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Sequential Nonlinear Mapping versus Simultaneous One

Algirdas Mykolas MONTVILAS
Institute of Mathematics and Informatics
Goštauto 12, LT-2021 Vilnius, Lithuania
e-mail: montvila@ktl.mii.lt

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Abstract. In the paper two methods for data structure analysis and visualisation are presented: the simultaneous nonlinear mapping (Sammon, 1969) and the sequential one (Montvilas, 1995). These two methods were compared according ability to map the data on the plane, mapping accuracy and a mapping time. It was showed that the sequential nonlinear mapping has some bigger total mapping error but needs considerable less calculation time than that of the simultaneous one. Examples are given.

Key words: simultaneous nonlinear mapping, sequential nonlinear mapping, accuracy, comparison.

1. Introduction

The nonlinear mapping of data from L-dimensional space to two-dimensional space is very important for the visualisation of data, their clustering, classification and for other data structure analysis. The *simultaneous* nonlinear mapping (Sammon, 1969) allows to map simultaneously all the data being already at a disposal. The *sequential* nonlinear mapping (Montvilas, 1995) do that in a real time. Furthermore it can be successfully used for sequential detection of states of a dynamic system, which states are described by many parameters (Montvilas, 1999).

The essence of any nonlinear mapping is to preserve the inner structure of distances among the parameter's vectors being in L-dimensional space after mapping them to two-dimensional space.

A heuristic relaxation method (Chang and Lee, 1973) maps a frame of M points and after that pairs of remaining points are considered in some order at every step (iteration). This method requires a smaller memory space than that of Sammon's one.

A triangular method of the *sequential* mapping (Lee *et all.*, 1977) preserves only two distances to vectors previously mapped and, in addition, it uses the spanning tree, so it makes the mapping dependent on the history, hence it is usable only for very special tasks.

In the paper two methods: simultaneous nonlinear mapping (Sammon, 1969) and sequential nonlinear mapping (Montvilas, 1995) are compared according ability to map the data on the plane, mapping accuracy and a mapping time.

It was showed that sequential nonlinear mapping has slightly bigger total mapping error but needs many times less calculation time. Thus, even having all the data already one can recommend to use the sequential nonlinear mapping for data structure analysis especially when there is a large amount of the data.

For the first we present these two methods for comparison them.

2. Simultaneous Nonlinear Mapping

This method for the analysis of multivariate data was presented by Sammon (1969). The algorithm is based upon a point mapping of N L-dimensional vectors from the L-space to a lower-dimensional (frequently two-dimensional) space such that the inherent structure of the data is approximately preserved under the mapping.

Suppose that we have N vectors of parameters in an L-dimensional space. Let's designate them by X_i, $i = 1, \dots, N$. The corresponding vectors in the two-dimensional space we designate by Y_i, $i = 1, \dots, N$. The distance between the vectors X_i and X_j in the L-space we define by d^*_{ij} and the distance between the corresponding vectors Y_i and Y_j in two-dimensional space define by d_{ij}. This algorithm uses the Euclidean distance measure because there is no a priori knowledge concerning the data. An initial two-space configuration for the Y vectors are better to choose along a descending diagonal (Sammon, 1969) and denote as follows:

$$Y_1 = \begin{bmatrix} y_{11} \\ y_{12} \end{bmatrix}, \quad Y_2 = \begin{bmatrix} y_{21} \\ y_{22} \end{bmatrix}, \quad \cdots, \quad Y_N = \begin{bmatrix} y_{N1} \\ y_{N2} \end{bmatrix}. \tag{1}$$

Now one can compute all the distances d^*_{ij} and d_{ij}, which are then used to define the error E, which represents how well the configuration of N points in the two-space fits the N points in the L-space:

$$E = \frac{1}{\sum_{i<j}^{N} d^*_{ij}} \sum_{i<j}^{N} \frac{\left(d^*_{ij} - d_{ij}\right)^2}{d^*_{ij}}. \tag{2}$$

Note that the error is a function of the $2 \times N$ variables y_{pq}, $p = 1, \dots, N$ and $q = 1, 2$. Now one have to change the two-space configuration so as to decrease the error. A steepest descent procedure to search for a minimum of the error is used.

The mapping error after the r-th iteration:

$$E(r) = \frac{1}{C} \sum_{i<j}^{N} \left[d^*_{ij} - d_{ij}(r)\right]^2 / d^*_{ij}, \tag{3}$$

where

$$C = \sum_{i<j}^{N} d^*_{ij},$$

and

$$d_{ij}(r) = \sqrt{\sum_{k=1}^{2} \left[y_{ik}(r) - y_{jk}(r)\right]^2}.$$

The new two-space configuration at time $r+1$ is given by

$$y_{pq}(r+1) = y_{pq}(r) - (MF) \cdot \Delta_{pq}(r), \tag{4}$$

where

$$\Delta_{pq}(r) = \frac{\partial E(r)}{\partial y_{pq}(r)} \Big/ \left| \frac{\partial^2 E(r)}{\partial y_{pq}^2(r)} \right|, \tag{5}$$

and *MF* is the "magic factor" which was determinated empirically to be between 0.3 and 0.4. The partial derivatives are given by

$$\frac{\partial E}{\partial y_{pq}} = \frac{-2}{C} \sum_{\substack{j=1 \\ j \neq p}}^{N} \left(\frac{d_{pj}^* - d_{pj}}{d_{pj}^* d_{pj}} \right) (y_{pq} - y_{jq}), \tag{6}$$

$$\frac{\partial^2 E}{\partial y_{pq}^2} = \frac{-2}{C} \sum_{\substack{j=1 \\ j \neq p}}^{N} \frac{1}{d_{pj}^* d_{pj}} \left[\left(d_{pj}^* - d_{pj}\right) - \frac{\left(y_{pq} - y_{jq}\right)^2}{d_{pj}} \left(1 + \frac{d_{pj}^* - d_{pj}}{d_{pj}}\right) \right]. \tag{7}$$

All points in two-dimensional space have to be different. This prevents the partials from "blowing up" (Sammon, 1969).

The simultaneous nonlinear mapping works excellent when the number of vectors N is not large, and the mapping error E increases by increasing N. The second restriction is an ability to work having already all the data, so it can not work in a real time. In addition, the mapping result depends on the initial conditions (Sammon, 1969). The sequential nonlinear mapping is free from that.

3. Sequential Nonlinear Mapping

The sequential nonlinear mapping uses the technique similar to that of simultaneous one with some peculiarities (Montvilas, 1995). The method requires at the beginning for the existence of earlier mapped vectors. Hence the mapping procedure consists of two stages. At the first stage one have to carry out the nonlinear mapping of M vectors simultaneously where M is approximately equal (but not necessary) to the number of clusters or the states of a dynamic systems being supervised (Montvilas, 1999). The simultaneous nonlinear mapping is used for that. At the second stage one can map sequentially the received parameter vectors and, in such a way, to work in a real time for a practically unlimited time.

In order to formalise the method we designate by N the number of the sequentially received vectors of parameters. Thus, let us have $M+N$ vectors in the L-space. We designate them by X_i, $i=1,\ldots,M$; and X_j, $j=M+1,\ldots,M+N$. The initial M vectors are already simultaneously mapped into two-dimensional vectors Y_i, $i=1,\ldots,M$. Now we need to sequentially map the L-dimensional vectors X_j into two-dimensional vectors Y_j, $j=M+1,\ldots,M+N$, with respect to simultaneously mapped the M initial vectors. Here the simultaneous nonlinear mapping expressions will change into sequential nonlinear mapping expressions, respectively. First, before performing iterations it is expedient to put every two-dimensional vector being mapped into the same initial conditions, i.e., $y_{jk}=C_k$, $j=M+1,\ldots,M+N$; $k=1,2$. It is advisable to put C_k close to the average of simultaneously mapped M initial vectors. Note that in the case of simultaneous mapping of the first M vectors, the initial conditions are chosen along the descending diagonal (Sammon, 1969). Let the distance between the vectors X_i and X_j in the L-space be defined by d_{ij}^X and on the plane – by d_{ij}^Y, respectively. This algorithm uses the Euclidean distance measure as well, because, if we have no a priori knowledge concerning the data, we would have no reason to prefer any metric over the Euclidean metric. For computing the mapping error of distances E_j, $j=M+1,\ldots,M+N$, we choose the expression which reveals the largest product of the error and partial error (Duda and Hart, 1973). For the correct mapping we have to change the position of every mapped vector Y_j, $j=M+1,\ldots,M+N$, on the plane in such a way that the error E_j would be minimal. This is achieved by using the steepest descent procedure. After the r-th iteration the error of distances will be:

$$E_j(r)=\frac{1}{\sum_{i=1}^{M}d_{ij}^X}\sum_{i=1}^{M}\frac{\left[d_{ij}^X-d_{ij}^Y(r)\right]^2}{d_{ij}^X},\quad j=M+1,\ldots,M+N; \tag{8}$$

here

$$d_{ij}^Y(r)=\sqrt{\sum_{k=1}^{2}\left[y_{ik}-y_{jk}(r)\right]^2},\quad i=1,\ldots,M;\quad j=M+1,\ldots,M+N. \tag{9}$$

During the $r+1$-iteration coordinates of the mapped vectors Y_j will be

$$y_{jk}(r+1)=y_{jk}(r)-\mathbf{F}\cdot\Delta_{jk}(r),\quad j=M+1,\ldots,M+N;\quad k=1,2; \tag{10}$$

where

$$\Delta_{jk}(r)=\frac{\partial E_j(r)}{\partial y_{jk}(r)}\Big/\left|\frac{\partial^2E_j(r)}{\partial y_{jk}^2(r)}\right|. \tag{11}$$

F is the factor for correction of the coordinates an its defined empirically to be **F**=0.35,

$$\frac{\partial E_j}{\partial y_{jk}} = H \sum_{i=1}^{M} \frac{D \cdot C}{d_{ij}^X \cdot d_{ij}^Y}, \tag{12}$$

$$\frac{\partial^2 E_j}{\partial y_{jk}^2} = H \sum_{i=1}^{M} \frac{1}{d_{ij}^X \cdot d_{ij}^Y} \left[D - \frac{C^2}{d_{ij}^Y} \left(1 + \frac{D}{d_{ij}^Y} \right) \right], \tag{13}$$

$$H = -\frac{2}{\sum_{i=1}^{M} d_{ij}^X}; \quad D = d_{ij}^X - d_{ij}^Y; \quad C = y_{jk} - y_{ik}.$$

When the mapping error $E_j(r) < \varepsilon$, $j = M+1, \dots, M+N$, where value of ε depends on the nature of data, the iteration process is over and the result is shown on the PC screen. In order to have an equal computing time for each mapping we can execute a constant number of iterations R. Minimum necessary value of the M is obtained in (Montvilas, 1995).

The mapping results of the sequentially receiving parameter vectors are independent on the mappings of the earlier received vectors (independence on the history).

4. Comparison of Simultaneous and Sequential Methods

The simultaneous nonlinear mapping and the sequential one had been constructed using the same technique. Both of them use the same distance measure, the steepest descent procedure, similar but not the same mapping error expression.

For the first we have to ascertain that the simultaneous nonlinear mapping works only having all the data at its disposal. Therefore for sequential data structure analysis one can use only the sequential nonlinear mapping procedure.

The *theoretical* comparison of these two methods according accuracy is impossible because of absolute value of the second derivation of mapping error E in expressions (5) and (11).

Concerning the mapping accuracy we can accomplish an experiment by mapping the same data using both the simultaneous nonlinear mapping and the sequential one. Let's have 30 vectors consisting of six parameters (Table 1).

According the experiment these vectors belong to five classes (Table 2).

For this investigation it was used 100, 200 and 500 iterations R. In Fig. 1 the result of mapping vectors into two-dimensional space using the *simultaneous* nonlinear mapping is presented at $R = 500$.

In the Fig. 2 the result of mapping the same data at $R = 500$ using the *sequential* nonlinear mapping is presented. The first $M = 5$ vectors mapped simultaneously are denoted by mark $\times$ with an index that means the vector's number, and the remainder $N = 25$ vectors mapped sequentially are denoted by mark $+$ with the respective index.

Table 1

30 vectors for the first experiment

Vect.	Parameters					
No	1	2	3	4	5	6
1	101.0	205.0	307.0	508.0	604.0	206.0
2	106.0	203.0	302.0	501.0	603.0	205.0
3	108.0	202.0	304.0	502.0	607.0	208.0
4	103.0	208.0	305.0	505.0	609.0	204.0
5	105.0	201.0	308.0	507.0	608.0	202.0
6	101.1	205.0	307.0	507.7	604.0	206.0
7	101.0	205.1	307.2	508.0	604.0	206.3
8	101.2	205.0	307.0	508.2	604.0	206.1
9	101.3	205.1	307.1	507.9	603.9	205.0
10	106.1	203.1	302.0	501.0	603.0	205.1
11	105.9	203.1	302.1	500.9	603.1	204.9
12	105.8	203.0	302.2	501.2	603.2	205.0
13	105.8	203.1	302.2	501.5	603.0	205.5
14	108.5	202.0	304.2	502.0	607.0	208.0
15	108.0	202.2	304.2	502.3	607.1	208.1
16	108.0	202.0	304.0	502.0	608.0	208.2
17	107.9	201.8	303.8	501.8	606.4	207.9
18	102.9	207.7	304.5	504.7	608.7	203.9
19	103.0	207.8	305.5	504.9	609.1	204.1
20	102.9	207.9	304.9	505.0	609.2	204.0
21	103.1	208.1	304.8	505.2	609.0	204.0
22	104.9	201.2	308.1	507.1	609.2	202.1
23	106.0	201.0	308.0	507.5	608.0	202.5
24	105.0	201.0	309.0	507.2	607.5	202.0
25	105.1	201.1	308.1	507.0	608.0	201.9
26	105.0	200.8	308.8	506.9	607.8	201.9
27	104.8	201.2	308.2	506.5	607.0	201.7
28	105.9	202.9	301.7	500.9	602.1	204.8
29	105.5	202.0	301.5	501.4	603.0	204.1
30	101.7	205.5	306.0	509.0	604.0	206.0

Table 2

30 vectors distributed to five classes

Class	Vectors
1	1, 6, 7, 8, 9, 30
2	2, 10, 11, 12, 13, 28, 29
3	3, 14, 15, 16, 17
4	4, 18, 19, 20, 21
5	5, 22, 23, 24, 25, 26, 27

Now one can compare simultaneous and sequential mappings by calculating their total mapping errors after mapping. The same formula (2) was used for calculation of mapping error both for simultaneous mapping and for sequential one. The results at various amount of vectors and various number of iterations R are presented in Table 3 and showed in Fig. 3 for the case of $R = 500$.

Let's repeat a similar experiment using another kind of data: more widely distributed and having more vectors ($N = 50$) consisting of six parameters, too (Table 4).

They are distributed to five classes as well (see Table 5).

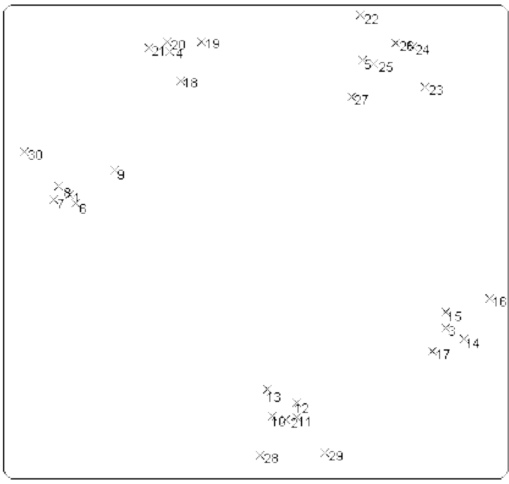

Fig. 1. The simultaneous nonlinear mapping.

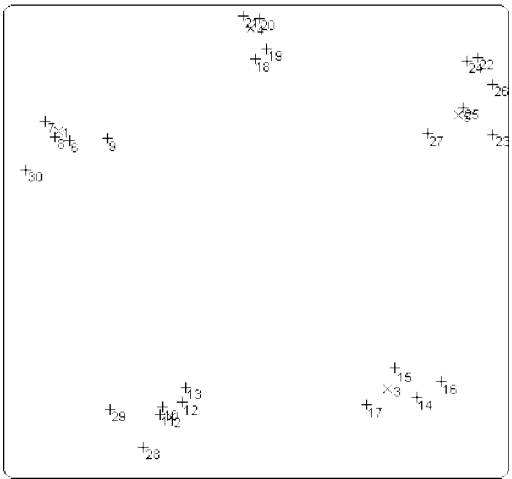

Fig. 2. The sequential nonlinear mapping.

The results of simultaneous and sequential mapping at $R = 500$ are presented in Fig. 4 and Fig. 5 respectively.

In Table 6 and Fig. 6 the results of mapping errors for the second experiment ($N = 50$) are presented analogous to Table 3 and Fig. 3 for the first experiment ($N = 30$).

The experiments using various sort of data show that both the simultaneous nonlinear mapping and the sequential one map the data onto the plane assorting them into 5 groups according experiment's conditions (data of 5 classes). In two cases the total mapping error of the sequential nonlinear mapping occur to be negligible less than that of the simultaneous one (Table 6, amount of vectors 6 and 50). It depends on the initial conditions and the sort of data. In the large

Table 3

Mapping errors dependence on amount of vectors

Amount of vectors	MAPPING ERROR					
	Simultaneous at iterations			Sequential at iterations		
	100	200	500	100	200	500
6	0.020316	0.020316	0.020316	0.030388	0.030388	0.030388
10	0.016469	0.016468	0.016468	0.033321	0.032869	0.032858
15	0.017295	0.013653	0.013613	0.024218	0.023999	0.023693
20	0.018497	0.017945	0.017944	0.025061	0.025094	0.025161
25	0.030821	0.030269	0.030268	0.031601	0.031434	0.031460
30	0.070796	0.030778	0.030777	0.033477	0.033354	0.033363

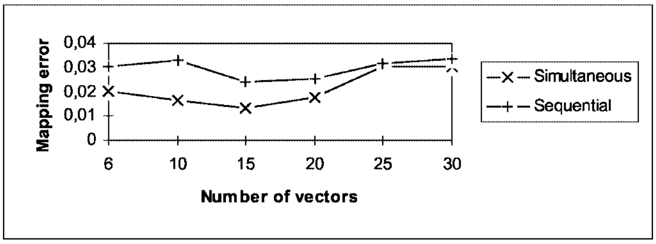

Fig. 3. Mapping errors dependence on amount of vectors.

Table 4

50 vectors for the second experiment

Vec. No	Parameters 1	2	3	4	5	6	Vec. No	Parameters 1	2	3	4	5	6
1	1.0	5.0	7.0	8.0	4.0	6.0	26	5.2	2.5	3.5	6.7	7.7	3.0
2	6.0	3.0	2.0	1.0	3.0	5.0	27	5.0	2.0	4.5	4.5	7.5	1.5
3	8.0	2.0	4.0	2.0	7.0	8.0	28	5.4	2.1	4.0	7.0	7.0	2.0
4	3.0	8.0	5.0	5.0	9.0	4.0	29	7.9	1.8	3.8	1.0	6.4	7.9
5	5.0	3.0	4.0	7.0	8.0	2.0	30	7.0	1.5	3.9	1.8	6.8	8.0
6	2.5	7.5	5.1	4.8	9.0	3.0	31	8.1	2.1	4.1	2.1	7.1	8.1
7	2.2	7.0	4.0	4.7	8.7	3.9	32	7.9	1.9	3.9	1.9	6.9	7.9
8	3.0	7.8	5.5	4.9	9.1	4.1	33	7.9	2.1	4.1	1.9	6.8	8.2
9	2.9	7.9	4.9	5.0	9.2	4.0	34	6.5	3.1	2.0	1.0	3.0	5.1
10	3.1	8.1	4.8	5.2	9.0	4.0	35	6.0	4.5	2.1	0.9	3.1	6.0
11	4.1	3.2	4.1	7.1	9.2	2.2	36	6.0	3.0	2.9	1.2	3.2	5.0
12	6.5	3.0	4.0	7.5	8.0	2.5	37	6.1	3.3	2.2	2.5	3.8	5.5
13	5.0	3.0	5.0	7.2	7.5	2.0	38	5.9	2.9	1.7	0.9	2.1	4.8
14	5.1	5.5	4.2	7.0	8.9	1.6	39	5.5	2.0	1.5	1.4	3.0	4.1
15	3.1	8.1	5.1	5.3	9.1	4.1	40	6.1	3.2	2.3	1.2	3.2	4.1
16	3.5	8.1	5.2	5.3	9.0	4.2	41	6.2	3.1	1.9	1.2	3.2	4.1
17	3.1	8.7	5.3	5.2	9.3	4.1	42	6.1	2.9	1.8	1.0	3.0	4.0
18	3.3	8.3	5.5	5.5	9.8	4.3	43	1.0	5.0	7.0	7.0	4.0	6.0
19	3.2	8.4	5.4	5.1	8.2	4.4	44	1.0	6.0	8.0	8.0	4.0	6.3
20	8.1	2.1	4.0	2.1	7.1	8.3	45	1.0	5.0	7.0	7.2	4.0	6.0
21	9.0	2.0	4.2	2.0	7.0	8.0	46	1.0	5.0	7.0	8.0	4.0	5.0
22	8.0	3.0	4.8	2.3	7.0	8.0	47	1.7	5.5	6.0	9.0	4.0	6.0
23	8.0	2.0	4.0	2.0	9.0	8.6	48	2.0	4.0	7.0	8.0	3.0	7.0
24	6.0	2.5	4.2	4.0	7.6	1.0	49	1.0	5.0	7.1	8.1	4.2	6.1
25	4.5	2.0	3.0	6.5	7.0	1.7	50	1.1	5.2	7.3	8.4	4.1	6.0

Table 5

50 vectors distributed to five classes

Class	Vectors
1	1, 43, 44, 45, 46, 47, 48, 49, 50
2	2, 34, 35, 36, 37, 38, 39, 40, 41, 42
3	3, 20, 21, 22, 23, 29, 30, 31, 32, 33
4	4, 6, 7, 8, 9, 10, 15, 16, 17, 18, 19
5	5, 11, 12, 13, 14, 24, 25, 26, 27, 28

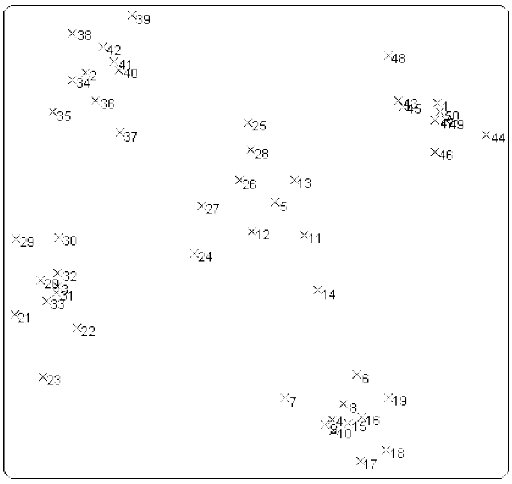

Fig. 4. The simultaneous nonlinear mapping, $N = 50$.

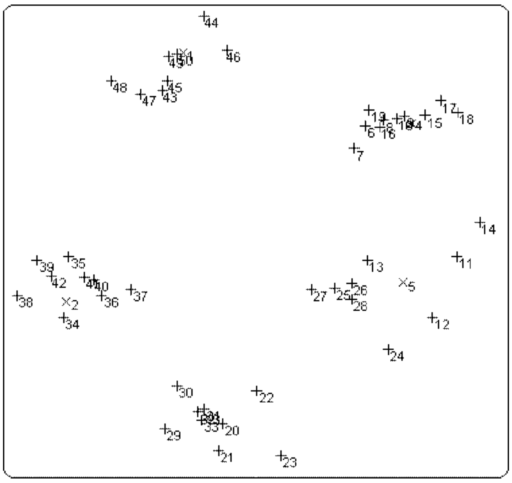

Fig. 5. The sequential nonlinear mapping, $N = 50$.

Table 6

Mapping errors dependence on amount of vectors

Amount of vectors	MAPPING ERROR					
	Simultaneous at iterations			Sequential at iterations		
	100	200	500	100	200	500
6	0.022116	0.022116	0.022116	0.021316	0.021320	0.021320
10	0.022495	0.022381	0.022376	0.030134	0.032440	0.031493
15	0.018129	0.017554	0.017543	0.033452	0.033934	0.033405
20	0.015397	0.015187	0.015186	0.037568	0.037778	0.037388
25	0.018013	0.018006	0.018006	0.039539	0.039541	0.039343
30	0.019077	0.018854	0.018781	0.043044	0.042962	0.042813
35	0.018624	0.016854	0.016853	0.037048	0.036743	0.036659
40	0.022577	0.022574	0.022574	0.031242	0.030911	0.030856
45	0.025473	0.025112	0.025104	0.028846	0.028684	0.028639
50	0.029817	0.029668	0.029666	0.029295	0.029335	0.029285

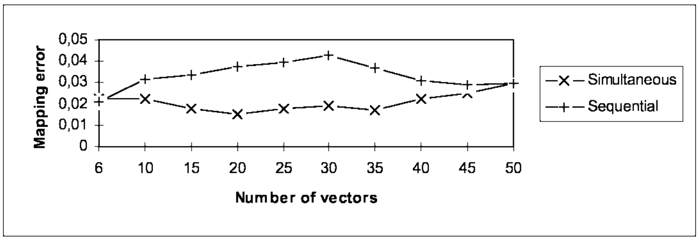

Fig. 6. Mapping errors for another experiment (N=50).

majority of experiments the sequential nonlinear mapping has some bigger total mapping error but always needs less number of iterations R. Its mapping error levels off at less R than that of the simultaneous one.

Comparison on calculation time. Calculation time depends on the number of distances between vectors which, on the other hand, depends on the number of vectors N. Hence one can write the calculation time for the simultaneous nonlinear mapping approximately to be $T_{sm} \approx N(N-1)/2$, and for sequential nonlinear mapping $T_{sq} \approx N{\cdot}S+S(S-1)/2$, respectively, where S – number of classes. In the Fig. 7 the relative calculation time at $S=5$ for one iteration is presented.

5. Discussions

Two methods for data structure analysis and visualisation are presented: the *simultaneous* nonlinear mapping and the *sequential* one. The sequential nonlinear mapping can work in a real time and its mapping results are independent on the history. These two methods were compared according ability to map the data onto the plane and the total mapping accuracy. In addition, relative mapping time dependence on number of vectors for one iteration was calculated.

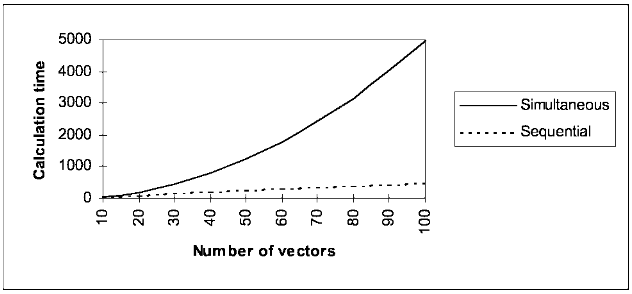

Fig. 7. Dependence of calculation time on the number of vectors.

The experiments show that the *sequential* nonlinear mapping maps the data well, though its total mapping error is bigger than that of the *simultaneous* one. However the *sequential* nonlinear mapping needs considerably less calculation time. In addition, the simultaneous mapping results depend on the initial conditions. Consequently, even having all the data already one can recommend to use for their mapping the *sequential* nonlinear mapping, especially when there is a large number of vectors being mapped.

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A.M. Montvilas is a doctor of technical sciences, a senior researcher of the Recognition Processes Department at the Institute of Mathematics and Informatics and an associate professor of the Radioelectronics Department at the Vilnius Gediminas Technical University. His research interests include processing of random processes, detection of dynamic system states and their changes, data visualisation, discrete signal processing, sequential nonlinear mapping.

Nuoseklus netiesinis atvaizdavimas prieš vienalaikį atvaizdavimą

Algirdas Mykolas MONTVILAS

Straipnyje pateikti du netiesinio atvaizdavimo metodai duomenų struktūros analizei bei vizualizavimui: Sammono (1969) vienalaikis ir Montvilo (1995) nuoseklusis. Šie metodai yra palyginti pagal atvaizdavimo tikslumą prie įvairių sąlygų bei skaičiavimo laiką. Parodyta, kad nuoseklus atvaizdavimo metodas nors ir turi kiek didesnę atvaizdavimo paklaidą, bet leidžia dirbti realiame laike, žymiai greičiau atvaizduoja duomenis į plokštumą bei reikalauja mažiau iteracijų. Visa tai ypač ryškėja didėjant duomenų kiekiui.

Todėl, netgi jau turint visus duomenys, rekomenduojama duomenų analizei naudoti *nuoseklų* netiesinį atvaizdavimą, ypač kai duomenų kiekis yra didelis. Pateikti pavyzdžiai.