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# Merge and chop in the computation for isotonic regressions

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**Abstract**

In this article the sufficient conditions for the merge and chop of domain partition sets during the computation for isotonic regressions are derived. The proposed merge-and-chop procedure yields exact isotonic regressions in finite steps when the orderings are of Type I or II defined in this paper. Simple tree orderings, umbrella orderings and simple orderings are of Type I or II. The paper also provides an example showing that the procedure works beyond Types I and II orderings.


*Keywords:* Isotonic regression; Lower set; Projection; Quasi-order; Upper set

## 1. Introduction

The Pool-Adjacent-Violator Algorithm (PAVA) for computing isotonic regressions by Ayer et al. (1955) works only for simple orderings. The iterative algorithm by Dykstra (1983) and extended by Dykstra and Boyle (1987) produces a sequence of functions that converges to the isotonic regression. Simple ordering and successive projection method still draw attentions, see Kearsley (2006). Thompson (1962) describes the Minimum-Violator Algorithm (MVA) that, just like PAVA, yields the exact isotonic regression in finite steps but works only for tree restrictions. This algorithm is recently implemented by Hansohm (2007) for hierarchical orderings.

Both PAVA and MVA involve the merge of "adjacent" points in the domain of a function. In this paper we study and derive the conditions for the merge of domain partition sets during the computation for isotonic regressions. To simplify the calculation sometimes part of the domain on which the values of the isotonic regression are already determined can be chopped off. Sufficient conditions for such operation are also investigated and established. Based on this study the merge-and-chop procedure is proposed. This procedure is an integrated merge-and-chop process in both upward and downward directions, and produces the exact isotonic regressions in finite steps for many commonly encountered orderings. In this paper Types I and II orderings are defined, and it is shown that the isotonic regressions associated with Types I and II orderings can be successfully computed by the merge-and-chop procedure. Umbrella orderings, simple tree orderings and simple orderings are all of Type I or II. In the implemented computer program the order types are automatically detected. The procedure, however, is carried out regardless of the order types. As shown in an example

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the success may be achieved even if the orderings are not of Type I nor of Type II since the success is also function dependent.

The preliminaries on isotonic regressions are reviewed in the next section. Sections 3 and 4 are on the merge and chop, respectively. The merge-and-chop procedure is introduced in Section 5. In Section 6 the implementation is discussed and a numeric example is presented. The comparisons with other computation methods and the conclusion remarks are placed in Section 7.

## 2. Isotonic regression

Quasi-order $\preceq$ is a transitive and reflexive binary relation on $\Omega = \{x_1, \ldots, x_n\}$. Let $L$ and $U$ be two subsets of $\Omega$. By the Definition 1.4.1 of Robertson et al. (1988) $L$ is a lower set if $x \in L$ is implied by $x \preceq y$ and $y \in L$, $U$ is an upper set if $y \in U$ is implied by $x \preceq y$ and $x \in U$. For weight function $w(x)$, $w(x_i) = w_i > 0$, and a given function $f(x)$, $f(x_i) = f_i$, set function $\mathrm{Av}(M|f, w) = \sum_{x_i \in M} f_i w_i / \sum_{x_i \in M} w_i$ gives the weighted average of $f$ on $M \subset \Omega$. With respect to the values of this set function in any collection of subsets of $\Omega$ there are maximum valued sets and minimum valued sets. But in the collection of all upper sets and in the collection of all lower sets the largest maximum valued upper set and the largest minimum valued lower set are unique. Since $\preceq$ confined on $M \subset \Omega$ is a quasi-order in $M$, lower sets, upper sets, maximum valued upper sets, minimum valued lower sets, the largest maximum valued upper set and the largest minimum valued lower set can be defined for subsets of $M$. A function $f$ is said to be isotonic if $f_i \leqslant f_j$ is implied by $x_i \preceq x_j$. Let $C$ be the collection of all isotonic functions on $\Omega$. Then $C$ is a convex cone in $R^n$. This cone is closed for the norm induced from the inner product $\langle f, g \rangle = \sum_{x_i \in \Omega} f_i g_i w_i$.Thus there is a unique function $f^* \in C$ that minimizes $\| f - g \|$ over all $g \in C$. This function is the projection of $f$ onto $C$, denoted by $f^* = P_C(f)$, and is called the isotonic regression of $f$. It is well known that $f^* = P_C(f)$ if and only if $f^* \in C$, $\langle f - f^*, f^* \rangle = 0$ and $\langle f - f^*, g \rangle \leqslant 0$ for all $g \in C$, see Zarantonello (1971, Lemma 1.1). The next theorem summarizing other well known facts is placed here without a proof.

**Theorem 1.** *Suppose $t$ is one of the values $f^* = P_C(f)$ assumes, and $T$ is the level set of $f^*$ at level $t$, i.e., $T = \{x : f^*(x) = t\}$. Then the followings hold*:

(a) $t = \mathrm{Av}(T|f, w)$.
(b) *$T$ is the largest maximum valued upper set in* $\{x : f^*(x) \leqslant t\}$.
(c) *$T$ is the largest minimum valued lower set in* $\{x : f^*(x) \geqslant t\}$.

In this paper it is assumed that $\mathcal{T} = \{T_1, \ldots, T_m\}$ is the collection of all level sets of $f^* = P_C(f)$ in which $T_i = \{x : f^*(x) = t_i\}$, $i = 1, \ldots, m$. Clearly $\mathcal{T}$ is a partition of $\Omega$. By (a) of Theorem 1 the isotonic regression of $f$ is completely determined by this partition.

## 3. Merge

Matrix $A = (a_{ij})_{n \times n}$, where $a_{ij} = 1$ if $x_i \preceq x_j$, and $a_{ij} = 0$ otherwise, gives all order pairs, and is called the all-order matrix. Order pair $x_i \preceq x_j$ is a base-order if it is not implied by the reflexivity nor by the transitivity. Matrix $B = (b_{ij})_{n \times n}$, where $b_{ij} = 1$ if $x_i \preceq x_j$ is a base order, and $b_{ij} = 0$ otherwise, is called the base-order matrix. A quasi-order can be defined by its all-order matrix, base-order matrix or any matrix $G = (g_{ij})_{n \times n}$, where $g_{ij} = 0$ or1, and $B \leqslant G \leqslant A$ component wise. For example

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad G = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

define the same umbrella ordering $x_1 \preceq x_2 \preceq x_3 \succeq x_4 \succeq x_5$.