

# Appendix to Generalized Isotonic Regression published in the Journal of Computational and Graphical Statistics

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## 1 Appendix

We need the following additional terminology: A group  $X$  *majorizes* (*minorizes*) another group  $Y$  if  $X \succeq Y$  ( $X \preceq Y$ ). A group  $X$  is a *majorant* (*minorant*) of  $X \cup A$  where  $A = \cup_{i=1}^k A_i$  if  $X \not\prec A_i$  ( $X \not\prec A_i$ )  $\forall i = 1 \dots k$ .

### Proof of Theorem 1:

We prove by contradiction. Assume there exists a union of  $K$  blocks in  $V$  in the optimal solution labeled  $\mathcal{M} = M_1 \cup \dots \cup M_K$  that get broken by the cut, with  $M_1$  and  $M_K$  as the minorant and majorant block in  $\mathcal{M}$ , and  $M_k^L$  and  $M_k^U$  as the groups in  $M_k$  below and above the cut. Define  $\mathcal{L}$  as the union of all blocks in  $V$  that lie “below” the algorithm cut,  $\mathcal{U}$  as the union of all blocks in  $V$  that lie “above” the algorithm cut. Further define  $A_K^L \subseteq \mathcal{L}$  ( $A_1^U \subseteq \mathcal{U}$ ) as the union of blocks along the algorithm cut such that  $A_K^L \succ M_K^L$  ( $A_1^U \prec M_1^U$ ). Figure 1 depicts an example of these definitions where  $A_1^U = A_1^L = A_K^U = A_K^L = \{\}$  for simplicity.

We first prove that  $w_{M_1} > w_V$ . First, consider the case  $A_1^U = \{\}$ . By convexity of  $f_i(\cdot)$  and summing over group  $M_1^U$ , we have

$$\sum_{i \in M_1^U} f_i(w_{M_1^U}) \geq \sum_{i \in M_1^U} f_i(w_V) + (w_{M_1^U} - w_V) \sum_{i \in M_1^U} \left. \frac{\partial f_i(\hat{y}_i)}{\partial \hat{y}_i} \right|_{w_V}.$$

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Definition of the weight operator gives

$$\sum_{i \in M_1^U} f_i(w_{M_1^U}) \leq \sum_{i \in M_1^U} f_i(w_V) \Rightarrow (w_{M_1^U} - w_V) \sum_{i \in M_1^U} \frac{\partial f_i(\hat{y}_i)}{\partial \hat{y}_i} \Big|_{w_V} \leq 0.$$

Finally, by the definition of the algorithm cut in (11) since no block exists below  $M_1^U$  to affect isotonicity,

$$\sum_{i \in M_1^U} \frac{\partial f_i(\hat{y}_i)}{\partial \hat{y}_i} \Big|_{w_V} \leq 0 \quad (1)$$

so that  $w_{M_1^U} \geq w_V$ . Since  $M_1$  is a block, we have  $w_{M_1^L} > w_{M_1^U}$ , and then

$$w_{M_1^L} > w_{M_1^U} > w_V \Rightarrow w_{M_1} > w_V.$$

For the case,  $A_1^U \neq \{\}$ , we have  $w_{M_1} > w_{A_1^U} > w_V$  with the first inequality due to optimality and the second follows directly the proof above replacing  $M_1^U$  by  $A_1^U$ . A proof for  $w_{M_K} < w_V$  follows a similar argument focusing on  $M_K^L$ . Putting this together gives  $w_{M_1} > w_V > w_{M_K}$ , which contradicts that  $M_1$  and  $M_K$  are blocks in the global solution, since by assumption then  $w_{M_1} < w_{M_K}$ . The case  $K = 1$  is also trivially covered by the above arguments. We conclude that the algorithm cannot cut any block. ■

### Proof of Theorem 2:

The proof is by induction. The base case, i.e., first iteration, where all points form one group is trivial. The first cut is made by solving linear program (11) which constrains the solution to maintain isotonicity.

Assuming that iteration  $k$  (and all previous iterations) provides an isotonic solution, we prove that iteration  $k + 1$  must also maintain isotonicity. Figure 2 helps illustrate the situation described here. Let  $G$  be the group split at iteration  $k + 1$  and denote  $A$  ( $B$ ) as the group under (over) the cut. Let  $\mathcal{A} = \{X : X \text{ is a group at iteration } k + 1, \exists i \in X \text{ such that } (i, j) \in \mathcal{I} \text{ for some } j \in A\}$  (i.e.,  $X \in \mathcal{A}$  border  $A$  from below).

Consider iteration  $k + 1$ . Denote  $\mathcal{X} = \{X \in \mathcal{A} : w_A < w_X\}$  (i.e.,  $X \in \mathcal{X}$  violates isotonicity with  $A$ ). The split in  $G$  causes the fit in nodes in  $A$  to decrease. Proof that

$$\sum_{i \in A} \frac{\partial f_i(\hat{y}_i)}{\partial \hat{y}_i} \Big|_{w_G} \geq 0$$

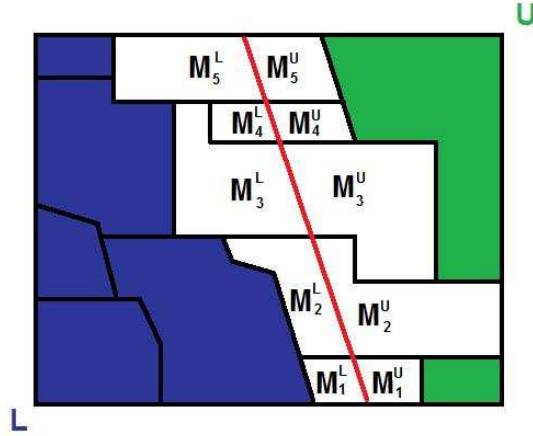


Figure 1: Illustration of proof of Theorem 1. Black lines separate blocks. The diagonal red line through the center demonstrates a cut of Algorithm 1.  $\mathcal{L}$  is the union of blue blocks below the cut and  $\mathcal{U}$  is the union of green blocks above the cut. White blocks are blocks that are potentially split by Algorithm 1. These blocks are split into  $M_1^L, \dots, M_5^L$  below the cut and  $M_1^U, \dots, M_5^U$  above the cut. In the proof,  $M_i = M_i^L \cup M_i^U \forall i = 1 \dots 5$ . The proof shows, for example, that if the algorithm splits  $M_1$  into  $M_1^L$  and  $M_1^U$  according to the defined cut in (11), then there must be no isotonicity violation when creating blocks from  $M_1^L$  and  $M_1^U$ . However, since  $M_1$  is assumed to be a block, there must exist an isotonicity violation between  $M_1^L$  and  $M_1^U$ , providing a contradiction.

follows the proof of (15) in Theorem 1 above so that  $w_A \geq w_G$ . We will prove that when the fits in  $A$  decrease, there can be no groups below  $A$  that become violated by the new fits to  $A$ , i.e., the decreased fits in  $A$  cannot be such that  $\mathcal{X} \neq \{\}$ .

We first prove that  $\mathcal{X} = \{\}$  by contradiction. Assume  $\mathcal{X} \neq \{\}$ . Denote  $k_0 < k + 1$  as the iteration at which the last of the groups in  $\mathcal{X}$ , denoted  $D$ , was split from  $G$  and suppose at iteration  $k_0$ ,  $G$  was part of a larger group  $H$  and  $D$  was part of a larger group  $F$ . It is important to note that  $X \cap (F \cup H) = \{\} \forall X \in \mathcal{X} \setminus D$  at iteration  $k_0$  because by assumption all groups in  $\mathcal{X} \setminus D$  were separated from  $A$  before iteration  $i$ . Thus, at iteration  $k_0$ ,  $D$  is the only group bordering  $A$  that violates isotonicity.

Let  $D_U$  denote the union of  $D$  and all groups in  $F$  that majorize  $D$ . By construction,  $D_U$  is a majorant in  $F$ . Hence  $w_{D_U} < w_{F \cup H}$  by Algorithm 1 and  $w_A < w_{D_U}$  by definition since  $w_{D_U} > w_D > w_A$ . Also by construction, any set  $X \in H$  that minorizes  $A$  has  $w_X < w_A$  (each set  $X$  that minorizes  $A$  besides  $D$  such that  $w_X < w_A$  has already been split from  $A$ ). Hence we can denote  $A_L$  as the union of  $A$  and all groups in  $H$  that minorize  $A$  and we have  $w_A > w_{A_L}$  and  $A_L$

is a minorant in  $H$ . Since  $A_L \subseteq H$  at iteration  $i$ , we have

$$w_{F \cup H} < w_{A_L} < w_A < w_{D_U} < w_{F \cup H}$$

which is a contradiction, and hence the assumption  $\mathcal{X} \neq \{\}$  is false. The first inequality is because the algorithm left  $A_L$  in  $H$  when  $F$  was split from  $H$ , and the remaining inequalities are due to the above discussion. Hence the split at iterations  $k + 1$  could not have caused a break in isotonicity.

A similar argument can be made to show that the increased fit for nodes in  $B$  does not cause any isotonic violation. The proof is hence completed by induction. ■

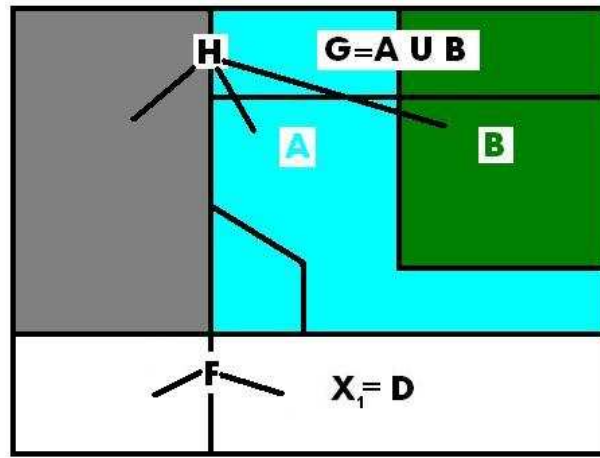


Figure 2: Illustration of proof of Theorem 2 showing the defined sets at iteration  $k + 1$ .  $G$  is the set divided at iteration  $k + 1$  into  $A$  (all blue area) and  $B$  (all green area). The group bordering  $A$  from below denoted by  $X_1$  (also referred to as  $D$  in the proof) is in violation with  $A$ . At iteration  $k_0$ ,  $G$  is part of the larger group  $H$  and  $X_1$  is part of the larger group  $F$ . At iteration  $k_0$ , groups  $F$  and  $H$  are separated. The proof shows that when  $A$  and  $B$  are split at iteration  $k + 1$ , no group such as  $X_1$  where  $w_{X_1} > w_A$  could have existed. In the picture,  $X_1$  must have been separated at an iteration  $k_0 < k + 1$ , but the proof, through contradiction, shows that this cannot occur.