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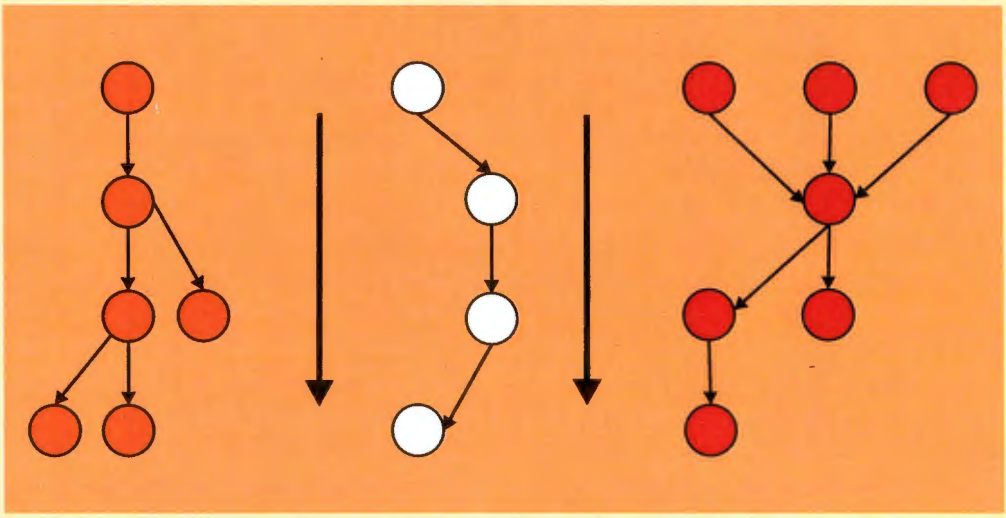
MULTICRITERIA ORDERING AND RANKING:
PARTIAL ORDERS, AMBIGUITIES AND APPLIED ISSUES



Jan W. Owsiński and Rainer Brüggemann
Editors

Warsaw 2008

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Theoretical Developments

Multicriteria Ordering and Ranking: Partial Orders, Ambiguities and Applied Issues
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Structural Constraints in the Optimization of Parameter Systems in Time Consuming Large Scale Computations

Lech P. Schulz

Adam Mickiewicz University, Department of Chemistry,
Grunwaldzka 6, 60-780 Poznan, Poland, (lsch@amu.edu.pl)

An approach to implicit structures of data constrained in computational procedures is presented herein. Transformations of them are looked for in order to obtain a desired effect of convergence in performed evaluations. First, a kinship between such structures has been elucidated by means of a resemblance comparator on weak Brouwerian lattices. Certain group representations introduced turned out to support suitable transformations imposed on the given set of data. An algorithm has been elaborated on the grounds of theoretical derivations. Data given by sets of multidimensional vectors were structured by associating elements of a Boolean ring (multidimensional bounded intervals) which enabled structural modifications. This yielded decreases of the function computed in an example of energy determination for the helium atom. The stabilization of data relationships was exercised in the course of computations. Skipping effect surpassing results of standard procedures circa 2500% has been shown and illustrated by relevant plots. The method is intended to open a way for a better efficiency in large scale computations, e.g., in many electron system evaluations with high accuracy. This should additionally be stressed that other approaches like extrapolations, genetic algorithms, etc. have not equally approved their power in resolving hard problems of efficient convergence predictions.

Keywords: optimization, convergence, resemblance, fuzzy set, large scale computations

1. Introduction

An insight into convergence of well known series close to the form of harmonic one is gained below for a preliminary illustration of the problem. Also, a concept

of resolving it is approximated in this way. The sequence, partial sums and sums are determined by the following formulas.

$$a_{ij} =: (-1)^{k_{i1}(j+1)} \frac{1}{j^{k_{i2}}} \quad , i = 1, 2, 3 \tag{1}$$

$$s_{in} =: \sum_{j=1}^{n} a_{ij}, \quad s_i =: \sum_{j=1}^{\infty} a_{ij} \quad , i = 1, 2, 3 \tag{2}$$

$$s_n =: s_{1n} + s_{2n} + s_{3n}, \quad s =: s_1 + s_2 + s_3 \tag{3}$$

Let parameters of the series be fixed

$$(k_{11}, k_{12}) =: (1, 1), \ (k_{21}, k_{22}) =: (1, 2), \ (k_{31}, k_{32}) =: (2, 2) \tag{4}$$

which leads to concrete evaluations

$$s_1 = \ln 2, \qquad s_2 = \frac{\pi^2}{12}, \qquad s_3 = \frac{\pi^2}{6} \tag{5}$$

Taking into account (4), two first series become alternating and an elementary property (Leibniz) claims that

$$a_{i1} + a_{i2} < s_{in} < a_{i1}, \text{ for } i = 1, 2, \ n \geq 3 \tag{6}$$

$$a_{i1} + a_{i2} < s_i < a_{i1}, \text{ for } i = 1, 2, \tag{7}$$

Thence,

$$1.25 + s_{3m} < s < 2 + \frac{\pi^2}{6}, \text{ for fixed } m \geq 3 \tag{8}$$

Fortunately, the exact values of sums s_i of (3) are known and inequalities (6), (7) play only an informing role. Otherwise, inequalities just considered could serve for an estimation of limits through calculations of finite sums

$$1.25 + s_{3m} < s_{1n} + s_{2n} + s_{3n} < 3.95, \text{ for fixed } m \geq 3 \text{ and } n \geq 3 \tag{9}$$

There is a structure associated to parameters (4)

$$u = [0,1] \times [0,1], \ v = [0,1] \times [0,2], \ w = [0,2] \times [0,2] \tag{10}$$

Calculate factors of differences between intervals of structure (10) as volumes of set theoretic symmetric differences, i.e.,

$$\mu(u\Delta v) = 1,\ \mu(u\Delta w) = 3,\ \mu(v\Delta w) = 2 \tag{11}$$

The same can be calculated for factors of similarity

$$\mu(u\cap v) = 1,\ \mu(u\cap w) = 1,\ \mu(v\cap w) = 2 \tag{12}$$

Using the numbers received, the resemblance of intervals considered can be assessed by formula $\rho(u,v) =: \mu(u\Delta v)/(\mu(u\Delta v) + \mu(u\cap v))$.

$$\rho(u,v) = 1/2,\ \rho(u,w) = 3/4,\ \rho(v,w) = \tfrac{1}{2} \tag{13}$$

Moreover, certain cumulative characteristics of the source structure can be determined, i.e.,

$$\frac{1+3+2}{(1+3+2)+(1+1+2)} = 0.6 \tag{14}$$

It can easily be seen that cumulative characteristics (14) is composed of summations of factors of differences and similarities respectively. Constant resultant ratio is not casual and its mathematical meaning will be explained below. The two dimensional intervals which constitute structure (10) have been pictured below in Fig. 1 by bold lines.

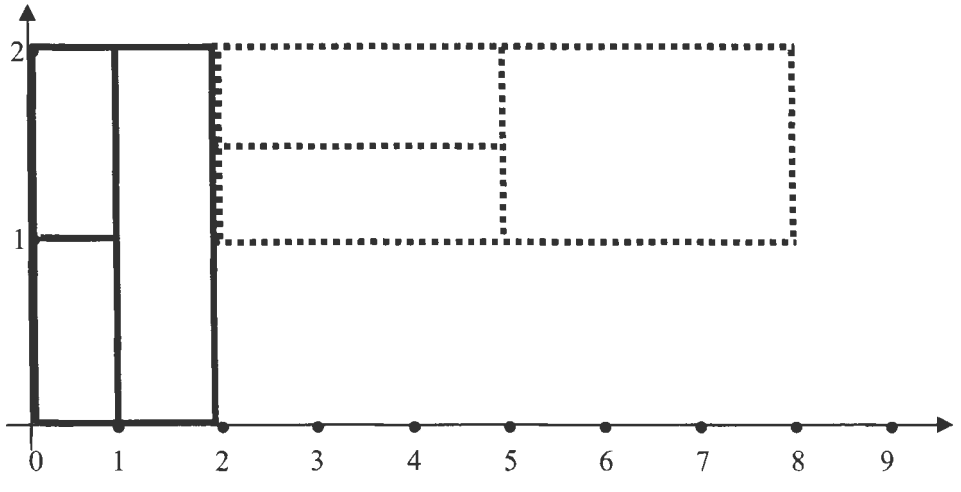

Figure 1. Structures associated to parameters (k_{t1}, k_{t2})

Consider other than (4) randomly chosen set of parameters

$$(2, 1/4), \quad (4, 1/2), \quad (3, 2) \tag{15}$$

There are no difficulties to check that distances (13) calculated for these new data are quite different from the previous evaluations, i.e., they equal 3/4, 11/12, and 10/13 respectively. Besides, cumulative characteristics under parameters (15) results in the ratio 24/29, which is different from the result obtained previously. Estimations of sums of series (2) or corresponding partial sums are not possible this time by means of inequalities mentioned above since two first series of (2) are divergent when parameters (15) are employed. An endeavour should be made to avoid random and unjustified trials.

Let another parallelism of transformations of structures associated with source parameters (4) and transformed ones be tested. For some mathematical reasons explained in the course of this paper parameters (4) and structure (10) will be transformed by operator ((3,2),(1/2,1)) in the following way

$$((3,2),(1/2,1)) \bullet (k_{t1}, k_{t2}) = (3 \cdot k_{t1}+2, (1/2) \cdot k_{t2}+1), \quad t = 1, 2, 3 \tag{16}$$

$$u' = [2,5] \times [1,3/2], \; v' = [2,5] \times [1,2], \; w' = [2,8] \times [1,2] \tag{17}$$

which is pictured by dotted line in Fig. 1.

As to the transformed structure (17), the results are as follows

$$\mu(u' \Delta v') = 3/2, \; \mu(u' \Delta w') = 9/2, \; \mu(v' \Delta w') = 3 \tag{18}$$

$$\mu(u' \cap v') = 3/2, \; \mu(u' \cap w') = 3/2, \; \mu(v' \cap w') = 3 \tag{19}$$

This a feature of comparisons just performed that mutual resemblance distances calculated for the source structure and the transformed one are the same.

$$\rho(u,v) = \rho(u',v') = 1/2, \; \rho(u,w) = \rho(u',w') = 3/4, \; \rho(v,w) = \rho(v',w') = \tfrac{1}{2} \tag{20}$$

Moreover, the cumulative characteristics of the source and transformed structures remain constant, i.e.,

$$\frac{3/2+9/2+3}{(3/2+9/2+3)+(3/2+3/2+3)} = 0.6 \tag{21}$$

Contrary to the case of parameters (15) which caused divergence of series considered, the new transformation (16) is leading to convergent species. However, constant values of conditions (20) and (21) do not afford sufficient criteria to

receive finite limits of series (2). For example, operator ((3,2),(1/2,–1)) applied to source parameters (4) yields new ones

$$(5,-1/2),\quad (5,0),\quad (8,0) \tag{22}$$

and a structure of the form

$$[2,5] \times [-1,-1/2],\ [2,5] \times [-1,0],\ [2,8] \times [-1,0] \tag{23}$$

Both characteristics (13) and (14) are saved for (23) but series (2) turn out divergent for actually transformed parameters. Observe that two dimensional intervals of (23) are placed in the fourth quadrant of the coordination system, while those of (17) accompanying convergence are of the first quadrant (see Fig. 1). Let this "first glance" feature be taken into account for framing a conjecture on the next operator supposed to make series convergent. Such operator suggested by transformation (16) can be of the form

$$((5,4),(1/3,2)) \bullet (k_{t1}, k_{t2}) = (5 \cdot k_{t1}+4, (1/3) \cdot k_{t2}+2) \tag{24}$$

The structure accompanying it is of the first quadrant and parameters transformed in this way lead to finite limits. Moreover, the rule can be generalized for arbitrary natural numbers m.

$$((2m+1,2m),(1/(m+1)),m)) \bullet (k_{t1}, k_{t2}) = ((2m+1) \cdot k_{t1}+2m, (1/(m+1)) \cdot k_{t2}+m) \tag{25}$$

where m = 0, 1, 2, ... There are no difficulties to check that all series (2) with parameters (25) are convergent and analogues of inequalities (6) and (7) hold. Numerical evaluations of sums in question acquire a better precision with growing m. Besides, invariant properties found by specific resemblance comparisons (13), (14) with the source structure are valid for transformations (25) as well. Thus, the convergence and accompanying resemblance relationships give rise to the conjecture that having some footstep premises like (16), a more efficient rule of transformations can be designed on the grounds of resultant estimations of similarity and differences between source and transformed structures. Following this way, a synergy with a more thorough theoretical insights is supposed to afford efficient ideas shedding a light on the nature of various kind convergence to be investigated.

2. Theoretical background

Lattice (A, $\vee$, $\wedge$) is a general algebraic structure involving two commutative semi-groups under operations $\vee$ and $\wedge$ such that absorption rules hold, i.e., $x \vee (x \wedge$

$y) = x = x \wedge (x \vee y)$ (Kuratowski and Mostowski, 1976). An operation called pseudo-difference can be determined in any lattice (Mc Kinsey and Tarski, 1960),

$$-^* : (x, y) \mapsto z \tag{26}$$

where z is the least element of all elements z′ satisfying condition

$$x \leq y \vee z' \tag{27}$$

where $x \leq y$ iff $x \wedge y = x$.

In the case, when pseudo-difference (1) is totally determined, i.e.,

$$\text{domain} -^* = A^2 \tag{28}$$

and there exists a unit under operation $\wedge$, then such lattice is said to be *Brouwerian* (Mc Kinsey and Tarski, 1960). If the existence of a unit is not necessarily assumed, such a lattice will be called a *weak Brouwerian lattice.*

Define symmetric pseudo-difference Δ^* on the weak Brouwerian lattices,

$$x \ \Delta^* y =: (x -^* y) \vee (y -^* x) \tag{29}$$

Let a general operation inspired by one of (29) be specified for lattices just considered

$$\Delta^\bullet : \mathbf{L}^2 \to \mathbf{L} \tag{30}$$

Function μ: $\mathbf{L} \to R^+$ is said to be *subtractive measure*, particularly $\Delta^\bullet$ - *subtractive measure*, provided that the following relationships are valid

$$\mu(a \ \Delta^\bullet b) = \mu(a \vee b) - \mu(a \wedge b) \quad \text{and} \tag{31}$$

$$\mu(a \ \Delta^\bullet c) \leq \mu(a \ \Delta^\bullet b) + \mu(b \ \Delta^\bullet c). \tag{32}$$

Note that each $\Delta^\bullet$ - subtractive property (31) implies μ to be symmetric and consistent with the lattice partial ordering of (27), i.e.,

$$\mu(a \ \Delta^\bullet b) = \mu(b \ \Delta^\bullet a) \quad \text{and if } a \leq b, \text{ then } \mu a \leq \mu b \tag{33}$$

This is a matter of fact that symmetric pseudo-differences (29) of weak Brouwerian lattices underlie examples of subtractive measures.

Owing to properties (31) and (32), subtractive measures admit comparisons between elements of a lattice by quantitative assessments of their relatedness via a pseudo-metric (metric) defined exclusively via subtractions $\Delta^\bullet$. Another more

universal tool has been employed (Schulz, 1991, 2003) in which both *factors* $\mu(a \Delta^{\bullet} b)$ and $\mu(a \wedge b)$ can efficiently contribute the resultant evaluations.

Generally, for any lattice $(\mathbf{L}, \vee, \wedge,)$ with a subtractive measure μ determined by means of operation $\Delta^{\bullet}$, there exists pseudo-metric

$$\rho_{\mu} : \mathbf{L} \times \mathbf{L} \rightarrow R^{+}$$

such that

$$\rho_{\mu}(a,b) =: \frac{\mu(a \Delta^{\cdot} b)}{C'\mu(a \wedge b) + C''\mu(a \Delta^{\cdot} b)} \tag{34}$$

for $(a,b) \in L^2 \setminus (\mu^{-1}(\{0\}) \times \mu^{-1}(\{0\}))$ and fixed positive real numbers $0 < C' \leq C''$, and

$\rho_{\mu}(a,b) = 0$

for $(a,b) \in \mu(\{0\}) \times \mu^{-1}(\{0\})$. Such a pseudo-metric is called a *resemblance comparator* herein and it can be a metric too under more specific structures.

Most often examples of weak Brouwerian lattices are afforded by Boolean rings of the form $(A, \Delta, \wedge)$ (Kuratowski and Mostowski, 1976), in which pseudo-difference and symmetric pseudo-difference become usual difference and symmetric difference of the rings in question. Values $\mu(a \Delta b)$ and $\mu(a \wedge b)$ are called respectively factors of differences (FD) and similarity (FS).

Certain group representations on Boolean rings with resemblance comparator will be introduced to support suitable transformations of data. Let $X =: (A,\cdot)$ and $X' =: (A, \cdot')$ be groups and

$$\pi : X \rightarrow \mathrm{Aut}X' \tag{35}$$

be a homomorphism into automorphisms of X', i.e., a representation of X on group X' (Lang, 2002). Then, semidirect product (Aschbacher, 1993).

$$\mathrm{Sd}(X, X', \pi) =: (A \times A', \cdot) \tag{36}$$

is a group on the Cartesian product $A \times A'$ such that $(x,x')\cdot(y,y') = (xy, x'(\pi x)y')$.

Moreover, a permutation representation of semidirect product on A' arises

$$T : \mathrm{Sd}(X, X', \pi) \rightarrow \mathrm{bij}A' \tag{37}$$

by means of assignment

$$T_{xx'}\, y' = x'\,(\pi x)y'. \tag{38}$$

For example, let multiplicative $Y =: (R^{*n}, \cdot)$ and additive $Y' =: (R^n,+)$ groups of real numbers be taken into account. Their elements are determined by operations

$$\alpha. : n \to R^*,\ \beta. : n \to R \tag{39}$$

for R^* denoting non-zero real numbers. The representation on additive group of R^n is given in a natural way by homomorphism

$$\sigma: (R^{*n}, \cdot) \to \mathrm{Aut}(R^n,+). \tag{40}$$

This yields a semi-direct product in virtue of (36).

$$\mathrm{Sd}(Y,Y',\sigma) =: (R^{*n} \times R^n, \cdot) \tag{41}$$

In the particular case, values of representation T of (37) establish a subgroup of the symmetry group on R^n. Consider some structure on subsets of R^n. There exists a Boolean ring $^{-}\mathrm{Itv}$ generated by bounded below and above intervals of the real line. For a.: $n \to {}^{-}\mathrm{Itv}$, products $\bigtimes_{i\in n} a_i$ generate Boolean ring $^{-}I \subseteq \mathrm{Pow}R^n$ consisting of finite unions of such products. For $\mathfrak{a} \subseteq I$ and $\mathfrak{a}$ finite, $\bigcup\mathfrak{a}$ is an element of ^{-}I. A semidirect product group action can easily be determined using representation T

$$(\alpha., \beta.) \bullet \bigcup\mathfrak{a} =: \bigcup_{w\in\mathfrak{a}} T_{\alpha.\beta.}(w) \in {}^{-}I. \tag{42}$$

Taking into account the above equality, there exists a corresponding permutation representation

$$\tau :\ \mathrm{Sd}(Y,Y',\sigma) \to \mathrm{bij}^{-}I \tag{43}$$

This correspondence naturally extends to the Boolean ring automorphisms, i.e., τ is a representation of semidirect product $\mathrm{Sd}(Y,Y',\sigma)$ on the ring in question.

$$\tau :\ \mathrm{Sd}(Y,Y',\sigma) \to \mathrm{Aut}({}^{-}I\ ,\ \Delta\ ,\ \cap) \tag{44}$$

Moreover, pseudometric automorphisms are constituted on this occasion as well, i.e.,

$$\tau:\ \mathrm{Sd}(Y,Y',\sigma) \to \mathrm{Aut}({}^{-}I;\ \rho_v) \tag{45}$$

The last condition shows that elements of Boolean ring ^{-}I can be conveyed along with resemblance relationships between them.

3. Algorithm

An often result of large scale computations leads to the immense collections of numerical data, which are cumbersome in clear interpretations. The case of a "black box" data sets is commonly encountered and poses the problem how to decipher the results received. This can reasonably be assumed that algorithms employed constrain some regularities in outputs of computations reflected in their structure. The general idea and mathematical details on related optimization have been described in Schulz (2003, 2008).

A problem related to the outlined theory emerges when one needs to evaluate data in order to reach an effect fulfilling a definite condition. For example, there is $m \times n$ matrix $[a_{ij}]$ given. The task is to find transformations

$$[a_{ij}] \mapsto [a'_{ij}] \tag{46}$$

such that ascribed real number values $f\,[a_{ij}]$ and $f\,[a'_{ij}]$ would satisfy a required relationship, e.g.,

$$f\,[a_{ij}] > f\,[a'_{ij}] \tag{47}$$

Since assignment f is often given indirectly via intricate computational procedures and there are many steps necessary to reach, e.g., minimum, transformation (46) is commonly performed by fitting matrix elements. Such a procedure consists in random trials (at least in a part) which takes much computational time surpassing even the efficiency of top power computers. In order to avoid difficulties of this kind, a concept of implicitly constrained structures has been elaborated

It is supposed that relationship (47) is fulfilled due to an implicit structure of coefficients a_{ij} of the matrix of data, which has been constrained, e.g., by computational procedures. A conjecture can be framed claiming that transformations (46) resembling such a source structure lead to the desired relationships. For each vector x. of R^n, in particular for any row (column) of matrix $[a_{ij}]$, there exists a closed n(m)-dimensional interval associated to x. in a natural way. Such intervals are elements of Boolean ring ^{-}I and they can mutually be compared. Moreover, there exist representations like (45), such they save

resemblance distances between all pairs of aforementioned intervals or indicate the ways of inducing likelihood for structures in question.

As usual, matrix data can equivalently be given as sets V of vectors of n-dimensional vector space R^n expressed by series of numbers $(a_{i1}, \ldots, a_{in})$. A direct way, employs *brute force* constraints (Powell's method, as usual) based on consecutive trials such that transformation

$$V \mapsto V' \tag{48}$$

is inevitably concluded, e.g., in the fall of, e.g., values of function E considered

$$E(V) > E(V') \tag{49}$$

like in general case (47) aforesaid.

Another way leads via an intermediate assignment of structures to data and reaching the desired energy evaluations due to the appropriate structural proximity. Structures suitable for analysis turn out Boolean rings, e.g., Boolean rings naturally generated by bounded intervals in R^n (i.e., open, half-open, closed, bounded below and above). Having a set of series of data V, one can ascribe a closed interval to each pair of fixed points of class $W = V \times V$. Simply, for $(a_{i1}, \ldots, a_{in})$, $(a_{j1}, \ldots, a_{jn}) \in V$, interval $[a_{i1}, a_{j1}] \times \ldots, [a_{in}, a_{jn}]$ is an element of the Boolean ring in which comparisons are to be performed. Thus, an enriched structure emerges on the distinguished vectors of W as illustrated in Fig. 2.

SCHEME OF DATA STRUCTURE AS A COMPLEX SYSTEM

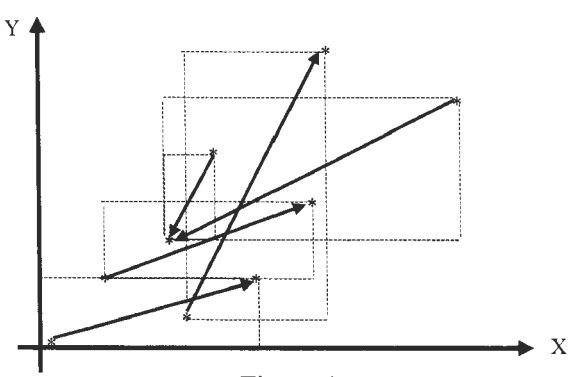

Figure 2.

W (a set of fixed vectors) F_W (the set of n-dimensional closed intervals) (50)

Due to the concept of constraining, appropriate kinships in the new structure ($F_{W'}$) achieved by transformations of data on the template (F_W) should lead to the desired decreases. This cannot be expected as automatically given, but a reasonable number of computational tests has shown essential skipping of procedures in comparisons with standard methods. A quantitative estimation of the kinship, i.e., a resultant assessment of mutual relationships between particular intervals has been accomplished by means of a resemblance comparator and a membership function by which a corresponding fuzzy set is defined (Schulz, 2003). This has been established in Schulz (1991) that a summation of factors of differences (FD) is again a factor of differences. Similarly, summation of factors of similarity (FS) is again a factor of this kind.

A cumulative resemblance contributed by factors of similarity and differences between all pairs of intervals of F_W ($F_{W'}$) yields a resultant characteristic of the investigated structure of parameters like in (14), i.e.,

$$dF_W =: \frac{\sum_{(a',a'')\in F_W \times F_W} FD(a',a'')}{\sum_{(a',a'')\in F_W \times F_W} FD(a',a'') + \sum_{(a',a'')\in F_W \times F_W} FS(a',a'')}. \tag{51}$$

If another set of data and vectors W′ is given, then resemblance $dF_{W'}$ of intervals $F_{W'}$ can be considered. Complex systems represented by pairs ($F_{W'}$, F_W) constitute a "*universe of discourse*" (Schulz (2003,2008)), elements of which are assessed by a membership function determined as follows

$$\gamma(F_{W'}, F_W) =: |\, dF_{W'} - dF_W \,|. \tag{52}$$

A stepwise procedure just described can be pictured in the following scheme.

$$\phi\colon V \mapsto F_W \quad \mapsto \quad F_{W'} \mapsto V'. \qquad \text{(adjustment: } \gamma(F_{W'}, F_W)\text{)} \tag{53}$$

Resolving the task of receiving diminished values, resemblance relationship γ (52) determined on complex system ($F_{W'}$, F_W) should be adjusted in a way leading to new evaluations

$$E'(V) =: E(\phi(V)) \tag{54}$$

which is to be accompanied by decrements under source value E(V), i.e.,

$$E'(V) < E(V). \tag{55}$$

Such an adjustment called optimization indicated in (53) can be accomplished using various resemblance based transformations of structures introduced (e.g., representation (45)) to produce the effect of energy decrease.

4. Computational experiments

An application presented here is oriented on the concrete problem of minimization of chemical particle energies. Evaluations of data by a general function f is specified as determinations of energy E in the case. Detailed descriptions of computational procedures can be found in Rychlewski and al. (2003).

ECG (Explicitly Correlated Gaussian functions) (Rychlewski and al., 2003) method employed for chemical particle energy computations runs through the stage of specific optimization. It is initially applied to randomly chosen set of parameters. Due to the algorithmic rules used and variational principle (establishing a threshold beyond of which the energy cannot be diminished), non-linear parameters of the best energy convergence are step by step selected. There is an indexed family of wave functions, as usual, involved

$$\Psi_k=\varphi(\alpha_{11k},.....,\alpha_{ijk},..). \tag{56}$$

In Powell's method, every optimizing step is made to reach the steepest descent in energy which decrement, however, is bounded below in virtue of the variational principle. Therefore, the initial, randomly generated set of coefficients determining wave functions (56) is transformed by consecutive extrapolations for each coefficient, simply by trial evaluations and verifications of the energy decreases. Helium atom has been used in the current work as the well elaborated species suitable for confrontations with alternative approaches to energy determinations.

As usual, cycles are distinguished at some stages of optimization. They include results of Powell's transformations for *all* non-linear coefficients of a fixed wave function basis set. Thence, differences between energies ascribed to particular cycles L and L′ can be determined,

$$\Delta E(L,L') =: E(L) - E(L'). \tag{57}$$

Formula (57) is a particular case of the general part, where sets of datum vectors V and V′ (48) play the role of cycles.

If adjustment indicated in (53) is applied, then transformations of another kind are involved. Starting from cycle L, the decreased energy has been determined independently of the Powell's method using only resemblance and fuzzy set based adjustments, as shown in the scheme mentioned. Thus, decreases of energy can be estimated in a new way,

$$\Delta E'(L) =: E(L) - E'(L). \tag{58}$$

The ratio of energy decreases estimates the relative efficiency for both cases, i.e.

$$\eta(L, L') =: \frac{E(L) - E'(L)}{E(L) - E(L')}. \tag{59}$$

Computations omitting the Powell's constraints are based on the conjecture that features of enriched data structure (e.g., as illustrated in Fig. 2) are coupled along with the growing number of cycles, and this fact does allow to succeed in adjustments.

In preliminaries, a test has been performed for checking do really any regularities can be observed in the sets of diminishing energy basis functions received by Powell's method. The results had shown that all mutual "bilateral" resemblance relationships between many dimensional intervals on the vectors of non-linear coefficients have mostly (more than 90%) values ranging from 0.9 to 1.0. This reveals a high level of diversification of structural elements, which supports the thesis on a deterministic character of the seemingly chaotic sets of data basis.

Next, computations have been performed in order to explain is the diminishing of energy possible at all by means of the new concept introduced. Energies have been computed for the early stage of optimization of non-linear coefficients for 1 - 10 cycles. Decreases of energy have been reached for all L of the diapason used, but up to L = 5, the values of the relative descents η (59) remained less than 1. This indicates that no skipping does occur in the relation to the Powell's method, if the constraints are not sufficiently advanced. The effect of skipping for $\eta \geq 1$ has been observed only after the 5^{th} step. Table 1 and Figs. 3 and 3a show detailed evaluations for consecutive cycles L = 1 – 10 and the effect in question. In view of applied aspects, a natural idea is emerging to check whether the skipping is possible when the cycles are not consecutive, but the leap L′ – L between evaluated cycles equals, e.g., 100 instead of 1 as in the previous case. The results obtained have been

gathered in Table 2 and depicted in plots of Figs. 4 and 4a. They confirm the ability of decreasing the energy in all cases for L = 100, 200, ..., 1000. Coefficient η remains less than 1 up to L = 400. Than it oscillates around 1 for L = 500, 600. A clear skipping appears for L exceeding approx. 650 cycles. This confirms the expectation framed by the conjecture that advancing in structural constraints by growing number of optimization cycles provides better conditions for adjustments of scheme (53). Since the behaviour of energy functions has been interpolated, as shown in plots, an insight in the intermediate evaluations for L = 910, 920, ..., 1000 has also been accomplished (see Table 3, Fig. 5a). Energy decrease $\Delta E'(L)$ has approximately constant value of 0.21 microhartree in this diapason and the skipping effect shows values exceeding circa 2500% over the sample of Powell's method determined for distinguished cycles.

Table 1. Energies determined by wave functions received by Powell's conjugated directions method and fuzzy set based resemblance of non-linear coefficient structures

(I)

Optimization cycle	Energy (hartree) E(L)	Energy for transformed wave function (hartree) E′(L)	Relative descents of transformed wave function $\eta(L,L')$ (×100%)
L / **L′**	Descents of energy under cycle L′ $\Delta E(L,L')(\times 10^6)$	Descents of energy under the source wave function $\Delta E'(L)(\times 10^6)$	
0	-2.903443242	-2.903504305	35
	172.672	61.063	
1	-2.903615914	-2.903622324	33
	19.335	6.410	
2	-2.903635249	-2.903637333	43
	4.810	2.084	
3	-2.903640059	-2.903641918	63
	2.972	1.859	
4	-2.903643031	-2.903644646	62
	2.600	1.615	
5	-2.903645631	-2.903647484	93
	1.988	1.853	
6	-2.903647619	-2.903649358	109
	1.597	1.739	
7	-2.903649216	-2.903651131	155
	1.235	1.915	
8	-2.903650451	-2.903652190	159
	1.092	1.739	
9	-2.903651543	-2.903653361	219
	0.831	1.818	
10	-2.903652374	-2.903653893	197
	0.771	1.519	

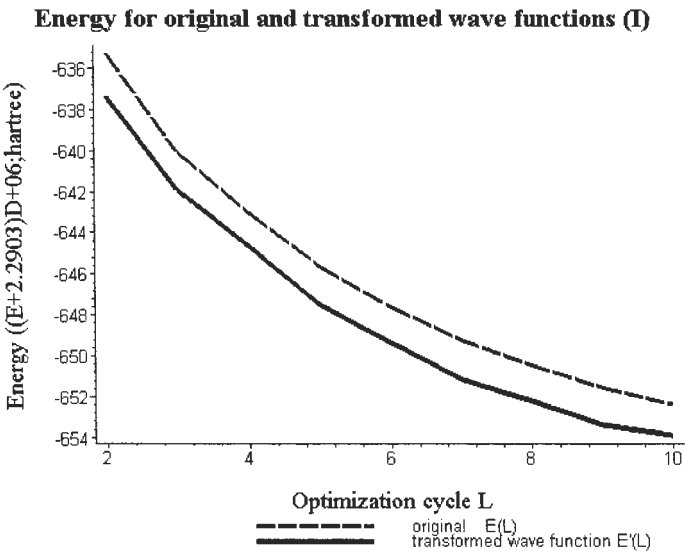

Figure 3.

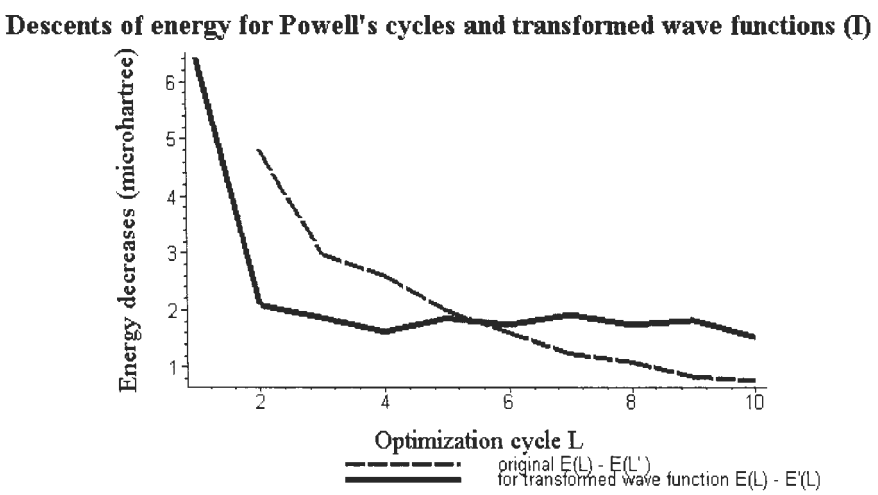

Figure 3a.

Table 2. Energies determined by wave functions received by Powell's conjugated directions method and fuzzy set based resemblance of non-linear coefficient structures

(II)

Optimization cycle	Energy (hartree) E(L)	Energy for transformed wave function (hartree) E′(L)	Relative descents of transformed wave function $\eta(L, L')$ (×100%)
L	Descents of energy under cycle L′ $\Delta E(L,L')(\times 10^6)$	Descents of energy under the source wave function $\Delta E'(L)(\times 10^6)$	
L′			
100	-2.903674003	-2.903676916057	25
	11.652	2.913	
200	-2.903685655	-2.903687366931	15
	11.408	1.711931	
300	-2.903697063	-2.903697349445	16
	1.799	0.286445	
400	-2.903698862	-2.903699080881	76
	0.287	0.218881	
500	-2.903699149	-2.903699363922	107
	0.200	0.214922	
600	-2.903699349	-2.903699556429	83
	0.251	0.207429	
700	-2.903699600	-2.903699798370	171
	0.116	0.198370	
800	-2.903699716	-2.903699915338	240
	0.083	0.199338	
900	-2.903699799	-2.903700003361	252
	0.081	0.204361	
1000	-2.903699880	-2.903700092034	
		0.212034	

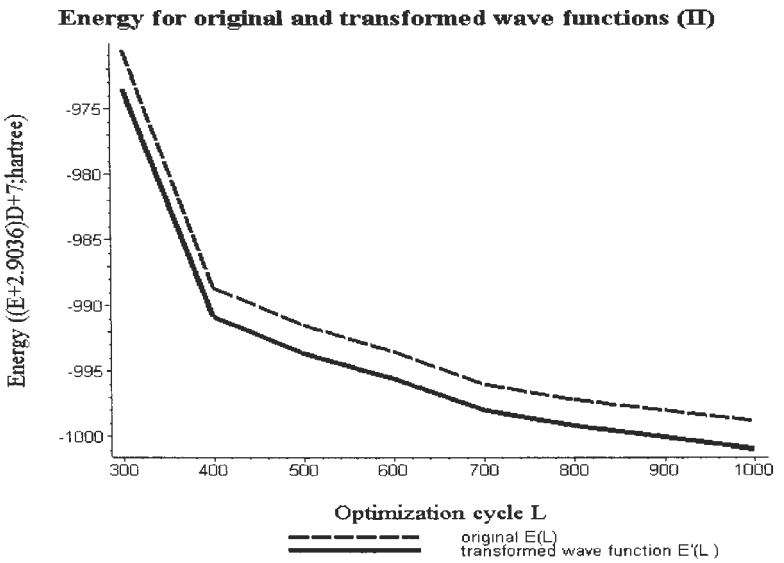

Figure 4.

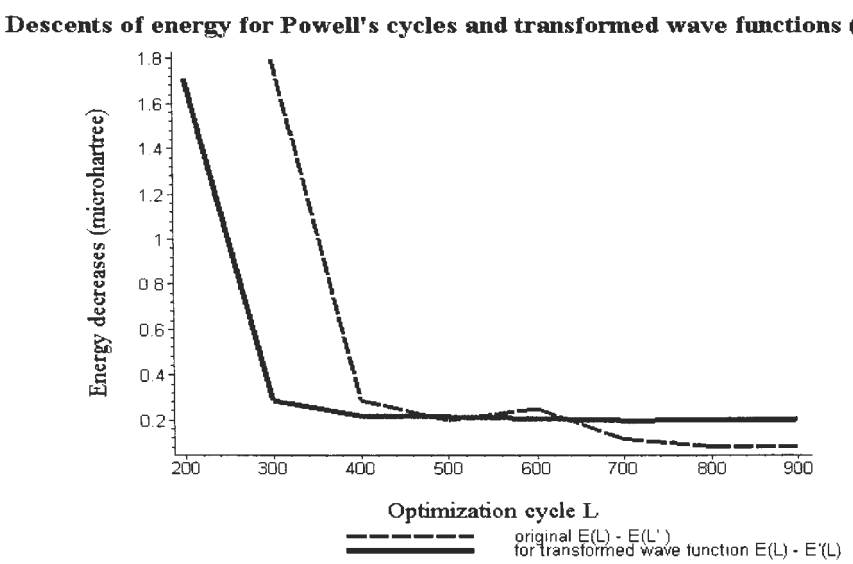

Figure 4a.

Table 3. Energies determined by wave functions received by Powell's conjugated directions method and fuzzy set based resemblance of non-linear coefficient structures

(III)

Optimization cycle	Energy (hartree) E(L)	Energy for transformed wave function (hartree) E′(L)	Relative descents of transformed wave function $\eta(L, L')$ (×100%)
L	Descents of energy under cycle L′	Descents of energy under the source wave function	
L′	$\Delta E(L,L')(\times 10^6)$	$\Delta E'(L)(\times 10^6)$	
900	-2.903699799	-2.903700003361	2555
	0.008	0.204361	
910	-2.903699807	-2.903700012913	2574
	0.008	0.205913	
920	-2.903699815	-2.903700022083	2958
	0.007	0.207083	
930	-2.903699822	-2.903700029819	2598
	0.008	0.207819	
940	-2.903699830	-2.903700039132	2614
	0.008	0.209132	
950	-2.903699838	-2.903700046418	2877
	0.007	0.201418	
960	-2.903699845	-2.903700054812	1648
	0.012	0.197812	
970	-2.903699857	-2.903700068447	2543
	0.008	0.203447	
980	-2.903699865	-2.903700075159	3002
	0.007	0.210159	
990	-2.903699872	-2.903700084062	2651
	0.008	0.212062	
1000	-2.903699880	-2.903700092034	
		0.212034	

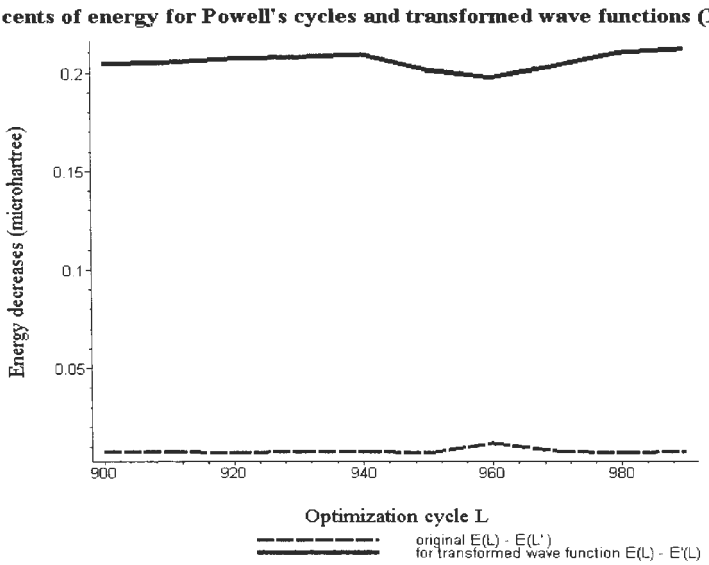

Figure 5a.

5. Discussion and conclusions

It can easily be observed that constant value of energy decrease (approx. 0.2 microhartree) occurs not only for advanced numbers of cycles (L = 900 – 1000), but this value emerges already on starting points of the skipping effect, i.e., for L = 400 or more. Following the hypothesis on the constrained structure, this is supposed that underlying structure of non-linear coefficients, owing to which the energy can be diminished, does undergo a stabilization and further constraints do not improve results. Values of relative descents η are increasing due to the more narrow intervals of energy falls caused by the Powell's procedures. Such a stabilization can especially be useful in computational pressing of high accuracy results since the classical procedures are extremely time consuming just on the stages for large number of cycles L.

Classical methods of the search for minima of molecular energy with high accuracy turn out insufficient in quantum-chemical computations. A non-standard approach combined with fuzzy set based structural constraints of data reveals significant efficiency when the data structures are transformed in accord to some resemblance rules. This unveils the role of structures constrained. The results

indicate that computationally grounded coefficients reflect features of structured systems deciding about desired properties such as minima of energy. Owing to this, when performing computational adjustments prompted by representations like (45), the effect surpassing desired descents of classically computed energies has been reached. Besides, the approach elaborated turns out more efficient for rapid computations of appropriate modifications of wave functions (basis sets) than standard approaches. Further investigations are oriented on expanding both theoretical and computational knowledge and experience, in order to find precise information on implicit structural characteristics responsible for the skipping effects*.

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This book is a collection of papers, prepared in connection with the 8th International Workshop on partial orders, their theoretical and applied developments, which took place in Warsaw, at the Systems Research Institute, in October 2008. The papers deal with software developments (PYHASSE and other existing software), theoretical problems of ranking and ordering under various assumed analytic and decision-making-oriented conditions, as well as experimental studies and down-to-earth pragmatic questions.

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