

MONOTONE REGRESSION

JAN DE LEEUW

Abstract. This is an entry for The Encyclopedia of Statistics in Behavioral Science, to be published by Wiley in 2005.

In linear regression we fit a linear function $y = \alpha + \beta x$ to a scatterplot of n points (x_i, y_i) . We find the parameters α and β by minimizing

$$\sigma(\alpha, \beta) = \sum_{i=1}^n w_i (y_i - \alpha - \beta x_i)^2,$$

where the w_i are known positive weights.

In the more general nonlinear regression problem we fit a nonlinear function $\phi_\theta(x)$ by minimizing

$$\sigma(\theta) = \sum_{i=1}^n w_i (y_i - \phi_\theta(x_i))^2$$

over the parameters θ . In both cases, consequently, we select the minimizing function from a family of functions indexed by a small number of parameters.

Date: March 27, 2004.

Key words and phrases. monotone regression, optimal scaling, multidimensional scaling.

In some statistical techniques low-dimensional parametric models are too restrictive. In nonmetric multidimensional scaling [3], for example, we can only use the rank order of the x_i and not their actual numerical values. Parametric methods become useless, but we still can fit the best fitting monotone (increasing) function non-parametrically. Suppose there are no ties in x , and the x_i are ordered such that $x_1 < \dots < x_n$. In monotone regression we minimize

$$\sigma(z) = \sum_{i=1}^n w_i (y_i - z_i)^2,$$

over z , under the linear inequality restrictions that $z_1 \leq \dots \leq z_n$. If the solution to this problem is \hat{z} , then the best fitting increasing function is the set of pairs (x_i, \hat{z}_i) . In monotone regression the number of parameters is equal to the number of observations. The only reason we do not get a perfect solution all the time is because of the order restrictions on z .

Actual computation of the best fitting monotone function is based on the theorem that if $y_i > y_{i+1}$ then $\hat{z}_i = \hat{z}_{i+1}$. In words: if two consecutive values of y are in the wrong order, then the two corresponding consecutive values of the solution \hat{z} will be equal. This basic theorem leads to a simple algorithm, because knowing that two values of \hat{z} must be equal reduces the number of parameters by one. We thus have a monotone regression problem with $n - 1$ parameters. Either the elements are now in the correct order, or there is a violation, in which case we can reduce the problem to one with

$n - 2$ parameters. And so on. This process always comes to an end, in the worst possible case when we only have a single parameter left, which is obviously monotone.

We can formalize this in more detail as the up-and-down blocks algorithm of [4]. It is illustrated in the table below, in which the first row is y . The first violation we find is $3 > 0$, or 3 is not up-satisfied. We merge the two elements to a block, which contains their weighted average $\frac{3}{2}$ (in our example all weights are one). But now $2 > \frac{3}{2}$, and thus the new value $\frac{3}{2}$ is not down-satisfied. We merge all three values to a block of three and find $\frac{5}{3}$, which is both up-satisfied and down-satisfied. We then continue with the next violation. Clearly the algorithm produces a decreasing number of blocks. The value of the block is computed using weighted averaging, where the weight of a block is the sum of the weights of the elements in the block. In our example we wind up with only two blocks, and thus the best fitting monotone function \hat{z} is a step function with a single step from $\frac{5}{3}$ to 4.

y	2	3	0	6	6	0
	2	$\frac{3}{2}$	$\frac{3}{2}$	6	6	0
	$\frac{5}{3}$	$\frac{5}{3}$	$\frac{5}{3}$	6	6	0
	$\frac{5}{3}$	$\frac{5}{3}$	$\frac{5}{3}$	6	3	3
\hat{z}	$\frac{5}{3}$	$\frac{5}{3}$	$\frac{5}{3}$	4	4	4

Table 1. Computing Monotone Regression

This is also illustrate in the figure below. The line through the points x and y is in blue. This is obviously the best possible fitting function. The best fitting monotone function, which we just computed, is in red.

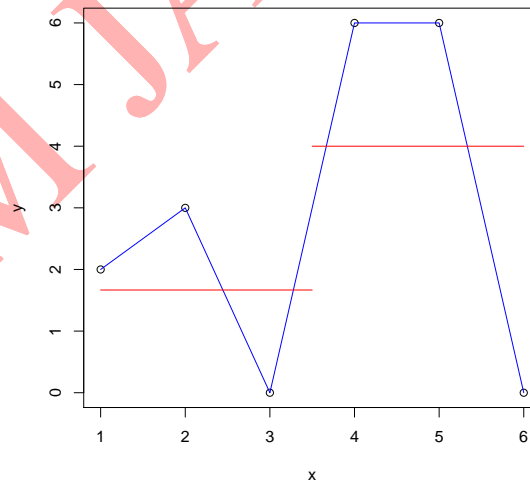


Figure 1. Plotting Monotone Regression

If x has ties, then this simple algorithm does not apply. There are two straightforward adaptations [2]. In the primary approach to ties we start our monotone regression with blocks of y values corresponding to the ties in x . Thus we require tied x values to correspond with tied z values. In the secondary approach we pose no constraints on tied values, and it can be shown that in that case we merely have to order the y values such that they are increasing in blocks of tied x values. And then we perform an ordinary monotone regression.

We finally mention that monotone regression can be generalized in two important directions. First, basically the same algorithm can be used to minimize any separable function of the form $\sum_{i=1}^n f(y_i - z_i)$, with f any convex function with its minimum at zero. For instance, f can be the absolute value function, in which case we merge blocks by computing medians instead of means. And second, we can generalize the algorithm from weak orders to partial orders in which some elements cannot be compared. For details see [1].

References

- [1] R.E. Barlow, R.J. Bartholomew, J.M. Bremner, and H.D. Brunk. *Statistical Inference under Order Restrictions*. Wiley, New York, 1972.

- [2] J. De Leeuw. Correctness of Kruskal's Algorithms for Monotone Regression with Ties. *Psychometrika*, 42:141–144, 1977.
- [3] J. B. Kruskal. Multidimensional Scaling by Optimizing Goodness of Fit to a Nonmetric Hypothesis. *Psychometrika*, 29:1–27, 1964.
- [4] J.B. Kruskal. Nonmetric Multidimensional Scaling: a Numerical Method. *Psychometrika*, 29:115–129, 1964.

Department of Statistics, University of California, Los Angeles, CA 90095-1554

E-mail address, Jan de Leeuw: deleeuw@stat.ucla.edu

URL, Jan de Leeuw: <http://gifi.stat.ucla.edu>

FROM JAN'S DESK