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INTERPOLAZIONE STATISTICA NON ISOTONICA DI DATI STRATIGRAFICI

STATISTICAL NON-ISOTONIC INTERPOLATION OF STRATIGRAPHIC DATA

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Sommario

Questa tesi tratta il problema della regressione non lineare e non monotona di diversi data-set tramite il metodo di regressione statistica bivariata, usato insieme ad una semplice trasformazione per rendere i dati monotoni. Si introduce quindi un algoritmo efficiente per la trasformazione, insieme al metodo di regressione statistica bivariata. L'algoritmo è quindi applicato a differenti data-set non monotoni, su cui sarà poi usato il metodo di regressione statistica non monotona, seguita da una trasformazione inversa per ottenere il modello del data-set. Il metodo di regressione non isotonica proposto è applicato ad una collezione di dati riguardanti le stratigrafie di atomi di stronzio.

Abstract

This thesis deals with the problem of nonlinear, non-monotonic regression of different data-sets by the statistical bivariate regression method used together with a simple transformation to make data monotonic. The present paper introduces an efficient algorithm to perform the transformation to be paired with a statistical bivariate regression method. The algorithm is then applied to different non-monotonic data-sets, which are subsequently treated with the statistical bivariate regression method, followed by an inverse transformation to obtain a model of the data-set. The proposed novel non-isotonic regression model is applied to a collection of data about strontium isotope stratigraphy.

Chapter 1

Introduction

Every experiment or phenomenological study produces a set of data. When this set is not non-monotonic it is hard to obtain a model of the data and to infer the value of missing records by interpolation. One solution is to infer a functional relationship between variables using regression analysis [8, 9, 10], which is an application of information processing of paramount importance [1, 3, 12, 14, 15, 17, 19, 20]. The present research takes its moves from the isotonic statistical bivariate regression (SBR) method presented in [11] (which was successfully applied to estimate the glomerular filtration rate in kidneys). Previous comparative studies [9, 11] have clearly shown how statistical regression implemented by look-up tables is much faster in execution than traditional techniques while affording the same modeling/regression abilities.

Since isotonic regression is based on the assumption that the variables stay in a monotonic relationship, the SBR method cannot work on data sets that are not monotonically increasing nor decreasing. A possible remedy is to use a transformation to achieve the monotonization of these data sets, which is the subject of the present research. In the chapter 2 a non-linear transformation is presented: it transforms an original data set so that the relation between the dependent variable and the independent variable looks monotonic. Chapter 3 contains a summary of the SBR method that will be applied to the data set after such transformation. After using the SBR method to infer a model, the inverse transformation described in Chapter 2 is applied to obtain a non-monotonic model. In Chapter 4 some results of numerical tests are illustrated and discussed.

A regression problem that motivated the present research endeavour is marine stratigraphy as confronted in [16]. Marine stratigraphy is at the heart of geology and deals with the study of marine deposits over ages of the earth [4, 5, 6]. The principal aim of stratigraphy is to produce a time scale to date geological processes by arranging rocks in chronological order on the basis of their inorganic and organic characteristics [18].

Absolute radiometric dating is the base for investigating the gross speed of processes such as tectonic movements or organic evolution [18]. The dataset analyzed through non-isotonic regression as well as the results of regression are explained in the chapter 5.

Chapter 6 concludes the thesis.

Chapter 2

Proposed transformation

The present chapter shows a novel transformation that will be used before the SBR method. It arises from the definition of increasing monotone function: a function $h : [a,\ b] \to \mathbb{R}$ is called increasing monotone if, for each $x_1 \leqslant x_2$, i have that $h(x_1) \leqslant h(x_2)$. A differentiable function is increasing monotone if an only if $h'(x) > 0$ (the prime $'$ denotes differentiation) for any $x \in [a,\ b]$.

Assume that a function $f : [a,\ b] \to \mathbb{R}$ is not monotonic: a non-linear transformation that makes it monotone increasing is defined as

$$h(x) := r \int_a^x \exp\left(c\, f'(\xi)\right) d\xi + f(a), \tag{2.1}$$

where $r, c > 0$ are constants. In fact, $h'(x) = r \exp(c\, f'(x))$ is positive for every x. The domain of the function h stays $[a,\ b]$, while its co-domain is $[f(a), \infty)$. The transformation (2.1) admits an exact inverse

$$f(x) = \frac{1}{c} \int_a^x \log\left(\tfrac{1}{r} h'(\xi)\right) d\xi + f(a). \tag{2.2}$$

The transformation exploits the exponential function that for any value gives a number larger than zero. So i have a sum of positive values and i obtain an ever increasing result.

A finite data-set is a set of pairs

$$\mathbb{D} := \{(x_1, y_1), (x_2, y_2), (x_3, y_3), \ldots, (x_n, y_n)\}, \tag{2.3}$$

where x_i denotes a sample of the independent variable, y_i a sample of the dependent variable, and n denotes the number of samples. Further, i assume that all the x_i values are unique (no repetitions) and that the pairs in $\mathbb{D}$ are sorted in ascending order according to the x_i values.

The (2.1) may be adapted to a finite data-set as follows:

$$z_i = \begin{cases} y_1, & \text{for } i = 1, \\ z_{i-1} + r \exp\left(c \, \frac{y_i - y_{i-1}}{x_i - x_{i-1}}\right)(x_i - x_{i-1}), & \text{for } i > 1, \end{cases} \tag{2.4}$$

where the pairs (x_i, z_i) constitute the monotonic dataset obtained from the transformation, namely

$$\mathbb{M} := \{(x_1, z_1), (x_2, z_2), (x_3, z_3), \dots, (x_n, z_n)\}. \tag{2.5}$$

The inverse transformation is achieved by

$$y_i = \begin{cases} z_1, & \text{for } i = 1, \\ y_{i-1} + \frac{1}{c}(x_i - x_{i-1}) \log\left(\frac{1}{r} \frac{z_i - z_{i-1}}{x_i - x_{i-1}}\right), & \text{for } i > 1. \end{cases} \tag{2.6}$$

The exponent of e is the difference between two adjacent values in $\mathbb{D}$. Through the inverse, on the other hand, the sign of this difference is maintained thanks to the natural logarithm of two adjacent points of the transformation. In order to be functional, the first point of the transformed function and the original function coincide. This is the initial point where it should be iteratively applied the transformation for the others points.

The proposed formula considers the finite difference $x_i - x_{i-1}$ as an approximation of the differential dx. The constants r and c are fundamental. They allow us to control the range of monotonic data so that they do not grow or decrease too quickly.

In tests presented in the Chapter 4 the value of r is constantly set to 0.1. The value of c, indeed, is modified several times with values between 0.001 to 0.0000001 to compare the various results obtained. As i shall see in Chapter 4 the value of c is very important when the inverse will be applied to the interpolated data with SBR.

A proposed pseudo-code of monotonicity transformation is outlined in the Algorithm 1. Line 1: the call to the function requires as arguments the x and y arrays that

Algorithm 1 Pseudo-code to implement the transformation (2.4).

```
1: function MONO(r, c, x, y)
2:     z_1 ← y_1
3:     i ← 2
4:     while i ⩽ length(x) do
5:         Δx_i ← x_i − x_{i−1}
6:         Δy_i ← y_i − y_{i−1}
7:         z_i ← z_{i−1} + r ∗ exp(c ∗ Δy_i/Δx_i) ∗ Δx_i
8:         i ← i + 1
9:     return z
```

will be transformed and the constants for control of the range, r and c. Lines 2-3: there is defined the point for starting an iterative cycle based on the value of index i. Lines 4-8: the monotonic transformation is computed. Line 9: The array z is returned as output of the function.

The Algorithm 2 shows a pseudo-code to implement the inverse of the transformation in Algorithm 1. Line 1: the call to the function requires as arguments the x and z

Algorithm 2 Pseudo-code to implement the transformation (2.6).

1: **function** INVMONO(r, c, x, z)

2: $y_1 \leftarrow z_1$

3: $i \leftarrow 2$

4: **while** $i \leqslant \text{length}(x)$ **do**

5: $\Delta x_i \leftarrow x_i - x_{i-1}$

6: $\Delta z_i \leftarrow z_i - z_{i-1}$

7: $y_i \leftarrow \Delta x_i * \log((\Delta z_i / \Delta x_i)/r)/c + y_{i-1}$

8: $i \leftarrow i + 1$

9: **return** y

arrays that may be transformed back to non monotonic data and the constants for control of the range, r and c that are necessarily the same as in the direct processing. Lines 2-3: definitions of the point for starting an iterative cycle based on the value of index i. Lines 4-9: the inverse of monotonic transformation is computed. Line 10: The array y is returned as output of the function.

Chapter 3

Statistical bivariate regression

Statistical bivariate regression (SBR) is a mathematical method that allows to deduce the value of missing points between adjacent pairs of points (x_i, y_i), thus obtaining a mathematical model. It is an improvement over isotonic regression.

In the paper [11] it was presented an algorithm that estimates the cumulative distribution function (CDF) of the set x. The inverse cumulative distribution function ((INVCDF)) of the y set is used by the algorithm to obtain the sought model. This algorithm can work only on monotonic data. A pseudo-code for the SBR procedure is shown in the Algorithm 3. In the pseudo-code, q_x denotes a set of query-points where

Algorithm 3 Pseudo-code to implement statistical bivariate regression.

```
function SBR(x, y, q_x)
    P_x ← CDF(x, q_x);
    q_y ← INVCDF(y, P_x)
    return q_y
```

the model is needed to be inferred, while the set q_y denotes the corresponding response. In other words, the set q_x contains values of the independent variable that were not observed, hence that do not belong to the set x and the procedure SBR infers the corresponding values of the dependent variable. For a detailed explanation of the underlying theory, interested readers might consult the published paper [11].

Chapter 4

Numerical experiments

This chapter discusses the results of several numerical tests. The numerical tests were performed on synthetic as well as real-world data drawn from public repositories.

4.1 Un-blended and blended methods

Once the SBR method is used on a monotonic data set, the inverse of the transformation is applied on interpolated data.

In the tests that follow i can clearly see how, directly applying the inverse transformation to the obtained numerical model, for constant c values up to 10^{-3}, it is obtained an incorrect model compared to the original: the new data do not homogeneously respect the distances relative to those of the original set. This problem disappeared for constant c values smaller than 10^{-4} and the correct model obtained never changes with the decreasing of c.

In this report, the direct application of the INVMONO function to the model is called *un-blended method*. In addition, another solution is proposed, which is referred to as *blended method*. This method consists in gathering the x and q_x sets (respectively, the original data and the query point) into $\hat{x}$ and then gathering the y and q_y sets (respectively original data and the algorithmic response to query points) into $\hat{y}$. By applying the INVMONO function to the pair $(\hat{x}, \hat{y})$, i get a model that contains information from both the original data-points as well as the point inferred by the SBR procedure. Recovering the results of de-monotonization corresponding to the query points (q_x, q_y) i get the model i are looking for. From the following tests it will be clear how for any value of the constant c, the blended method is always effective.

4.2 Specifications of data sets used in the experiments

Several data sets, each exhibiting different features, will be used as tests of the monotonicity transformation and SBR method applied together in combination. At the end of each test there is a comparison between the blended method and un-blended method results.

The Figure 4.1 shows the data sets on which the behavior of monotonic transformation and SBR method were tested.

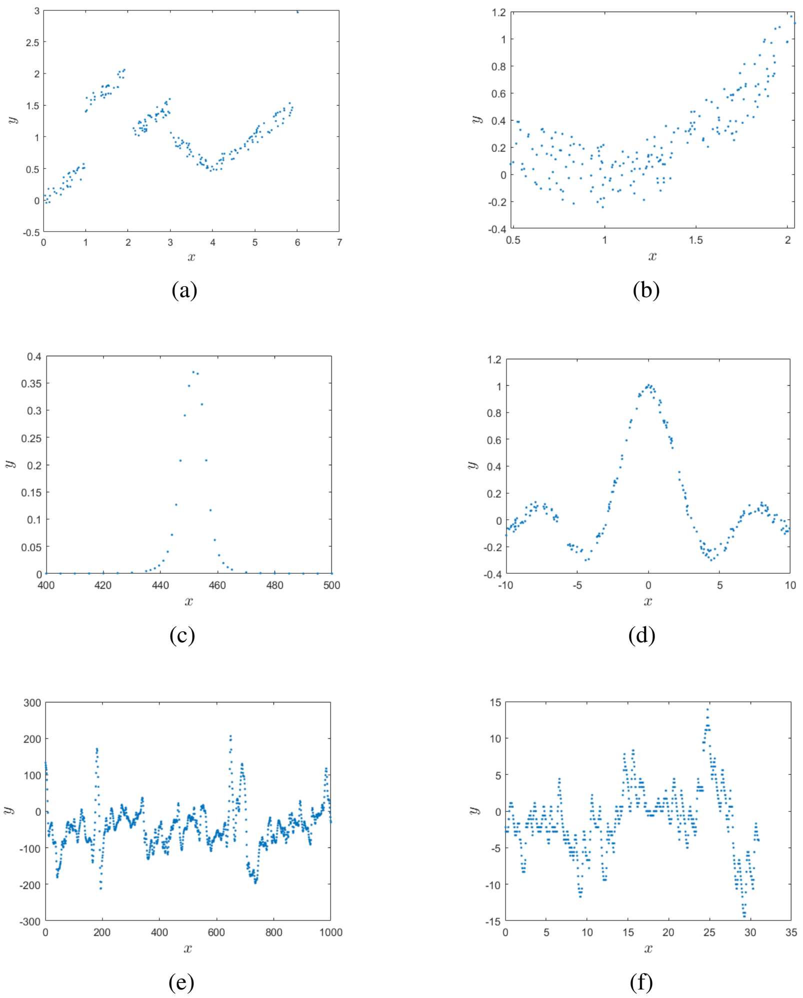


Figure 4.1: Graphical illustration of the three synthetic and three real-world data sets used in the numerical experiments: (a) Dataset 1; (b) Dataset 2; (c) Dataset 3; (d) Dataset 4; (e) Dataset 5; (f) Dataset 6.

These data sets have been borrowed from the article [9]. Some specifications about these data are as follows:

- The Dataset 1, Dataset 2 and Dataset 4 are synthetically generated data that exhibit specific features. The Dataset 1 was generated to as to exhibit a discontinuous dependency between the independent variable x and the dependent variable y as well as moderate noise. The Dataset 2 was designed on the basis of a quadratic dependency and large additive noise. The Dataset 4 was designed on the basis of a moderately noisy, oscillating (cardinal-sine-type) dependency.

- The Dataset 3 was downloaded from the repository described in [7] and is the result of a NIST study involving circular interference transmittance. It has been chosen because it contains only 35 records for a comparison with other large data sets.

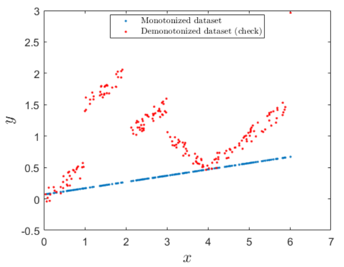
- The Dataset 5 arises from an electrocardiogram (ECG) readout. The x variable represents a data-sample (or temporal) index, while the y variable represents an ECG voltage reading. This dataset contains 1000 sample pairs.

- The Dataset 6 is a real-world data set of temperature readings (in Celsius scale) taken every hour at the Logan Airport for the entire month of January 2011. This dataset contains 744 sample pairs.

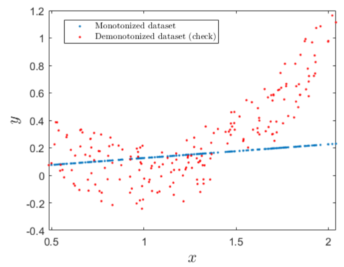
The real-world data sets exhibit large variability in the variables' ranges. All numerical experiments were performed on a MATLAB® platform.

4.3 Results of the monotonization function

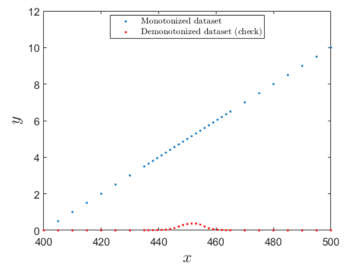
In this section the results of the monotonic transformation are illustrated through numerical examples. The Figure 4.2 shows the results of monotonization applied to the Data sets 1 to 6. In the figures, blue points denote transformed data while red points denote the results of the inverse transform. These results were obtained by setting $c = 0.0001$.



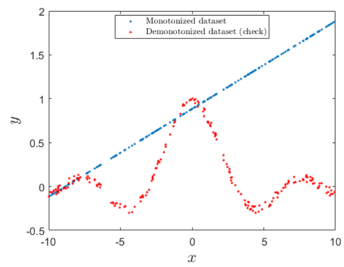
(a)



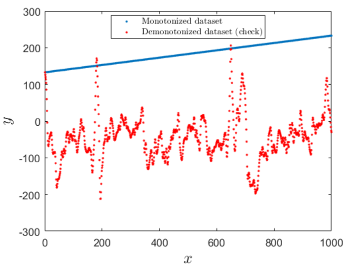
(b)



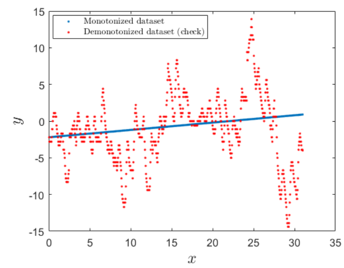
(c)



(d)



(e)



(f)

Figure 4.2: Results of monotonization/demonotonization applied to: (a) Data set 1, (b) Data set 2, (c) Data set 3, (d) Data set 4, (e) Data set 5, (f) Data set 6.

In all the figures the red points coincide with the original data-points, confirming that the monotonization/demonotonization cascade is an approximate identity. It is interesting to observe that, with the very low value of the constant c taken, the monotonized data distribute along a straight line.

4.4 Results of statistical bivariate regression on monotonized data

This section illustrates the results of statistical bivariate regression. In the Figures 4.3, blue points indicate monotonic data obtained with the previous transformation, while red circles denote the results of the interpolation performed by the SBR procedure. In

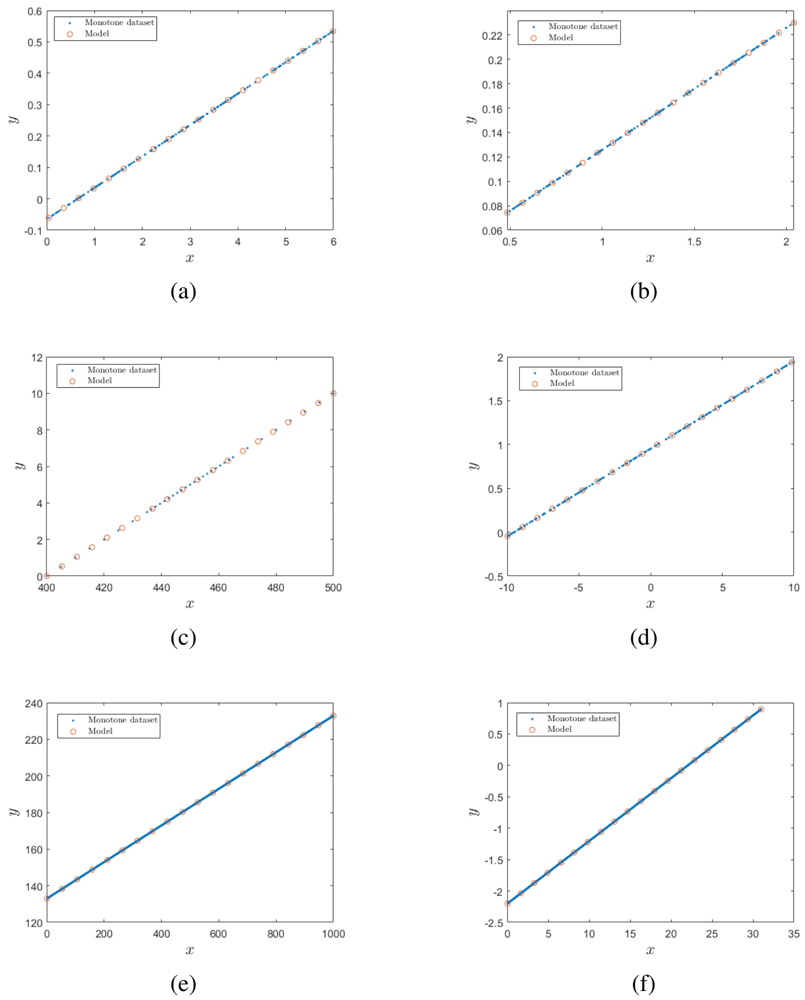


Figure 4.3: Result of statistical bivariate regression by the SBR method applied to: (a) Data set 1, (b) Data set 2, (c) Data set 3, (d) Data set 4, (e) Data set 5, (f) Data set 6.

all experiments, a value $c = 0.0001$ was used. In all experiments the result of statistical modeling look coherent with the monotonized data.

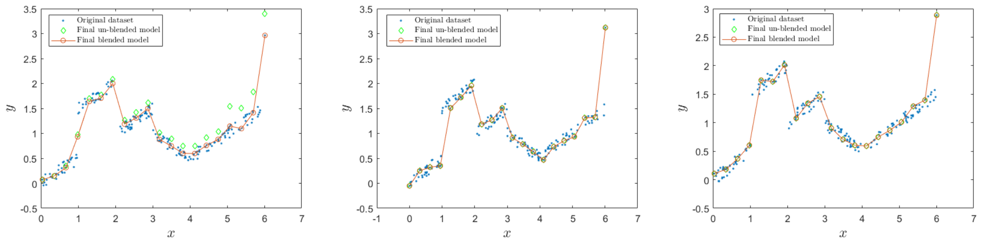
4.5 Final results of original data regression

In the last phase of the tests the blended and un-blended methods to achieve de-monotonization were compared. Three different values of the constant c were chosen, namely $c = 0.0001$, $c = 0.00001$ and $c = 0.000001$.

The Figure 4.4 shows the results obtained on the Data Set 1.

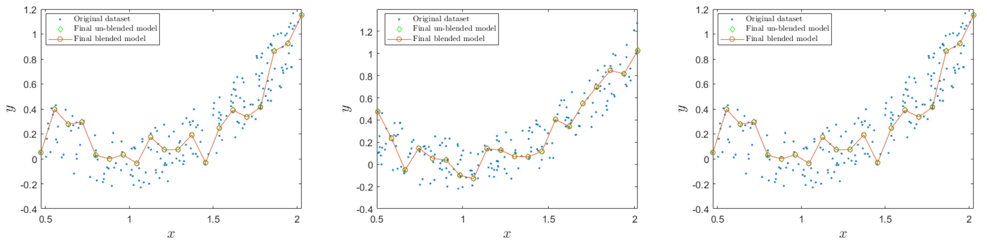
The Figure 4.5 shows the results obtained on the Data Set 2.

The Figure 4.6 shows the results obtained on the Data Set 3.



(a) (b) (c)

Figure 4.4: Results of non-isotonic modeling obtained on the Data set 1 with $r = 0.1$ and: (a) $c = 0.0001$, $c = 0.00001$, (c) $c = 0.000001$.

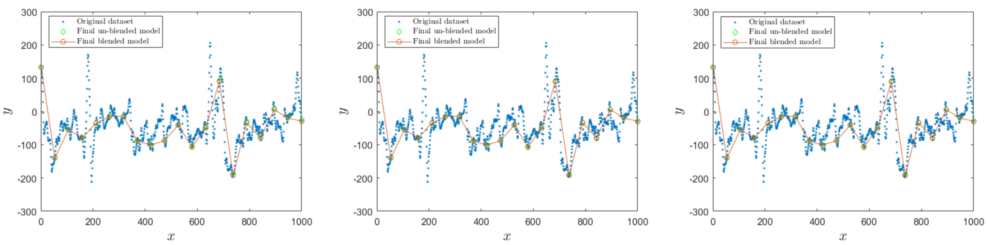


(a) (b) (c)

Figure 4.5: Results of non-isotonic modeling obtained on the Data set 2 with $r = 0.1$ and: (a) $c = 0.0001$, $c = 0.00001$, (c) $c = 0.000001$.

The Figure 4.7 shows the results obtained on the Data Set 4.

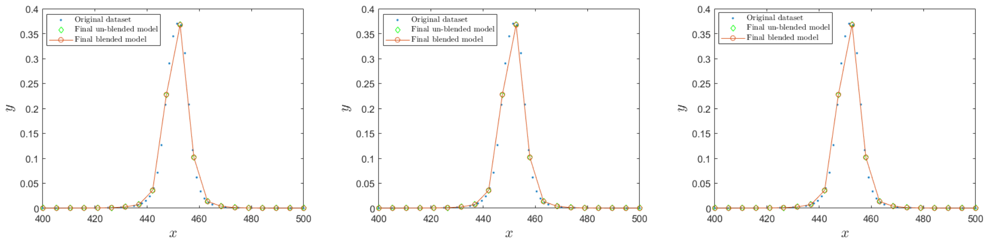
The Figure 4.8 shows the results obtained on the Data Set 5.



(a) (b) (c)

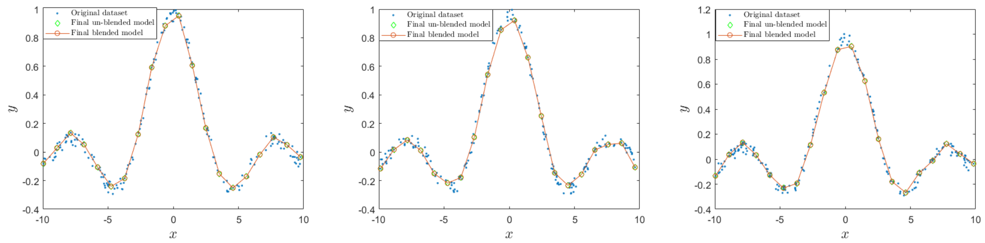
Figure 4.8: Results of non-isotonic modeling obtained on the Data set 5 with $r = 0.1$ and: (a) $c = 0.0001$, $c = 0.00001$, (c) $c = 0.000001$.

The Figure 4.9 shows the results obtained on the Data Set 6.



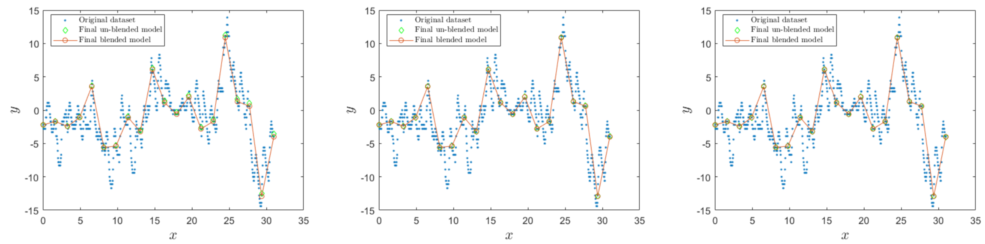
(a) (b) (c)

Figure 4.6: Results of non-isotonic modeling obtained on the Data set 3 with $r = 0.1$ and: (a) $c = 0.0001$, $c = 0.00001$, (c) $c = 0.000001$.



(a) (b) (c)

Figure 4.7: Results of non-isotonic modeling obtained on the Data set 4 with $r = 0.1$ and: (a) $c = 0.0001$, $c = 0.00001$, (c) $c = 0.000001$.



(a) (b) (c)

Figure 4.9: Results of non-isotonic modeling obtained on the Data set 6 with $r = 0.1$ and: (a) $c = 0.0001$, $c = 0.00001$, (c) $c = 0.000001$.

It is very clearly noticed, especially in Datasets 1, 2, 5 and 6, that the un-blended-based model deviates from the original one, while it will coincide with blended model for very small values of the constant c.

Chapter 5

Application to strontium isotope stratigraphy

The present chapter deals with an application of the proposed non-isotonic regression method to a collection of Strontium isotope stratigraphic data from a study by McArthur, Howarth and Bailey [16], where the author refer to this collection with the name of "*V3*". The purpose of the study by McArthur and coworkers was to compile a table that affords assigning numerical ages to sediments based on concentration of radioactive Strontium isotopes ^{87}Sr/^{86}Sr.

The *V3* dataset comes in pairs of 3401 records of the type (x_i, y_i), where the variable x denotes the age of a sediment, expressed in Ma ('mega-annum' corresponding to a period of 1 million years) and the variable y denotes the ratio ^{87}Sr/^{86}Sr of Strontium isotopes [2]. The dataset *V3* is indeed incomplete, since 11 records are missing a y value and one record presents a 0 value in the y attribute.

In order to apply the devised non-isotonic regression method to this dataset, the collection need to be fixed. As i can see from the expression (2.4) this method cannot be applied in the presence of more records that present the same value in the x attribute, therefore, as a first fix, all those values have been replaced with a pair (x,$\bar{y}$) where the x is unchanged and the $\bar{y}$ is the mean value taken among all records whose x attribute was repeated. Furthermore, incomplete records were removed from *V3* to realize the regression exercise. After this pre-processing, the dataset reduced to 3389 pairs.

In the following, i will show the result of the non-isotonic regression method applied to the reformed *V3*. The interpolation covers only the range $0 - 509$ Ma as in the study by McArthur, Howarth and Bailey.

The Figure 5.1 shows the results obtained on the whole dataset.

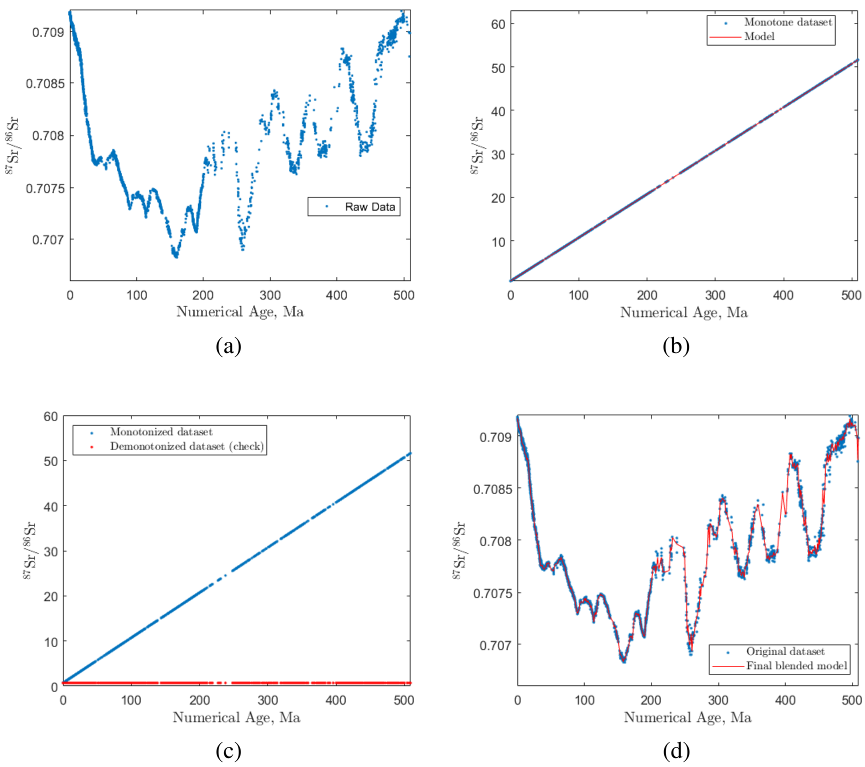


Figure 5.1: Results of non-isotonic modeling obtained on *V3* with $r = 0.1$ and $c = 0.1$ (range $0 - 509$ Ma). The bottom-right panel shows the numerical model superimposed to the raw data.

In order to get more details about the evolution of the fitting, following [16], i have divided the interval $0 - 509$ Ma into several sub-intervals and focused the view on each of them.

The Figure 5.2 shows the results obtained on the first half ($0 - 210$ Ma). In three out of four graphs, the data-points are pretty dense, hence the statistical regression method, which bases on the probability distribution of the data, possesses enough information to infer a data model. In the graph corresponding to the interval $30 - 70$ Ma, the data-points are less dense and the algorithm can only produce a coarse model of the relationship between the dependent and the independent variable.

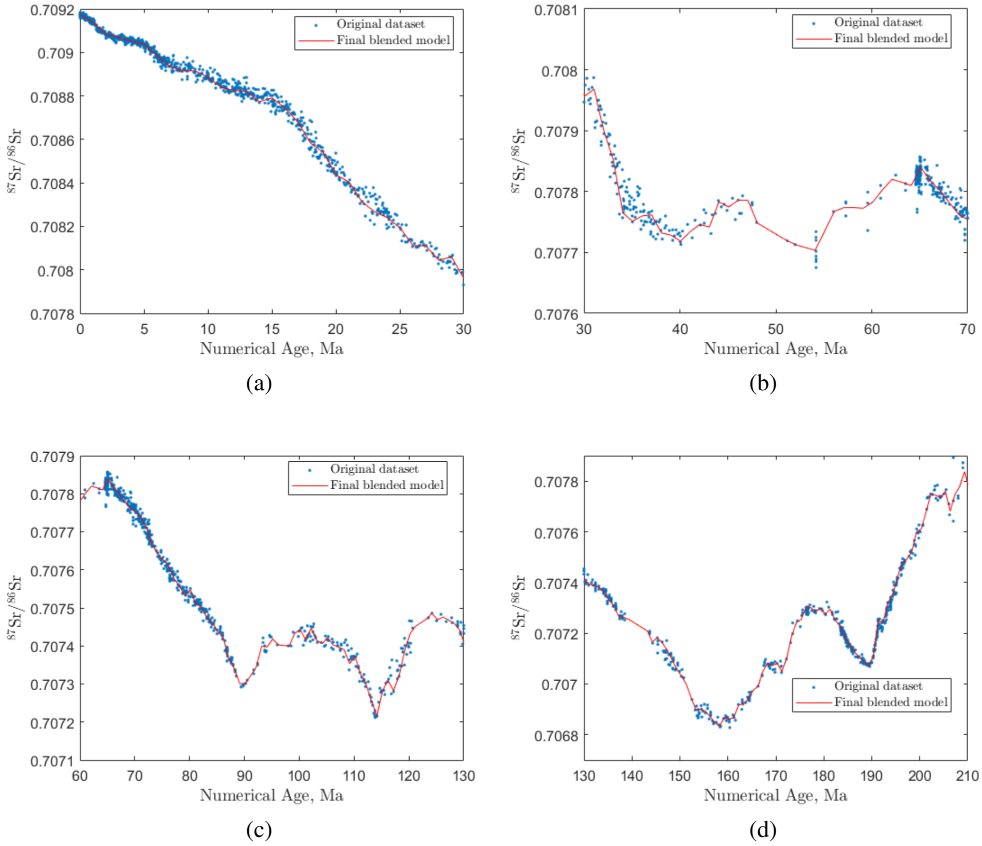


Figure 5.2: Results of non-isotonic modeling obtained on *V3*: First four subintervals, two of which are slightly overlapping as in [16]. Only incomplete records have been omitted from the graphs.

The Figure 5.3 shows the results obtained on the second half (200 – 509 Ma). As already noted, wherever the data-points are scarce, the regression algorithm can only produce a coarse model. It is also interesting to observe how the regression algorithm ignores some data-points, as it happens for example to some data-points in the interval 360 – 370 Ma, treating them as outliers.

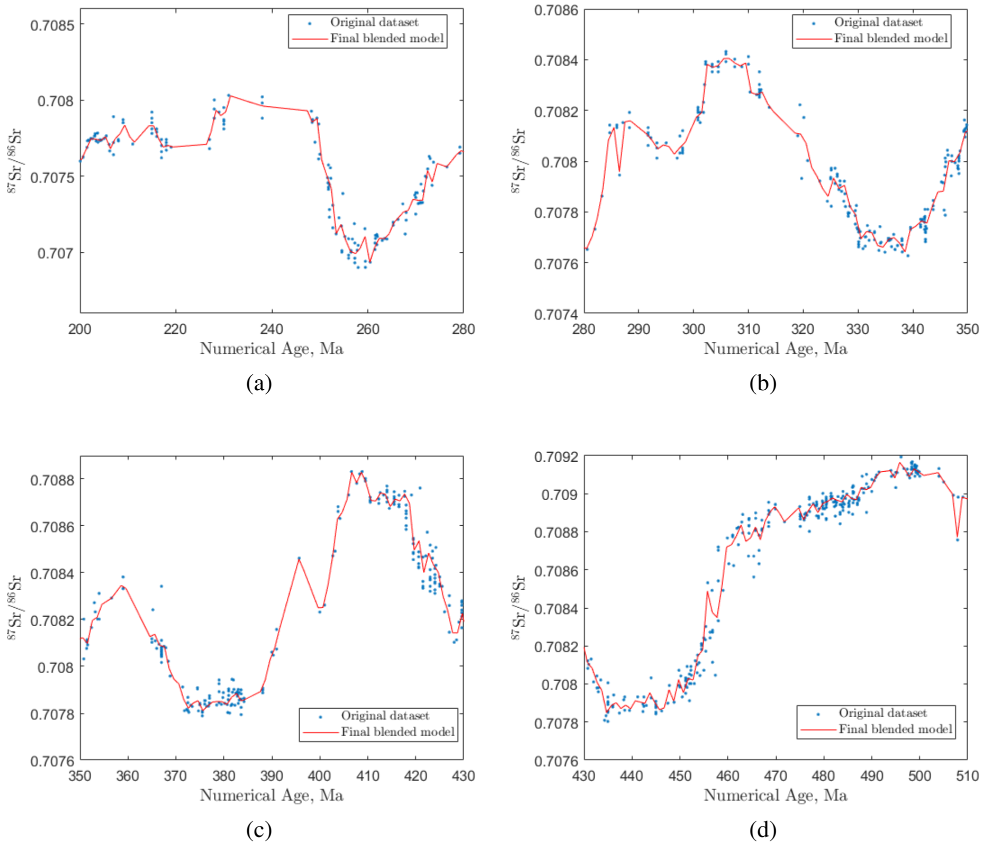


Figure 5.3: Results of non-isotonic modeling obtained on *V3*: Last four subintervals. The interval 200 – 210 Ma was repeated to get a clearer vision of the graphs, as in [16]. Only incomplete records have been omitted from the graphs.

For comparison purposes, the non-isotonic regression method is contrasted with the LOWESS method on the Strontium dataset. The LOWESS method is a nonparametric regression technique that is clearly explained on another article of McArthur and Howarth [13].

The LOWESS fit gives three graphs according to the mean of the model, its maximum and its minimum. The Figure 5.4 compares estimations provided by the devised statistical regression method and by the LOWESS method.

As it may readily be observed, the line output of the statistical regression method discussed in the present work agrees pretty well with the ‘Min LOWESS’ inference, except perhaps for a point around 220 Ma, where statistical regression seem to adhere more closely to the data than the LOWESS prediction, for the interval 230 – 250 Ma, where the LOWESS method predicts some spikes, while our method predicts a flatland,

and for a point around 400 Ma where, the Min LOWESS curve looks pretty smooth, while the curve pertaining to our method presents a spike.

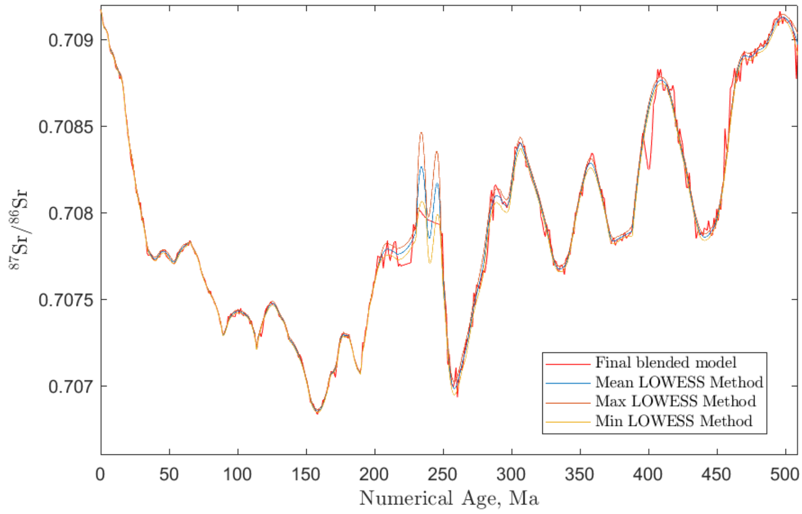
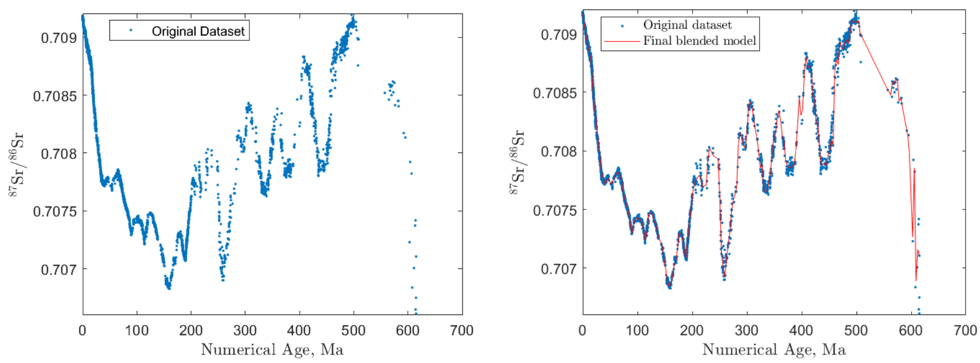


Figure 5.4: Comparison of the non-isotonic regression method and the three estimations gotten by the LOWESS method.

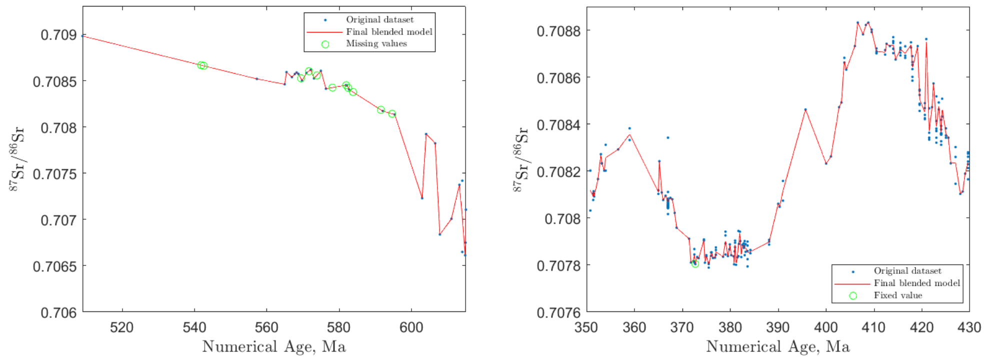
Since the *V3* data table extends to more than 600 Ma its age span, i have also tried to extend the model using the records of all the numerical ages even if they were further than 509 Ma. The Figure 5.5 represent the non-isotonic regression method applied to the whole dataset. The data appear not particularly well-tamed in the interval 500 – 600 Ma and are quite scarce, therefore the regression algorithm tries to fit them as well as it can returning a zig-zagging line.



(a) (b)

Figure 5.5: Results of non-isotonic modeling obtained on *V3* (whole range).

In addition, the missing values in the *V3* dataset have been filled-in as a result of interpolation by the regression model. The Figure 5.6 focuses the view on the missing records, and the Table 5.1 contains their numerical values.



(a) (b)

Figure 5.6: Representation of the missing values on *V3*: (a) Records that are missing a y attribute, (b) Record with a 0 in the y attribute.

Numerical age (Ma)	541.8	542.5	569.4	571.6	573.8	578.1
Strontium isotopes ratio	0.7087	0.7087	0.7085	0.7086	0.7086	0.7084
Numerical age (Ma)	581.9	582.5	583.8	591.5	594.6	372.7
Strontium isotopes ratio	0.7085	0.7084	0.7084	0.7082	0.7081	0.7078

Table 5.1: The table reports pairs of values that fill-in gaps in *V3*. The first 11 columns refer to missing values, the last column refers to the pair (x, y) that had the original y attribute equal to 0.

Chapter 6

Conclusion

This paper dealt with the problem of nonlinear, non-monotonic regression by the principles of isotonic statistical bivariate regression. Since isotonic regression may only cope with monotonic relationships, the present paper introduced an efficient algorithm to perform a reversible data-transformation to convert non-monotonic data to monotonic ones. Upon performing statistical regression by an isotonic regression technique previously devised by the author, the obtained monotonic data model is brought back to its original domain by applying a reversed transformation.

The devised algorithm was applied to different non-monotonic data-sets, either synthetic and natural, to test its capabilities and to investigate the sensitivity of the method to different choices of the free parameters.

In addition, the proposed novel non-isotonic regression method was applied to a collection of data about Strontium-isotope-based marine stratigraphy and the obtained results were compared to those obtained by a LOWESS method. The results of this comparison revealed that the devised non-isotonic statistical bivariate regression method compares favorably with the LOWESS method as it infers a model which appears yo be more adherent to the data and less bound by smoothness/continuity constraints. By applying the inferred model as an interpolation tool, the proposed method was also shown to be able to fill-in gaps in the original data sets.

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