeneboom and Jongbloed (2014). Also, Guntuboyina and Sen (2018) review risk bounds, asymptotic theory, and algorithms in common nonparametric shape-restricted regression problems in the context of least squares optimization. Among the most recent developments on algorithms for isotonic regression with partially ordered covariates, Kyng et al. (2015) and Stout (2015) provide fast algorithms for isotone regression under different loss functions using the representation of a partial order as a directed acyclic graph. Recent advances on asymptotic theory for isotonic regression include Han et al. (2017), giving rates for least squares isotonic regression on the unit cube of arbitrary dimension, and Bellec (2018), considering
isotonic, unimodal, and convex regression in the context of total orders. Another recent interest is the regularization of isotonic regression on multiple variables with Luss and Rosset (2017) proposing a method via range restriction on the solution to the regression problem.

2 Functionals and consistent loss functions

We start with the definition of a functional via an identification function.

**Definition 2.1.** A function $V: \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ is called an identification function if $V(\cdot, y)$ is increasing and left-continuous for all $y \in \mathbb{R}$. Then, for any finite and nonnegative measure $P$ on $\mathbb{R}$, we define the functional $T$ induced by an identification function $V$ as

$$T(P) = [T_P^-, T_P^+] \subseteq [-\infty, +\infty] = \bar{\mathbb{R}}$$

where the lower and upper bounds are given by

$$T_P^- = \sup \{x : V(x, P) < 0\} \text{ and } T_P^+ = \inf \{x : V(x, P) > 0\},$$

using the notation $V(x, P) = \int_{-\infty}^{\infty} V(x, y) \, dP(y)$.

Defining functionals for any finite and nonnegative measure, as opposed to merely probability distributions, is a minor detail that simplifies notation when joining and intersecting data subsets. Except in the case of the null measure, any finite and nonnegative measure can be replaced with its corresponding probability distribution, without any change to the functional values.

All new results in this paper are concerned with probability distributions $P$ with finite support, and therefore, existence of integrals is always guaranteed. The following example and Proposition 2.4 hold for more general types of distributions given that the relevant integrals exist. We leave these obvious generalizations up to the reader and assume from now on that all probability distributions considered have finite support.

Note that $T_P^-$ can take the value $-\infty$ and $T_P^+$ can take the value $+\infty$. In the subsequent results, we repeatedly refer to the smallest or largest element of a finite set where one of the elements could be $\pm \infty$. We still write min and max of the set but this quantity could be $\pm \infty$.

**Example 2.2.** Let $\alpha, \tau \in (0, 1)$, and let $P$ denote a probability distribution.

(a) Consider the identification function $V(x, y) = \mathbb{1}_{\{x > y\}} - \alpha$, then

$$V(x, P) = \mathbb{E}_P V(x, Y) = P(Y < x) - \alpha,$$

and

$$T(P) = [\sup\{x : P(Y < x) < \alpha\}, \inf\{x : P(Y < x) > \alpha\}]$$

is the set of all $\alpha$-quantiles of $P$. 

(b) Consider the identification function \( V(x, y) = 2 \mathbb{1}\{x > y\} - \tau |(x - y)| \), then

\[
\mathbb{E}_P V(x, Y) = 2(1 - \tau) \int_{-\infty}^{x} (x - y) \, dP(y) + 2 \tau \int_{x}^{\infty} (x - y) \, dP(y).
\]

The unique solution in \( x \) for the equation \( \mathbb{E}_P V(x, Y) = 0 \) is the \( \tau \)-expectile \( e_\tau(P) \). In particular, for \( \tau = \frac{1}{2} \) we obtain \( V(x, y) = x - y \) and thus \( T(P) = \{ \mathbb{E}_P(Y) \} \).

In the later proofs, we use three implications of Definition 2.1 repeatedly to establish order relationships between the variable in the first argument of \( V \) and the functional of an empirical distribution. To facilitate reference, we note these statements explicitly,

\[
\begin{align*}
V(x, P) = 0 & \implies x \in T(P), \quad (5) \\
V(x, P) > 0 & \implies x > \sup T(P) = T^+_P, \quad (6) \\
V(x, P) < 0 & \implies x \leq \inf T(P) = T^-_P. \quad (7)
\end{align*}
\]

Lemma 2.3 shows that a generalized version of the Cauchy mean value property, used to define functionals in Robertson and Wright (1980), holds for any functional we consider in this paper. This suggests that our results are less general, unless it can be proven that every Cauchy mean value function can be defined in terms of an identification function. On the other hand, in contrast to Robertson and Wright (1980), we treat set-valued functionals and their boundaries rigorously, and retain a higher level of generality in that regard.

**Lemma 2.3.** Let \( P, Q \) be finite and nonnegative measures on \( \mathbb{R} \). Then,

\[
\min\{T^-_P, T^+_Q\} \leq T^-_{P+Q} \leq T^+_{P+Q} \leq \max\{T^-_P, T^+_Q\}.
\]

**Proof.** The statement follows from Definition 2.1. The second inequality is trivial. For the first inequality, and \( x < \min\{T^-_P, T^+_Q\} \), we have \( V(x, P) < 0 \) and \( V(x, Q) \leq 0 \), hence \( V(x, P + Q) < 0 \). A similar argument applies to the third inequality. \( \square \)

The definition of a functional in terms of an identification function comes with a straightforward construction principle for large classes of loss functions. In a nutshell, a continuous oriented identification function defines a functional via its unique root in the first argument, a first-order condition. By integration, corresponding loss functions inherit the consistency for the functional, i.e., the minimum expected loss is attained by any member in \( T(P) \). The loss functions defined in Proposition 2.4 are the most basic, in the sense that they are a result of integration with respect to the Dirac measure at a given threshold \( \eta \in \mathbb{R} \). A similar result has also been discussed in Dawid (2016) and Ziegel (2016).
Proposition 2.4. Let $V$ be an identification function, $T$ be the induced functional, and $\eta \in \mathbb{R}$. Then the elementary loss function $S_\eta: \bar{\mathbb{R}} \times \mathbb{R} \to \mathbb{R}$ given by

$$S_\eta(x, y) = (\mathbbm{1}\{\eta \leq x\} - \mathbbm{1}\{\eta \leq y\})V(\eta, y)$$

is consistent for $T$ relative to the class $\mathcal{P}$ of probability distributions with finite support. That is,

$$\mathbb{E}_P S_\eta(t, Y) \leq \mathbb{E}_P S_\eta(x, Y)$$

for all $P \in \mathcal{P}$, all $t \in T(P)$ and all $x \in \bar{\mathbb{R}}$.

Proof. Let

$$d(\eta) = \mathbb{E}_P S_\eta(t, Y) - \mathbb{E}_P S_\eta(x, Y) = (\mathbbm{1}\{\eta \leq t\} - \mathbbm{1}\{\eta \leq x\})V(\eta, P).$$

If $V(\eta, P) = 0$ then $d(\eta) = 0$. If $V(\eta, P) < 0$ it follows from (7) that $\eta \leq t$ and therefore $d(\eta) \leq 0$. If $V(\eta, P) > 0$ it follows from (6) that $\eta > t$ and therefore $d(\eta) \leq 0$.

As an immediate consequence of the consistency of elementary loss functions for the functional $T$, we have that all loss functions in the class $S$ defined at (4) are also consistent for the functional $T$. This result exemplifies an important line of reasoning used multiple times in this paper: A property of $S_\eta$ that holds for all $\eta \in \mathbb{R}$ translates to the class $S$.

The importance of the construction in Proposition 2.4 lies in the postponing of integration, or, in other words, applying Fubini in a double integration (with respect to $P$ and to $H$), and then showing the property of consistency for the integrand $S_\eta$ for each $\eta$ rather than for the original loss function which is the integral of $S_\eta$ with respect to $dH(\eta)$.

3 Results for total orders

3.1 Min-max and max-min solutions

Suppose that we have observations $(z_1, y_1), \ldots, (z_n, y_n)$, and let $P$ denote their empirical distribution. Throughout this section, we assume that the covariates $z_1, \ldots, z_n$ are equipped with a total order, and that the indices are chosen such that $z_1 < z_2 < \cdots < z_n$. Repeated observations can also be easily accommodated as explained in Remark 3.1 below.

We aim to find an increasing function $g: \{z_1, \ldots z_n\} \to \bar{\mathbb{R}}$ that minimizes

$$\mathbb{E}_P S_\eta(g(Z), Y) \quad \text{for all } \eta \in \mathbb{R},$$

where the random vector $(Z, Y)$ has distribution $P$. Any increasing function $\hat{g}$ solving this optimization problem is a solution to the isotonic regression problem that is optimal with respect to all scoring functions in the class $S$, simultaneously.
Condition (8) is equivalent to minimizing $\mathbb{E}_P \mathbb{1}\{\eta \leq g(Z)\}V(\eta, Y)$ for all $\eta \in \mathbb{R}$. We can rephrase the minimization problem to reflect the way in which we prove the main result: For a given $\eta \in \mathbb{R}$, we have to find an index $i \in \{1, \ldots, n+1\}$ that minimizes

$$s_i(\eta) = v_{i:n}(\eta) = \sum_{\ell=i}^{n} V(\eta, y_\ell).$$

Thereby, we obey the condition

$$\{z : g(z) \geq \eta\} = \{z_i, \ldots, z_n\},$$

implied by the monotonicity constraint on $g$. This index search needs to be conducted for every $\eta \in \mathbb{R}$ separately. In a nutshell, we find the generalized inverse to an optimal solution. Afterwards, we define the overall minimizing function $\hat{g}$.

From now on, we assume that all indices $i, j \in \{1, \ldots, n+1\}$ unless specified otherwise.

Remark 3.1. The assumption that the ordering $z_1 < \cdots < z_n$ is strict is non-restrictive. Given a series of observations $(z'_1, y_1), \ldots, (z'_m, y_m)$ with non-strictly ordered or unordered $z'_i$, we can choose $z_1 < \cdots < z_n < z_{n+1} = \infty$ such that $\{z'_1, \ldots, z'_m\} \subseteq \{z_1, \ldots, z_n\}$. We define the empirical counting measure for the index range from $i$ to $j$ by

$$P_{i:j}(B) = \sum_{\ell=i}^{j} \sum_{k=1}^{m} \mathbb{1}\{z_\ell = z'_k\} \mathbb{1}\{(z'_k, y_k) \in B\},$$

with the corresponding integral of the identification function being equal to the following sum,

$$V(\eta, P_{i:j}) = v_{i:j}(\eta) = \sum_{\ell=i}^{j} \sum_{k=1}^{m} \mathbb{1}\{z_\ell = z'_k\} V(\eta, y_k).$$

For condition (8), we write the empirical probability distribution as $P(B) = P_{1:n}(B)/m$. The subsequent arguments leading to an optimal solution rely solely on the identification sum $v_{i:j}(\eta)$ and the functional $T(P_{i:j})$, where we dealt with the dependence on the number of observations for each unique value of $z_\ell$ in the above generalization.

We begin by introducing sets consisting of minimizing indices. For $\eta \in \mathbb{R}$, let $I(\eta)$ denote the set of indices $i$ minimizing $s_i(\eta)$, and define $\mathcal{I} = \bigcup_{\eta \in \mathbb{R}} I(\eta) \subseteq \{1, \ldots, n+1\}$ That is, $i \in \mathcal{I}$ if and only if there exists an $\eta \in \mathbb{R}$ such that

$$s_i(\eta) \leq s_j(\eta) \quad \text{for all } j.$$

The following proposition is immediate.
Lemma 3.4. Let \( \eta \in \mathbb{R} \). The inclusion \( i \in I(\eta) \) holds if and only if,
\[
\begin{align*}
v_{i;(j-1)}(\eta) &\leq 0 \quad \text{for all } j > i, \\
v_{j;(i-1)}(\eta) &\geq 0 \quad \text{for all } j < i.
\end{align*}
\]
If \( j > i \) and \( v_{i;(j-1)}(\eta) = 0 \), then \( j \in I(\eta) \). Analogously, if \( j < i \) and \( v_{j;(i-1)}(\eta) = 0 \), then \( j \in I(\eta) \).

The following proposition is a key observation to show optimality of the min-max and max-min solution. We relate the threshold \( \eta \in \mathbb{R} \) to the minimal and maximal elements of the functional \( T \) on subsets of the data. We write \( T_{i;j}^- = T_{i;j}^* = \inf T(P_{i;j}) \) and \( T_{i;j}^+ = T_{i;j}^{**} = \sup T(P_{i;j}) \).

Proposition 3.3. Let \( \eta \in \mathbb{R} \), and \( i \in I(\eta) \). Then,
\[
\begin{align*}
\max_{j < i} T_{j;(i-1)}^- &\leq \eta \leq \min_{j > i} T_{i;(j-1)}^+, \\
\max_{j < i, j \notin I(\eta)} T_{j;(i-1)}^+ &< \eta \leq \min_{j > i, j \notin I(\eta)} T_{i;(j-1)}^-.
\end{align*}
\]

Proof. For all \( j < i \), we have \( v_{j;(i-1)}(\eta) \geq 0 \). For all \( j > i \), we have \( v_{i;(j-1)}(\eta) \leq 0 \). Both inequalities are strict when \( j \notin I(\eta) \). Equations (5) – (7) imply the result. \( \square \)

Figure 1 illustrates the statement in Proposition 3.3.

Lemma 3.4. (a) For all \( \eta \in \mathbb{R} \), \( I(\eta) \) is a set of consecutive indices in \( \mathcal{I} \). In other words, if \( i, j \in I(\eta) \) and \( i < i_0 < j \) such that \( i_0 \notin I(\eta) \), then \( i_0 \notin \mathcal{I} \).

(b) The functions
\[
\eta \mapsto \min I(\eta) \quad \text{and} \quad \eta \mapsto \max I(\eta)
\]
are increasing.

(c) Suppose that \( \eta_m \uparrow \eta \) and \( i \in I(\eta_m) \) for all \( m \in \mathbb{N} \). Then, \( i \in I(\eta) \).

Proof. (a) Suppose the contrary: There exists an \( \eta' \neq \eta \) such that \( i_0 \in I(\eta') \). If \( \eta' < \eta \), we have that \( v_{i;(i_0-1)}(\eta') \geq 0 \). Similarly, since \( i_0 \notin I(\eta) \) it holds that \( v_{i;(i_0-1)}(\eta) < 0 \). This contradicts the monotonicity assumption for the first argument of \( V \). The argument against an \( \eta' > \eta \) such that \( i_0 \in I(\eta') \) works similarly.

(b) Let \( \eta < \eta' \) and suppose the contrary: Let \( i = \min I(\eta) \) and \( i' = \min I(\eta') \) such that \( i > i' \). Then, \( i' \notin I(\eta) \), and we have \( v_{i';(i-1)}(\eta') \leq 0 \) and \( v_{i';(i-1)}(\eta) > 0 \), contradicting the monotonicity assumption for the first argument of \( V \). The argument for \( \eta \mapsto \max I(\eta) \) works similarly.
Figure 1: **Separation into quadrants.** For a sample of 9 data points, the graph illustrates the functional value (expectation) on relevant subsets of the data for a given $\eta$. The expectation value (vertical location of a brown line) is above or below $\eta$ when the corresponding subsample extends (horizontal extension of a brown line) to the right or left of the minimizing index, respectively.
Therefore, \( \{ \eta \} \) among all increasing functions \( \eta \) such that \( \iota \). Proposition 3.5. monotone functions are characterized by their superlevel sets. Proof. Due to the monotonicity and left-continuity of \( \iota \), i.e., with \( g(z) \geq \eta \) for all \( z \in \{ z(\eta), \ldots, z_n \} \) for all \( \eta \in \mathbb{R} \), must be an optimizing solution. In fact, this solution is unique for a given \( \iota \) because monotone functions are characterized by their superlevel sets.

**Proposition 3.5.** Let \( \iota : \mathbb{R} \rightarrow \{1, \ldots, n+1\} \) be an increasing, left-continuous function such that \( \iota(\eta) \in I(\eta) \). Then, the function \( \hat{\iota} : \{z_1, \ldots, z_n\} \rightarrow \mathbb{R} \) given by

\[
\inf \{ \eta : \iota(\eta) > \ell \} = \hat{\iota}(z) = \max \{ \eta : \iota(\eta) \leq \ell \}
\]

(9)
is the unique function that satisfies

\[
\{ z : g(z) \geq \eta \} = \{ z(\eta), \ldots, z_n \} \quad \text{for all } \eta \in \mathbb{R},
\]

among all increasing functions \( g : \{z_1, \ldots, z_n\} \rightarrow \mathbb{R} \).

**Proof.** Due to the monotonicity and left-continuity of \( \iota : \mathbb{R} \rightarrow \{1, \ldots, n+1\} \), we have \( \inf \{ \eta : \iota(\eta) > \ell \} = \max \{ \eta : \iota(\eta) \leq \ell \}, \ell = 1, \ldots, n \). The monotonicity of \( \hat{\iota} \) follows from the monotonicity of \( \iota \) and the fact that \( \{z_1, \ldots, z_n \} \) is ordered. Let \( \eta' \in \mathbb{R} \). Then,

(i) \( \hat{\iota}(z) \geq \eta' \implies \iota(\hat{\iota}(z)) \geq \iota(\eta') \implies \ell \geq \iota(\eta') \),

(ii) \( \hat{\iota}(z(\eta')) = \max \{ \eta : \iota(\eta) = \iota(\eta') \} \geq \eta' \).

Therefore, \( \{ z : \hat{\iota}(z) \geq \eta' \} \subseteq \{ z(\eta'), \ldots, z_n \} \subseteq \{ z : \hat{\iota}(z) \geq \eta' \} \) where the first inclusion follows by (i) and the second by (ii). Uniqueness of \( \hat{\iota} \) follows because increasing functions are characterized by their superlevel sets.

In Figure 2 we give an example for a collection of 6 data points. The example illustrates how the values \( \hat{\iota}(z), \ell = 1, \ldots, n \), can be determined from the epigraph of the function \( \eta \mapsto z(\eta) \).

Now, we can state and show our main result which is that \( \hat{\iota} \) coincides with or is bounded by a min-max and max-min solution.

**Proposition 3.6.** Let \( \ell \in \{1, \ldots, n\} \) and let \( \hat{\iota} \) be a solution to the isotonic regression problem. Then,

\[
\min \max_{j \geq \ell} T^-_{ij} \leq \hat{\iota}(z) \leq \max \min_{i \leq \ell} T^+_{ij}.
\]
Figure 2: **Graph of \( \hat{g} \).** For a sample of 6 data points, the values of \( \hat{g}(z) \) for \( z = z_1, \ldots, z_6 \) are shown in red. The epigraph of the function \( \eta \mapsto z_{i(\eta)} \) is shown in grey, where \( T \) is chosen as the median functional to choose \( i(\eta) \).
Proof. Applying the first set of bounds from Proposition 3.3 to the formula for \( \hat{g} \) at (9) yields

\[
\inf_{i:\eta(i) > \ell} \max_{i < \iota(\eta) - 1} T^-_{i;\iota(\eta) - 1} \leq \hat{g}(z\ell) \leq \max_{i:\eta(i) \leq \ell} \min_{j > \iota(\eta) - 1} T^+_{\iota(\eta) - 1},
\]

The lower bound is bounded below by \( \min_{j \geq \ell} \max_{i \leq j} T^-_{ij} \), and the upper bound is bounded above by \( \max_{i \leq \ell} \min_{j \geq i} T^+_{ij} \).

The max-min inequality implies that for functionals \( T \) that always map to singletons, e.g., the expectation or expectile functionals, the lower and upper bound in Proposition 3.6 are equal. Otherwise, when the functional \( T \) is not always a singleton, a similar statement can be made where the choice of \( \iota \) determines whether \( \hat{g} \) pointwise attains the minimal or maximal elements of the functional.

Proposition 3.7. Let \( \ell \in \{1, \ldots, n\} \).

(a) If \( \iota(\eta) = \min I(\eta) \) for all \( \eta \in \mathbb{R} \), then,

\[
\hat{g}(z\ell) = \min_{j \geq \ell} \max_{i \leq j} T^+_{ij} = \max_{i \leq \ell} \min_{j \geq i} T^+_{ij}.
\]

(b) If \( \iota(\eta) = \max I(\eta) \) for all \( \eta \in \mathbb{R} \), then,

\[
\hat{g}(z\ell) = \min_{j \geq \ell} \max_{i \leq j} T^-_{ij} = \max_{i \leq \ell} \min_{j \geq i} T^-_{ij}.
\]

Proof. The proof works the same way as the proof of Proposition 3.6 but using second set of bounds in Proposition 3.3. This is possible because in (a) we have that for \( j < \iota(\eta) \) it holds that \( j \not\in I(\eta) \) and in (b), for \( j > \iota(\eta) \) we know that \( j \not\in I(\eta) \).

Let us denote the solution in part (a) of Proposition 3.7 by \( g^+ \) and the one in part (b) by \( g^- \). Clearly, it always holds that \( g^- \leq g^+ \). It is a natural question whether any increasing function \( g \) that satisfies \( g^- \leq g \leq g^+ \) is also a minimizer of the criterion (8). It turns out that the answer is negative; see Moesching and Duembgen (2019, Remark 2.2, Example 2.4). The following proposition provides a simple sufficient criterion for \( g \) to also be a solution. In the case of quantiles and for the classical asymmetric linear loss, the same result is shown in Moesching and Duembgen (2019, Lemma 2.1). Note that in Proposition 3.8 it is not required that \( g^- \), \( g^+ \) are the solutions from Proposition 3.7 as long as they satisfy \( g^- \leq g^+ \).

Proposition 3.8. Let \( g^-, g^+ \) be two solutions to the isotonic regression problem, that is, minimizers of (8), and suppose they satisfy \( g^- \leq g^+ \). Let \( \hat{g} \) be increasing, \( g^- \leq \hat{g} \leq g^+ \), and suppose that \( g^+(z\ell) = g^+(z\ell') \), \( g^-(z\ell) = g^-(z\ell') \) for some \( \ell < \ell' \) implies \( \hat{g}(z\ell) = \hat{g}(z\ell') \). Then, \( \hat{g} \) is also a minimizer of (8), that is, a solution to the isotonic regression problem.
**Proof.** For $\eta \in \mathbb{R}$, define $\iota(\eta) := \min\{\ell : \hat{g}(z_{\ell}) \geq \eta\}$, and analogously $\iota^-(\eta)$ and $\iota^+(\eta)$ with $\hat{g}$ replaced by $g^-$ and $g^+$, respectively. The functions $\iota$, $\iota^-$, $\iota^+$ are increasing and left-continuous. For $\iota^-$, $\iota^+$ it holds that $\iota^-(\eta), \iota^+(\eta) \in I(\eta)$. For all $\ell \in \{1, \ldots, n\}$, we have that

$$g^-(z_{\ell}) = \max\{\eta : \iota^-(\eta) \leq \ell\} \leq \hat{g}(z_{\ell}) = \max\{\eta : \iota(\eta) \leq \ell\} \leq g^+(z_{\ell}) = \max\{\eta : \iota^+(\eta) \leq \ell\},$$

therefore, $\iota^+(\eta) \leq \iota(\eta) \leq \iota^-(\eta)$ for all $\eta \in \mathbb{R}$. It remains to show that $\iota(\eta) \in \mathcal{I}$. This follows from the following two observations.

First, if

$$\hat{g}(z_{\ell}) = \max\{\eta : \iota(\eta) \leq \ell\} = \max\{\eta : \iota(\eta) \leq \ell'\} = \hat{g}(z_{\ell'})$$

for some $\ell \leq \ell'$, then $\iota(\eta) \not\in (\ell, \ell')$. Second, if $g^-(z_{\ell}) < g^-(z_{\ell+1})$ or $g^+(z_{\ell}) < g^+(z_{\ell+1})$, then $\ell + 1 \in \mathcal{I}$. 

The proof of Proposition 3.8 shows that $\hat{g}$ may jump at points $z_{\ell}$ where $g^+$ and $g^-$ do not jump as long as $\ell \in \mathcal{I}$, that is, as long as $\ell$ is a minimizing index for some $\eta$. The following Proposition 3.9 characterizes the possible additional jumps of $\hat{g}$.

**Proposition 3.9.** Let $g^-, g^+$ be two solutions to the isotonic regression problem, and suppose that for some $i, j \in \{1, \ldots, n\}, i < j$,

$$\eta^- := g^-(z_i) = g^-(z_j) < g^+(z_i) = g^+(z_j) =: \eta^+.$$

Furthermore, assume it holds that, for $i > 1$, $g^-(z_{i-1}) \neq g^-(z_i)$ or $g^+(z_{i-1}) \neq g^+(z_i)$, and, for $j < n$, $g^-(z_j) \neq g^-(z_{j+1})$ or $g^+(z_j) \neq g^+(z_{j+1})$. Then, for $\ell \in \{i+1, \ldots, j\}$, we have $T^-_{i:(\ell-1)} \leq \eta^-$ if and only if $\ell \in I(\eta)$ for all $\eta \in (\eta^-, \eta^+)$. 

**Proof.** Throughout the proof, we assume that $k \in \{1, \ldots, n+1\}$, and we use Proposition 3.2 repeatedly.

We will first argue that $T^+_{i:k} \geq \eta^+$ for $k > i$, and that $T^-_{k:j} \leq \eta^-$ for $k < j$.

The assumptions ensure that there are $i^- \leq i$, $i^+ \leq i$ such that $i^- \in I(\eta^-)$, $i^+ \in I(\eta^+)$, and $\min\{i^-, i^+\} = i$. If $i^+ = i$, then $v_{i:k}(\eta^+) \leq 0$ for all $k > i$, hence $T^+_{i:k} \geq \eta^+$. If $i^- = i$ and $i^+ < i^-$, then $v_{i^+:i^+-1}(\eta^+) \geq v_{i^+:i^+-1}(\eta^-) \geq 0$ but also $v_{i^+:i^+-1}(\eta^+) \leq 0$. Therefore, $v_{i:k}(\eta^+) = v_{i+:k}(\eta^+) \leq 0$ for all $k > i$, and again $T^+_{i:k} \geq \eta^+$.

The assumptions also imply that there are $\eta^- > \eta^-$, $j^- \geq j$, $\eta^+ > \eta^+$, $j^+ \geq j$ such that $j^- + 1 \in I(\eta)$ for all $\eta \in (\eta^-, \eta^-]$, $j^+ + 1 \in I(\eta)$ for all $\eta \in (\eta^+, \eta^+]$, and $\min\{j^-, j^+\} = j$. If $j = j^-$, then $v_{k:j}(\eta) \geq 0$ for all $k \leq j$, $\eta \in (\eta^-, \eta^+]$, hence $T^-_{k:j} \leq \eta$. If $j = j^+$ and $j^- > j^+$, then $v_{j^+ + j^-}(\eta^-) \leq 0$ for $\eta \in (\eta^+, \eta^+]$, and due to the monotonicity of $V$ also for $(\eta^-, \eta^-]$. Also, $v_{j^+ + j^- - j}(\eta) \geq 0$ for $\eta \in (\eta^-, \eta^-]$. Therefore, $v_{k:j}(\eta) = v_{k:j^-}(\eta) \geq 0$ for all $k \leq j$, $\eta \in (\eta^-, \eta^-]$, and again $T^-_{k:j} \leq \eta^-$. In summary, $T^-_{k:j} \leq \eta^-$ for all $k \leq j$. 

14
For the first part of the result, let $\ell \in \{i + 1, \ldots, j\}$ such that $T^-_{i, \ell - 1} \leq \eta^-$. By Lemma 2.3, we have $T^+_{i, k} \leq \max\{T^-_{i, (\ell - 1)}, T^+_{i, k}\}$ for all $k \geq \ell$. Since $T^+_{i, k} \geq \eta^+$ and $T^-_{i, (\ell - 1)} \leq \eta^-$, we have $T^+_{i, k} \geq \eta^+$ and $v_{i, k}(\eta) \leq 0$ for all $\eta \leq \eta^+, k \geq \ell$. Similarly, by Lemma 2.3, we have $T^-_{k, j} \geq \min\{T^-_{k, (\ell - 1)}, T^+_{k, j}\}$ for all $k \leq \ell - 1$. Since $T^-_{k, j} \leq \eta^-$ and as shown above $T^+_{k, j} \geq \eta^+$, we have $T^-_{k, (\ell - 1)} \leq \eta^-$ and $v_{k, (\ell - 1)}(\eta) \geq 0$ for all $\eta > \eta^-$, $k \leq \ell - 1$. Hence, we have $\ell \in I(\eta)$ for all $\eta \in (\eta^-, \eta^+]$.

To prove the converse, note that $\ell \in I(\eta)$ for all $\eta \in (\eta^-, \eta^+]$ implies $v_{\ell, (\ell - 1)}(\eta) \geq 0$ for all $\eta \in (\eta^-, \eta^+], k < \ell$. Hence, in particular, $v_{\ell, (\ell - 1)}(\eta) \geq 0$ and $T^-_{\ell, (\ell - 1)} \leq \eta$ for all $\eta \in (\eta^-, \eta^+]$, and, therefore, $T^-_{i, (\ell - 1)} \leq \eta^-$.

\[\square\]

### 3.2 Pool-adjacent-violators algorithm

As in Section 3.1, the PAV algorithm takes observations $(z_1, y_1), \ldots, (z_n, y_n)$, with $z_1 < \cdots < z_n$ and can be generalized as detailed in Remark 3.1. Its starting point is the finest partition $Q_0 = \{\{1\}, \ldots, \{n\}\}$ of the index set $\{1, \ldots, n\}$, and a corresponding function $g_0: \{z_1, \ldots, z_n\} \to \mathbb{R}$ satisfying

$$g_0(z_\ell) \in T(P_{\ell, \ell}).$$

If possible, an increasing function has to be chosen. The algorithm then iteratively considers pooling adjacent elements $Q_1$ and $Q_2$ in the current partition, where “adjacent” means that the largest element of $Q_1$, $Q_1^+ = \max Q_1$, is the predecessor (in terms of the natural numbers) of the smallest element of $Q_2$, $Q_2^- = \min Q_2$.

Pooling adjacent partition elements is considered necessary when $T^-_{Q_1^+ - 1, Q_1^+} > T^+_{Q_2^- - 1, Q_2^-}$ (strong adjacent violators), it is considered invalid when $T^+_{Q_1^+, Q_1^+} < T^-_{Q_2^- - 1, Q_2^-}$; and optional otherwise (weak adjacent violators). The early stopping criterion is the existence of an increasing function $g_{PAV}: \{z_1, \ldots, z_n\} \to \mathbb{R}$ that is constant on each element of the current partition $Q_{PAV}$ and satisfies

$$g_{PAV}(z_\ell) \in T(P_{Q^-_{\ell}, Q^+}) \quad \text{for all } Q \in Q_{PAV}, \ell \in Q,$$

that is, when no further pooling is necessary. The late stopping criterion is reached when no weak adjacent violators remain. The first and most apparent property we observe is that for all $\ell \in \{1, \ldots, n\}$, $Q_1, Q_2 \in Q_{PAV}$, $Q_1^- \leq \ell \leq Q_2^+$, we have

$$T^-_{Q_1^- - 1, Q_1^+} \leq g_{PAV}(z_\ell) \leq T^+_{Q_2^- - 1, Q_2^+},$$

since otherwise either $g_{PAV}$ is not increasing or the condition \[10\] is violated. Definition 2.1 and its implications \[5\]–\[7\] allow for an immediate proof of an additional property of $Q_{PAV}$:

**Proposition 3.10.** Let $Q$ be a partition of $\{1, \ldots, n\}$ found by the PAV algorithm, $Q \in Q$, and $j \in Q$. Then,

$$T^-_{j, Q^+} \leq T^-_{Q^-_{\ell}, Q^+} \leq T^+_{Q^-_{\ell}, Q^+} \leq T^+_{Q^-_{\ell}, j}.$$
Proof. The second inequality is trivial. For the first inequality, suppose the contrary: There exist \( \eta \in \mathbb{R}, j \in Q \) such that \( T^+_j, Q^- > \eta > T^-_j, Q^+ \). This implies that \( j > Q^- \) and \( v_{Q^- - j}(\eta) \geq 0 > v_{j, Q^+}(\eta) \), hence \( v_{Q^+ - (j-1)}(\eta) > 0 \). Therefore, \( T^+_{j, (j-1)} < \eta < T^-_{j, Q^+} \), which means that \( Q \) can be seen as the result of an invalid pooling of \( \{Q^-, \ldots, j-1\} \) and \( \{j, \ldots, Q^+\} \). A similar argument applies to the third inequality.

To show the connection between a valid solution by the PAV algorithm and the score optimizing solution \( \hat{g} \) in Section 3.1, we define

\[
\iota_{PAV}(\eta) = \min\{k : \eta \leq g_{PAV}(z_k)\}.
\]

Plugging \( \iota_{PAV} \) into the definition of \( \hat{g} \) recovers \( g_{PAV} \),

\[
\hat{g}(z_\ell) = \max\{\eta : \iota_{PAV}(\eta) \leq \ell\}
= \max\{\eta : \eta \leq g_{PAV}(z_\ell)\} = g_{PAV}(z_\ell).
\]

In order to show that \( g_{PAV} \) solves the isotonic regression problem, it remains to be shown that \( \iota_{PAV}(\eta) \in I(\eta) \) for all \( \eta \in \mathbb{R} \).

Proposition 3.11. Let \( \eta \in \mathbb{R} \), then \( \iota_{PAV}(\eta) \in I(\eta) \).

Proof. Let \( \eta \in \mathbb{R} \). We combine Proposition 3.10, the statement (11), and the defining equation (12). As a result, for all \( j, k \in \{1, \ldots, n+1\}, j < \iota_{PAV}(\eta) < k \), we have \( T^-_{j, \iota_{PAV}(\eta)} \leq g_{PAV}(z_{\iota_{PAV}(\eta)-1}) \leq \eta \leq g_{PAV}(z_{\iota_{PAV}(\eta)}) \leq T^+_{\iota_{PAV}(\eta), (k-1)} \), hence \( v_{\iota_{PAV}(\eta)-1}(\eta) \geq 0 \geq v_{\iota_{PAV}(\eta), (k-1)}(\eta) \). The statement follows from Proposition 3.2.

As a closing side note, we point out that \( \iota_{PAV} \) corresponds to coarsest partition that allows the solution \( g_{PAV} \). Any weak adjacent violators on which \( g_{PAV} \) takes the same value have been pooled.

4 Generalization to partial orders

In the first part of this paper, we considered a series of observations \((z_\ell, y_\ell)\), where \( \ell = 1, \ldots, n \) and the set \( \{z_1, \ldots, z_n\} \) was totally ordered. In this section, we solve the isotonic regression problem (8) assuming only a partial order on the covariates \( \{z_1, \ldots, z_n\} \). It is not restrictive to assume that \( z_1, \ldots, z_n \) are pairwise different.

Repeated observations can be accommodated as detailed in Remark 3.1.

The considerations in Section 3.1 lead to the formulation of an optimization problem, i.e., the minimization of

\[
s_i(\eta) = v_{i:n}(\eta) = \sum_{\ell=1}^n V(\eta, y_\ell)
\]

16
over all $i \in \{1, \ldots, n+1\}$. The dependency on $z_1, \ldots, z_n$ and $\hat{g}$ seemingly vanishes, but remains encoded in the index set $\{1, \ldots, n+1\}$ and in the link to $\eta$ via an optimizing function $\iota: \mathbb{R} \rightarrow \{1, \ldots, n+1\}$ such that
\[
\{z : \hat{g}(z) \geq \eta\} = \{z_{\iota(\eta)}, \ldots, z_n\}.
\]
In the second part, we now generalize the index set $\{1, \ldots, n+1\}$ and the function $\iota$ in order to accommodate partially ordered sets $\{z_1, \ldots, z_n\}$.

As a generalization, we introduce sets of indices $x \subseteq \{1, \ldots, n\}$ to replace single indices $i \in \{1, \ldots, n+1\}$. We consider a set $\mathcal{X} \subseteq \mathcal{P}(\{1, \ldots, n\})$, where $\mathcal{P}$ denotes the power set. The set $\mathcal{X}$ consists of all index subsets corresponding to the admissible superlevel sets for an increasing function $g$ imposed by the partial order on $\{z_1, \ldots, z_n\}$. A set $x \in \mathcal{X}$ is characterized by the property that if $z \in x$ and $z \leq z'$, then $z' \in x$. This implies that $\mathcal{X}$ is closed under union and intersection.

Consequently, we replace the function $\iota: \mathbb{R} \rightarrow \{1, \ldots, n+1\}$ with a function $\xi: \mathbb{R} \rightarrow \mathcal{X}$, that maps $\eta$ to a minimizing set of indices in $\mathcal{X}$ for the objective
\[
s_x(\eta) = v_x(\eta) = \sum_{\ell \in x} V(\eta, y_\ell). 
\quad (13)
\]
Let $X(\eta)$ denote the set of index sets $x \in \mathcal{X}$ minimizing $s_x(\eta)$.

**Example 4.1.** We choose $\mathcal{X}$ as the image of $\{1, \ldots, n+1\}$ under the one-to-one mapping
\[i \mapsto \{k \in \{1, \ldots, n\} : k \geq i\}.\]

In combination with the function $\xi: \mathbb{R} \rightarrow \mathcal{X}$ that satisfies
\[
\{z_{\iota(\eta)}, \ldots, z_n\} = \{z_{\ell} : \ell \in \xi(\eta)\},
\quad (14)
\]
we can embed the results from Section 3 into the more general setting of a partial order on the covariates.

The generalization of Proposition 3.3 follows directly.

**Proposition 4.2.** Let $\eta \in \mathbb{R}$, $x \in X(\eta)$. Then, subject to $x' \in \mathcal{X}$,
\[
\max_{x' \supseteq x} T^-_{x' \setminus x} \leq \eta \leq \min_{x' \subseteq x} T^+_{x' \setminus x},
\]
\[
\max_{x' \supseteq x, x' \notin X(\eta)} T^+_{x' \setminus x} \leq \eta \leq \min_{x' \subseteq x, x' \notin X(\eta)} T^-_{x' \setminus x}.
\]

**Proof.** For all $x' \supseteq x$, we have $v_{x' \setminus x}(\eta) \geq 0$. For all $x' \subset x$, we have $v_{x' \setminus x}(\eta) \leq 0$. If $x' \notin X(\eta)$, then both inequalities are strict. Equations (5)–(7) imply the result. □

Equation (14) demonstrates that instead of an increasing function $\iota: \mathbb{R} \rightarrow \{1, \ldots, n+1\}$ such that $\iota(\eta) \in I(\eta)$ for all $\eta \in \mathbb{R}$, we are now interested in a decreasing function $\xi: \mathbb{R} \rightarrow \mathcal{X}$ in the sense that for $\eta' > \eta$ it holds that $\xi(\eta') \subseteq \xi(\eta)$. Furthermore, $\xi(\eta) \in X(\eta)$ should hold for all $\eta \in \mathbb{R}$. The following lemma guarantees the existence of such a function $\xi$. 17
Lemma 4.3. Let \( \eta, \eta' \in \mathbb{R} \), \( x \in X(\eta) \). Then the following statements hold:

(a) If \( \eta' > \eta \), then there exists an \( x' \in X(\eta') \) such that \( x' \subseteq x \).

(b) If \( \eta' < \eta \), then there exists an \( x' \in X(\eta') \) such that \( x' \supseteq x \).

Proof. For the proof of part (a), suppose the contrary: For all \( x' \in X(\eta') \) we have that, either, (i) \( x' \supseteq x \), or, (ii) there is no nesting relationship between \( x' \) and \( x \).

Then, \( x \notin X(\eta') \). Note that \( X(\eta') \) is non-empty. We now take any \( x' \in X(\eta') \).

If (i) holds, then \( v_{x' \setminus x}(\eta') < 0 \) and \( v_{x' \setminus x}(\eta) \geq 0 \), creating a contradiction to the monotonicity in the first argument of the identification function.

If (ii) holds, then \( x \cap x' \subsetneq x \), which implies \( x \cap x' \notin X(\eta') \), hence \( s_{x'}(\eta') < s_{x \cap x'}(\eta) \). Also, \( x \in X(\eta) \) implies \( s_{x}(\eta) \leq s_{x \cup x'}(\eta) \). Since \( x' \setminus (x \cap x') = x' \setminus x = (x \cup x') \setminus x \), we have \( v_{x' \setminus x}(\eta') < 0 \) and \( v_{x' \setminus x}(\eta) \geq 0 \), creating a contradiction to the monotonicity in the first argument of the identification function.

The proof of part (b) is analogous to part (a). \( \square \)

Because \( X \) is the set of possible superlevel sets induced by the partial order on \( \{z_1, \ldots, z_n\} \) it always holds that \( \{z_1, \ldots, z_n\} \in X \) and \( \emptyset \in X \). The set \( X \) is a lattice and together with the subset relation has a bottom and top element. As \( \eta \) increases, \( \xi \) follows one of the totally ordered paths through the lattice; see Figure 3 for an illustration. The existence of a minimizing path through the lattice, that is \( \xi(\eta) \in X(\eta) \) for all \( \eta \in \mathbb{R} \) is a consequence of Lemma 4.3. In Figure 3 the direction of movement through the lattice as \( \eta \) increases is illustrated by arrows. The left-continuity of these paths in \( \eta \in \mathbb{R} \) follows with the same argument as in the proof of Lemma 3.4 and is essentially just a consequence of the left-continuity of the identification function \( V \).

The functions \( \xi \) are in one-to-one correspondence to the solutions \( \hat{g} \) of the isotonic regression problem. The following proposition is analogous to Proposition 3.5 and allows to recover \( \hat{g} \) from \( \xi \).

Proposition 4.4. Let \( \xi : \mathbb{R} \rightarrow X \) be a decreasing, left-continuous function such that \( \xi(\eta) \in X(\eta) \). Then, the function \( \hat{g} : \{z_1, \ldots, z_n\} \rightarrow \mathbb{R} \) given by

\[
\inf\{\eta : \ell \notin \xi(\eta)\} = \hat{g}(z_\ell) = \max\{\eta : \ell \in \xi(\eta)\} \quad (15)
\]

is the unique function that satisfies

\[
\{z : g(z) \geq \eta\} = \{z_\ell : \ell \in \xi(\eta)\} \quad \text{for all } \eta \in \mathbb{R},
\]

among all increasing functions \( g : \{z_1, \ldots, z_n\} \rightarrow \mathbb{R} \).

Proof. The left-continuity and monotonicity of \( \xi : \mathbb{R} \rightarrow X \) implies (15).
The monotonicity of \( \hat{g} \) follows from the monotonicity of \( \xi \) and the fact that each path through the lattice is totally ordered. Let \( \eta' \in \mathbb{R} \). Then,

(i) \( \hat{g}(z_\ell) \geq \eta' \Rightarrow \xi(\hat{g}(z_\ell)) \subseteq \xi(\eta') \Rightarrow \ell \in \xi(\eta') \).

(ii) For any \( \ell \in \xi(\eta') \) : \( \hat{g}(z_\ell) = \max\{\eta : \ell \in \xi(\eta)\} \geq \eta' \).

Therefore, \( \{z : \hat{g}(z) \geq \eta'\} \subseteq \{z_\ell : \ell \in \xi(\eta')\} \subseteq \{z : \hat{g}(z) \geq \eta'\} \) where the first inclusion follows by (i) and the second by (ii). Uniqueness of \( \hat{g} \) follows because increasing functions are characterized by their superlevel sets.

As a generalization of Proposition 3.6, we can provide min-max and max-min bounds on solutions to the isotonic regression problem.

**Proposition 4.5.** Let \( \ell \in \{1, \ldots, n\} \) and let \( \hat{g} \) be a solution to the isotonic regression problem. Then, subject to \( x, x' \in \mathcal{X} \),

\[
\min_{x' : \ell \notin x' \cup x \supseteq x} \max_{x : \ell \in x} T^-_{x \setminus x'} \leq \hat{g}(z_\ell) \leq \max_{x : \ell \in x} \min_{x' : \ell \not\in x' \cup x \supseteq x} T^+_{x' \setminus x'}.
\]

**Proof.** Applying the first set of bounds from Proposition 4.2 to the formula for \( \hat{g} \) at (15), we obtain

\[
\inf_{\eta : \ell \notin \xi(\eta)} \max_{x \supseteq \xi(\eta)} T^-_{x \setminus \xi(\eta)} \leq \hat{g}(z_\ell) \leq \max_{\eta : \ell \in \xi(\eta)} \min_{x' \subseteq \xi(\eta)} T^+_{x' \setminus \xi(\eta)}.
\]

The lower bound is bounded from below by \( \min_{x' : \ell \notin x'} \max_{x \supseteq x'} T^-_{x \setminus x'} \), and the upper bound is bounded from above by \( \max_{x'' : \ell \in x''} \min_{x' \subseteq x''} T^+_{x' \setminus x''} \).
In the case of partial orders on the covariates, it is also possible to define minimal and maximal solutions. Recall that, analogously to \( I(\eta) \), we defined \( X(\eta) \) as the set of index sets \( x \in \mathcal{X} \) minimizing \( s_x(\eta) \) at (13). Now, let

\[
X^- (\eta) = \{ x \in X(\eta) : \exists x' \in X(\eta) \text{ such that } x' \subseteq x \},
\]

\[
X^+ (\eta) = \{ x \in X(\eta) : \exists x' \in X(\eta) \text{ such that } x' \supseteq x \}
\]

denote the sets of minimal and maximal elements of \( X(\eta) \), respectively. In order to prove an analogous statement to Proposition 3.7, we need the following lemma on a modified max-min inequality.

**Lemma 4.6.** Let \( \ell \in \{1, \ldots, n\} \) and let \( T_x \) map to a singleton for all \( x \in \mathcal{X} \). We identify \( T_x \) with its unique element. Then, subject to \( x, x' \in \mathcal{X} \),

\[
\max \min_{x, x' \in \mathcal{X}} T_{x \setminus x'} \leq \min \max_{x, x' \in \mathcal{X}} T_{x \setminus x'}.
\]

**Proof.** Let \( x'' \in \mathcal{X} \) such that \( \ell \notin x'' \), then

\[
\max \min_{x, x' \in \mathcal{X}} T_{x \setminus x'} \leq \max_{x, x' \in \mathcal{X}} T_{x \setminus (x \setminus x'')} \leq \max_{x, x' \in \mathcal{X}} T_{x \setminus x''}.
\]

Since \( \mathcal{X} \) is closed under intersection, we have \( \max_{x, x' \in \mathcal{X}} \min_{x, x' \in \mathcal{X}} T_{x \setminus x'} \leq \max_{x, x' \in \mathcal{X}} T_{x \setminus x''} \) for all \( x'' \in \mathcal{X} \) such that \( \ell \notin x'' \). \( \square \)

**Proposition 4.7.** Let \( \ell \in \{1, \ldots, n\} \), and let \( \xi : \mathbb{R} \rightarrow \mathcal{X} \) be decreasing and left-continuous.

(a) If \( \xi(\eta) \in X^+(\eta) \) for all \( \eta \in \mathbb{R} \), then, subject to \( x, x' \in \mathcal{X} \),

\[
\hat{g}(z_\ell) = \min \max_{x, x' \in \mathcal{X}} T^+_{x \setminus x'} = \max \min_{x, x' \in \mathcal{X}} T^+_{x \setminus x'}.
\]

(b) If \( \xi(\eta) \in X^-(\eta) \) for all \( \eta \in \mathbb{R} \), then, subject to \( x, x' \in \mathcal{X} \),

\[
\hat{g}(z_\ell) = \min \max_{x, x' \in \mathcal{X}} T^-_{x \setminus x'} = \max \min_{x, x' \in \mathcal{X}} T^-_{x \setminus x'}.
\]

**Proof.** The proof follows using Lemma 4.6 and applying the same steps as in the proof of Proposition 4.5 to the second set of bounds in Proposition 4.2. \( \square \)

In order prove the existence of a function \( \xi \) (and thus \( \hat{g} \)) that solves the isotonic regression problem, we need that \( \mathcal{X} \) is closed under union and intersection. This property is heavily used in the proof of Lemma 4.3.

We could also start with a set \( \mathcal{X} \) of subsets of \( \{z_1, \ldots, z_n\} \) that are interpreted as the admissible superlevel sets of the function \( g \) that is to be fitted. If \( \mathcal{X} \) is closed under union and intersection, then \( \mathcal{X} \) induces a partial order on \( \{z_1, \ldots, z_n\} \) by Birkhoff’s Representation Theorem; see for example Gurney and Griffin (2011). Consequently, the optimal function \( \hat{g} \) always exists and is increasing.

Starting with \( \mathcal{X} \), one could formulate different constraints than isotonicity on \( g \) as long as they can be formulated in terms of restrictions on admissible superlevel sets. Examples are unimodality or quasi-convexity. Generally, there is no solution that is simultaneously optimal with respect to all elementary loss functions; see Section 5 for examples in the case of a unimodality constraint.
Figure 4: **Possible Modes.** For a sample of 4 data points, the five possible choices $m_1, \ldots, m_5$ for the mode, and the corresponding subdivision into isotonic and antitonic part for the functions $\hat{g}_1, \ldots, \hat{g}_5$ are marked.

### 5 Unimodal Regression

It is astonishing that in isotonic regression, there exists a solution that is simultaneously optimal for all loss functions in the class $\mathcal{S}$ which exhausts all consistent loss functions for the functional $T$ in many relevant examples. One might wonder whether this is still fulfilled for slightly adapted shape constraints. Unimodality is a shape constraint closely related to isotonicity. One estimation procedure is to take a mode between two consecutive observations and then split the dataset in two. On the subset preceding the mode an isotonic regression is performed and on the data following the mode an antitonic regression is performed. This procedure is then repeated for any possible choice of mode, as illustrated in Figure 4. Finally the optimal function is chosen by selecting the one with minimal loss. The reason for the mode to be chosen outside of $\{z_1, \ldots, z_n\}$ is to avoid ambiguity. If the mode is fixed on observation $z_i$, $1 < i < n$, then the isotonic regression on $\{z_1, \ldots, z_i\}$ and the antitonic regression on $\{z_i, \ldots, z_n\}$ might yield two different values for $\hat{g}(z_i)$.

Fixing mode $m_i$ and applying our method to $\{z_1, \ldots, z_{i-1}\}$ and $\{z_i, \ldots, z_n\}$ with isotonicity and antitonicity, respectively, as shape constraints yields a function $\hat{g}_i: \{z_1, \ldots, z_n\} \to \mathbb{R}$ that is optimal for any consistent loss function for functional
The question arises whether there is one mode \( m_i \) such that the corresponding \( \hat{g}_i \) dominates all other functions \( \hat{g}_j, j \neq i \). It turns out that this is generally not the case.

To give an example, we consider four observations \((z_1, y_1), \ldots, (z_4, y_4)\) with \( z_1 < \cdots < z_4 \) and \((y_1, \ldots, y_4) = (9, 9, 0, 10)\), and let \( P \) denote the corresponding empirical distribution. We choose the expectation functional as the regression target, and consider modes \( m_1, \ldots, m_5 \) with \( m_1 < z_1 < m_2 < z_2 < \cdots < z_4 < m_5 \). For modes \( m_1 \) and \( m_3 \), the unimodal approach yields the PAVA partitions \( Q_{m_1} = Q_{m_3} = \{\{z_1, z_2\}, \{z_3, z_4\}\} \), and for mode \( m_2 \), we obtain the PAVA partition \( Q_{m_2} = \{\{z_1\}, \{z_2\}, \{z_3, z_4\}\} \). But for this specific data example all three modes yield the same function i.e., \( \hat{g}_1 = \hat{g}_2 = \hat{g}_3 \). For modes \( m_4 \) and \( m_5 \), we obtain the partitions \( Q_{m_4} = Q_{m_5} = \{\{z_1, z_2, z_3\}, \{z_4\}\} \) and therefore \( \hat{g}_4 = \hat{g}_5 \). The functions \( \hat{g}_1, \ldots, \hat{g}_5 \) are illustrated in Figure 5.

Solution \( \hat{g}_i, 1 \leq i \leq 5 \), dominates all other \( \hat{g}_j, j \neq i \), if

\[
E_{P^* \eta}(\hat{g}_i(Z), Y) \leq E_{P^* \eta}(\hat{g}_j(Z), Y) \quad \text{for all } \eta \in \mathbb{R}, j \neq i.
\]

It can be seen that this condition is not fulfilled by plotting the expected elementary scores for \( \hat{g}_1, \ldots, \hat{g}_5 \); see Figure 6. This visual method of comparing forecasts is
Figure 6: **Murphy Diagram.** The Murphy diagram comparing the expected elementary scores of $\hat{g}_1, \ldots, \hat{g}_5$ for $\eta \in \mathbb{R}$ given realizations $(y_1, \ldots, y_4) = (9, 9, 0, 10)$.

called a Murphy diagram and was introduced by [Ehm et al.](#) (2016).

Hence, in unimodal regression there is not necessarily a solution $\hat{g}_i$ that simultaneously minimizes all consistent loss functions for a functional $T$. This agrees with our findings in Section 4 because the set $\mathcal{X}$ is not closed under union and intersection. Indeed, it holds that $\{z_1\}, \{z_4\} \in \mathcal{X}$ but $\{z_1, z_4\} \notin \mathcal{X}$. Therefore, the existence of a decreasing function $\xi: \mathbb{R} \to \mathcal{X}$ is not guaranteed.

**References**

Ayer, M., Brunk, H. D., Ewing, G. M., Reid, W. T. and Silverman, E. (1955). An empirical distribution function for sampling with incomplete information. *Ann. Math. Statist.*, 26, 641–647.

Barlow, R. E., Bartholomew, D. J., Bremner, J. M. and Brunk, H. D. (1972). *Statistical Inference Under Order Restrictions*. Wiley, London.

Bartholomew, D. J. (1959a). A test of homogeneity for ordered alternatives. *Biometrika*, 46, 36–48.
Bartholomew, D. J. (1959b). A test of homogeneity for ordered alternatives. II. *Biometrika*, 46, 328–335.

Belloc, P. C. (2018). Sharp oracle inequalities for least squares estimators in shape restricted regression. *Ann. Statist.*, 46, 745–780.

Brümmer, N. and Du Preez, J. (2013). The PAV algorithm optimizes binary proper scoring rules. Available at arXiv:1304.2331.

Brunk, H. D. (1955). Maximum likelihood estimates of monotone parameters. *Ann. Math. Statist.*, 26, 607–616.

Dawid, A. P. (2016). Contribution to the discussion of “Of quantiles and expectiles: Consistent scoring functions, Choquet representations and forecast rankings” by Ehm, W., Gneiting, T., Jordan, A. and Krüger, F. *J. R. Stat. Soc. Ser. B. Stat. Methodol.*, 78, 505–562.

Ehm, W., Gneiting, T., Jordan, A. and Krüger, F. (2016). Of quantiles and expectiles: Consistent scoring functions, Choquet representations and forecast rankings. *J. R. Stat. Soc. Ser. B. Stat. Methodol.*, 78, 505–562.

Gneiting, T. (2011). Making and evaluating point forecasts. *J. Amer. Statist. Assoc.*, 106, 746–762.

Groeneboom, P. and Jongbloed, G. (2014). *Nonparametric estimation under shape constraints*. Cambridge University Press, New York.

Guntuboyina, A. and Sen, B. (2018). Nonparametric shape-restricted regression. *Statist. Sci.*, 33, 568–594.

Gurney, A. J. T. and Griffin, T. G. (2011). Pathfinding through congruences. In *Relational and Algebraic Methods in Computer Science*, vol. 6663. Springer, Heidelberg, 180–195.

Han, Q., Wang, T., Chatterjee, S. and Samworth, R. J. (2017). Isotonic regression in general dimensions. Available at arXiv:1708.09468.

Kyng, R., Rao, A. and Sachdeva, S. (2015). Fast, provable algorithms for isotonic regression in all $L_p$-norms. In *Advances in Neural Information Processing Systems 28*. Curran Associates, Inc., Red Hook, 2719–2727.

Luss, R. and Rosset, S. (2017). Bounded isotonic regression. *Electron. J. Stat.*, 11, 4488–4514.

Miles, R. E. (1959). The complete amalgamation into blocks, by weighted means, of a finite set of real numbers. *Biometrika*, 46, 317–327.
Moesching, A. and Duembgen, L. (2019). Monotone least squares and isotonic quantiles. Available at arXiv:1901.02398.

Newey, W. K. and Powell, J. L. (1987). Asymmetric least squares estimation and testing. *Econometrica*, 55, 819–847.

Patton, A. J. (2019). Comparing possibly misspecified forecasts. *J. Bus. Econom. Statist.* Forthcoming.

Polonik, W. (1998). The silhouette, concentration functions and ML-density estimation under order restrictions. *Ann. Statist.*, 26, 1857–1877.

Robertson, T. and Wright, F. T. (1973). Multiple isotonic median regression. *Ann. Statist.*, 1, 422–432.

Robertson, T. and Wright, F. T. (1980). Algorithms in order restricted statistical inference and the Cauchy mean value property. *Ann. Statist.*, 8, 645–651.

Savage, L. J. (1971). Elicitation of personal probabilities and expectations. *J. Amer. Statist. Assoc.*, 66, 783–801.

Stout, Q. F. (2015). Isotonic regression for multiple independent variables. *Algorithmica*, 71, 450–470.

van Eeden, C. (1958). *Testing and Estimating Ordered Parameters of Probability Distributions*. Mathematical Centre, Amsterdam.

Ziegel, J. F. (2016). Contribution to the discussion of “Of quantiles and expectiles: Consistent scoring functions, Choquet representations and forecast rankings” by Ehm, W., Gneiting, T., Jordan, A. and Krüger, F. *J. R. Stat. Soc. Ser. B. Stat. Methodol.*, 78, 505–562.