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# *Editors' Remarks*

## *Of Many Worlds in this World*

*By Margaret Cavendish*

***********************************************************

Just like as in a Nest of Boxes round,
Degrees of Sizes in each Box are found:
So, in this World, may many others be
Thinner and less, and less still by degree:
Although they are not subject to our sense,
A World may be no bigger than Two-pence.
NATURE is curious, and such Works may shape,
Which our dull senses easily escape:

For Creatures, small as Atoms, may be there,
If every one a Creature's Figure bear.
If Atoms Four, a World can make, then see
What several Worlds might in an Ear-ring be:
For, Millions of those Atoms may be in
The Head of one small, little, single Pin.
And if thus small, then Ladies may well wear
A World of Worlds, as Pendents in each Ear

***********************************************************

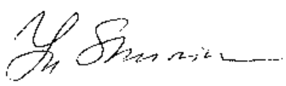
Margaret Cavendish♥ (1661–1717)

This 15th volume No.1 presents the papers on the actual topics such as **Applied Statistics and Operations Research**, **Quantum Chemistry**, **Information Processing**, **Nanodevices and Nanomaterials**, **Nanothinking and Nanoeducation**. As to *'nano'* activities of the journal we consider this field of our interests very essential both from the point of nanotechnology development and nanothinking shaping. These publications carry out not only scientific tasks but also an important social function.

Our journal policy is directed on the fundamental and applied sciences researches, which are the basement of a full-scale modelling in practice.

This edition is the continuation of our publishing activities. We hope our journal will be interesting for research community, and we are open for collaboration both in research and publishing. This number continues the current 2011 year of our publishing work. We hope that journal's contributors will consider the collaboration with the Editorial Board as useful and constructive.

**EDITORS**



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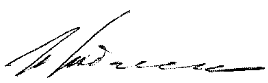

**I.V. Kabashkin**

♥ **Margaret Cavendish, Duchess of Newcastle-upon-Tyne** (1623–15 December 1673) was an English aristocrat, a prolific writer, and a scientist. Born **Margaret Lucas**, she was the youngest sister of prominent royalists Sir John Lucas and Sir Charles Lucas. Cavendish was a poet, philosopher, writer of prose romances, essayist, playwright and, some say, a tireless self-publicist, publishing under her own name at a time when most women writers published anonymously. Her writing addressed a number of topics, including gender, power, manners, scientific method, and animal protection. Her romance, *The Blazing World*, is one of the earliest examples of science fiction.

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# COLLECTIVE INTERACTION IN ION TRACK ELECTRONICS

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The capability of a multitude of parallel electroactive nanostructures in a given substrate to show collective interactions has been examined. Specifically, we consider here electroactive nanostructures as well as (a) electrolyte-filled current spike-emitting latent ion tracks in thin polymer foils and (b) metal cluster-filled etched ion tracks in the TEMPOS structures (i.e. in thin $SiO_2$ layers on Si substrates). Whereas the electroactive nanostructures are usually operated in the first case by application of a sinusoidal voltage at low frequency to trigger the current spike emission, TEMPOS structures are usually operated by applying a constant voltage to them.

An electroactive nanostructure can influence the performance of neighbouring nanostructures by modifying the entrance or exit potentials (or both) of the latter one, via lateral charge exchange through the common front or backside conductors or contacts. For the two cases considered here, this leads to two different effects:

(a) The collective interaction of many current spike-emitting latent tracks in electrolytic ambient leads to pulse-locked synchronization as predicted by Neural Network theory;

(b) In TEMPOS structures with etched tracks in $SiO_2$ on Si, with metal nanocluster coverage of both the oxide layer and the track walls, with at least two contacts on the oxide surface and one on the Si substrate, and with the insulator/semiconductor interface exhibiting two extreme states of resistivity (a high and a low Ohmic one), the collective track interaction can induce negative differential resistances.

This is the consequence of a chain reaction triggered by spontaneous opening of previously closed (or closing of previously open) neighbored tracks. Periodic repetition of such opening/closing processes leads to self-pulsating devices. It is suggested to modify these interacting track systems further, to develop more sophisticated, yet unknown electronic devices. Combined with the known possibilities of physical/chemical/biological sensing and logic decision-making of track-based structures, a challenging new field of unconventional solid and liquid electronic devices based on collective interactions appears to emerge.

***Keywords:*** *electroactive nanostructures, ion track electronics, physical/chemical/biological sensing*

## 1. Introduction: Collective Interaction of a Multitude of Objects

In systems with a multitude of interacting individual objects new properties, which the individuals themselves do not possess, may develop. These emerging collective effects can exhibit a level of sophistication higher than the individual objects capabilities themselves, which is considered primarily to be due to the communication between these individuals. In the general case, the communication between the individuals takes place in both directions. It may be transferred by acoustic, visual, pressure, electric, phonetic, social, economic, psychological, etc. signals. The amount and the quality of the collective interaction depend on:

a) the capability and readiness of the individuals to accept communication;
b) the type, quality and variation of their individual capability to "digest" the received information, i.e. to draw logic conclusions from it;
c) the individual's response to the received signals by communicating with the other individuals, their strength of response and their capability to express the information to be transferred;
d) the quality, intensity and type of the interaction, and the type of communication (e.g., whether it is parallel or asynchronous etc.);
e) the number of actively communicating units;
f) the range up to which other communicating individuals can be reached.

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To facilitate our basic understanding, in this work we try to minimize the preconditions for the emergence of the collective effects. Therefore, such advanced features as the capability to store the collectively obtained expertise, to inherit, plan or learn new types of behavior, to define rules for communication and to build up communication hierarchies are neglected. This means, we assume the interacting objects to possess only one input channel each for the incoming information (which may stem either from other objects or from external sources such as sensors), to be capable to make decisions on the basis of the obtained information, and to possess only one output channel for communication of their decisions to other objects. The decisions made by the individual objects should be preferably logic ones, based on mathematical, physical, or chemical correlations.

## 2. Ion Track-Based Electroactive Nanostructures

The objects treated in this work are swift heavy ion tracks – either as-obtained by ion irradiation or subsequently modified – embedded in two different types of systems. When applying a voltage to these tracks, they eventually show interesting electroactive properties and are therefore denoted here as ElectroActive NanoStructures (EANS).

a) The first system consists of one or two thin polymeric foils with latent ion tracks that separate a vessel filled with electrolytes into two or three parts, respectively. A sinusoidal low frequency voltage of sufficient intensity is applied to this vessel via two inert electrodes. Then, the electrolyte-immersed latent tracks often respond with current spike emission to the applied voltage [1, 2]. Alternatively, EANS can also be produced by etching these tracks towards funnel-type shapes [3]. These tracks are used to combine current pulsation emission with current rectification – the latter due to the asymmetric track shapes which give rise to internal asymmetric electrostatic fields [4, 5]. Such {electrolyte/irradiated polymer} configurations were denoted earlier as "$E^3T$" (Electronics made of Electrolyte-filled Etched Tracks) [6]. The used latent tracks were obtained by swift heavy ion irradiation (typically ~ 100 MeV to a few GeV of Ar…U projectiles, from a suitable high energy accelerator) of suitable polymer foils (typically PET or PC). The latent tracks have effective radii for electrolyte penetration in the order of a few nm; the diameters of the etched ion tracks that we used ranged up to ~ 20…50 nm. Their length is given by either the range of the used swift heavy ions or by the thickness of the layer/foil/membrane in which they are formed (typically ~ 2…50 μm) and their areal density is usually in the order of $10^{6 \ldots 10}$ $cm^{-2}$. All tracks in the polymer foils are parallel to each other. In all $E^3T$ arrangements, all tracks in contact with electrolytes are exposed to the same externally applied potential.

b) The other, more complex system consists of a bilayer structure with a Si substrate and a swift heavy ion-irradiated ~ 100 nm thick top layer. The tracks formed by ion irradiation of that top layer (at fluencies of typically ~ $10^{8 \ldots 10}$ $cm^2$ and energies between ~ 20 MeV and a few GeV) impose an overall asymmetry of the electronic properties onto quite a number of materials. The emerging tracks in them often distinguish markedly from their environment so that they are well-defined EANS. These structures had been denoted as "TEAMS" (tunable electronically anisotropic material on semiconductor) structures [7]; typical examples for the materials of the layers are organometals and fullerite [8, 9].

If, for contrast, the top layer consists of ion irradiated and subsequently etched $SiO_2$ or SiON, onto which dispersed metallic or semiconducting (e.g. Ag, Au, $TiO_2$,…) nanoclusters or other materials (e.g. $C_{60}$, porphyren etc.) were deposited, one uses to denote the corresponding structures as "TEMPOS" (Tunable Electronic Material with Pores in Oxide on Semiconductor) structures [10–13]. We are restricted in this work by metal nanocluster coverages. Usually both the TEAMS and TEMPOS structures are equipped with 3 contacts, two on the thin surface layer and another one on the silicon substrate. The voltage can either be applied to one surface and the back contact. Alternatively, the voltage can also be applied via two contacts on the surface. Then, the third contact serves for tuning these devices. This geometrical configuration ensures that all neighbouring tracks in a TEAMS or TEMPOS structure are subject to different potentials, in contrast to the $E^3T$ case. Depending on the charge injection/extraction into/from the {layer/Si} interface of these structures, the interface can either be in a well-conducting or a highly resistive state. The possibility of switching between these two working states is one of the characteristic properties of these structures.

We have chosen swift heavy ion tracks as EANS for this work as they fulfill the requirements defined above, i.e., they have an input channel, they can make logic decisions and they have an output channel. More specifically, their input feature consists of the acceptance of some voltage signal applied to them, their decision-making features consist of:

1) the analysis of the sign of incoming charge carriers (rectification in the case of diodelike EANS):
2) the acceptance or rejection of an incoming signal in respect to its polarity (eventually in relation to a preset threshold)

and

3) the adjustment of the diode resistance to the applied voltage, according to the I/V relation of the said diode (which may be e.g., quadratic or exponential), and the output feature consists of the transmission of currents of well-adjusted heights (which includes zero currents).

These EANS, if properly designed, can even be made tunable by any physico-chemical parameter (such as voltage, light, magnetic fields, temperature, ambient gases, biomaterials etc.), so that the collective effects emerging from them (such as negative differential resistances (NDR), synchronous oscillations etc., see below) are tunable. For simplification, we will restrict our discussion to the resistive properties of EANS only. Similar argumentation can also be made on their capacitive properties.

## 3. Communication between Electroactive Nanostructures

EANS-EANS (i.e. here: inter-track) interaction can be implemented in several ways.

a) In the simplest case, the medium between two communicating EANS has a constant resistivity R. Here, R can be near-zero (metallic contact between EANS), near-infinity (insulating connection), or it can have any positive value (semiconducting or electrolytic connection).
b) The medium between two communicating EANS can have a variable conductivity. This is implemented by, e.g., resistive sensor materials, where the resistivity depends on the impact of radiation, temperature, chemical or biological parameters, etc.
c) In addition to the above-mentioned conductive properties, the medium can also have capacitive properties. For applied DC voltage, these capacitive properties signify a transient memory effect; for applied AC voltage it signifies reduced resistance and a phase shift. Such a type of inter-track contact can be employed by capacitor-like layers of the type: {nanocomposites of metal or semiconductor}/{insulator ($SiO_2$, polymer,..)}.
d) The medium between two communicating EANS can have both conductive and amplifying properties. This may be implemented by flat transistors deposited lithographically [13] on the surface to amplify the track-track communication. The amplification can be externally controlled by the gates of the corresponding transistors. (In fact the latter described systems, though not yet having been verified technologically, are expected to have the best functionality, as they are employed by nature in the human brain. Here, the synapses, i.e., the interaction points between two different dendrites (i.e., input/output channels of neurons) are tuned by an external control system of lower operation frequency (the glions or astrocytes), so that interneuron signals can be reduced or amplified.)

## 4. Elemental Cells of EA/S Communication

The different functionalities of these two systems introduced above lead to the introduction of two different types of elemental cells for communication.

### 4.1. $E^3T$ Communication

Due to the good mobility of ions in electrolytes, the cloud of charge carriers emerging one from a track into its electrolytic neighbourhood upon current spike emission can extend rather far, even within short time. Consequently, the charge cloud of one track may readily mix with that one of another spike-emitting track. This is what we interpret as track communication. Indeed, it is this overall charge exchange between many tracks, which leads to a neural network-type behaviour of the whole track assembly within a given domain. According to the rules of Neural Network theory [15, 16], this collective interaction leads to a synchronization of the current spike emission of all tracks at a fixed phase ("phase-locked synchronization").

The maximum time, available for the charge cloud dispersion, is given by the half period of the applied sinusoidal voltage. The mean free path-length of ions within this time, $\lambda$, defines the size of the domain within which unlimited inter-track communication is possible. Two different domains on a polymer foil will still have some limited information exchange if they are sufficiently close to each other; however, the larger the distance, the less becomes the inter-domain communication. In our previous work [2] we found typical domain sizes of 20…30 $mm^2$, corresponding to $\lambda \sim 3$ mm.

### 4.2. Teams/Tempos Communication

The different geometrical configuration leads to a different charge carrier behaviour. Charges injected from the power supply (suppose at positive potential) at a given contact point on the surface will spread radially on the surface around that contact. Whenever they meet an etched track, they will be driven through that track towards the conducting interface (and further to the Si substrate), if an attractive potential (suppose: a negative one) was applied to the latter one. The same happens if the charges are not brought from the outside to the surface, but through a track which is on a potential (suppose: positive) different from that one of its neighboring tracks (suppose: negative). The more far away one track is from the point of charge injection, the lower is its chance to be still reached by some of the previously injected charges. Based upon network theory as developed by Barabasi-Albert [17], a circular 'radius of influence' (ROI) around a given contact point for insertion of a current $I_0$ has been defined by the distance r from a contact point at which an initial current $I_0$ has dropped to the value $I_0/1000$ [18] (see Fig. 1a). The size of the ROIs depends on the working states of the ion track diodes; for closed diodes the ROIs are markedly larger than for open ones. However, in the frame of this work, only open track diodes are of interest as only they can contribute to the collective interactions. In this case, the ROI for typical TEMPOS structures is in the order of S µm or so [18].

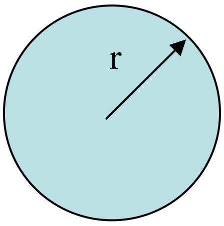


*Figure 1a.* The elemental cell of inter-track-communication. In the case of TEAMS/TEMPOS structures, r = ROI is the radius of the region of interconnection (shown here). Alternatively, for $E^3T$ systems, r can be replaced by λ, to describe a neural network domain

Depending on the type of track distribution, two cases must be distinguished: (a) random track distributions (such as usually obtained by swift heavy ion irradiation) and (b) regularly spaced track distributions (such as obtained by sequential ion-by-ion writing or as obtained by the use of self-organizing nanopores). The probability distributions $P_0(r)$ to find nodes at large distances r are the same for both cases, but deviations occur for very small distances r. Whereas, for random track distributions, P(r) is always positive even for the smallest values of r, there exists a cutoff for the case of regularly spaced tracks which is given by the inter-track distance. However, as our interest focuses on long-range track communication to maximize the collective interactions in a track system, we can neglect these details here.

## 5. Modification of EA/S Intercommunication by Additional Wiring

A consequence of the limited mean free ionic path-length λ in $E^3T$ systems, and of the limited radius of influence ROI in TEAMS/TEMPOS systems is that only a fraction of the available total device area of larger samples is used for intercommunication of the electroactive tracks. The possibility to simply enlarge the actively intercommunicating sample area by increasing λ or ROI, respectively, is usually limited by the system physical restrictions. Therefore, another way is discussed here, namely the interconnection of spatially separated domains (or regions of interaction) by additional wires. This idea has its biological counterpart in the dendrites of the neurons in the human nerve system which are known to connect cells or cell clusters with each other, with up to about 2 m distance.

Let us consider here a simple case: let us connect two elemental cells (i.e. neural network domains in the case of $E^3T$ or two regions of interaction in the case of TEAMS/TEMPOS structures) spaced by a distance d by a wire, as shown in Fig. 1b. Let us also assume that this wire is covered by an insulator except for its end points so that track intercommunication is restricted to only these cells and does not take place in between them. Then one should expect that, for the example of TEAMS/TEMPOS structures, this case should be approximately equivalent to that of only one ROI but with double track density, hence $P(r) = 2 \cdot P_0(r)$, with $P_0(r)$ being the probability distribution of the elemental cell of communication. P(r) is independent of the distance d.

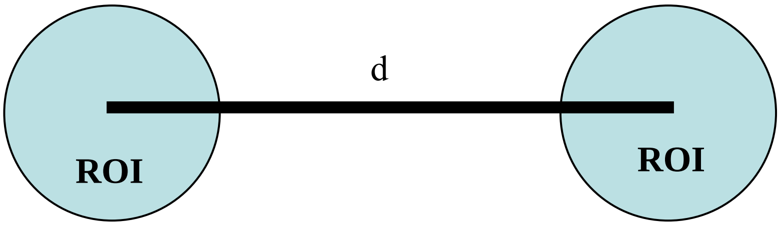


*Figure 1b.* The simplest case of an advanced system of track-track-communication, shown here for TEAMS/TEMPOS systems: two elemental cells connected by a wire of length d; wire insulated in between the ROIs. Consideration of domain interconnections in $E^3T$ systems is analogous

To check this assumption, we made a first test experiment. For this sake 12 µm thick PET foil of 1 $cm^2$ area with $4x10^9$ tracks/$cm^2$ was covered by a mask so that everything was shielded apart from two 1 $mm^2$ large test areas A and B at a distance of about 5 mm (Figs. 2d, e).

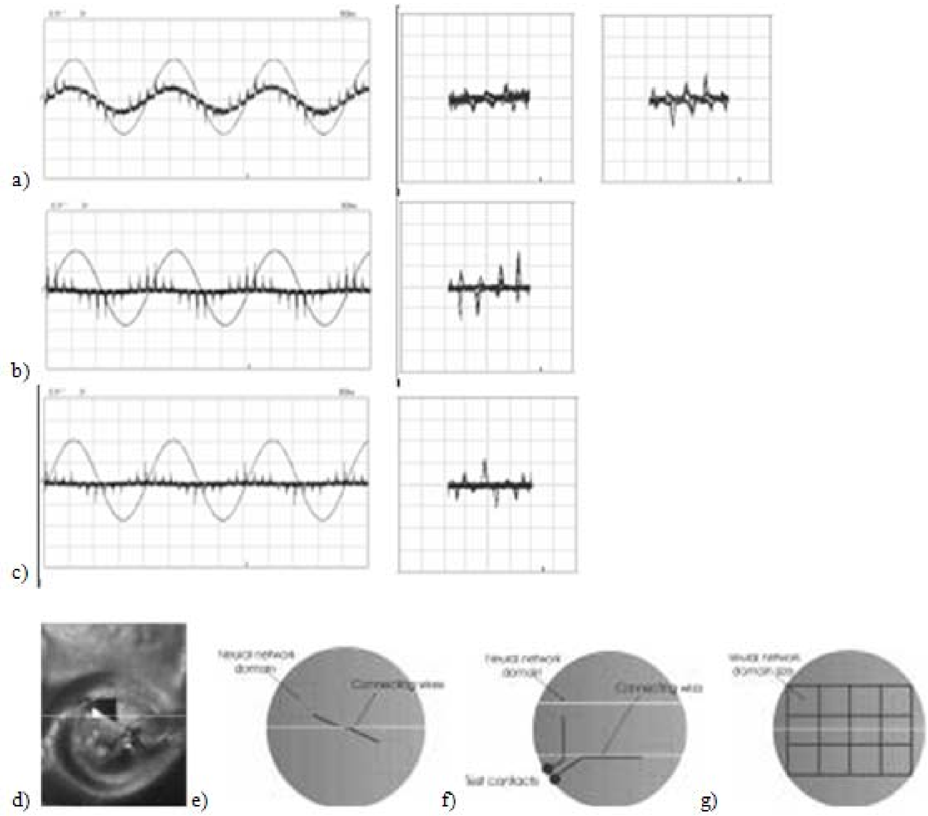


*Figure. 2.* First test experiment for interconnection of two spatially separated cells A and B:

a) spiky currents through cell A (left and center) and cell B (right). Shown are both the time dependence of current and voltage (left) and the corresponding current/voltage plots (center, right);
b) both test areas A and B exposed simultaneously to the applied voltage;
c) same as b), but additionally connection of A and B by a thin Cu wire. Scales: voltage: 3V/div, current: 0.1 µA/div, time: 500 ms/div;
d) Picture of the mask on the track-containing polymer foil with two selected domains and a thin copper wire connecting them, after removal from the experiment;
e) principle sketch of that setup;
f) and g): suggestions for future experiments on this system;
f) extracting both test area potentials for their external manipulation by, e.g. transistors, sensors etc.;
g) printing a conducting grid with mesh size = neural network domain diameter should enable one to synchronize larger sample areas

After immersing this masked foil as usual into electrolytes in our measuring chamber and applying a sinusoidal voltage, current spike emission occurred. As both the test areas A and B are smaller than the average domain size, all spikes emitted from all tracks are well synchronized so that the 4 peaks in the current/voltage plots which are theoretically expected for individual tracks show also up rather clearly here (Fig. 2a). The I/U plots of both test areas A and B are similar to each other as concerns the spike positions, but they distinguish somewhat in the spike intensity spectra (Fig. 2a, center and right). This may be due to slight differences in the geometry and position of the selected areas.

When both test areas are exposed to the applied voltage simultaneously, the spike spectrum becomes increasingly sharp and the spike heights are about equal to the sum of both components A and B (Fig. 2b). Also, the overall spike characteristics simplifies insofar as now the positions of the positive and negative spikes become the same.

However, when – for else unchanged geometry – an additional thin Cu wire connects both areas A and B, the spectrum gets considerably distorted: the spike heights become smaller, their height distribution changes and the positions of the negative and positive spikes differ now from each other (see Fig. 2c).

This fact clearly indicates that by additional wiring one is capable to influence the interaction of two spatially separated domains. However it appears that the result of this manipulation is not that simple as originally expected; connecting two cells by an additional wire does not simply double the signal height while leaving everything else unchanged. The reason is that the information exchange paths are not the same in both cases. Suppose the area of a small elemental cell (i.e. with area being much smaller that that of the neural network domain size), is just doubled, then every track can still communicate with every track individually, hence the overall information exchange just doubled: $\Sigma_{1n}\, c_i + \Sigma_{1n}\, c_i = \Sigma_{12n}\, c_i$ , with $c_i$ being the information exchange current from track i to all its neighbours and n being the total number of tracks in the cell. However, additional wiring between spatially distant cells signifies that now $\Sigma_{1n}\, c_i + \Sigma_{1n}\, c_i \neq \Sigma_{12n}\, c_i$ , as all the intercommunication paths $c_{AB,i}$ between the individual tracks i of both cells A an B (in total: $\Sigma_{1n}\, c_{AB,i}$ ) are missing. Apparently, this loss of information cannot be compensated fully by just equalizing the sums $S_A = \Sigma_{1n}\, c_{A,i}$ and $S_B = \Sigma_{1n}\, c_{B,i}$ of both cells.

Nevertheless we think that cell interconnection by wiring may be useful as it definitely increases the overall intercommunicating area – though at the expense of the loss of long-distance individual track intercommunication, which apparently the collective long-distance intercommunication cannot compensate fully. From this point of view, we suggest to design more sophisticated wiring configurations such as illustrated in Figs. 1c-e and 2f-g, for a sake of developing more advanced intercommunication systems. In the following we restrict our discussion to TEAMS/TEMPOS structures only; the $E^3T$ case can be treated analogously.

Star-like communication patterns, n elemental cells connected by wires: This case is approximately (i.e. while loosing all individual long-distant inter-track communications) equivalent with the one having only one ROI but with n times the track density: $P(r) = n\, P_0(r)$ with n/2 being the number of star pattern branches. P(r) is independent of distance d (Fig. 1c).

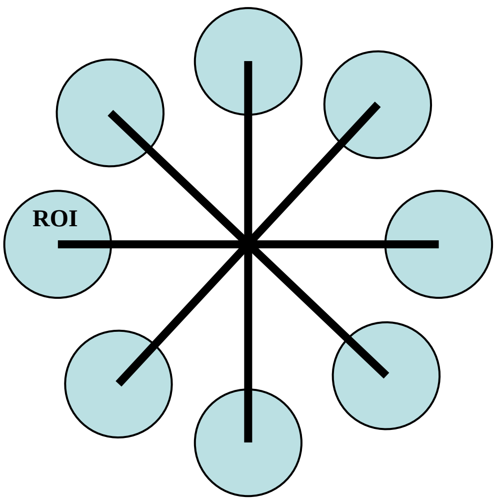


*Figure 1c.* Advanced system of track-track communication: n elemental cells connected by wires of length d to a star pattern. Shown here for the TEAMS/TEMPOS case only

Pointwise connection of k elemental cells by a wire: Also, this case (Fig.1d) is approximately equivalent to the one having only one ROI but with k times the track density: $P(r) = k\,P_0(r)$, i.e., it does not matter at which distance and according to which geometry the elemental cells of communication are connected with each other.

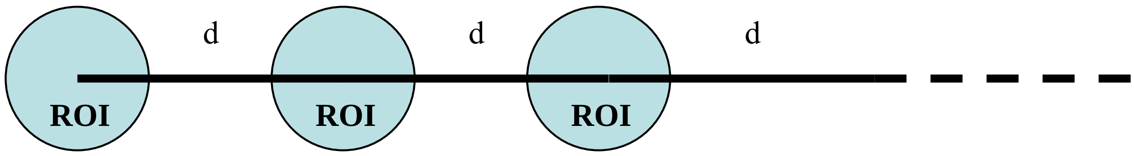


*Figure 1d.* Advanced system of track-track communication: k elemental cells connected sequentially by a wire

Connection of two elemental cells and the area in between them: This modifies P(r) so that, additionally to two halves $P_0(r)/2$, one has to add a term which is proportional to the connection length d: $P(r) = P_0(r) + \alpha d$, where the factor α can be derived easily from the network theory. Consequently, when linear ROIs are connected with each other according to a star-like pattern: $P(r) = n\,(P_0(r) + \alpha d)$, with d being the wire length and n/2 being the number of star branches, each point within this star pattern can communicate with another point of the same star pattern at least via the overall signals of each individual cell.

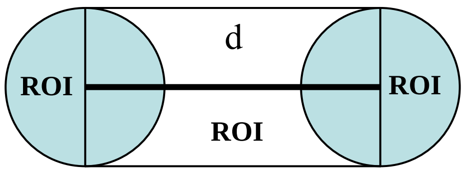


*Figure 1e.* Advanced system of track-track communication: linear expansion of an elemental cell by an overall conducting wire

Optimization of P(r) with the help of line patterns: Hence, for σ stars (or lines) being present per unit area, the probability distribution becomes: $P(r) = \sigma\ n\ (P_0(r) + \alpha d)$. To optimize P(r), it will be necessary to have many stars with many long arms, i.e., σ, n and d should be large. These stars can be arranged in 3 different configurations:

a) the individual star (or line) patterns do not touch each other. In this case, there does not exist any direct information exchange between the individual star patterns, hence any larger-scale communication between the stars (lines) is suppressed. In contrast, there exists a multitude of localized individual information transfers per star pattern;
b) the individual star patterns are connected with each other by at least one wire. Then, all star patterns form one common system of information exchange;
c) the individual star patterns are not directly connected with each other by conducting wires, but their ROIs overlap. Then, all star patterns form a common system of information exchange, but information exchange within each individual star pattern is favored to information exchange between neighboring star patterns.

## 6. Different Qualities of Communication

Several cases offer different qualities of communication:

**Case 0:** Here, no object communicates with the other, hence, information exchange has no meaning and consequently no collective interaction takes place.

**Case I:** Here, all objects follow exclusively a prescribed behaviour without any deviation. In such case, no useful communication is possible due to the virtual identity of all objects and hence, no peculiar collective behaviour can develop.

**Case II:** Here, all objects communicate with each other within a limited range (i.e., contact only with the nearest neighborhood as described in section 4.1). Two possibilities are shown up: (a) the communication of all objects is, in principle, of equal importance, or, (b) not all objects have equal importance, but the communication of some is weighed higher than that of others. In these cases, the information exchange is largely limited to the more important objects, the influence of others becoming negligible. Consequently, the amount of collective interaction will be reduced.

**Case III:** Here, all objects communicate equally strongly with each other; no preference of any object is made. This yields the maximum degree of information exchange. However, as both the quality and direction of the acquired collective information are not weighed, the collective interaction suffers from unpredictable statistical fluctuations and may, thus, eventually even deteriorate the behaviour of the whole system, instead of improving it. Therefore, some kind of superimposed additional regulating authority may be advantageous.

Drawing the conclusion, one may find the optimum collective interaction somewhere in between Cases II and III.

### 6.1. Application to Collective EA/S Electronics

**Case 0:** In this case all EANS are completely decoupled from each other by belonging to separate electronic circuits parallel to each other. As there does not exist any communication in this case, it is of no interest for this work.

**Case I:** This case is implemented by track-track interconnections of very high conductivity so that all EANS are forcefully set to equal potential upon application of an external voltage. Due to zero potential difference, no EANS can communicate with another one; no collective interaction takes place. Then, the sum of all parallel EANS behaves just as one very big electroactive nanostructure. This case is favoured in technology for ion track enabled multiple wire interconnects in printed circuit boards where a given signal should be transferred without any deviation from the input [19]. Fig. 3 illustrates such case in the $E^3T$ electronics. Though, metal-clad EANS exhibit good and stable diode properties, no other electronic effect is found to show up.

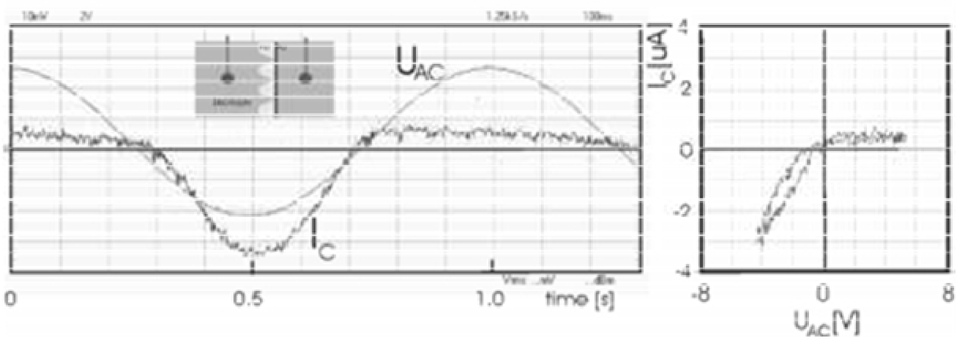


*Figure 3.* Electronic behaviour of a track-containing membrane with thin metal coating (~50nm Au) immersed in electrolyte (see insert): good and stable diode behaviour is recorded, but no collective effects are shown up. $4x10^6$ EANS/cm$^2$ in a 10 µm thick PET foil, embedded in water. 10 V peak-to-peak sinusoidal voltage (1 Hz) has been applied. Such diodes exhibit long-lasting stability

**Case II:** This case is implemented by highly resistive track-track interconnections which make some track-to-track intercommunication possible. In comparison to the above Case I in which any diode-diode communication is suppressed, Case II may be considered as somewhat better. Due to the rather short range of influence of a given track in TEAMS/TEMPOS structures, as given by the 1/r – probability distribution of Ohmic interconnectivities (resulting from the Barabasi-Albert network theory) [17], only nearest neighbouring tracks communicate with each other reasonably. Tracks at a longer distance are decoupled from each other (Fig. 5a) so that direct collective interactions are restricted to a marginal part of the sample defined by the ROI. However, information can be communicated sequentially from the ROI of a given track to the ROI of a neighbouring track, if the given information (in the form of transferred charges) is strong enough not to be annihilated immediately. This is how collective effects such as NDRs [20, 21] and pulsations emerge from the contemporary TEMPOS and $E^3T$ devices.

The collective EANS-EANS interaction can be influenced by different obstacles in the current paths, e.g., by thin layers of insulators, nonlinear resistances, resistive sensors etc., either within the EANS or in between them. Fig. 4 shows such an example for an $E^3T$ structure.

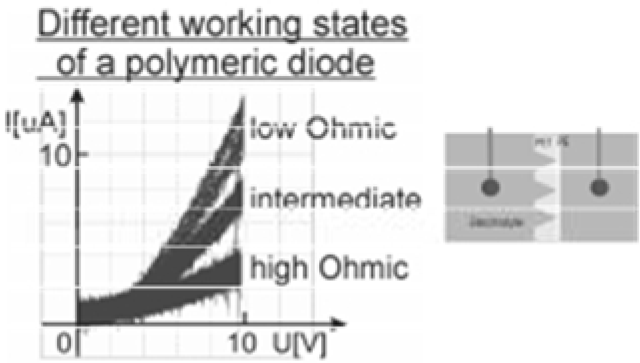


*Figure 4.* Electronic behaviour of an etched track-containing (4 x $10^6$ $cm^{-2}$) 10 µm thick PET foil clad with a ~ 50 nm thick layer of polyethylene (PE), immersed in electrolyte (here: deionized water), see insert. During track etching, the irradiated PET zones are removed, however not the irradiated PE. As a result, the etched tracks are covered with a thin insulating membrane on one side. Though at low applied voltages nearly no response is observed, currents start flowing when field effects play a role at elevated voltages. The characteristic of this membrane is quite unstable, exhibiting collective effects such as NDRs and sporadic jumps between multiple working states. 10 V peak-to-peak sinusoidal voltage (1 Hz) has been applied, ~ 100 sweeps are superimposed

Ion tracks emerge from statistical ion impact into the targets. Hence they will, at higher fluencies, start overlapping. The overlapping tracks are larger in diameter than the individual ones; hence after filling with (semi)conducting material, the corresponding EANS will have higher conductivity and therefore, will dominate over their non-overlapping neighbours. This means, with increasing ion fluence (i.e., track density) we have the transition from the abovementioned possibility (a) (equal importance of all objects) towards possibility (b) (few objects weigh more than others). The first case – equal importance of all objects – can either be accomplished by using etched ion tracks at low fluence or by producing nanopores at regular distances via nanolithography.

When these few highly conducting entities start determining the overall communication, the other non-overlapping higher-resistant single track EANS will yield only some 'background noise' to this communication. Therefore, it may happen that, at the onset of track overlapping, the overall amount of communication starts collapsing, due to the rather small number of such dominant track diodes. Hence, it appears that, in order to obtain a high degree of collective interaction, track overlapping should be avoided.

**Case III:** We assume that, the larger the number of neighbouring tracks is with which a given track can communicate, the larger will become the overall collective interaction of the track system. A larger number of tracks that can be reached for communication can be obtained in two ways:

(a) increase the track density;

(b) increase the range of the conducting paths from one track to another.

We can rule out (a) as according to the above section, an increase in track density will lead to the emergence of a higher degree of ion track overlapping which appears to be detrimental for an increase in collective interactions. The other case signifies that one should establish long-range order in communication. This is not trivial as the natural probability distribution of track-track connectivity follows a 1/r relation, i.e., leads to short-range order. In order to overcome this problem, one should artificially establish a network of long-range wires from one track to the other as sketched in Figs. 5b. Though this has – apart from the above-mentioned test experiment – not yet been verified technologically, such networks have, however, been implemented in nature already since long, e.g., by dendrites which connect even distant neurons with each other. It is expected that, similarly in this case, the longer range of the communication network would lead to a much higher degree of information exchange and collective interaction. As in planar systems such as TEMPOS structures, the number of interconnected EANS increases with the square of communication range, the amount of collective interaction is expected also to increase with the square of the communication range. (As in spatial systems such as the human brain, the number of neurons interconnected via the very long dendrites increases even with the cube of communication range, the collective interaction becomes tremendous; this explains why spatial construction principles were chosen for the design of biological neural systems.)

No such long-range inter-track connectors have yet been employed. One may speculate that they could be obtained by:

a) growing a fibrous network of conducting carbon nanotubes – first attempts in this directions have already been reported in literature;
b) producing bio-hybrides by fixing natural nerve cells at the track positions and letting them grow dendrites. Possibly the dendrite growth can be influenced by putting the adequate potentials onto those tracks which the growing dendrites should reach. If this bio-approach works, one could possibly use these cells themselves for permanent communication. This task is, however, not trivial, as the living cells require special care concerning food, waste removal, adequate temperature, humidity, sterility etc., and dendrite growth requires typically at least a month;
c) in contrast, one could think at using the formed dendrites just as templates for interconnecting wire production. This may be accomplished by sacrificing the nerve cells by doping them and their dendrites with a very high amount of metal (e.g., Ag, Cu, Au,…) salts and thereafter reducing these salts to the corresponding metal to obtain a long-range network of biomimetic metallically conducting nanowires at the place where the dendrites were;
d) alternatively, one might think at enriching the dendrites with organic matter which in a later stage could be carbonized to yield conducting graphitic nanowires;
e) instead of following the above bio-technological approach, one could also think of producing the required long-distance connection network artificially by conventional techniques, e.g., by lithographic evaporation of a corresponding network of long wires through a mask.

In spite of its advantages, even Case III seems not to be the ideal working solution as in this case the collective interactions will be only randomly acquired and randomly directed, with hence eventually having only limited use. Therefore, the optimum system appears to have some kind of limited interaction with a superimposed independent regulating system. This could be implemented by putting some kind of switching points in between the long-range connection wires of different objects. These switching points would have not only the task to amplify the weak track-to-track connection signals, but they could also interfere the track-to-track communication by lowering or even suppressing unwanted information. For this sake, these switching centers should be connected to another network of interacting entities of a higher hierarchic level (Fig. 5c). In order to avoid any resonance catastrophes between these two systems, they should work with widely different time constants, i.e. different frequencies. Further, it should be guaranteed by proper design of this control system that it suppresses only unwanted track of intercommunication but not the valuable one.

Though, at present this suggestion still seems to be speculative due to the high complexity of two interacting nanoscale electronic systems on a planar substrate, one should keep in mind that this is exactly how nature works: in the human brain, the intercommunicating network of gluons or astrocytes, reacting $\sim 10^4$ times slower than the neurons, controls like an external regulating authority the neuron-neuron intercommunication via enhancing or reducing the number of messenger molecules in the synapses which are the dendrite-dendrite transition points. Therefore, one should at least try to define the utmost goal and direction of the present ion track electronics research.

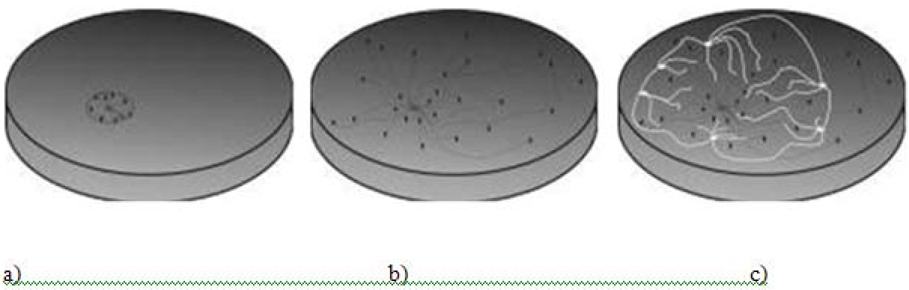


*Figure 5.* The different types of ion track electronics communication, a) Case II as implemented by contemporary TEAMS and TEMPOS structures: all neighbouring EANS within a certain ROI (see the circle) are influenced by a selected track (central spot in the figure); b) Case III, as possibly implemented in future by long-range connections; c) the future bio-inspired system of Case III with a superimposed regulating authority: one EAN system is controlled by another network (drawn as light lines) via certain "switching points" (light spots). Analogous considerations as for the TEAMS/TEMPOS structures described here also hold for $E^3T$ structures

## Conclusions

Based on the above considerations, we recommend the future research strategy to be the following:

1) get more systems operating with short-range order, i.e., of the type of Case II (Fig. 5a) by modifying the track-track interconnection – e.g., by depositing selected resistive materials (such as sensors, ion exchangers, ferrofluidics, nanocomposites, etc.) onto the sample;
2) verify the TEMPOS-like structures with very long track-to-track intercommunication lines according to Fig. 5b by connecting the EANS with (a) a lithographically deposited long wire network, (b) conducting inter-track CNTs, or (c) biologically created track-to-track interconnections as employed directly by dendrites or by inorganic replica derived from them, to pave the way towards more interacting systems according to Case III. By modification of the electronic properties of the inter-track communication lines, different types of collective track-track interaction should be obtained;
3) deposit controlling authorities in between the inter-track communication lines according to Fig. 5c. The nature of such controlling authorities can range from lithographically deposited thin film transistors or biosensors up to living nerve cells grown on the substrate in between the etched ion. In the latter case, their dendrites would be the natural interconnection lines even between distant EANS. Apart from this, it appears vital to develop the accurate simulation programs to make predictions on the detailed behaviour of these complex devices.

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# TYROSINE-TRYPTOPHAN COMPLEX: INTERMOLECULAR ELECTRON TRANSFER USING QUANTUM CHEMISTRY APPROACH

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This work is devoted to theoretical study of electron transfer (ET) processes between molecular pair of organic π-conjugated luminophores: tyrosine-tryptophan complex. Therefore, the rate of intermolecular ET is evaluated according to Fermi golden rule. Calculations are done using semi-empirical ZINDO approximation method, which is suitable for UV/Visible absorbance spectra calculation.

***Keywords:*** *Organic luminophores, electron transfer, electronic states, Fermi golden rule*

## 1. Introduction

Electron transfer (ET) and energy transfer processes [1] are vitally important for entirety of biological structures. The processes lay on the base of such phenomena as photosynthesis [2] in plants and metabolism [3] in biological structures becoming an irreplaceable source of energy. However, the most biological structures are notable by complicity of their composition. Organic luminophores are constituent units of biological structures, which distinguish for their ability to luminescent at low and middle temperatures. These organic compounds allow the energy transfer processes between the separated parts of enzymes, cofactors, etc. The most valuable structures include π-conjugated molecular fragments, such as tyrosine and tryptophan derivatives.

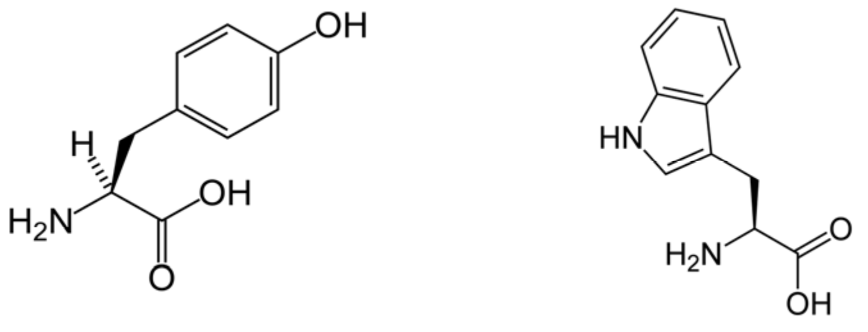
The possibility to apply non-invasive luminescence analysis methods for the complicated biological structures is tied up with an effective absorption of tyrosine and following electron transfer to tryptophan. The mentioned phenomenon is known from the middle 30s and could be used as a dynamic representation of the complicated relaxation processes.

This work is devoted to theoretical evaluation of intermolecular ET process of well known model system called tyrosine-tryptophan complex. Rate of ET process is calculated according to Fermi golden rule as process between one-particle resonance states, caused by electronic couplings.

## 2. Object of Investigation

Tyrosine (2-amino-3-(4-hydroxyphenyl) propanoic acid, Tyr) and tryptophan (2-amino-3-(1*H*-indol-3-yl) propanoic acid, Trp) molecules are well-known natural π-conjugated luminophores – see Fig. 1. Tyr-Trp molecular pair belongs to the class of 20 standard amino acids, which are essential for biological organisms [4]. Tyrosine molecule contains phenol fragment and tryptophan molecule correspondingly indole fragment.

Absorbance ranges of the molecules overlap, consequently, it becomes difficult to isolate contribution of pending molecules to the process in common spectra [5]. However, tryptophan has nearly five times higher maximum absorbance magnitude at 280 nm comparing to tyrosine and correspondingly 50…100 times more efficient quantum efficiency.




**Tyr** **Trp**

*Figure 1.* Tyrosine (Tyr) and tryptophan (Trp) molecules

It is known, that exciting a tryptophan molecule by laser with quite wide spectra range in Tyr-Trp complex leads to luminescence of both molecules, but more intensive luminescence of tryptophan molecule. What is more, an accurate excitation at 295–310 nm could eliminate tyrosine excitation.

We have examined Tyr-Trp complex of a sandwich type, when phenol and indole fragments are placed in parallel plane surface. Distance between planes contains 4.7 Å. Orientation of molecules is typical for pigment-protein complexes (see Fig. 2.)

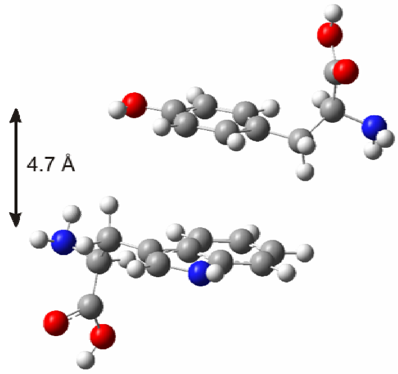



*Figure 2.* Typical Tyr-Trp complex. Intermolecular distance between plane surface 4.7 A

## 3. Theoretical Background

ET process estimation is performed according to the basic models of quantum chemical theory. Specifically, Fermi golden rule (Eq. 1) and Marcus theory [6] are used for evaluation of ET parameters. The dynamical process between two molecular systems, MS-1 and MS-2, respectively, is defined by rate *W*:

$$W = \frac{2\pi}{\hbar} S_{\alpha\beta}^2 \delta\left(E_\alpha - E_\beta\right), \tag{1}$$

where α and β represent the electronic states of the separated molecular systems, MS-1 and MS-2, respectively. Interaction between these MS could be expressed *via* intermolecular electronic coupling $S_{\alpha\beta}$ parameter:

$$S_{\alpha\beta} = \left\langle \alpha \middle| \hat{V} \middle| \beta \right\rangle, \tag{2}$$

where $\hat{V}$ represents a Hamiltonian of intermolecular interaction.

*Delta* function δ(x) used in Fermi golden rule expresses the strongest resonant condition (band half-width converges to zero). For ET process simulation purposes, we have replaced this expression by Gauss-shaped function containing half-width σ parameter which allows us to control the resonant conditions according to Marcus theory:

$$\delta\left(E_\alpha - E_\beta\right) \Rightarrow \frac{1}{2\pi\sigma} \exp\left(-\left(\frac{E_\alpha - E_\beta}{2\sigma}\right)^2\right). \tag{3}$$

Electronic states α and β of separated molecular systems, MS-1 and MS-2, respectively, belong to the one-particle state type according to Fermi golden rule definition. We have generated the molecular orbitals (MO) in the framework of atomic orbitals (AO). *Ab-initio* Hartree-Fock (HF) method allows expressing MO in a pure one-particle state manner. However, this exact assumption is not fully suitable for spectrometric tasks, for example, for definition and simulation of bathochromic shift of absorbance spectrum. Due to the practical needs, we decided to use another, less exact method as first assumption. We have used the one-particle state assumption when MO were generated using semiempirical ZINDO but not classical *ab-initio* HF method.

Mainly, semi-empirical calculation methods [7] are applied for the quantum molecular process simulations. Then theoretical results are compared to the experimental data in order to understand physical nature of pending process.

In our case, theoretical and experimental absorbance spectra were compared with a quite high accuracy. Consequently, semi-empirical method ZINDO [8] (Zerner intermediate neglect of differential overlap), suitable for UV/VIS absorbance spectra simulations, was selected.

Our calculations are done applying semi-empirical ZINDO method, which is suitable for UV/VIS absorbance spectra simulation. Spectroscopic state as multiparticle state is constructed as a set of several one-particle states. Therefore, calculations are performed using several highest occupied molecular orbitals (MO), up to ten, and the same number of the lowest virtual MO.

Calculations are done using programming package *NUVOLA* [9] and quantum chemistry tool *GAUSSIAN03*[10]. ZINDO routine (including singlets only) was used for absorption spectra simulation.

## 4. Main Electronic Transitions of Spectroscopic Importance

Intermolecular ET process starts from an electronic excitation of MS-1 system (donor) into LUMO (and higher). Each MS was described using the model of MO in the framework of separated AO. Three main types of electronic transitions $S_0 \rightarrow S_1$, $S_0 \rightarrow S_2$, $S_0 \rightarrow S_3$ were analyzed and pictured in a form of schematic Jablonski diagrams. Fig. 3 and Table 1 represent the electronic transitions in Tyr molecule, MS-1, after excitation. Spectroscopic transition $S_0 \rightarrow S_n$ could be characterized using several parameters: energy $E$ and oscillator strength $f$. However, spectroscopic transition is combined of several one-particle transitions (HOMO-$N_1$) →(LUMO + $N_2$) with corresponding weight coefficient $k$ (total number of MO is equal to sum of $N_1$ and $N_2$). Population schema of $S_1$, $S_2$, $S_3$ spectrometric states allow us to conclude that only two MO (37, [LUMO + 1] and 38, [LUMO + 2]) could be used in the intermolecular ET process.

Fig. 4 represents simulated UV/VIS absorbance spectrum separate tyrosine and tryptophan molecules. Absorption of Tyr in the low energy region 4.2 eV is per order more effective that Tpr. The main ET events occur after excitation of Tyr into electronic band of 4.2 eV (according to the simulated spectrum). The mentioned simulation of Tyr absorbance is in a good agreement with the experimental data [11, 12].

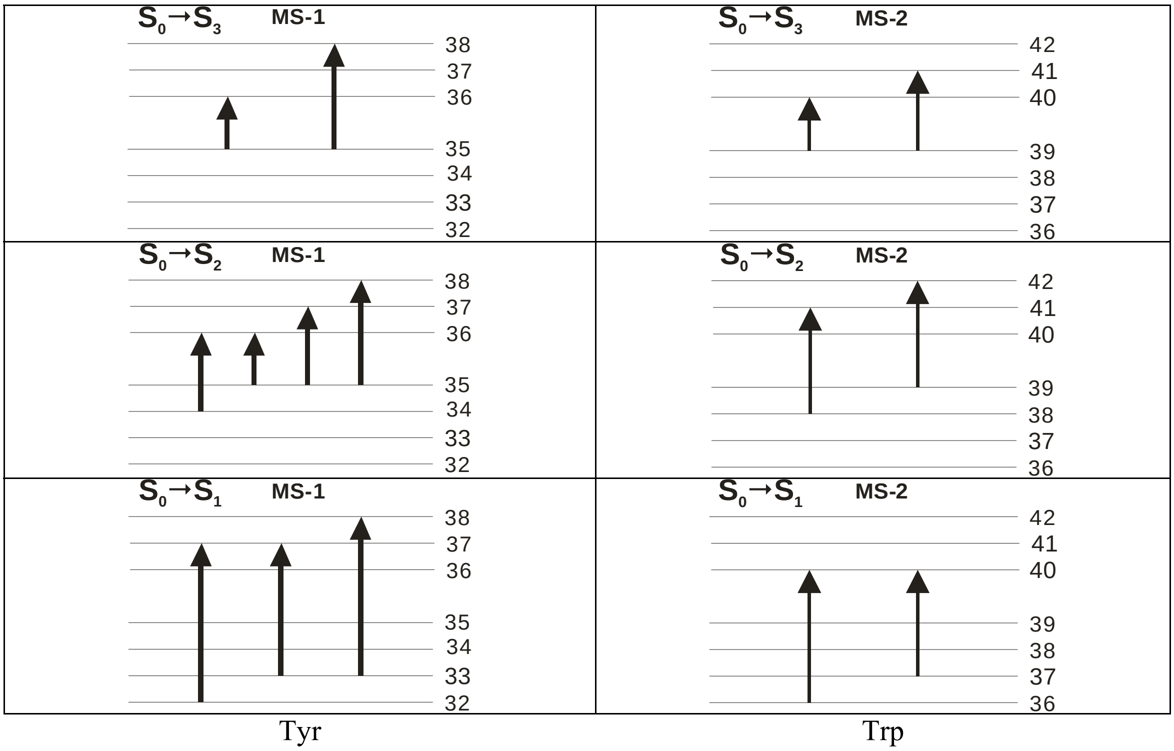



*Figure 3.* One-particle state distribution and corresponding electronic transitions near HOMO-LUMO region of Tyr-Trp structure (Tyr, MS-1, and Trp, MS-2, molecules).Population schema of $S_1$, $S_2$, $S_3$ spectrometric states. Arrows represent the strongest transitions between HOMO and lower and LUMO and higher levels (HOMO-LUMO separated by gap)

**Table 1.** Calculated electronic transition parameters of tyrosine. *Gaussian*-03, ZINDO, singlets only

| Electronic transition | Energy $E$ (eV) | Osc. Strength $f$ | MO/ character | coefficient $k$ | Transition dipole moment (D) | | | CT type |
|---|---|---|---|---|---|---|---|---|
| | | | | | $X$ | $Y$ | $Z$ | |
| $S_0 \rightarrow S_1$ | 3.8643 | 0.0004 | HOMO-2→ LUMO+1 | 0.59046 | -0.0586 | 0.0215 | 0.0227 | π-π* |
| $S_0 \rightarrow S_2$ | 4.1463 | 0.0932 | HOMO-1→ LUMO | -0.26572 | -0.1791 | -0.9018 | 0.0932 | π-π* |
| | | | HOMO→ LUMO | 0.40200 | | | | |
| | | | HOMO→ LUMO+1 | 0.24667 | | | | |
| | | | HOMO→ LUMO+2 | 0.42722 | | | | |
| $S_0 \rightarrow S_3$ | 4.4509 | 0.2452 | HOMO→ LUMO | 0.53110 | -1.3908 | 0.2763 | -0.4875 | π-π* |
| | | | HOMO→ LUMO+2 | -0.37928 | | | | |

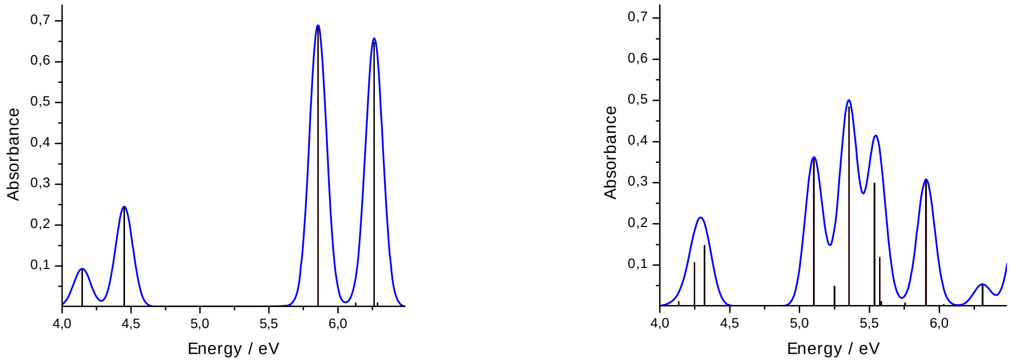



*Figure 4.* Simulated absorption spectrum of Tyr (MS-1, left) and Trp (MS-2, right). ZINDO transitions (vertical lines) and corresponding Gauss-shaped bands, bandwidth 500 $cm^{-1}$

## 5. Intermolecular Distribution of Electron Transfer Ratio

Fig. 5 represents the spectral distribution of ET ratio for the mentioned structure – Tyr-Trp complex. The ET processes start from states 38, [LUMO + 2]. Tyr-Trp complex contains neighbour molecules separated by a short distance (up to 4 Å). In that case Tyr-Trp complex expresses the effective ET process (ET ratio in range $10^{10}..10^{11}$ Hz). In case when an intermolecular distance is long (up to 10 Å), the ET process is ineffective (ratio decreases to 100 Hz).

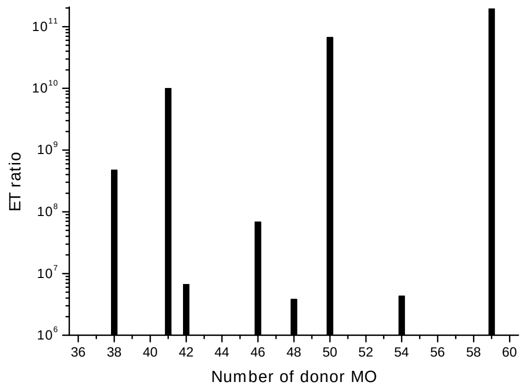



*Figure 5.* Spectral dependence of ET ratio (calculated using Eq. 1) on MO number of donor molecule Tyr

Fig. 6 represents 2D map of the intermolecular ET ratio distribution and the corresponding intermolecular charge transition simulated for [LUMO + 2]→ [LUMO + 2] ET processes. Orientation of monomers in tyrosine (MS-1)-tryptophan (MS-2) complex was used as showed in Fig. 2. The charge-donor atoms are colored in black, and the charge-acceptor atoms – in white, respectively. The significant electron transfer occurs in complex: from Trp (14 carbon atom) to Tyr (18 and 24 carbon atoms).

**38→42, [LUMO+2]→ [LUMO+2]**

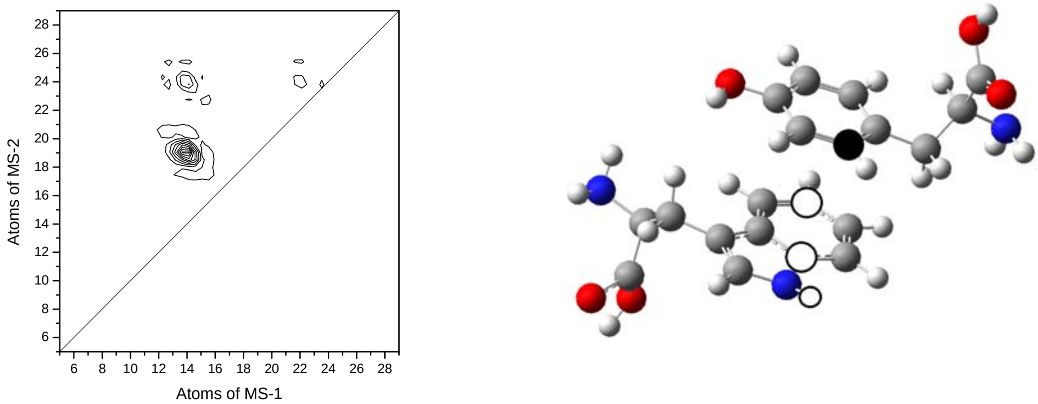



*Figure 6.* 2D map of the intermolecular ET ratio distribution (left) and the corresponding intermolecular electron transition (right) simulated for [LUMO + 2]→ [LUMO + 2] ET processes. Tyrosine (MS-1)-tryptophan (MS-2) complex. The electron-donor atoms are colored in white, and the electron-acceptor atoms – in black, respectively

## 6. Discussion

π-conjugated systems usually are potential charge donors, especially in case when significant electronic overlap occurs. In case of Tyr-Trp complex, this condition plays an essential role, and Tyr-Trp complex represents the alternated derivative where the monomers are separated by distance ~4, 7 Å – two fragments of different MS are placed "face-to-face". Only one significant intermolecular transition, 38→42, [LUMO + 2] →[LUMO + 2] could be used for modeling. No significant differences was found using HF/6-311G simulation routine in comparison to ZINDO.

Fig. 6 represents one of CT events attributed to the strong CT complex (distance ~ 4, 7 Å, orientation of propanoic acid fragments 180 deg).

The provided simulation qualitatively confirms the experimental phenomena of ET in Tyr-Trp complex and also could be useful for analyzing many pigment-protein complexes where ET occurs additional, non-trivial effects.

## Conclusion

Analysis of ET processes in tyrosine-tryptophan complex was done using quantum chemistry methods. The main results are presented in the form of ET rate spectral redistributions. The process between the separated parts of a molecular system was evaluated with accuracy of value of each atom parameter, and it is enough for modeling many photophysical and photochemical reactions. It is determined, that the most probable electron transfer acquires between the phenol ring of tyrosine molecule and the benzene fragment of tryptophan molecule, that proved the tentative expects on this problem. It was concluded that using the semi-empirical ZINDO method allows us to estimate the ET conditions in case, when the intermolecular distance is up to 5 Å.

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# CONSTRUCTION REGRESSION DEPENDENCIES IN R ENVIRONMENT

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The considerable quantity of publications about significant opportunities statistical and free-of-charge R environment makes pay to it the most steadfast attention. In the present work the review of the user opportunities of language and R environment is done. An explanation of the structure of the environment and detailed elaboration of some opportunities will allow the user to get more deeply and more quickly skills of work in environment R. From the other side, the basic applicability of R environment is reduced to realization of classical and modern statistical methods. The problem of construction nonlinear regression dependences of dependent variable Y on independent variable X remains topical. On an example of this class of problems we show the opportunities of the language means of R environment for their solution. In the work the so-called nuclear construction tools of nonlinear regresses are discussed, their comparison with usual estimations of a method of the least squares is done. For realization of such nuclear estimations modern means of environment R, which are reduced to an opportunity of a choice at a program level the so-called "width of a window" – bandwidths, which allows receiving nuclear regression estimation in the "best" image, are used.

***Keywords:*** *R environment, regression analysis, nuclear estimations*

## 1. Introduction

Now the significant amount of publications [1, 2, 3] about the opportunities of the language and the software of R environment for the statistical analysis of data forces researchers to pay the most steadfast attention to it. R environment is freely distributed according to license GNU (General Public Licence), it is developed and accompanied by statisticians group, known as R Development Core Team [5]. R is a system for statistical analyses and graphics. R is both a software and a language considered as a dialect of the S language created by the AT&T Bell Laboratories. S is available as the software S-PLUS commercialised by Insightful [7]. There are important differences in the designs of R and S. But R users may benefit from a large number of programs written for S and available on the internet [8].

R has many functions for statistical analyses and graphics; the latter are visualized immediately in their own window and can be saved in various formats (jpg, png, bmp, ps, pdf, emf, pictex, xfig; the available formats may depend on the operating system). The results of a statistical analysis are displayed on the screen; some intermediate results (P-values, regression coefficients, residuals and etc.) can be saved, written in a file, or used in subsequent analyses. The power of R environment is supported with such objects as functions and packages (group of functions) and we consider how it works for solution statistical problems.

## 2. Structure and Usability of R Environment

When R is running, variables, data, functions, results, etc, are stored in the active memory of the computer in the form of objects. The user can do actions on these objects with operators (arithmetic, logical, comparison and etc.) and functions (which are themselves objects). All the actions of R are done on objects stored in the active memory of the computer: no temporary files are used (Fig. 1). The readings and writings of files are used for input and output of the data and results. The user executes the functions via some commands. The results are displayed directly on the screen, stored in an object, or written on the disk (particularly for graphics). Since the results are themselves objects, they can be considered as data and analysed as such. Data files can be read from the local disk or from a remote server through the Internet.

The basic applicability of R environment is implementation of classical and modern statistical methods. Some of these means are built in the basic set R, but many of them are delivered as packages using Comprehensive R Archive Network (CRAN) [6], enough unique resource in the Internet. Now it is known more than 2400 packages delivered with R which contain the modern means of solution of various statistical problems.

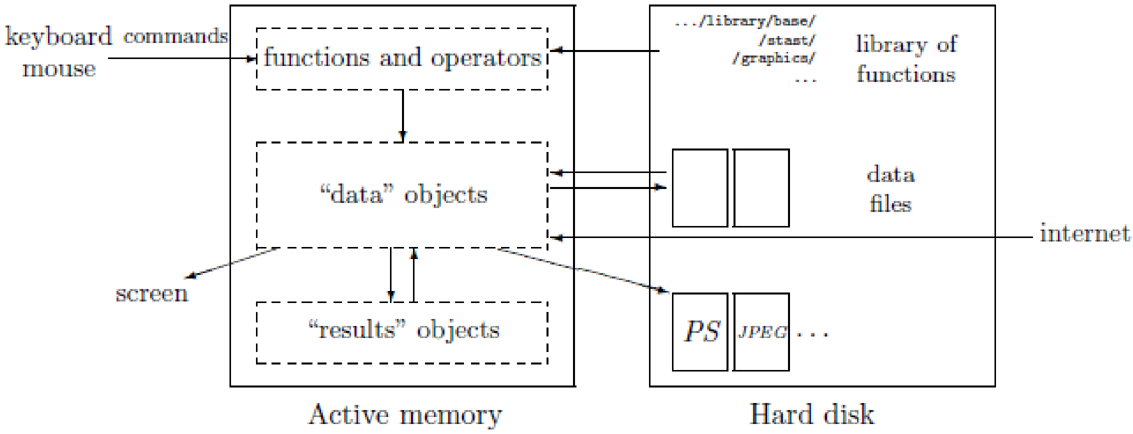


*Figure 1.* A schematic view of how R works

The following screen (Fig. 2) lists the standard packages which are distributed with a base installation of R. Some of them are loaded in memory when R starts; this can be displayed with the function *search()*, the other packages may be used after being loaded ( for example, package *grid* with the command *library(grid)*), the list of the functions in a package can be displayed with the *library(help = grid)* or by browsing the help.

| Package | Description |
|---|---|
| base | base R functions |
| datasets | base R datasets |
| grDevices | graphics devices for base and grid graphics |
| graphics | base graphics |
| grid | grid graphics |
| methods | definition of methods and classes for R objects and programming tools |
| splines | regression spline functions and classes |
| stats | statistical functions |
| stats4 | statistical functions using S4 classes |
| tcltk | functions to interface R with Tcl/Tk graphical user interface elements |
| tools | tools for package development and administration |
| utils | R utility functions |

*Figure 2.* Basic R packages

Many contributed packages add to the list of statistical methods available in R. They are distributed separately, and must be installed and loaded in R. A complete list of the contributed packages, with descriptions, is on the CRAN Web site. Several of these packages are recommended since they cover statistical methods often used for the data analysis. The recommended packages are often distributed with a base installation of R. They are briefly described (Fig. 3).

It is the main advantage of the R environment – placing functions in the libraries, which are collected in packages and are automatically available through the Internet in a global network of CRAN servers. There are two other main repositories of R packages: the Omegahat Project for Statistical Computing [9], which focuses on web-based applications, and interfaces between the software and the languages, and the Bioconductor Project [10] specialized in bioinformatic applications (particularly for the analysis of microarray data).

| Package | Description |
|---|---|
| boot | resampling and bootstraping methods |
| class | classification methods |
| cluster | clustering methods |
| foreign | functions for reading data stored in various formats (S3, Stata, SAS, Minitab, SPSS, Epi Info) |
| KernSmooth | methods for kernel smoothing and density estimation (including bivariate kernels) |
| lattice | Lattice (Trellis) graphics |
| MASS | contains many functions, tools and data sets from the libraries of "Modern Applied Statistics with S" by Venables & Ripley |
| mgcv | generalized additive models |
| nlme | linear and non-linear mixed-effects models |
| nnet | neural networks and multinomial log-linear models |
| rpart | recursive partitioning |
| spatial | spatial analyses ("kriging", spatial covariance, ...) |
| survival | survival analyses |

*Figure 3.* Recommended R packages

R could seem to be too complex for a non-specialist. This may not be true actually. But the following table gives an overview of the type of objects representing data.

| Object | Mode |
|---|---|
| vector | Numeric, character, complex, logical |
| factor | Numeric, character |
| array | Numeric, character, complex, logical |
| matrix | Numeric, character, complex, logical |
| data frame | Numeric, character, complex, logical |
| time set | Numeric, character, complex, logical |
| list | Numeric, character, complex, logical, function, expression |

It is clear that manipulation of such objects requires detailed knowledge of the language and enough programmers' skills.

The initial organization of the environment in which the operators of the language are carried out in lines, from a command line, looks rather unusual. There are many publications [3] where updating environment the various routine operations are automated and the graphic environments are offered. One of such GUI (Graphical User Interface) for R is R Commander [11]. Only those features are simplified:

- The R Commander provides several ways to get data into R. To enter data directly via New data set. This is a reasonable choice for a very small data set. To import data from a plain-text ("ascii") file or the clipboard, from another statistical package (Minitab, SPSS, or Stata), or from an Excel, Access, or dBase data set. To read the data set that is included in an R package, either typing the name of the data set (if you know it), or selecting the data set in a dialog box.
- The R Commander menus can be used to produce a variety of numerical summaries and graphs.
- Several kinds of statistical models can be fit in the R Commander using the menu items. Models: linear models, generalized linear models, multinomial logic models, and proportional-odds models. Double-clicking on a variable in the variable-list box copies it to the model formula. The row of buttons above the formula can be used to enter operators and parentheses into the formula. You can also type directly into the formula fields, and indeed have to do so, for example, to put a term such as *log(income)* into the formula. You can type an R expression into the box labelled Subset expression; if supplied, this is passed to the subset argument of the *lm* function, and is used to fit the model to a subset of the observations in the data set.

In the next screenshot (Fig. 4) you can see how the work in R environment in some cases can be simplified using R commander.

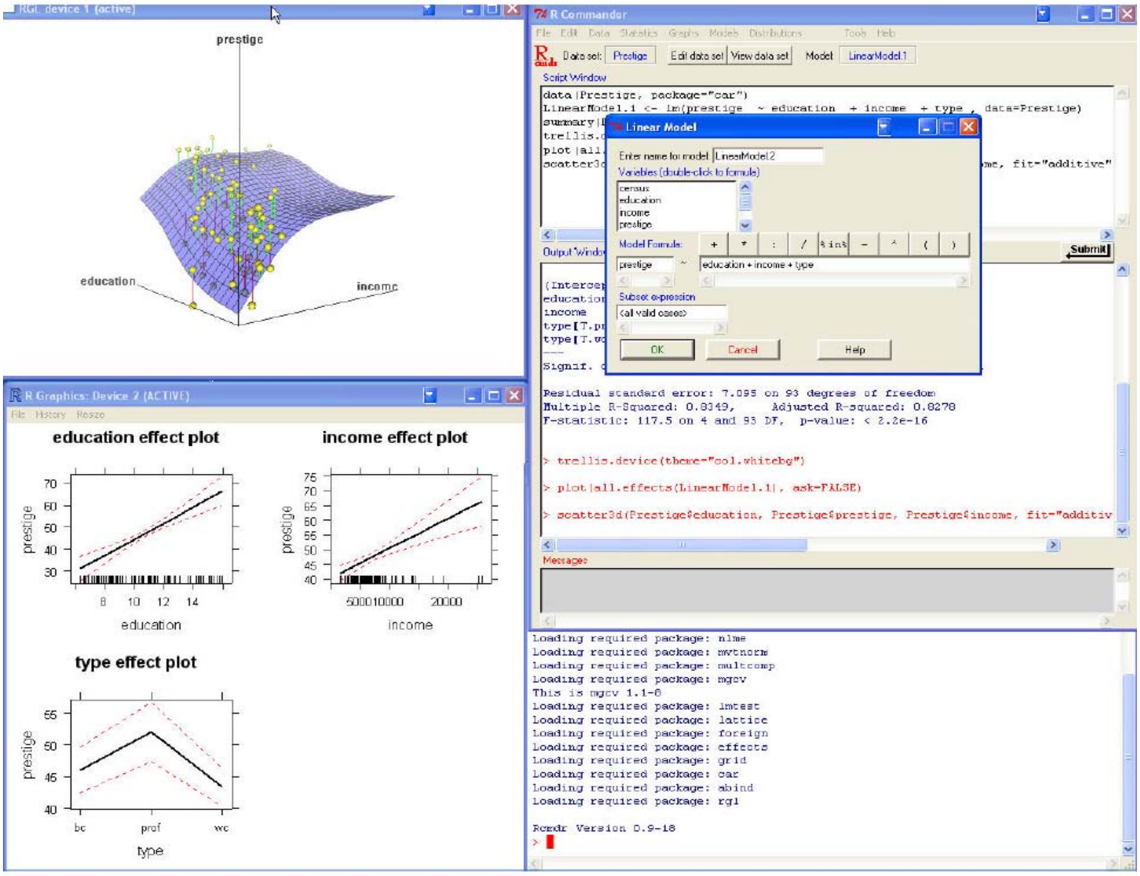


*Figure 4.* A view of how R Commander works

The next GUI for R is Java GUI for R – speak Jaguar (JGR) [11]. JGR provides only those features (Fig. 5): Console with several not valuable conveniences, Editor, Objects browser, Package manager, Spread sheet for manipulation with data and Help system.

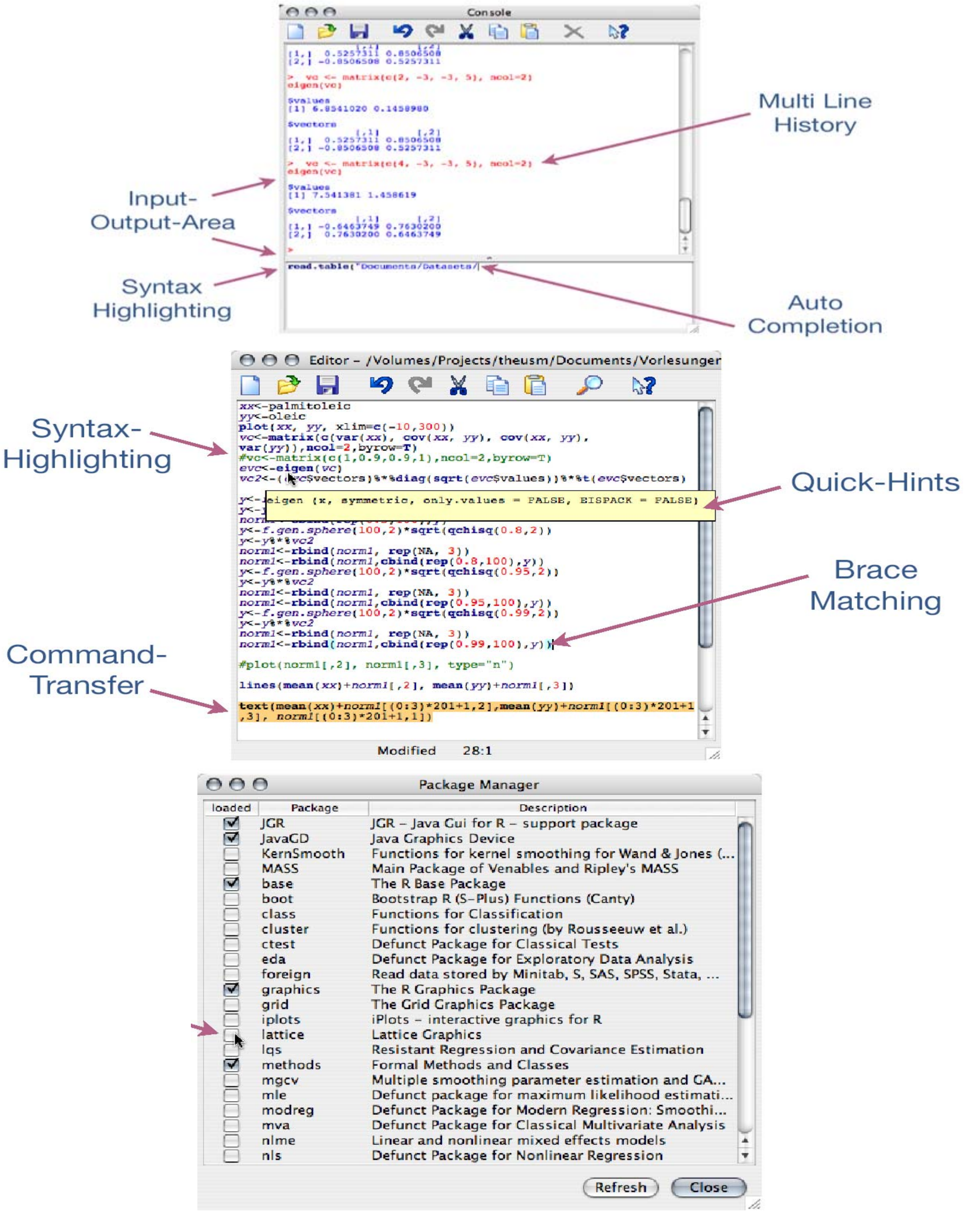


*Figure 5*. Screenshots of JGR user interface

So the functionality of the JGR package expands R environment and simplifies the packages control but the necessity of elaborate programming is still here. The GUI interfaces for R seem still have the problem oriented nature and it will be so in the future.

## 3. Application of the Language R for the Solving the Statistical Problems, Construction of Nonlinear Regression Dependences

As it was already mentioned, the basic applicability of R environment is reduced to employment of classical and modern statistical methods. In this connection it is possible to remind, that the problem of construction nonlinear regression dependences of the dependent variable Y on independent variable X remains rather actual [13, 14] and it is one of the central one in a number of statistical problems. On an example of this class of problems we will show the opportunities of the language means of R environment of the solution of similar problems. In work the so-called nuclear construction the tools of nonlinear regresses [4, 14] are discussed, their comparison with usual estimations of a method of the least squares is done. For realization of such nuclear estimations the modern means of environment R which are reduced, in particular, to an opportunity of a choice at a program level the so-called "width of a window", bandwidth – sizes, which allow receiving regression nuclear estimation in the "best" image, are used. So, the further results are based on the consideration of an exact example of the nonlinear dependence Y from the independent variable X, thus we were limited to the detailed consideration of only one example by virtue of the limited opportunities of present clause.

Let us notice further, that quite often it is possible to postulate the so-called regression equation of relative between the dependent variable Y and the independent variable X of a kind

$$Y = f(X,\theta) + \varepsilon, \tag{1}$$

where $\varepsilon$ – some random variable having at everyone X=x distribution with a mathematical expectation $M(\varepsilon) = 0$ and a variation $D(\varepsilon) = \sigma^2$, $f(X,\theta)$ – some known smooth function depending on a vector of explaining variables X = $(x_1, x_{2,} ... x_k)$ and a vector of parameters $\theta = (\theta_1, \theta_2, ..., \theta_p)$.

The standard way of a finding a vector of unknown parameters, as is known [13], is reduced to the minimization of the sum of squares of discrepancies – to usage of the method of the least squares (MLS) that is reduced to minimization of the function of a kind

$$S(\theta) = \sum_{i=1}^{n} (Y_i - f(x_i,\theta)^2 , \tag{2}$$

where *n* – number of observations of dependent variable Y from a vector of explaining variables.

To find estimation $\hat{\theta}$ on MLS we should differentiate (2) on $\theta$ and equate the left parts to 0 for reception of the so-called system p normal equations. Difficulties of the solution for the received system of the normal equations are well-known, and for its solution it is necessary to use the iterative methods, moreover, the difficulties are aggravated with that there can be a set of stationary values of function $S(\theta)$. As opposed to the classical method of the least squares, considered above, it is possible to paraphrase a little in some cases required regression equation of relationship between the dependent variable Y and the vector of explaining variables X and to reduce to model of a kind

$$Y = m(X) + \varepsilon, \tag{3}$$

where $\varepsilon$ – some random variable having at everyone X = x distribution with a mathematical expectation $M(\varepsilon) = 0$ and a variation $D(\varepsilon) = \sigma^2$, m(X) – some smooth function.

By definition, the conditional average of a continuous random variable can be presented thus

$$M(Y|X = x) = \int yg(y/x)dy = \int y\frac{f(x,y)}{f(x)}dy = m(x), \tag{4}$$

where g (y/x) – conditional density of the random variable Y at fixed value X = x, and f (x, y) joint density of random variables X, Y.

The estimation of a conditional average turns out replacement of unknown functions of density joint and marginal distributions, f (x, y) and f (x), their "good" estimations. Thus "good" estimation of a conditional average is the nuclear estimation (5), which detailed design is described, for example, in works [4, 14]. It allows reducing the estimation of conditional average Y at everyone x to an estimation of a kind:

$$\hat{m}(x) = \frac{\sum_{i=1}^{n} Y_i K(\frac{X_i - x}{h})}{\sum_{i=1}^{n} K(\frac{X_i - x}{h})}, \tag{5}$$

where K(z) – value of function of density of standard normal distribution in a point z.

In table 1 the given sample dependences of the variable Y from x are presented in the assumption that true dependence looks like

$$Y = \frac{\theta_1 x}{(\theta_2 + x)} + \varepsilon \cdot \qquad (6)$$

**Table 1.** Dependence Y from x for model (6)

| x | 2 | 2 | 0.667 | 0.667 | 0.4 | 0.4 | 0.286 | 0.286 | 0.222 | 0.222 | 0.2 | 0.2 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Y | 0.0615 | 0.0527 | 0.0334 | 0.0258 | 0.0138 | 0.0258 | 0.0129 | 0.0183 | 0.0083 | 0.0169 | 0.0129 | 0.0087 |

It is necessary to receive an estimation of parameters of this nonlinear model by means of method of the least squares, and it is possible to emphasize, that the search of the parameters of model is carried out on small sample and that is characteristic for some practical problems. Methodologically, first of all, there arises a problem of choice of initial approaches for correct finding the estimations of the parameters on a method of the least squares. In this connection, rejecting ε in model 6, we can receive the system of the equations of a kind

$$Y_i x_i = \theta_1 x_i - Y_i \theta_2, \; i = 1, 2, \ldots n, \; n = 12.$$

Designating a required vector $\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}$ and using the solution of plural linear regression, we shall receive $\theta = (Z^T Z)^{-1} Z^T U = \begin{pmatrix} 0.084 \\ 1.031 \end{pmatrix}$, where $Z = \begin{pmatrix} x_1 & -Y_1 \\ \ldots & \ldots \\ x_n & -Y_n \end{pmatrix}, U = \begin{pmatrix} Y_1 x_1 \\ \ldots \\ Y_n x_n \end{pmatrix}$.

Having received the initial approach, we use the standard method of search of such estimations of parameters of model (6) which minimize the value of discrepancy (2). Taking private derivatives on the parameters in (2) and having equated them to zero, we shall receive the corresponding system of the equations of a kind

$$\begin{cases} \sum\limits_{i=1}^{n} \left(\frac{x_i y_i}{x_i + \theta_2}\right) - \theta_1 \sum\limits_{i=1}^{n} \frac{x_i^2}{(x_i + \theta_2)^2} = 0 \\ \sum\limits_{i=1}^{n} \left(\frac{x_i y_i}{(x_i + \theta_2)^2}\right) - \theta_1 \sum\limits_{i=1}^{n} \frac{x_i^2}{(x_i + \theta_2)^3} = 0 \end{cases} . \qquad (7)$$

The numerical solution of this system of the equations in R at presence of the initial approaches $\theta = \begin{pmatrix} 0.084 \\ 1.031 \end{pmatrix}$ gives the final solution of a kind $\theta = \begin{pmatrix} 0.10564 \\ 1.70269 \end{pmatrix}$. The list of R commands for the solution of system of the equations (7) is as follows:

```
library("rootSolve")
xt<-c(2,2,0.667,0.667,0.4,0.4,0.286,0.286,0.222,0.222,0.2,0.2)
yt<-c(0.0615,0.0527,0.0334,0.0258,0.0138,0.0258,0.0129,0.0183,0.0083,0.0169,0.0129,0.0087)
model<-function(o)  c(
F1=-sum(xt*yt/(xt+o[2])) + sum(o[1]*(xt^2)/((xt+o[2])^2)),
F2=-sum(xt*yt/((xt+o[2])^2)) + sum(o[1]*(xt^2)/((xt+o[2])^3)))
MRres<-multiroot(model,c(0.08,1))
yregr <- function(x){
MRres$root[1]*(x/(MRres$root[2]+x))}
plot(xt,yt)
points(xt,yt, col='red',bg='red',pch=21)
lines(xt,yregr(xt), col = 'blue', lty = "dotted")
```

Classical regression dependence can be presented now as: $YR(x) = 0.1056 \dfrac{x}{(1.702 + x)}$.

In Figure 6 the corresponding regression smoothing for the given correlation field is presented.

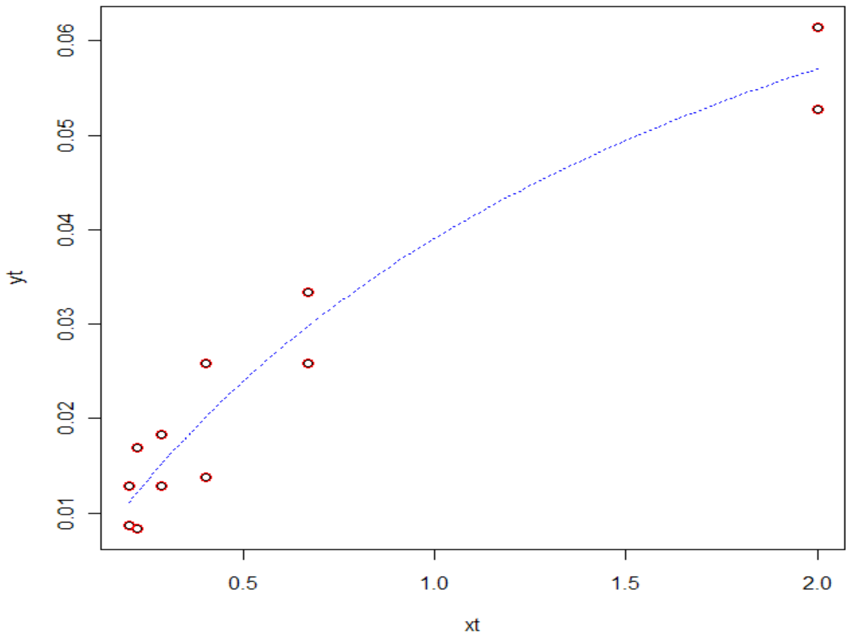


*Figure 6.* Field of variability and corresponding classical regression for the model (6)

As opposed to the classical regression, the nuclear regression as it was marked earlier, is reduced to the implementation of the formula (5) where all is simple enough except for a choice of a step h. A key to carrying out the further researches connected with a nonparametric nuclear estimation is the choice of size h – width of a window (bandwidth). There were many works connected with an optimum choice of width of a window from which, certainly, it is possible to allocate works [4, 14]. The authors offer various algorithms of a choice h in them, thus they concentrate the attention on the algorithm cross-validation. The merit of the authors of the specified works is reduced to that they bring theoretical algorithms of a choice of width of a window to application of convenient programs in the practical plan. All these programs are realized in the package *np*. We shall give an example applications of the key function *npregbw()* (Nonparametric Regression Bandwidth Selection) from the package, providing a choice optimum size of width of a window by the consideration of our model (6):

```
library(np)
x1<-c(2,2,0.667,0.667,0.4,0.4,0.286,0.286,0.222,0.222,0.2,0.2)
y1<c(0.0615,0.0527,0.0334,0.0258,0.0138,0.0258,0.0129,0.0183,0.0083,0.0169,0.0129,0.0087)
m1<-npregbw(formula=y1~x1,tol=0.1,ftol=0.1)
m1
Regression Data (12 observations, 1 variable(s)):x1
Bandwidth(s): 0.1379053
Regression Type: Local-Constant
Bandwidth Selection Method: Least Squares Cross-Validation
Formula: y1 ~ x1
Bandwidth Type: Fixed
plot(m1,xlim=c(0,2),ylim=c(0,0.1))
points(x1,y1,cex=1.25,col="red")
```

In Figure 7 below the curve of nuclear smoothing for data of table 1 with optimum choice of a step h = 0.138 is presented.

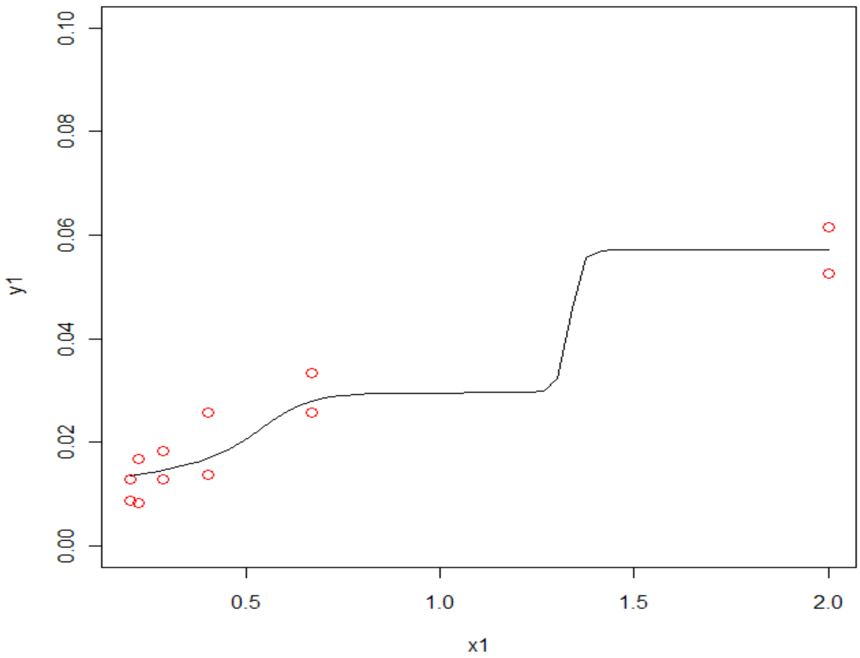


*Figure 7.* Sample sheet and nuclear regression (a continuous line) with optimum step h = 0.138

In our work some analysis of the chosen smoothing dependences connected both with a choice of value of a step h, and with research of the quality of smoothing at increased size of sample is done. In the beginning we have a sample of volume $n = 20$ from model 6, simulated at true parameters $\theta_1 = 1, \theta_2 = 2$. In Figure 8 the corresponding correlation field and smoothing regression dependence on the base MLS is presented.

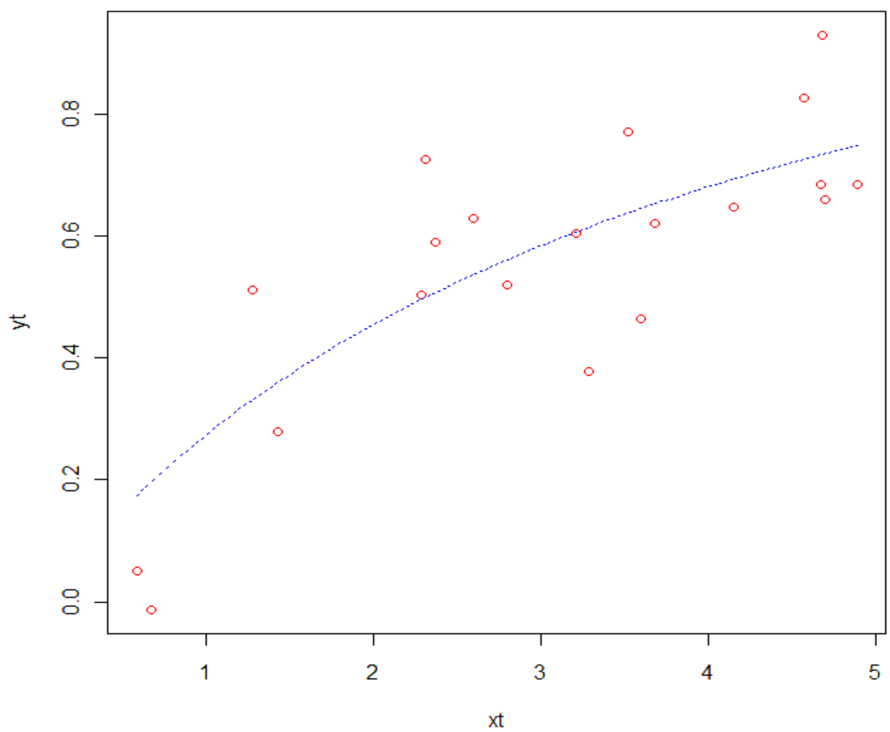


*Figure 8.* Field of variability and corresponding classical regression for the model (6) at volume of sample n = 20

In Figure 9 the nuclear smoothing curve received in the process of using the formula (5) and optimum chosen size of a step h = 0.508 is presented.

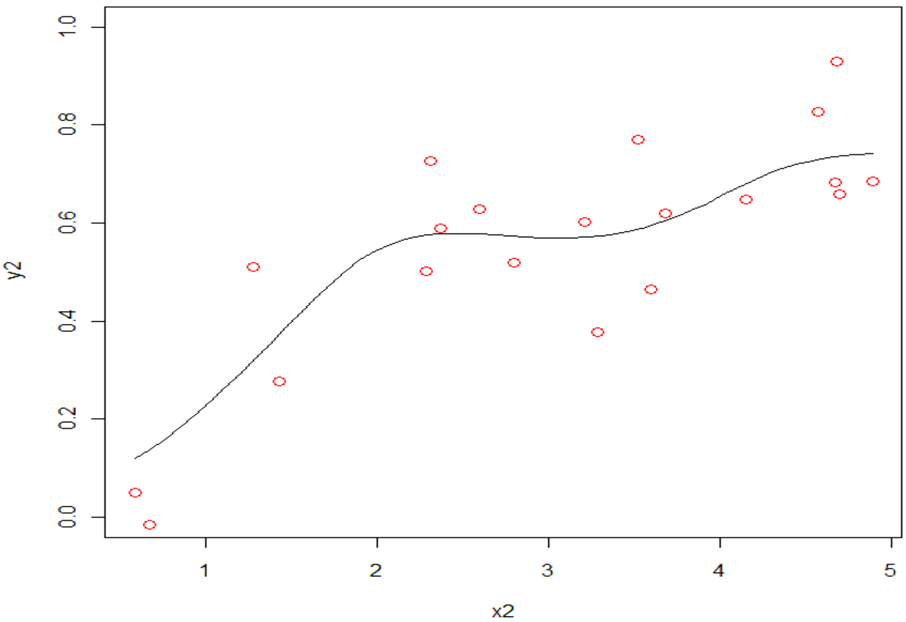


*Figure 9.* Field of variability and corresponding nuclear regression for the model ( 6) at volume of sample n = 20 and an optimum step h = 0.508

Let us notice, that even visually the optimality of a choice of a step h = 0.508 is visible.

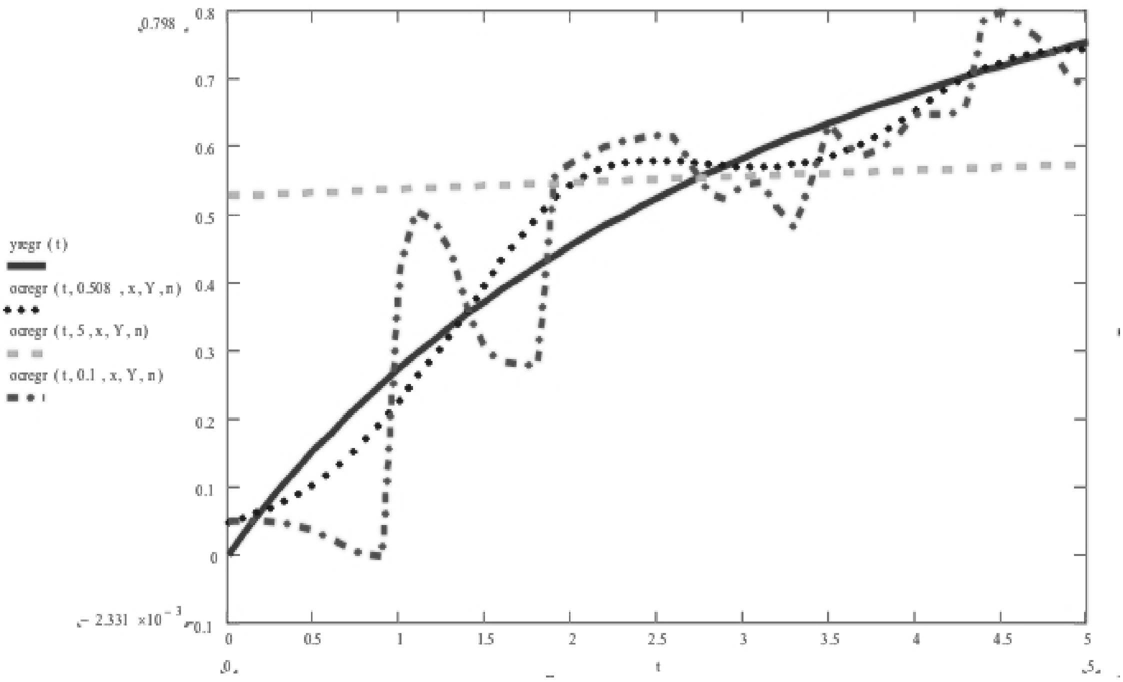


*Figure 10.* Smoothing curves: red continuous – regression on MLS, a dark blue dotted line – nuclear smoothing at an optimum step h = 0.508, a green dotted line – nuclear excessive smoothing at h = 5, an purple dotted line-insufficient nuclear smoothing at h = 0.1

From the above-stated it is possible to make a conclusion, that undr the conditions when it is difficult to employ the method of the least squares, the method of nuclear smoothing in some cases can be not the worst alternative. Apparently, especially evidently it will be shown at rather great volume of sample observations. In Figure 11 the simulated sample in volume n = 200 for model (6) is presented and corresponding classical regression dependence has been received.

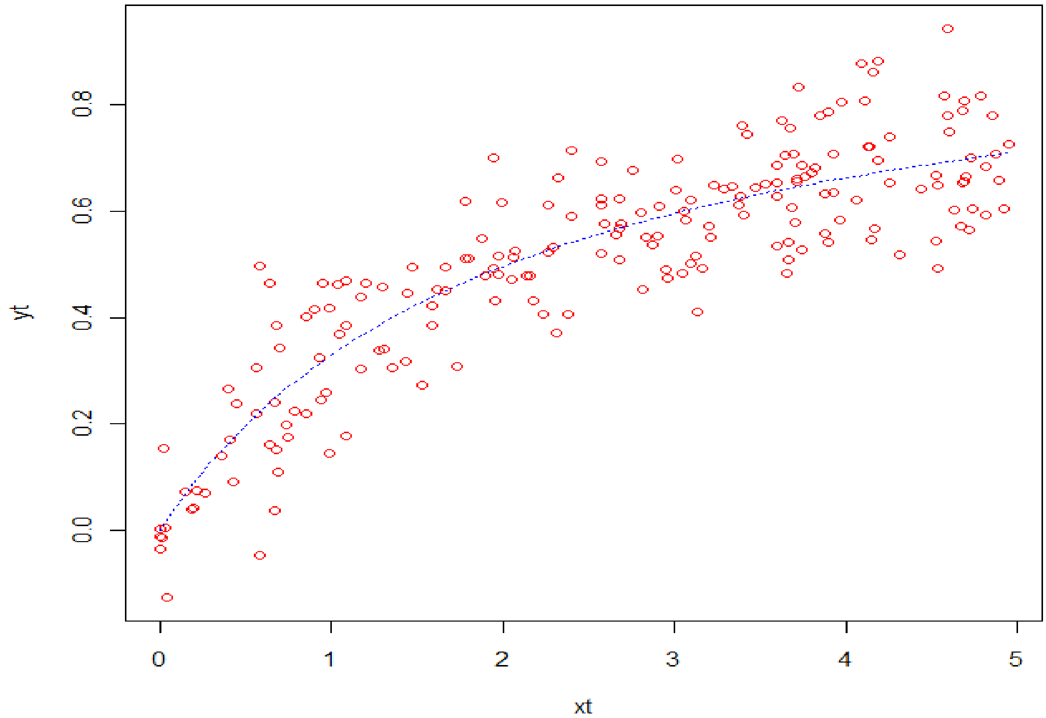


*Figure 11.* Field of variability and corresponding classical regression for the model (6) at volume of sample n = 200

In Figure 12 the corresponding nuclear smoothing dependence for the same data is presented at volume of sample n = 200.

Comparing Figures 11 and 12, we see the comprehensible enough coincidence of the regression curve MLS with corresponding nuclear smoothing.

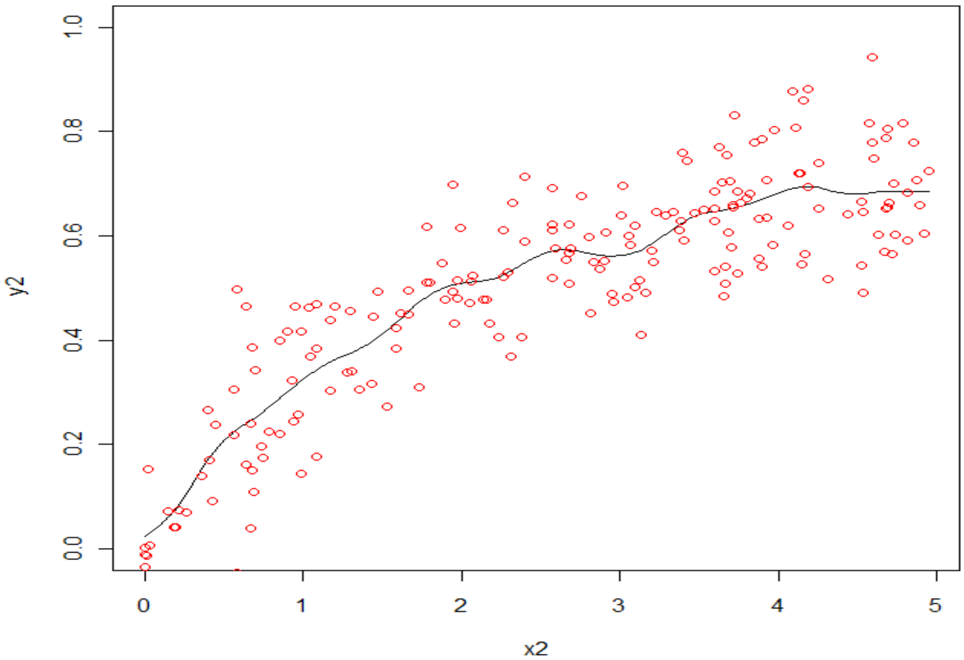


*Figure 12.* Field of variability and corresponding nuclear regression for the model (6) at volume of sample n = 200

## Conclusions

The usage of various statistical procedures and methods in practical activities by many engineers demands the universal employment of the qualitative software. Such characteristic is deserved with R environment. In the present work the authors bring to a focus to the user's opportunities and structure of R environment suitable for the solution of a wide class of statistical problems. The attention is paid to such facts as the function environment, every possible modification of the environment, and in the whole it can facilitate the user's work. From the other hand, the exact approach to the solution of an actual statistical problem – construction on sample data nonlinear regression model by means of R environment is presented in this work. The comparative analysis of the construction of the models of nonlinear regression, by means of the classical regression and with the use of the nuclear regression, is shown on an exact example. Under the conditions of nonparametric models the employment of the nuclear approach is obviously reasonable. On the other hand, even at presence of the parametrical model it is possible to use the nuclear regression, if difficulties of implementation of the parametrical model (for example, a choice initial approach) take place. The difference between the applications of both approaches is levelled off, as shown in the study, by increased volume of sample data. The use of R for the solution of similar problems is difficult to overestimate. Convenient software of a choice of an optimum weight step h in the formula of nuclear smoothing and the modern graphic interface allow the user to reach the demanded result of data smoothing.

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# METHODOLOGY OF RISK DETERMINATION BASED ON MULTI-CRITERIA RISK ANALYSIS AS A PART OF LOGISTICAL LEADERSHIP

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Logistical Leadership defines that the purposeful and well-founded evaluation of conditions might take place before any decision has been made. It is particularly important in case of handling security elements of the state, society or infrastructure. It has to be underlined that the meaning of infrastructure security has changed and has to be understood as much broader spectrum of interdependent branches, starting from the raw material, transportation and energy producing elements and finishing with providing telematic monitoring, banking or state governing element functionality. The cornerstone of decision making in such environment is the exploration of the risks and the consequences as well as the necessity of taking into consideration all possible risks even before any element has been created. Methodology is the way of combining theoretical and practical measures with the aim to create a systematic approach for achieving the set goal or for accomplishing the given tasks. Methodology renders practical recommendations how to answer the following questions: 1) what to do for practical solving the problem? 2) how to perform these practical activities? 3) how to evaluate the process and its credibility? and 4) how to analyze the results?

By specifying the tasks of such methodology and concentrating attention on the problems in safety and security areas, the detailed answers to the above mentioned questions have been given through an overview of a scientific research called "Substantiation of the decision making process on the basis of multi-criteria risk analysis with the aim of solving defence related tasks" (AZPC – 02/01-2009; ISBN 9984-625-23-0). Therefore the presented methodology defines only the sequence of the activities to be performed as well as renders the procedural references for the risks determination in the safety and security areas on the basis of experts' conclusions, although taking into account that the methodology can, under equal conditions, be used by any decision-maker who personally can undertake an expert responsibility.

The methodology could be eventually divided into three main parts:

1. Problem formulation
2. Assembling a group of experts
3. Identification, analysis and evaluation of risks

The concluding part, namely the development of the proposals for the decision making on the basis of the safest alternative, hasn't been considered as a dependent part of the methodology, but is (has to be) the product of its utilization.

***Keywords:*** *logistic management, decision making, risk management, methodology of risk determination*

## 1. Introduction

An unambiguous conclusion sequentially drown after an analysis of the decision making procedures in context of the idea of the Logistical Leadership, especially in the area of safety and security, makes to believe that a risk determination stage must be regarded as an absolute necessity and an inseparable part of any decision making. It means that for providing a decision maker with possibility to take a qualitative and trustworthy decision, a qualitative risks determination phase must be accomplished. A systematic and scientifically proved approach to the risks determination based on the theoretical formulations as well as on the practical experiences can be integrated in one methodology.

With aim to come to a common understanding it needs to be underlined that for the correct determination of risks in safety in security area it is necessary:

1. To identify the security aspects, its importance to the society and the level of safety and security to be kept;
2. To build up a group of experts, that runs the threats analysis and defines the risks connected with each threat;
3. To arrange the risks in accordance with their significance;
4. To analyse the identified risks and group them for estimation of the complete probability, identifying the significance of each risk in each group;
5. To calculate the probability of implementing each risk and to estimate the possibility of the threat implementation in the given area of security;

6. To arrange the threats in accordance with their significances in the given area of security and to estimate the common security level as a possibility of realisation of the identified threats;

7. To work out recommendations and to deliver the results of the risks determination to the responsible person (institution).

The first of the above mentioned tasks should be accomplished by the responsible person himself. It is again his own responsibility to appoint a decision maker (institution) as well as to define the definite tasks and the main criteria. From this perspective selection of experts and formation of experts' group for analysis of the threats, determination of the risks and their significances are the areas of the responsibility of a decision maker (institution).

The group of experts will be tasked to conduct the threats analysis, to determine all the possible risks of each threat and to arrange them in accordance with their significances separately for each threat.

Depending on the characters of the determined risks, a new group of experts can be formed with the aim to solve the similar tasks connected to a separate group of risks.

The decision making, though it is the area of responsibility of a decision maker, deeply depends on the quality of the expertise, namely – on the quality of the risk determination and the level of competency of experts. That is why the choice of experts and determination of their level of competency is so important.

Although the methodology has been built on the assumption that there has to be a separate decision maker (institution) that will draw the exact decisions and work out recommendations for implementing the accepted alternative, it is absolutely possible that these tasks can be passed to the group of experts as well. In contrast, the methodology can be used with the same efficiency if the responsible person (institution) has the necessary qualifications and is able to take the responsibility of solving all the tasks (that can be solved by the group of experts) by him/her self.

## 2. Choice of Experts

Regarding to the fact that the legislation of the Republic of Latvia does not content any regulations prescribing the use of the experts with an aim to provide the quality of the process of decision making, it is each institution own responsibility and right to detect the qualification of the specialists, to choose one and to involve him/her as an expert into a process of making an expertise without coordinating such efforts with a higher authority or other institutions.

If the decision about the necessity of conducting an expertise and formation of an expert group has been taken, there will be need of implementation of choicen procedures and a list of possible candidates will have to be drawn up. The main condition under which a specialist can be added to the list of expert-candidates is his/her voluntarily expressed wish to become an expert.

Depending on the foundation of an expertise the number of the involved expert can vary from 5 and up to 30 people. The result of an expertise may influence the already taken decision as well as may ask to take a decision that will either cause changes in the law system or will violate some norms of legislation. That is why, the more serious consequences a decision can cause, the more experts have to be involved into the expertise. Sequentially, a primer (documents-based) expert-candidate selection has to be conducted with the aim to form a group of expert-candidates that numerically is at least two times larger than the decided number of experts.

In the branches, where some areas of expertise are covered by an expert-candidate's area of responsibility, but the candidate has no professional qualification, the expert candidate has to argue additionally his/her wish to become an expert.

Additional arguments for the choice of experts:

– Candidate's previous positive experience in conducting expertise in the given area;

– The quantity and the quality of the published candidate's works in the area of the expertise (taking into account the frequency and the expertise related subjects of those publications);

– Additional formal qualifications of the candidate in the areas very close or similar to the area of the expertise.

These below mentioned additional arguments may not be taken as a part of the evaluation of a candidate's competency and may not influence the process of choosing a candidate:

– Recommendations from any higher-positioned officials (excluding possible consultations about necessity of tasking an expert in addition to his/her main job);

– Recommendations from any persons who can be interested in the results of the expertise (including prospective consumers of the products of the expertise);

– Recommendations from the supervisor or any one involved into the process of administration of the choice of the candidates;

– Not-written recommendations.

If there is no any necessity for the additional arguments for accomplishing of an expert-candidate's competency evaluation, this candidate can participate in the selection regardless of the restrictions above.

The head of the managing group conducting selection should have the right to ask for additional arguments, if he finds it appropriate.

The responsible person (institution) that has requested the expertise can delegate authority to the head of the managing group conducting selection and assign him/her as a manager of the whole process of expertise. In this regard it is necessary to underline that the manager will have only support and administration authority.

The second phase of the selection is selection of the experts from the pool of the experts-candidates. To choose the experts from the expert-candidates, a practical experts' evaluation procedure is to be applied. To assure the maximum efficiency of the evaluation process, it is divided into two interconnected measures:

– A self-evaluation of each expert-candidate;

– A cross-evaluation among the experts-candidates.

The quality of an expert can be found out of the self-evaluation data. The results of some researches showed that people, conducting self evaluation of competency, perform an evaluation that is very close to the real one, although they have at the same time tendency to evaluate their own abilities higher then their colleagues' abilities. The worst evaluated individuals usually do not know that they have been counted as incompetent specialists. The paradox is, that without knowing this evaluation they continue to act as specialists and exactly their incompetence does not allow them to recognise that they act incorrectly. The situation when the colleagues evaluate an individual as an incompetent, but the individual evaluates him/her-self as a specialist, proves that this individual may solve some problems inadequately and his expert quality is doubtful.

If the experts-candidates know each other well, they can conduct evaluations easily. In other cases, when the expert candidates are not familiar with each other (neither personally nor on the base of publications) they may need some time and specially created conditions to get acquainted with each other. To solve this problem the head of the managing group must organize a simulated problem expertise, in the procedure of which the experts-candidates will have duty to show their knowledge and experience in the given area and to pursue an active, real participation in solving the simulated problem. The cross-evaluation questionnaire will be filled in on the base of the results of the simulation.

The duty of the head of the managing group is to draw the experts-candidates attention to the fact that the most important thing during the simulation is to get the knowledge about other experts-candidates rather than to get "the right result".

To simplify and to standardize the process of self- and cross-evaluations, a specific template has been worked out. The template (Table 1) is divided into two parts, where the first part is about self-evaluation and the second- about evaluation of other experts-candidates.

**Table 1.** Expert's questionnaire

| No | Self-evaluation criteria | points | No | Experts-candidates | points |
|---|---|---|---|---|---|
| 1. | Competency | | 1. | | |
| 2. | Creativity | | 2. | | |
| 3. | Attitude to the expertise | | 3. | | |
| 4. | Conformism | | 4. | | |
| 5. | Ability to analyze and think "out of box" | | 5. | | |
| 6. | Ability to think constructively | | …. | | |
| 7. | Ability to apply self-criticism | | | | |
| 8. | Co-operation skills | | | | |
| $k_{self}$(don't fill-in, has to be filled in by the person responsible for the selection) | | ....... | | | |
| Expert-candidate<br>……………………………………<br>20...... "___ ." ___________ | | | | | |
| | | | | | |
| | | | | | |
| | | | | | |
| | | | | | |
| | | | ..... | | |

Granting the evaluation points has to take place on the base of the proposed standards for the levels of the qualities (Table 2), with use of only the natural digits (1; 2; 3... but not 1,5; 2,7 or similar), and on the base of clarification of self-evaluation criteria (Table 3).

The 10-point evaluation standard is to be applied both for the self-evaluation and for the cross-evaluation, with the only difference that the cross-evaluation has to be done as the only one mark assigned for each expert-candidate, but self evaluation substitutes all the self-evaluation criteria and will be estimated by the person responsible for the selection.

**Table 2**. Expert quality evaluation classification

| Points | Expert's quality classification | Explanation of the classifications |
|---|---|---|
| 9,0-10,0 | Excellent | Extremely good evaluation for conducting an expertise successfully |
| 8,0-8,9 | Exceptionally good | Sufficiently good evaluation for conducting an expertise successfully |
| 7,0-7,9 | Very good | |
| 6,0-6,9 | Good | Partly sufficient evaluation for conducting an expertise successfully |
| 5,0-5,9 | Barely good | |
| 4,0-4,9 | Satisfactory | |
| 3,0-3,9 | Barely satisfactory | Insufficient evaluation for conducting an expertise successfully |
| 2,0-2,9 | Poor | |
| 1,0-1,9 | Very poor | |

**Table 3.** Self-evaluation criteria

| Criteria | Explanation | Comments |
|---|---|---|
| Competency | Qualification and knowledge in the given area | The evaluating ability, the level of education, experience and not least timeframe of being involved into processes in the given area are determinant |
| Creativity | Ability to solve a problem in a smart manner | Solution for a problem is usually hidden under "visible surface", that is why a creative approach is a necessity |
| Attitude to the expertise | Wish or partial wish to conduct an expertise | A specialist usually has a lot to do in his working place. Additional tasks can lead to a physical or emotional exhaustion. A negative attitude to these tasks (expertise) can affect the result distractedly, and influence the quality as well as the credibility of an expertise |
| Conformism | The influence from the prominent figures to an expert judgments and decisions, i.e. instability of an expert's position/judgments | It is desirable that each expert conducts his duties as much independently as possible, because an optimal solution can be found only by means of comparison of all the different ways of solving the problem |
| Ability to analyze and think "out of the box" | Wide knowledge about the area of an expertise and ability to analyze and to evaluate the popular statements | Only wide knowledge without critical attitude to the generally obtained information will not cause any trustable conclusions. By use of the common knowledge only, only the common problems can be solved |
| Ability to think constructively | Pragmatic way of thinking | An expert has to take a decision that can be enforced in reality. A conclusion without connection to the reality will make no sense |
| Ability to apply self-criticism | Ability to see things and to analyze information from a position of objective consideration | Ability to apply self-criticism proves an expert's potentiality to concentrate on the given task using different and effective approaches. Application of self-control augments probability that the decision, drawn by an expert, has the high level of credibility |
| Co-operation skills | Ability to communicate with other experts and to accept their arguments | These skills are very important in case of an open collective discussion. Atmosphere inside the group of expert will directly influence the effectiveness of their work as well as the result of an expertise. This criterion could be excluded in case if an expertise is independently conducted by each expert |

Receiving the filled-in templates the person responsible for the selection has to ensure that the data will be correctly transferred into a consolidated experts-candidates evaluation form (Table 4).

A unique self-evaluation result $k_{self.}$ is to be calculated as an average of all the points from the self-evaluation criteria list. It is calculated with help of formula (1)

$$k_{self.} = \frac{\sum t}{n}, \qquad (1)$$

where $K_{self.}$ – self-evaluation coefficient, $t$ – self-evaluation points of one criterion, $n$ – number of criteria (usually 8 or 7).

A collective cross evaluation coefficient $k_{col.}$ of an expert can be calculated similarly, assigning ***t*** as an evaluation of an expert-candidate by another expert-candidate and ***n*** as the number of experts-candidates minus 1.

The results have to be mirrored in the same consolidated experts-candidates evaluation form (Table 4). (The results in the Table 4 are given only for demonstration purpose).

**Table 4.** Consolidated experts-candidates evaluation form

| No | Expert candidate | Evaluation points | | | | | | | | | | | | | | $k_{col.}$ | $K_{self.}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A. | 7 | 9 | 8 | 6 | 6 | 5 | 9 | 8 | 9 | 6 | 6 | 8 | 8 | 8 | 7.4 | 7,4 |
| 2 | B. | 8 | 8 | 7 | 5 | 6 | 9 | 7 | 7 | 9 | 5 | 6 | 8 | 8 | 8 | 7.2 | 7,5 |
| 3 | C. | 6 | 6 | 7 | 8 | 8 | 9 | 7 | 7 | 9 | 5 | 6 | 7 | 6 | 9 | 7.1 | 7,3 |
| 4 | D. | 9 | 8 | 7 | 7 | 9 | 8 | 7 | 6 | 9 | 8 | 7 | 9 | 9 | 5 | 7.7 | 8,2 |
| 5 | E. | 5 | 5 | 7 | 9 | 6 | 8 | 7 | 6 | 9 | 7 | 7 | 9 | 5 | 5 | 6.8 | 8,1 |
| 6 | F. | 8 | 8 | 9 | 7 | 6 | 5 | 7 | 6 | 9 | 6 | 9 | 9 | 7 | 6 | 7.3 | 8 |
| 7 | G. | 8 | 8 | 6 | 9 | 6 | 6 | 7 | 9 | 6 | 8 | 8 | 8 | 5 | 7 | 7.2 | 7,7 |
| 8 | H. | 7 | 7 | 4 | 5 | 7 | 5 | 7 | 7 | 6 | 9 | 8 | 8 | 6 | 7 | 6.6 | 7,2 |
| 9 | I. | 7 | 6 | 7 | 8 | 7 | 5 | 7 | 5 | 6 | 7 | 8 | 5 | 6 | 7 | 6.5 | 7,5 |
| 10 | J. | 6 | 7 | 7 | 8 | 7 | 5 | 7 | 7 | 6 | 5 | 5 | 5 | 7 | 8 | 6.4 | 7 |
| 11 | K. | 8 | 9 | 8 | 6 | 8 | 7 | 7 | 7 | 6 | 7 | 5 | 8 | 9 | 6 | 7.2 | 7,2 |
| 12 | L. | 8 | 9 | 8 | 6 | 9 | 6 | 7 | 8 | 8 | 6 | 7 | 7 | 8 | 6 | 7.4 | 7,6 |
| 13 | M. | 7 | 7 | 7 | 9 | 8 | 5 | 7 | 5 | 7 | 6 | 5 | 6 | 6 | 8 | 6.6 | 7 |
| 14 | N. | 9 | 9 | 9 | 7 | 8 | 8 | 7 | 6 | 7 | 8 | 9 | 8 | 9 | 7 | 7.9 | 8,3 |
| 15 | O. | 9 | 7 | 7 | 8 | 6 | 8 | 7 | 6 | 7 | 7 | 6 | 9 | 6 | 7 | 7.1 | 8 |

A common evaluation of qualities of an expert-candidate can be calculated by use of formula (2)

$$k_{exp.} = 0{,}4k_{self.} + 0{,}6k_{col.}, \tag{2}$$

where $k_{exp}$ is the common expert-candidate evaluation coefficient, $k_{self..}$ is the self-evaluation coefficient, $k_{col.}$ is the collective cross-evaluation coefficient.

The most common situation is that an evaluation from colleagues' side defines more precisely the competency of a specialist, but will be incorrect in connection with his/her qualities that depend on his/her psychological type. Usually colleagues know each other pretty well. However, some (even one) mistakes can cause very negative perception of a specialist, that consequentially will cause decreasing of the level of his/her evaluation. Observations testify that it is much easier to lose one's professional credibility among colleagues than to regain it.

To calculate an expert-candidate evaluation relativity coefficient the formula (3) is to be used

$$V_i = \frac{T_i}{T_1}, \tag{3}$$

where $V_i$ – an expert-candidate relative evaluation coefficient, $T_1$ – the biggest (among experts-candidates) transitional indicator, $T_i$ – an expert's transitional indicator.

But the transitional indicator T is to be calculated using formula (4),

$$T_i = 50 + \frac{k_i - \overline{k}}{0{,}1\sigma}, \tag{4}$$

where $T_i$ is the transitional indicator of an expert-candidate, $k_i$ is the evaluation coefficient of an expert-candidate, $\overline{k}$ is the average of the evaluation coefficients of the same group (M), $\sigma$ is the standard deviation of evaluation coefficients of the same group (SD; 0,5 is normal).

Formula (4)is to be used for calculation of both transitional indicators $T_{self.}$ (using $k_{self.}$) and $T_{col}$. (using $k_{col}$ ).

By use of formula (2) (replacing "k" coefficients accordingly by "T" indicators) a common transitional indicator $T_i$ is to be calculated.

Taking the biggest $T_i$ as $T_1$ (so this expert-candidate's relative evaluation coefficient $V_i$ will be equal to "1") other $V_i$ are to be calculated using formula (3)

**Table 5**. Cumulative Table of Coefficients and Transitional indicators

| No | Expert candidate | $K_{self}$ | $K_{col}$ | $K_{exp}$ | $T_{self}$ | $T_{col}$ | $T_i$ | $V_i$ |
|---|---|---|---|---|---|---|---|---|
| 1. | A. | 7.4 | 7.4 | 7.4 | 45.22 | 57.00 | 52.29 | 0.77 |
| 2. | B. | 7.5 | 7.2 | 7.32 | 47.61 | 52.43 | 50.50 | 0.75 |
| 3. | C. | 7.3 | 7.1 | 7.18 | 42.83 | 50.15 | 47.22 | 0.70 |
| 4. | D. | 8.2 | 7.7 | 7.9 | 64.35 | 63.84 | 64.04 | 0.95 |
| 5. | E. | 8.1 | 6.8 | 7.32 | 61.96 | 43.31 | 50.77 | 0.75 |
| 6. | F. | 8 | 7.3 | 7.58 | 59.56 | 54.72 | 56.66 | 0.84 |
| 7. | G. | 7.7 | 7.2 | 7.4 | 52.39 | 52.43 | 52.42 | 0.77 |
| 8. | H. | 7.2 | 6.6 | 6.84 | 40.44 | 38.74 | 39.42 | 0.58 |
| 9. | I. | 7.5 | 6.5 | 6.9 | 47.61 | 36.46 | 40.92 | 0.60 |
| 10. | J. | 7 | 6.4 | 6.64 | 35.65 | 34.18 | 34.77 | 0.51 |
| 11. | K. | 7.2 | 7.2 | 7.2 | 40.44 | 52.43 | 47.63 | 0.70 |
| 12. | L. | 7.6 | 7.4 | 7.48 | 50.00 | 57.00 | 54.20 | 0.80 |
| 13. | M. | 7 | 6.6 | 6.76 | 35.65 | 38.74 | 37.51 | 0.55 |
| 14. | N. | 8.3 | 7.9 | 8.06 | 66.74 | 68.41 | 67.74 | 1.00 |
| 15. | O. | 8 | 7.1 | 7.46 | 59.56 | 50.15 | 53.92 | 0.80 |
| | $\overline{k}$ (M) | 7.6 | 7.1 | | | | | |
| | σ (SD) | 0.42 | 0.44 | | | | | |

The person responsible for the selection enters the data to the Cumulative Table of Coefficients and Transitional indicators (Table 5), calculates all the relative evaluation coefficients $V_i$ and selects the experts on the base of their relative evaluation coefficients (e.g. (usually) experts with a $V_i > 0,7$). These experts will proceed with conducting the expertise (The data in the Table 5 referring to the data in the Table 4. The data are used for illustration purpose only).

The $V_i$ coefficient can serve as a reason for granting the certificate of expert in the given area. The certificate can be granted only to the experts that have got, e.g., $V_i > 0,7$

With the aim to provide the most objective results of the expertise the chosen experts may stay uninformed about the expert evaluation results.

The Vn coefficient will also be used during the analysis of results of the expertise, but only on the purpose of estimation of the individual results founded by each expert and it is about how the most trustable results can be obtained.

The quality of the expertise will never be better than quality of the group of experts. Assuming, that under the most optimal conditions the quality of expertise can reach it utmost and so can be equal to the quality of the group of experts; it is possible to estimate an indicator of the quality of expertise (formula (5))

$$Q_{\exp} = \frac{\sum_{i=1}^{n} k_{\exp,i} V_i}{n}, \qquad (5)$$

where $Q_{\exp}$ is the indicator of the quality of expertise (10 points system); $k_{exp,i}$ is the common evaluation coefficient of the chosen expert; $V_i$ is the relative evaluation coefficient of the chosen expert; $n$ is the number of the chosen experts.

According to the above mentioned illustration (tables Nr. 4 and Nr. 5) only 9 experts of the 15 obtained the $V_i$ coefficient higher than 0.7. After calculation of the $Q_{exp}$ with using the data of evaluations of the 9 experts, the result 6.24 is obtained. It corresponds to the evaluation "Good" (Table 2) or describes the utmost quality of the formed group of experts as "Partly sufficient for conducting an expertise successfully".

To achieve any higher quality level of expertise the selection of experts must be done more carefully. Another way of checking the quality is to conduct evaluation of the experts one more time, but only for the chosen experts and after the real expertise has been conducted, so the experts will have better knowledge about each other.

## 3. Risks Determination on the Base of Multi-Criteria Risks Analysis

Nowadays, the decision making is mostly conducted on the base of models instead of real situations. It allows investigating the real process in more detailes, simultaneously avoiding any unnecessary expenditure and not least – it can help to prepare plans for diminishing the influence of the possible consequences. A natural demand is that the models have to be utmost identical to the reality. The three main stages of such decision-making are:

- Creation of the model;
- Choice of criteria for analysis and conduction of expertise;
- Evaluation of the results of the expertise and search for an optimal decision.

If the created model has all characteristics of the real situation and participation of the decision-maker in the process of creation of the model is not necessary, the decision-maker also can only give the task and receive the ready-for-implementation solutions.

If the model consists of many interconnected areas, there will be a necessity to define criteria for each of them and to accomplish several more complicated analyses that:

- have unique structure and there are no any statistical data proving correlation between criteria;
- cannot be carried out at the moment of decision making due to the lack of information about possible consequences (can be predicted only by human been on the base of experience and intuition).

Formation of a qualitative group of experts can partly solve the problem of multi-criteria analysis, but at the same time raises the problem of organisation of a qualitative expertise. Usually each expert has his/her own opinion. That is why in many cases a conference or a meeting of the experts can be organized with the aim to discuss all possible alternatives. In some cases it gives a positive result and allows finding a common or a compromise solution, although this approach has some positive sides as:

- each expert can express and prove his own idea;
- each expert can obtain information about others experts' ideas;

it has also negative sides as well:

- too high influence from the side of notorious specialists (experts) that can suppress others' ideas;
- inadequate waste of time in situation when each expert keeps his own, possibly controversial position;
- high possibility of a premature decision based only on principle of majority, when some experts can even decide to quit.

To create a systematic approach to the conduction of the expertise the three-stage procedure is developed:

- Outset data definition;
- Determination and analysis;
- Summing-up and recommendations to the decision-maker.

**At the First Stage** it is necessary: – to define and prepare the list of the criteria; – to work out or to co-ordinate the evaluation steps and; – to aggregate accessible information.

The following factors can be mentioned as criteria to be added into the list:

- Security risks;
- Environmental and ecological risks;

- Political and social risks;
- Risks connected with utilisation of some technical and innovative methods;
- Risks connected with manufacturing and economic activities;
- Commercial or financial risks, etc.

The classification is not full and is proposed on the base of short overview of obviously detected threats for any society. The exact list of threats and their criteria as well as the level of significance of these criteria have to be determined by the experts themselves.

With the aim to illustrate the utilisation of the methodology and to draw parallels to the theory of probability, the following evaluation has been proposed for using as an example.

One of the pretty known tasks is to define the safest route for transportation from point A to point B (1.A-C-B, 2.A-D-B, 3.A-G-B etc.). Consequently, there is the task to determine **what the risk of an accident on the first route from point A to point B is.**

The experts have completed the list of the mutually independent criteria that form a full group of the risks (hypothetic risks H) connected to:

H1 – driver (R-I);
H2 – car (R-II);
H3 – condition and furniture of the road (R-III);
H4 – traffic intensity (R-IV);
H5 – meteorological conditions during transportation (R-V).

According to the theory of probability an event occurs if at least one of the hypothetical risks from the full group of risks becomes the reality. In our example it means that an event, like accident on the road, can occur if one or more of this group of risks components take place. There is no reason to speculate about incompatibility or about equal possibility to take place among these risks; however it is clear that they are independent from each other. Then we can count as the probability of an accident depends on the 5 inter-independent hypothesises (H1, H2, H3, H4 un H5) and so the probability **P** of an event **A** (road accident) – **P(A)** can be calculated in accordance with the formula of the complete probability:

$$P(A) = \sum_{i=1}^{n} P(H_i)\, P(A/H_i). \tag{6}$$

The probability of an event “A” for independent hypothesises Hi is the sum of multiplications between the unconditional probability of each hypothesis P(Hi) and conditional probability P(A/Hi). The conditional probability $P(A/H_i)$ characterizes the possibility of a road accident under the condition that the hypothesis Hi takes place and it can be labelled as a coefficient of significance of this hypothesis $\mathbf{w_i}$. As it has been mentioned before, all the hypothesis form the full group of events, that is why the condition $\sum_{i=1}^{n} P(A/H_i) = \sum_{i=1}^{n} w_i = 1$ has to be kept.

To calculate the complete probability, the probability of each hypothesis has to be defined. To define the probability of each hypothesis, the experts need to make a full list of inter-independent sub-criteria for the each hypothetic criterion Hi.

For example, for the hypothesis H1 – “driver”, the group of experts agreed about following list of sub-criteria:

R-I1 – alcohol or drug influenced;
R-I2 – inadequate health condition;
R-I3 – tiredness/exhaustion;
R-I4 – nervousness/frustration;
R-I5 – insufficient driving experience;
R-I6 – regular sidetrack attention.

Insufficient confidence about one of the criteria, lack of information or differences in opinions, or any other reasons can cause further extension of any of sub-criteria or one of sub-criterion as deep as it needed. E.g. the experts do not agree upon arrangement of the sub-criteria of the criterion **RI-6 *„ Regular sidetrack attention”*** that was divided into the next level sub-criteria:

R-I1r1 – passenger;
R-I1r2 – mobile phone;
R-I1r3 – manipulation with radio;
R-I1r4 – necessity to observe an object beside the road.

In this case the new developed multi-criteria risks analysis method or DVM (Dynamic Verification Method) is to be applied to find the coefficient of significance $\mathbf{w_i}$.

DVM can be utilised as a universal methodology in any cases and is designed for using experts' individually made evaluations, but in case of experts unity a more simple – the arrangement method that is based on the Fishburn's formula (10) (see also remarks after a "*" sign in paragraph "the fourth step" of DVM) can be used as well, instead of the first two steps of the DVM.

DVM tailored for using of four steps of evaluation.

The first step is the simple arrangement of the criteria by determination of priority of each criterion in comparison with others of the same group. After arrangement, each criterion receives **Wp** points, that can be calculated by use of the following formula:

$$W_p = N - I + 1, \quad (7)$$

where N is the quantity of criteria/sub-criteria; i is the number of criterion in the priority list.

The second step is evaluation of the significance of each criterion. In reality it is the answer to the questions: – how it is important to observe this risk; – how it can influence the development of a normal process or situation; – what heavy consequences can be caused in case if the risk takes place?

With the aim to standardize evaluation of the significance of the criteria, the 10-point verification system has been developed and is presented in the table 6 below.

**Table 6**. The levels of significance of risks

| Points | (RIS) Risk Significance | Explanation |
|---|---|---|
| 10 | Critical | High possibility of inadmissibly heavy consequences in case of realisation of the risk. Elimination of the consequences asks for abundant recourses (time and finance) |
| 9 | Utmost | |
| 8 | High | A possibility of serious consequences in case of implementation of the risk. Elimination of the consequences asks for some additional recourses (time and finance) |
| 7 | Higher than medium | |
| 6 | Medium | |
| 5 | Considerable | Expected level of possibility of tangible consequences in case of implementation of the risk. Some additional activities have to be performed with aim to reduce the influence of consequences |
| 4 | Medium considerable | |
| 3 | Barely considerable | Expected level of the daily risk that usually does not bring any serious consequences |
| 2 | Low | |
| 1 | Very low | |

The results from the second level of evaluation can be used for performing arrangement of the next level criteria in situations when common understanding about the list of criteria has been achieved but there are still different positions about the arrangement of the criteria. In this case the sum of values of $W_{p_i}\ RIS_i$ of the same criterion from each table filled in by the experts is to be divided by the sum of all $\sum_{i=1}^{n} W_{p_i}\ RIS_i$ from all the tables containing the same group of criteria. The result reflects the value of $w_i$ of the given criterion. So:

$$W_i = W_{p_i}\ \mathrm{RIS_i} / \sum_{i=1}^{n} W_{p_i}\ RIS_i\ , \quad (8)$$

where $W_i$ is the coefficient of significance of the criterion; $\sum_{i=1}^{n} W_{p_i}\ RIS_i$ is the sum of all $W_{p_i}\ RIS_i$ for the same group criterion. $\sum_{j=1}^{m} (\sum_{i=1}^{n} W_{p_i}\ RIS_i)_j$ is the sum of all $\sum_{i=1}^{n} W_{p_i}\ RIS_i$ for the same group of j-criteria.

The third step is calculation of the probability of the risk. Calculation of the probability is not the subject of this methodology, because the methods of such calculation are already known and depend on the choice of an expert that is his/her own responsibility. *It has to be underlined that the probability is separately calculated only on the lowest/deepest level of the expanded criteria, where an expert can determine it by usage of statistic data or calculate mathematically or define it on the base of personal experience*, taking into account that values from 0–0,25 describe low level of the risk; 0,26–0,4 – medium; 0,41–0,7 – high; and 0,71–1,0 – critical.

Going through these three levels it is remarkable that there was no single word about the recourses needed to diminish the risks or to prevent the factors of the risks from their employment. It is obvious that these resources can also characterize the risks; however, they are the part of the area of risks prevention – the area that is closely connected with an after-expertise phase. Although it belongs to the area of responsibility of the person responsible for the expertise, an additional expertise can be organized separately (or as an independent part of the organized one) with aim to provide him/her with necessary support in this area as well.

The fourth step is to be conducted by the group, managing the expertise. The group has to consolidate all the data and calculate all the cumulative values of risks taking into account the relative evaluation coefficient $V_i$ of each expert by use of formula:

$$P(X_i) = \frac{\sum (p(x_i)/V_i)}{n}, \quad (9)$$

where $P(X_i)$*is the* the cumulative probability of the risk, $p(x_i)$ is the probability calculated by "*i*" expert; $V_i$ is the relative evaluation coefficient; *n* is the number of the experts (received evaluations).

If experts have agreed about the arrangement of the N criteria the simplified method of calculating wi with help of formula of Fishburn (10) can be used (example of calculation is in Table 7). Using this methods experts are to arrange the criteria after their significance in sequence $w_1 > w_2 > w_3 > w_4 > .... > w_n$ so a criterion $P(A/H_i)$ value $w_i$ can be calculated using formula:

$$w_i = \frac{2(N - i + 1)}{(N + 1)N}, \quad (10)$$

where $w_i$ is the coefficient of significance of the criterion; *N* is the quantity of the criteria; *i* is the number of a criterion in the arrangement.

So, when all the criteria have been defined the experts can proceed with the next stage. During the second stage the experts act individually and pass all the results to the person responsible for the expertise. However, it cannot exclude the possibility of organising necessary meetings between them or ask for consultations with others institutions.

During **the Second stage** the experts analyse and evaluate the criteria from the approved list as well as search for necessary information with the aim to determine all the risks and to evaluate all the criteria with the utmost accuracy. The results are to be analysed and the necessity of a deeper evaluation is to be declared by the managing group. On the base of the defined criteria the sub-criteria may be formulated, and approved after a common discussion among experts. The arrangement and determination of the coefficient of significance are evaluated by use of the DVM method, except the situation when experts agree upon an arrangement.

For calculation of a safety indicator of a criterion it is necessary to form the list of all the elements /sub-criteria composing one whole group. Next step is to arrange these sub-criteria according to the experts' evaluation and calculate their coefficient of significance $w_i$, that will be used for calculation of the complete probability (formula 6).

By arranging all the criteria/sub-criteria in reducing priority, the coefficient $w_i$ describes how the risk can be realized or the situation can be influenced in the most simple way.

Let us imagine that experts agreed about the previously considered example with N = 5 criteria (H1, H2, H3, H4 and H5), and ordered those in the same sequence (in reality the experts have to arrange them according to the results of the evaluation) thereby defined their priority and accomplished their arrangement (it is how the table 7 is filled in) as well as calculated their coefficient of significance by use of formula of Fishburn (10). In this case the coefficients of significances $w_i$ correspond to the utmost entropy of the object of research.

**Table 7.** Common table of arrangement of criteria with examples

| **Common table of arrangement of criteria** | | |
|---|---|---|
| **i** | **Criteria** | **wi** |
| 1 | H1 – driver (R-I) | 0,33 |
| 2 | H2 – car (R-II) | 0,27 |
| 3 | H3 – condition and furniture of the road (R-III) | 0,2 |
| 4 | H4 – traffic intensity (R-IV) | 0,13 |
| 5 | H5 – meteorological conditions during transportation (R-V) | 0,07 |

Continuing with evaluation of each hypothesis, experts are to determine the conditional probability P(A/Hi). This can be done by level gradual evaluation of criteria and sub-criteria (coefficient of significance $w_i$ of hypothesises hi (R-I1, R-I2, ...)) down to the lowest level where probabilities of single risks can be found on the base of statistic data, or calculated mathematically, or estimated from the position of personal experience. (The cells "$p_i = P(R_i)$" in tables 10;11 and 12 are filled in by use of this method). The methods of estimation of probability are not described in this methodology because they are widely known and choice of the most appropriate is the responsibility of experts themselves.

**Table 8.** Expert's individual table of evaluation of criteria (risks)

| **Expert's individual table of evaluation of criteria (risks)**<br>**Expert:................................................** | | | | | | | |
|---|---|---|---|---|---|---|---|
| **Nr.** | **Title of criterion/sub-criterion $r_i$** | **$Wp_i$** | **$RIS_i$ (points)** | **$Wp_i\ RIS_i$** | **$w_i = (P(R\text{-}I/R_i) = Wp_i\ RIS_i / \Sigma Wp_i\ RIS_i$** | **$p_i = P(R_i)$** | **$P(r_i) = P(R_i)\ P(R\text{-}I/R_i)$ (Probability of risk of sub-criterion $R_i$ of criterion R-I)** |
| 1 | $r_1$ | | | | | | |
| 2 | $r_2$ | | | | | | |
| .... | ...... | | | | | | |
| i | $r_i$ | | | | | | |
| .... | ...... | | | | | | |
| N | $r_N$ | | | | | | |
| | | $\Sigma\ Wp_i\ RIS_i$ = | | ........... | $P(R\text{-}I) = \sum P(Ri)\ P(R\text{-}I/R_i) = \sum w_i \times p_i$ = | | |
| Data............................ | Signature of expert.................................... | | | | | | |

Processing the data of the higher (less detailed) level of criteria occurs on the base of the results of evaluation of the lower level criteria, but by use of the same level of the coefficient of significance.

With aim to provide a proper processing all necessary data each expert fills-in the Expert's individual table of evaluation of the criteria (risks) (Table 8), or the Unified table of expert's evaluation of criteria (risks) (Table 9).

**Table 9.** Unified table of expert's evaluation of criteria (risks)

| **Unified table of expert's evaluation of criteria (risks)**<br>**Expert:................................................** | | | | |
|---|---|---|---|---|
| **$i_{(1\text{-}N)}$** | **Titles of risks of criteria/sub-criteria** | **Coefficient of significance of the risk wi = $P(R\text{-}I/R_i)$** | **Unconditional probability of the risk $P(R_i) = p_i$** | **Complete probability of the risk P(Ri) $P(R\text{-}I/R_i)$** |
| | | | | |
| | | | | |
| | | | | |
| | | | | |
| | | | | |
| | | | | |
| | $P(R\text{-}I) = \sum P(Ri)\ P(R\text{-}I/Ri) = \sum wi \times pi$ = | | | |
| Data............................ | Signature of expert .................................... | | | |

An expert individually evaluates all the criteria and sub-criteria, fills-in his/her working table (8) and calculates all the necessary data that allow estimating the probability of the corresponding criterion probability.

To illustrate an "A" expert's work (with expert's coefficient $V_i = 0.77$ (look in table 5)), the above mentioned example about the risks of a road accident during travel from point A to point B through point C.

Expert „A" evaluated **„Regular sidetrack attention"** criterion on the base of already defined sub-criteria:

R-I1r1 – passenger;
R-I1r2 – mobile phone;
R-I1r3 – manipulation with radio;
R-I1r4 – necessity to observe an object beside the road,

as well as received all necessary statistical information that helped to calculate the unconditional risks ($p_i = P(R_i)$) of those sub-criteria. On the base of these data the table 10 is filled in (the data are used only for illustration purpose).

**Table 10.** Example of filled-in Expert's individual table of evaluation of criteria (risks)

| No | Title of criterion/sub-criterion $r_i$ | $Wp_i$ | $RIS_i$ (points) | $Wp_i$ $RIS_i$ | $w_i = (P(R\text{-}I/R_i) = Wp_i RIS_i / \Sigma Wp_i RIS_i$ | $p_i = P(R_i)$ | $P(r_i) = P(R_i) P(R\text{-}I/R_i)$ (Probability of risk of sub-criterion $R_i$ of criterion R-I) |
|---|---|---|---|---|---|---|---|
| 1 | R-I1r2 – mobile phone | 4 | 5 | 20 | 0.38 | 0.2 | 0.08 |
| 2 | R-I1r3 – manipulation with radio | 3 | 7 | 21 | 0.40 | 0.4 | 0.16 |
| 3 | R-I1r4 – necessity to observe an object beside the road | 2 | 4 | 8 | 0.15 | 0.2 | 0.03 |
| 4 | R-I1r1 – passenger | 1 | 3 | 3 | 0.06 | 0.1 | 0.01 |
| | | $\Sigma$ $Wp_i$ $RIS_i$ = | | 52 | $P(R\text{-}I) = \sum P(Ri) P(R\text{-}I/Ri) = \sum w_i \times p_i =$ | | **0.28** |

Further the expert work is organized similarly.

<u>**During the Third stage**</u> the cumulative probability of each hypothesis is to be estimated on the base of valuations conducted by the experts taking into account experts' individual relative evaluation coefficient $V_i$ (formula (9)). For example, the "A" expert's estimated result 0,28 at the end will be used for further calculations as 0,37 (0,28/0,77 = 0,37), and so the final (cumulative) probability of risk connected to this hypothesis will be calculated i.a.w. formula (9) (and result will be, for example, 0,1 – see Table 11).

Taking into account the fact that experts agreed upon the arrangements of the criteria of higher level, the risks connected with these criteria are calculated on the base of significances found i.a.w. formula (10).

**Table 11**. Example of the filled in unified table of expert's evaluation of criteria (risks) for R-I criteria

| $I_{(1\text{-}N)}$ | Titles of Ri sub-criteria of R-I criteria | Coefficient of significance of the risk $w_i = P(R\text{-}I/R_i)$ | Unconditional probability of the risk $P(R_i) = p_i$ | Complete probability of the risk $P(Ri)\, P(R\text{-}I/R_i)$ |
|---|---|---|---|---|
| 1 | Risk that driver is influenced by alcohol or drug R-I1 | 0,28 | 0,05 | 0,014 |
| 2 | Risk that driver is in an inadequate health condition R-I2 | 0,24 | 0,01 | 0,0024 |
| 3 | Risk of driver's tiredness/exhaustion R-I3 | 0,19 | 0,15 | 0,0285 |
| 4 | Risk of driver's nervousness/frustration R-I4 | 0,14 | 0,01 | 0,0014 |
| 5 | Risk that driver has insufficient driving experience R-I5 | 0,10 | 0,02 | 0,002 |
| 6 | Risk that driver paid regular sidetrack attention R-I6 | 0,05 | <u>*0,1*</u> | 0,005 |
| | | $P(R\text{-}I) = \sum P(R_i) P(R\text{-}I/R_i) = \sum w_i \times p_i =$ | | **0,0533** |

The same procedure is used for calculation of probability of risks bound to other R-N criteria P(R-II), P(R-III), P(R-IV) un P(R-V), that also are accordingly consolidated into the table (see Table 12) for further calculations. On the base of these data and by using the formula of the complete probability (6) the probability of the risk of a road accident during travel from point A to point B through point C can be calculated, taking the significance coefficients $w_i$ as the conditional probability P(A/Hi).

**Table 12.** Example of the filled in unified table of expert's evaluation of criteria (risks) for R-N criteria

| $i_{(1-N)}$ | Titles of R-I, R-II, R-III, R-IV and R-V sub-criteria of the criterion R(A) | Coefficient of significance of the risk wi = P(R-I/Ri) | Unconditional probability of the risk P(Ri)= pi | Complete probability of the risk P(Ri) P(R-I/Ri) |
|---|---|---|---|---|
| 1 | Risks connected to the driver (R-I) | 0,33 | **0,0533** | 0,0176 |
| 2 | Risks connected to the car (R-II) | 0,27 | 0,0355 | 0,0096 |
| 3 | Risks connected to the condition and furniture of the road (R-III) | 0,2 | 0,003 | 0,0006 |
| 4 | Risks connected to the traffic intensity (R-IV) | 0,13 | 0,009 | 0,0012 |
| 5 | Risks connected to the meteorological conditions during transportation (R-V) | 0,07 | 0,0014 | 0,0001 |
| P(R-I) = ∑ P(Ri) P(R-I/Ri) = ∑ wi x pi = | **0,0291** | | | |

The result of the estimations shows that the risk of the road accident during the travel from point A to point B through point C is R(A) = 0,029. It means that travelling safety can be easily found as a probability P = 1 – R(A) = 0,971. In other words there is possibility of a road accident (A-C-B trip) roughly about 3 cases from 100 and the main causes for such accident can be: an unqualified driver; or technical problems with car; or bad conditions of the road.

The same estimations and analysis have to be conducted for all the routes, and then the comparison between all final results will give the answer to the question about which route is the safest one. And last but not the least – one more time – it is necessary to pay attention to the fact that the quality of this expertise corresponds to the utmost quality of the formed group of experts that got the evaluation "Good" or is described as "Partly sufficient for conducting an expertise successfully".

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# SINGULAR VALUE DECOMPOSITION OF IMAGES WITH THE SIMPLE ELEMENTS

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Simple image elements are analyzed by singular value method. Analytical results for a few matrix forms are received. Nonequivalence of image diagonal and parallel elements is shown. Division into sub-blocks method is used in order to eliminate noise in the case of diagonal clustering.

***Keywords:*** *singular value decomposition, matrix, eigenvectors*

## 1. Introduction

Singular Value Decomposition (SVD) technique is widely used in the signal and image processing [1] including a noise reduction [2].

Any real positively defined matrix $m \times n$ can be decomposed uniquely as

$$A = USV^T , \tag{1}$$

$U$ is an orthogonal ($m\times m$) matrix ($U^TU = I$) and $V$ is an orthogonal ($n\times n$) matrix. $S$ is a ($m\times n$) matrix whose off-diagonal elements are 0's [3]:

$$S = \begin{bmatrix} S_r & 0 \\ 0 & 0 \end{bmatrix}, \tag{2}$$

$$S_r = diag(\sigma_1, \sigma_2, \dots, \sigma_r). \tag{3}$$

The diagonal elements are arranged so that

$$\sigma_1 \ge \sigma_2 \ge \dots \ge \sigma_r \ge 0 \tag{4}$$

and $\sigma_{r+1}, \sigma_{r+2}, \dots, \sigma_n = 0$ .

The equation (1) can be rewritten in explicit form:

$$A = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \dots \quad \mathbf{u}_n] \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^T \\ \mathbf{v}_2^T \\ \vdots \\ \mathbf{v}_n^T \end{bmatrix}, \tag{5}$$

or

$$A = \mathbf{u}_1\sigma_1\mathbf{v}_1^T + \mathbf{u}_2\sigma_2\mathbf{v}_2^T + \dots + \mathbf{u}_n\sigma_n\mathbf{v}_n^T = \sum_{i=1}^{r} \mathbf{u}_i\sigma_i\mathbf{v}_i^T . \tag{6}$$

The columns of $U$ are called the left singular vectors and they form an orthonormal basis. The rows of $V^T$ contain the elements of the right singular vectors. The above mentioned vectors are defined by the equations [4]:

$$A^T \mathbf{u}_i = \sigma_i \mathbf{v}_i , \tag{7}$$

$$AA^T \mathbf{u}_i = \lambda_i \mathbf{u}_i , \tag{8}$$

$$A^T A\mathbf{v}_j = \lambda_j \mathbf{v}_j . \tag{9}$$

The SVD is frequently used in digital signal processing as a method for noise reduction. The central idea is to represent the noisy signal by a matrix *A* (caterpillar approach [5]). After computing the SVD one can dismiss small singular values of *A* which usually represent the noise. Given one retain *k* singular values, the denoised signal is stored in $A_k$ [2].

## 2. Simple Image Elements SVD

In spite of a large number of publications in this field, several points still require further discussion. In image processing the image matrix is converted to a numerical matrix and all processing is carried out with numbers – singular values and vector components. Some additional information about SVD may be obtained by using analytical approach.

Let us consider a SVD of simple image elements: diagonal, horizontal and vertical lines. As image elements they are equivalent (lines) but their SVD transformations are essentially different. In order to preserve diagonals all singular matrix values are necessary, but at the same time the horizontal and vertical lines need only one singular value (and corresponding vectors).

The first matrix we choose in the form

$$A = \begin{bmatrix} a & 0 & b \\ 0 & a & b \\ b & b & a \end{bmatrix} . \tag{10}$$

SVD example of matrix *A* is shown in Fig. 1.

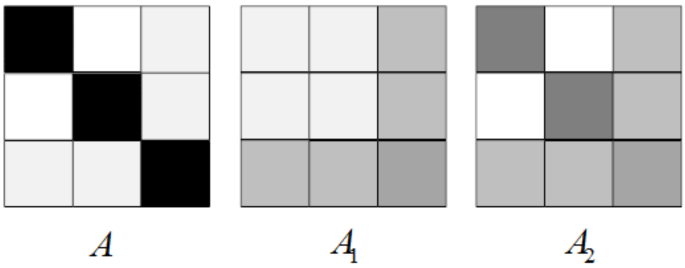


*Figure 1.* $A_1$ – only first singular value preserved, $A_2$ – two singular values preserved (MatLab)

One can get (using the symbolic programs Maple and Maxima) an analytical result for *A* (10).
$AA^T$ and $A^TA$ are:

$$AA^T = \begin{bmatrix} a & 0 & b \\ 0 & a & b \\ b & b & a \end{bmatrix} \cdot \begin{bmatrix} a & 0 & b \\ 0 & a & b \\ b & b & a \end{bmatrix} = \begin{bmatrix} a^2+b^2 & b^2 & 2ab \\ b^2 & a^2+b^2 & 2ab \\ 2ab & 2ab & a^2+2b^2 \end{bmatrix}, \tag{11}$$

$$A^T A = \begin{bmatrix} a^2+b^2 & b^2 & 2ab \\ b^2 & a^2+b^2 & 2ab \\ 2ab & 2ab & a^2+2b^2 \end{bmatrix}, \tag{12}$$

and eigenvalues (*A* is symmetrical):

$$\lambda_1 = a^2 + 2\sqrt{2}ab + 2b^2 , \tag{13}$$

$$\lambda_2 = a^2 , \tag{14}$$

$$\lambda_3 = a^2 - 2\sqrt{2}ab + 2b^2 . \tag{15}$$

Singular values are

$$\sigma_1 = \sqrt{\lambda_1} = \sqrt{a^2 + 2\sqrt{2}ab + 2b^2} = a + \sqrt{2}b , \tag{16}$$

$$\sigma_2 = \sqrt{\lambda_2} = a , \tag{17}$$

$$\sigma_3 = \sqrt{\lambda_3} = \sqrt{a^2 - 2\sqrt{2}ab + 2b^2} = a - \sqrt{2}b . \tag{18}$$

We assume $a \geq \sqrt{2}b$ . Singular matrix $S$ takes the form:

$$S = \begin{bmatrix} a+\sqrt{2}b & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a-\sqrt{2}b \end{bmatrix} . \tag{19}$$

At the next stage we calculate $V$ and $U$ eigenvectors. These can be orthonormalized by Gram-Schmidt orthogonalization [6]. Then we get $V^T$ and $U$:

$$V^T = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} \end{bmatrix} , \tag{20}$$

$$U = \begin{bmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{bmatrix} , \tag{21}$$

Matrix A is restored according to (1):

$$USV^T = \begin{bmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} a+\sqrt{2}b & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a-\sqrt{2}b \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} \end{bmatrix} =$$

$$= \begin{bmatrix} \frac{a+\sqrt{2}b}{4} + \frac{a-\sqrt{2}b}{4} + \frac{a}{2} & \frac{a+\sqrt{2}b}{4} + \frac{a-\sqrt{2}b}{4} - \frac{a}{2} & \frac{a+\sqrt{2}b}{2\sqrt{2}} - \frac{a-\sqrt{2}b}{2\sqrt{2}} \\ \frac{a+\sqrt{2}b}{4} + \frac{a-\sqrt{2}b}{4} - \frac{a}{2} & \frac{a+\sqrt{2}b}{4} + \frac{a-\sqrt{2}b}{4} + \frac{a}{2} & \frac{a+\sqrt{2}b}{2\sqrt{2}} - \frac{a-\sqrt{2}b}{2\sqrt{2}} \\ \frac{a+\sqrt{2}b}{2\sqrt{2}} - \frac{a-\sqrt{2}b}{2\sqrt{2}} & \frac{a+\sqrt{2}b}{2\sqrt{2}} - \frac{a-\sqrt{2}b}{2\sqrt{2}} & \frac{a+\sqrt{2}b}{2} + \frac{a-\sqrt{2}b}{2} \end{bmatrix} = \begin{bmatrix} a & 0 & b \\ 0 & a & b \\ b & b & a \end{bmatrix} . \tag{22}$$

For $A_1$ (only $\sigma_1$ is preserved) we get

$$A_1 = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \cdot \left(a + \sqrt{2}b\right) \cdot \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{a+b\sqrt{2}}{4} & \frac{a+b\sqrt{2}}{4} & \frac{a+b\sqrt{2}}{2\sqrt{2}} \\ \frac{a+b\sqrt{2}}{4} & \frac{a+b\sqrt{2}}{4} & \frac{a+b\sqrt{2}}{2\sqrt{2}} \\ \frac{a+b\sqrt{2}}{2\sqrt{2}} & \frac{a+b\sqrt{2}}{2\sqrt{2}} & \frac{a+b\sqrt{2}}{2} \end{bmatrix}, \qquad (23)$$

for $A_2$

$$A_2 = \begin{bmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} a+b\sqrt{2} & 0 \\ 0 & a \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{bmatrix} = \begin{bmatrix} \frac{3a+b\sqrt{2}}{4} & \frac{b\sqrt{2}-a}{4} & \frac{a+b\sqrt{2}}{2\sqrt{2}} \\ \frac{b\sqrt{2}-a}{4} & \frac{3a+b\sqrt{2}}{4} & \frac{a+b\sqrt{2}}{2\sqrt{2}} \\ \frac{a+b\sqrt{2}}{2\sqrt{2}} & \frac{a+b\sqrt{2}}{2\sqrt{2}} & \frac{a+b\sqrt{2}}{2} \end{bmatrix}. \qquad (24)$$

The analytical result corresponds to Fig.1. It is worth noting that only the first two singular values are necessarily to be preserved if $a = \sqrt{2}b$.

It can be shown that matrix *A* (10) gives the following singular values in *n* dimensional case

$$a + b\sqrt{n-1}, a, \ldots, a, a - b\sqrt{n-1}\ . \qquad (25)$$

In the above considered example the eigenvectors $\boldsymbol{u_i}$ and $\boldsymbol{v_i}$ do not depend on *a* and *b* values.

If we consider *b* elements in *A* as a noise of pure diagonal matrix we see that this noise cannot be eliminated by SVD because of clusterization of the diagonal elements (all elements in matrix *S* should be preserved). With this fact some problems arise in image processing by the SVD method. The clusterization of singular values (elements with the same value) in some sub-block of matrix *A* forbids the noise reduction in this sub-block. The only method in this case is to divide sub-block into smaller blocks and perform noise separation in these sub-blocks.

In the same manner we can analytically examine other symmetrical matrixes. If *A* is not symmetrical, eigenvalues contain *a* and *b* explicitly. A number of matrices can be examined analytically, for example

$$A = \begin{bmatrix} a & 0 & b \\ 0 & a & b \\ 0 & 0 & a \end{bmatrix}, \begin{bmatrix} a & 0 & 0 \\ b & a & 0 \\ 0 & 0 & a \end{bmatrix}, \begin{bmatrix} a & c & 0 \\ b & a & 0 \\ 0 & 0 & a \end{bmatrix}, \begin{bmatrix} la & 0 & 0 \\ b & ka & 0 \\ 0 & 0 & a \end{bmatrix}. \qquad (26)$$

## 3. Division into Sub-Blocks

Let us consider the numerical test matrix *A* (Fig. 2) and try to eliminate noise (grey color).

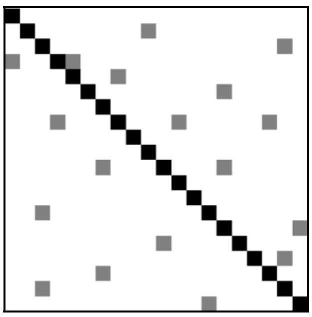

*Figure 2.* Matrix with noise (grey)

It is worth noting that blocks with clusters are not necessarily in the diagonal form (any permutation of columns and rows do not annihilate clusters). Divided into sub-blocks matrix is presented in Fig. 3.

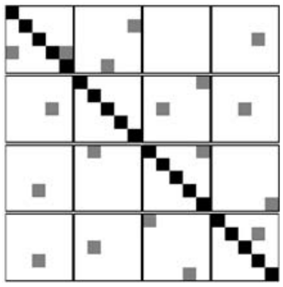

*Figure 3.* Matrix divided into blocks

After performing the SVD on each sub-block and retaining only the first singular value, we obtain a matrix, further denoted as *B*.

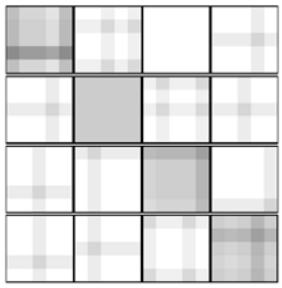

*Figure 4.* Matrix restored after SVD, only the largest singular value is preserved

We calculate Pearson correlation coefficient [7] according to

$$r = \frac{\sum_m \sum_n \left(A_{mn} - \overline{A}\right)\left(B_{mn} - \overline{B}\right)}{\sqrt{\left(\sum_m \sum_n \left(A_{mn} - \overline{A}\right)^2\right)\left(\sum_m \sum_n \left(B_{mn} - \overline{B}\right)^2\right)}}, \quad (27)$$

where $A_{mn}$ is an image $A$ with $m$, $n$ pixel intensity, $B_{mn}$ is an image $B$ with $m$ ,$n$ pixel intensity, $\overline{A}$ – $A$ is an image (matrix) averaged pixel value, $\overline{B}$ – $B$ is an image averaged pixel value.

Correlation coefficient values are given in the Table 1.

**Table 1.** Correlation coefficients

| **Sub-block *i/j*** | ***1*** | ***2*** | ***3*** | ***4*** |
|---|---|---|---|---|
| **1** | 0.2357 | 0.4955 | 1 | 0.5555 |
| **2** | 0.5555 | 8.0059e-017 | 0.4955 | 0.5555 |
| **3** | 0.5555 | 0.5555 | 0.1416 | 0.5555 |
| **4** | 0.5555 | 0.5555 | 0.4955 | 0.1416 |

In the sub-blocks with correlation coefficient $r > 0.4$ all pixel values are assigned the average background pixel value, these sub-blocks contain only noise. Sub blocks with $r < 0.4$ remain unchanged.

In Fig. 5 we show only sub-blocks where full SVD is necessary.

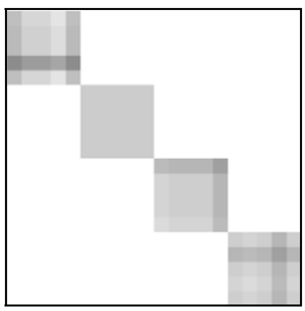

*Figure 5.* Only subblocks where full SVD is necessary to be performed

After performing the procedure described above, we obtain the restored (denoised) matrix *A* (image) (Fig. 6).

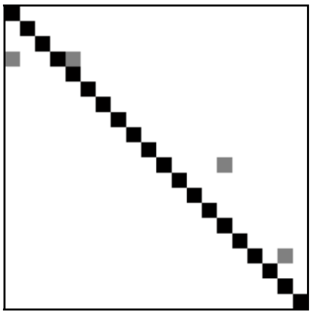

*Figure 6.* Denoised matrix *A*

## Conclusions

It is shown that analytical SVD performed on simple matrices with diagonal, horizontal and vertical elements can give some additional insight into the image processing with SVD, especially in the case when the diagonal elements are clustered.

A simple sub block SVD method which permits to overcome the clustering problems is presented.

## Acknowledgements

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# NANOTHINKING AS AN ESSENTIAL COMPONENT OF SCIENTIFIC COMPETENCE AND SOCIAL RESPONSIBILITY IN THE 21$^{ST}$ CENTURY SOCIETY

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Around the world, the pace, complexity and social significance of technological changes are increasing. Striking developments in such areas as computer and communications technology, biotechnology and nanotechnology are finding applications and producing far-reaching effects in all spheres of business, government, society and the environment. However, the far-reaching social consequences are often not understood until after new technologies become entrenched. Historically this has resulted in important lost opportunities, significant social and environmental costs and channeling societal development down long-term unhealthy paths. Knowing how to live together healthily, safely, and humanely in society is certainly a worthwhile cause. It is also a real challenge for those who educate young citizens of today. This paper outlines how nanotechnology education can be considered to be a fundamental discipline of the 21$^{st}$ century educational systems for supporting the development of responsible citizenship, since it touches the most significant areas of the wellbeing of every citizen – health, safety and security, and the environment – which occupy a privileged position in all cultures and all considerations. Citizenship education does not rest on the acquisition of explicitly theoretical knowledge. Rather, it targets the development of civic behaviour in all inhabitants of a given territory (one they identify with) and ultimately throughout the entire world.

***Keywords:*** *Nanothinking, nanoeducation, nanomanagement, nanochallenges, nanorisks*

## Introduction

One decade into the 21$^{st}$ century, people and governments worldwide face decisions on daily basis involving complex scientific considerations or innovations in technology. Decisions small and large – whether they are policy-makers' votes on a climate bill, biotech corporations considerations of potential product lines, consumers' choices of food purchases or educators' use of computers in the classroom – must incorporate a dizzying array of factors. The new participative democracy demands that citizens are asked to make judgments, and even vote, on subjects about which they know very little – the desirability of cloning animals and human beings, creating novel biological organisms, manipulating matter at an atomic scale, nuking your enemies, eugenics, genetic engineering, GM food, nanoproducts, and other great moral and economic questions of the day. Therefore, educational systems have to produce a steep increase in citizens' intellectual potential in order to provide sane answers to such deep philosophical questions, previously the domain of university researchers.

Educational environment is becoming a new supercomplex system with a constantly changing intellectual pattern. It has been predicted that today school-leavers will have many careers – not just jobs, over their lifetimes, and that more than 50% of the jobs they will be doing do not exist yet. But one thing is certain – they will be doing knowledge jobs, intellectually more demanding and almost certainly involving interaction with technologies far more sophisticated than those existing at present. ***Mindpower*** is replacing ***manpower***.

Still, the structure of our universities has changed very little in the past fifty years; they are still organized in the traditional fields with little or no horizontal structures. In materials science, as in many other fields, much of the most exciting discovery potential is located at the boundaries between traditional disciplines. Already today, many novel multifunctional nanomaterials, advanced nanodevices, new nano-based products and processes are designed and developed by team efforts of materials scientists working with chemists, biologists, physicists, information technology experts, and engineers. It is thus apparent that we need to create new types of universities, which have 'departments without walls' [1, 3].

## 1. Nanotechnology as an Imperative for Educational Redesign

Rapid technological changes have dramatically altered our educational needs. The simplest explanation for the current need of educational change is that we, as society, have outgrown our educational systems disseminating core knowledge and building the basic skills. With the advent of the information age, and now the beginning of new technologies age, the educational model of today no longer meets our societal needs. In fact, it is limiting the ability of teachers and students to adapt to the 21$^{st}$ century.

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## Nanothinking and Nanoeducation

Nanotechnology is an exciting area of scientific research and development that is truly multidisciplinary. The prefix '*nano*' originates from the Greek word meaning 'dwarf'. In science it means one billionth ($10^{-9}$) of a meter, which is tiny, only the length of ten hydrogen atoms, or about one hundred thousandth of the width of a hair!

Nanotechnology is not really anything absolutely new. In one sense, it is the natural continuation of the miniaturization revolution that we have witnessed over the last decade, where millionth of a meter ($10^{-6}$ m) tolerances in engineered products have become commonplace. A good example of the application of nanotechnology is a mobile phone, which has changed dramatically in a few years – becoming smaller and smaller, while paradoxically growing cleverer and faster – and cheaper!

What is new, though, is the multidisciplinary approach and the ability to 'see' these entities and to manage them. Although scientists have manipulated matter at the nanoscale for centuries, calling it physics or chemistry, it was not until a new generation of microscopes were invented in IBM, Switzerland, in the late 1980s that the world of atoms and molecules could be visualized and managed. Now biologists can discuss steric effects of cell membranes with chemists, while physicists provide the tools to watch the interaction *in vivo* - infra-red microscopes to study molecules and X-ray microscopes to study atomic structures and to handle even single atoms.

On a nanoscale, the properties of materials can be very different from those in bulk matter. The development of nanoscience will require the expertise of all scientists – from engineers to ecologists. **Nanoscience** can be defined as 'the multidisciplinary study of phenomena and manipulation of materials at atomic, molecular and macromolecular scales, in order to understand and exploit properties that differ significantly from those on a larger scale'[1]. The question arises, – why do the properties of materials become different on a nanoscale? There are two main reasons for it.

First, nanomaterials have, relatively, a larger surface area than the same materials in bulk matter. And, consequently, they become more chemically reactive, showing very useful physical and chemical properties such as strength, exceptional electric conductivity or resistivity, a high capacity for storing and transmitting heat. This is exemplified by the fine grained materials that we use in our daily lives, such as flour, which can become explosive in some circumstances. Nanomaterials can even modify their biological properties (with silver, for example, becoming bactericide on a nanoscale).

Second, below 50 nm, the laws of classical physics give way to quantum effects, causing different optical, magnetic and electrical behaviours of nanomaterials. These properties, however, can be difficult to control. For example, when nanoparticles touch each other, they can fuse, losing both their shape and those unusual properties, as magnetism – that scientists hope to exploit for a new generation of microelectronic sensors and devices. Therefore, **Nanotechnology** can be defined as the 'design, engineering, characterization, production and application of structures, devices and systems by controlling shape and size on a nanometer scale' [1]. Specific functionalities, therefore, can be achieved by reducing the size of the particles to 1–100 nm.

A concise definition is given by the US National Nanotechnology Initiative: '**Nanotechnology** is concerned with materials and systems whose structures and components exhibit novel and significantly improved physical, chemical, and biological properties, phenomena, and processes due to their nanoscale size. The goal is to exploit these properties by gaining control of structures and devices at atomic, molecular and supramolecular levels and to learn to efficiently manufacture and use these devices' [4]. This term can be applied to many areas of research and development – from medicine to manufacturing, to renewable energy, transport, computing, and even to textiles and cosmetics.

It can be difficult to think of and imagine exactly the invisible world of atoms and molecules to get a greater understanding of how it will affect our lives and the everyday objects around us, but the areas where nanotechnologies are set to make a difference are expanding alongside with the challenges they pose to society. Challenges in nanotechnologies can be presented in their hierarchical priorities (Fig. 1).

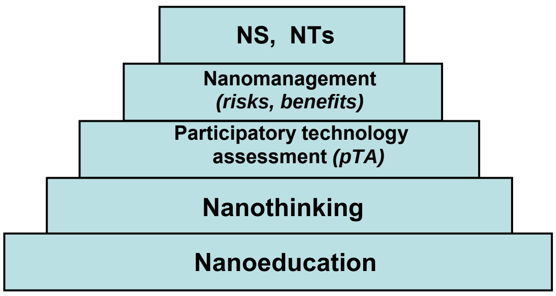



*Figure 1.* Nanochallenges hierarchy (T. Lobanova-Shunina, Yu. Shunin, 2010)

**Nanochallenges** comprise such basic areas as *nanoeducation, nanothinking, participatory technology assessment (pTA), and nanomanagement (incorporating risks and benefits).*

Already today, many novel multifunctional nanomaterials, advanced nanodevices, new nano-based products and processes are designed and developed by team efforts of materials scientists working with chemists, biologists, physicists, information technology experts, and engineers. Therefore, the appropriate education, which produces young top-notch scientists, is a big concern. It is thus apparent that we need to create new types of universities, which have *'departments without walls'*.

## 2. Valuable Contribution of Nanoeducation to the 21st Century Societal Consciousness and Social Responsibility

During the past 10 years, we have seeded many ideas into the global consciousness to stimulate preparation of our students for their future. The world is changing but our education matrix remains in the Industrial version of reality. We are neither even close to understanding, nor preparing our students for these major changes they will face in the next few decades. **Nanoeducation** is the new foundation for a new way of thinking, for the integration of all disciplines to expand our next generation students' knowledge base and prepare them for a very different future in a global society enhanced by all of the integrated science research now in process [2].

The rise of a highly networked global knowledge economy is changing the interface between scientists, researchers and the general public as consumers of new technologies, new materials and devices. Nanoeducation has to contribute to closing the gap between public rhetorical value and nanotechnology practice on decision-making policy.

Many companies throughout Europe and the world report problems in recruiting the types of graduates they need, as many graduates lack the skills to work in a modern economy. For majority of European universities to continue to compete alongside prestigious international institutions and programmes on nanomaterials, it is important to create educational systems that would provide a top-level education and the relevant skills mix and would cover education, training, sciences and technologies for research and have strong involvement by European industry.

The elements for such high-level education are

- multi-disciplinary skills;
- top expertise in nanomaterials science and engineering;
- literacy in complementary fields (physics, chemistry, biology);
- exposure to advanced research projects;
- literacy in key technological aspects; exposure to real technological problems;
- basic knowledge in social sciences, culture, management, ethics, foreign languages;
- literacy in neighbouring disciplines: international business, law, IT, etc;
- interlinkages between education, research and industrial innovation: students will be ready for what research and development will provide;
- sharing of post-docs, Masters and PhD students to foster the mobility of permanent researchers and professors between different institutions to create 'team spirit'.

Companies, universities, governments, research organizations and technical societies must all strive to define their roles in this partnership. The 'output' will be graduates with a new way of thinking, skillful manipulators, synthesizers and creators of new knowledge excellently equipped to solve future complex problems and to work collaboratively.

The option offered by a new era of emerging technologies to all of us on the planet today can be spelled out in the words: 'nanoeducation can be considered a privileged discipline for supporting the development of social consciousness and responsibility of citizens in the 21st century technologically empowered global society' [1].

## 3. Nanothinking as an Educational Concept of the 21st Century

Data saturation that accompanies the 'new technologies age' has fostered an ever-increasing interdependency between people. The pace of expected adaptation is accelerated to a pace that exceeds individuals' abilities to accommodate. Being on the receiving end of technologies deluge serves to undermine people's confidence and sense of personal responsibility giving rise to the sense of helplessness that many people feel as the world enters the 'age of interdependency'.

**Nanothinking** can serve as the antidote to the sense of helplessness since it is a concept for seeing the 'structures' that underlie complex processes, for a much better understanding how our organism works, and for discerning how to foster health, safety and the surrounding environment. Our life is reduced due to ignorance and neglect of the elementary things concerning our health. If we do not understand ourselves, we will not be able to change our life for the better.

**Nanothinking** is a comprehensive system thinking – the ability to think of, imagine and understand matter, structures and processes at an atomic and molecular levels; it is the ability to envision a nanophenomenon within the context of a larger whole. To **think nanoscalely** – means to put things into a nanoscale context and to establish the nature of their relationships within larger contexts [2]. To put it simply, it is the ability to understand in what way this tiny atomic and molecular world can have impact on us, on our health, on our safety and security, and on the environment we live in.

Contemporary top-level education envisions cause students think systemically – integrating not only macro-, micro-, but also the nano scale. **Nanothinking** offers a language that begins by restructuring the way how we think. It is a dynamic concept where practitioners are continually engaged in a process of 'seeing wholes' – a perspective that pays attention to the interrelationships and patterns of influence between constituent parts to foster the dissolution of compartmentalization of science and the corresponding compartmentalization of the mind .

Nanoscientists are now enthusiastically examining how the 'living world works' in order to find solutions to long-standing problems in the 'non-living world'. The way marine organisms build 'strength' into their shells or insects create the most amazing structures has lessons in how to engineer lightweight, tough materials for vehicles and other applications, or to improve the design and create even better structures for buildings and the environment. The way a leaf photosynthesizes can lead to techniques for efficiently generating, converting and storing renewable energy. Even how a nettle delivers its sting can suggest better vaccination techniques.

Natural systems provide us with solutions, but solutions are usually package solutions with concepts strongly interconnected one with the other. The problem is that too much of our thinking today in business – is poor business based on poor competence. We have knowledge and we have one market. The time has come to re-think the system. And if we are prepared to re-think (probably due to the crisis) the business world, we will be able to re-think how o put innovative structures and systems into the production process.

Education in this highly technological global economy has to play a double role. First, it has to provide a top-level, systemic, multidisciplinary education to graduates able to think innovatively and creatively. Second, to educate the general public, thus, shaping citizens' consciousness. Citizen thinking can be formed and improved through sustained and carefully crafted dialogue, which has to be integrated into educational communication practice.

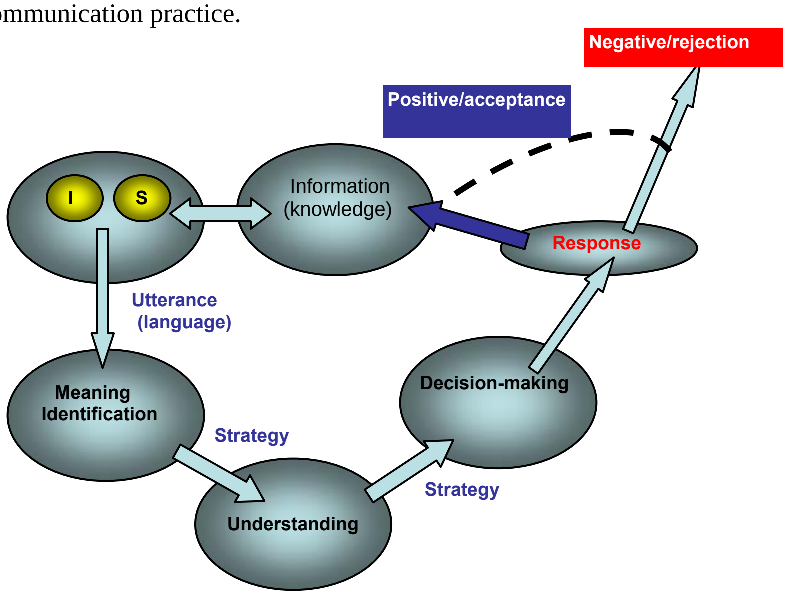



*Figure 2.* Language and understanding as major determinants for shaping consciousness

Educational communication has to contribute to developing a new way of thinking – the systemic thinking, with the main strategy – 'how to think' rather than 'what to think'. It is the privilege of a liberal university not to give the right answers to students but to put the right questions.

Educational communication, as human communication in general, can be defined (according to a German sociologist Niklas Luhman) in terms of interactive construction of meaning/thinking [3]. Thus, it can be presented as the unity of three components:

i) information – provided by teachers possessing knowledge;
ii) utterance – by means of language;
iii) understanding – a kind of created 'identical' thinking.

The acceptance or rejection of the receiver is added to this unity to continue communication and interaction (Fig. 2). Language, as the main method of communication, shapes our way of thinking and, consequently, our feeling and acting.

Anthony Giddens, a famous British sociologist, points out that people are always to some extent knowledgeable about what they are doing. Because people are reflexive and monitor the ongoing flow of information, activities, and conditions, they adapt their ways of thinking/actions to their evolving understanding (Figure 3). As a result, *knowledge changes human ways of thinking/activities, thus, shaping our consciousness*. Consciousness is not inherited or static. It rather becomes a reflective project – an endeavour, which we continuously work out and reflect on. It is not a set of observable characteristics of a moment, but becomes an account of a person's life.

Language, in this respect, can act as a constraint on action/way of thinking, but at the same time, it also enables action by providing common frames of mutual understanding [6].

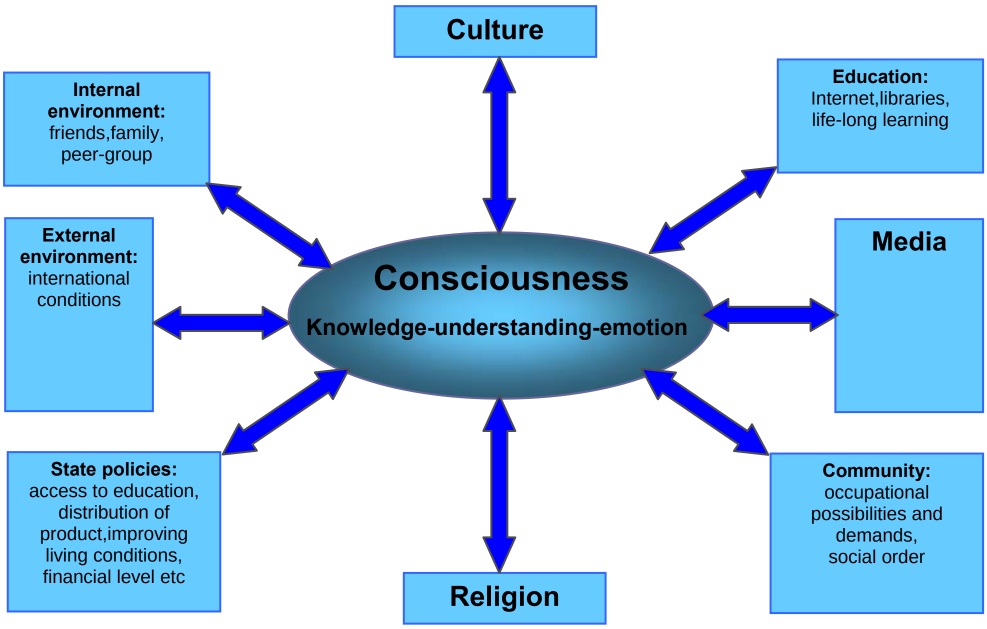



*Figure 3.* Shaping public consciousness. (T. Lobanova-Shunina, Yu. Shunin, 2010)

The development of a new way of thinking envisions bringing the practice of participatory technology assessment (pTA) into alignment with the realities of the 21st century technology – to create a 21st century educational model.

## 4. Citizen Participative Technology Assessment (pTA) – a Way of Developing the Scientific Competence

The ability to create novel biological organisms, manipulate matter at an atomic scale, or intervene significantly (and possibly irreversibly) in the earth climate system raises a host of ethical, social, legal and environmental questions that will require broad public discourse and debate.

As nanotechnology has emerged from the laboratory into industrial manufacture and commercial distribution, the potential for human and environmental exposure, and hence risk, has become both reality and priority. Scientists and researchers engaged in nanoscience and nanotechnology research and development constitute a relatively small group compared to the general public. However, the outcomes of their work – innovative materials, systems, devices and technologies have a strong impact on the life of every citizen and the whole human society.

The research into health, safety and the environmental implications of nanotechnology lacks strategic direction and coordination. As a result, researchers are unsure about how to work safely with new nanomaterials, nano-businesses are uncertain about how to develop safe products, and public confidence in the emerging applications is in danger of being undermined.

Nanotechnology presents both an unprecedented challenge and unparalleled opportunity for risk management. Existing risk management principles are inadequate, given pervasive uncertainties about risks, benefits and future directions of this rapidly evolving set of technologies. The health implications of nanoparticles are unknown, the ramifications may be profound, and only a lengthy and extensive research effort can assess the safety implications with any certainty.

In light of these developments, it is important that the relations between science, technology and society be given proper attention in the education of citizens. Citizenship is about taking an active part in society. It is about ensuring that everyone has the knowledge and skills to *understand*, *engage with* and *challenge* the main pillars of our democratic society – *politics*, *economy* and *law*. Democracies need active, informed and responsible citizens; citizens who are willing and able to take responsibility for themselves and their communities and contribute to the wellbeing and safety processes.

However, citizenship capacities do not develop unaided. They have to be learnt. If citizens are to become genuinely involved in public life and affairs, a more explicit approach to citizenship education and involvement is required to deal responsibly with new technologies.

In the first place, citizen civil rights include the ensuring of peoples' physical integrity and safety (as the condition of being protected against physical, social, financial, political, emotional, occupational, psychological, educational or other types or consequences of threats).

Technology assessment (TA) is a practice intended to enhance societal understanding of the broad implications of science and technology. This creates the possibility for citizens of the world to influence constructively technology developments to ensure better outcomes. Participatory technology assessment (pTA) enables the general public/laypeople, who are otherwise minimally represented in the politics of science and technology, to develop scientific competence and express informed judgments concerning complex topics, as well as, to make informed choices.

Since applications of nanotechnology quickly penetrate all sectors of life and affect our social, economical, ethical and ecological activities, citizens' acceptance is compulsory for further developments in the field of nanotechnology and its applications. Consequently, it is of the utmost importance to educate citizens, and to disseminate the results of nanotechnology development in an accurate and open way so that the general public will eventually transform their way of thinking to accept nanotechnology. In this endeavour, educational institutions have a pivotal role in developing pTA practices by:

- educating citizens (pupils, students) about science and technology;
- informing the public about the benefits and risks of nanomaterials and nanoproducts;
- evaluating, minimising, and eliminating risks associated with the manufacturing and use of nanomaterials and nanotechnology enabled products (risk assessment);
- exchanging with public authorities for the risk management of nanotechnologies.

In the process, pTA deepens the social and ethical analysis of technology, complementing the expert-analytic and stakeholder-advised approaches. The Internet and interactive TV capabilities can help pTA be more effective and cost-efficient and would also align with the policy-makers' initiatives to make them more transparent, accessible and responsive to societal concerns.

## 5. Responsible Nanomanagement as an Imperative Concept of the 21st Century

Nanotechnology is a radically new approach to manufacturing. It will affect so many sectors that failure to respond to the challenges will threaten the future competitiveness of a large part of the economy.

As nanotechnology has emerged from the laboratory into industrial manufacture and commercial distribution, the potential for human and environmental exposure, and hence risk, has become both reality and priority.

The research into health, safety and the environmental implications of nanotechnology lacks the strategic direction and coordination. As a result, researchers are unsure about how to work safely with new nonomaterials, Nanobusinesses are uncertain about how to develop safe products, and public confidence in the emerging applications is in danger of being undermined.

Nanotechnology presents both an unprecedented challenge and unparalleled opportunity for risk management. Existing risk management principles are all inadequate, given pervasive uncertainties about risks, benefits and future directions of this rapidly evolving set of technologies. The health implications of

Nanoparticles are unknown, the ramifications may be profound, and only a lengthy and extensive research effort can assess the safety implications with any certainty.

Yet the public, driven by heuristics such as Affect and Availability, is likely to stigmatize and reject this technology unless effective and credible risk management processes can be put into practice quickly. Because of the fact that traditional command and control regulation will be unable to fill this need, innovative approaches that are incremental, flexible and decentralized should be developed to fill the risk management gap.

Scientific and technological innovation now requires accompanying innovations in management mechanisms that place an emphasis on public engagement. In its turn, public policy has to be grounded on understanding the risks and benefits of new technologies to have practical impact on decision-making.

One of the most pertinent examples of a multi-stakeholder approach to voluntary nanotechnology regulation is the Foresight Institute, which was organized explicitly to provide a forum for public discussion of the risks and benefits of nanotechnology and to 'pave the way' for its societal acceptance. The institute members include scientists, engineers, business people, investors, ethicists, policy makers and lay people as well as firms. Thus, the organization represents a broad spectrum of stakeholders, interests and opinions to be at the forefront of public discussions of nanotechnology risks and benefits [5, 7].

Some engineered nanoparticles, including carbon nanotubes, although offering tremendous opportunities also may pose risks which have to be addressed sensibly in order that the full benefits can be realized. We have all already learned how to handle mobile phones, TVs, computers, electricity, gas, steam and even cars, airplanes in a safe manner because we need their benefits [2].

The same goes for engineered nanoparticles. Mostly they will be perfectly safe, embedded within other materials, such as polymers. There is some possibility that free nanoparticles of a specific length scales may pose health threats if inhaled, particularly at the manufacturing stage. Industry and governments are very conscious of this and are funding research into identifying particles that may pose a hazard to health or the environment, and how these risks may be quantified and minimized over the whole lifecycle of a given nanoparticle.

There is no doubt that nanotechnology has a great potential to bring benefits to the society over a wide range of applications, but it is recognized that care has to be taken to ensure these advances come about in as safe a manner as possible. We need to manage nanotechnologies making our life more intellectual, comfortable and safe.

## 6. Bringing the Spirit of Nanotechnology into the Classroom – Developing Scientific Competence: *Pilot Study*

With the aforementioned in mind, we launched a pilot study at Information Systems Management Institute (Riga, Latvia) in different groups of students comprising Information Technologies, Management, Tourism, and Design departments as well as international students enrolled in ISMA on the ERASMUS student exchange programme.

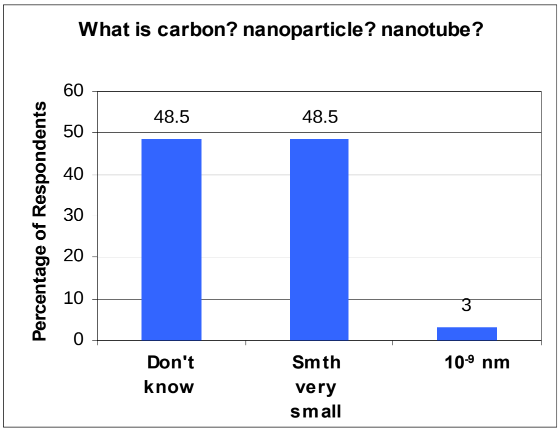
We have undertaken a set of researches into the nature of students' intellectual potential development in order to elicit their general knowledge of some basic scientific notions and their understanding of the utilitarian value of some scientific phenomena. The study envisioned providing the necessary knowledge, understanding and support to our students to be successfully introduced to the technologically empowered environment of today's life, to adjust and adapt in it.

The purpose of the pilot study was primarily to work with the delivery of the questionnaires and interview questions to determine what was required to elicit the quantity and quality of data needed to respond powerfully to the research question. As a result of four pilot undertakings – a fluid conversation with students, an interview, a questionnaire with a feedback analysis – a level of intimacy and trust was created that supported the process of gathering the quantity and quality data.

Our mission has a focus on introducing nanoscience curriculum into classrooms. In order to encourage students and teachers to understand the importance of this scale of science, they need to see that '***size matters***' in the unseen world of nature. This introduction to the 'unseen size of nature' can stimulate curiosity and a desire to learn more about their world through study with advanced microscopes that lead to an interest in chemistry, biology, physics, information technologies and other sciences.

The results of the study make us conclude that students' general knowledge of basic disciplines is rather restricted, sometimes rather obscure or fluid (Fig. 4).

What is more discouraging, the research has established that students do not possess the systemic vision of the sciences and the world. Their knowledge is compartmentalized – they are unable to relate physics to chemistry, to biology, etc. Hence is their low level of awareness of many innovations in science, and especially, in developments in the field of nanotechnology and its applications.



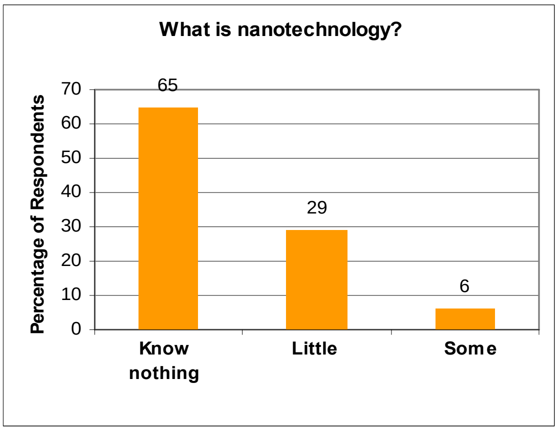




*Figure 4.* Students' general knowledge of basic sciences and nanotechnology in Latvia is low. Respondents were asked, What is carbon? Nanoparticle? Nanotube? Have you heard much about nanotechnology?'

This is mainly due to the inability to imagine the world at the nanoscale level. Hence is the fragile confidence in technological innovation and regulatory systems (Figs. 5, 6).

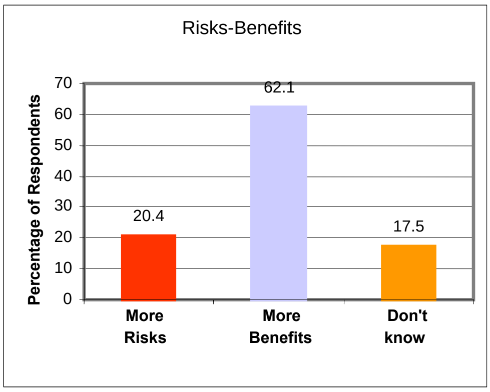



*Figure 5.* Respondents' impressions of the risks versus the benefits of nanotechnology (N = 103)

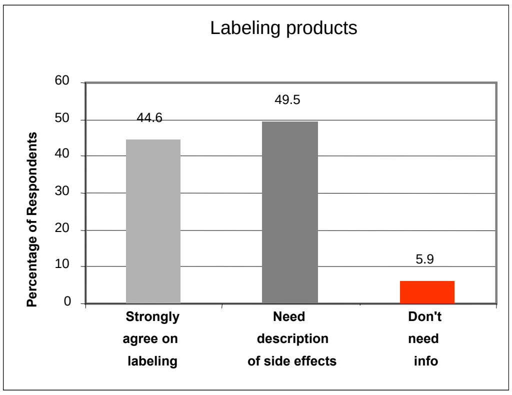



*Figure 6.* Consumers who support labelling the nanoproducts and are concerned about side effects (N = 103)

There might be objective and subjective reasons for the situation observed. Most higher education teachers feel that the knowledge the students gain at secondary school is not sufficient for a higher education institution. In particular, a Latvian scientist – professor of Latvian University Dmitry Babarykin – relates it to the decrease of general level of secondary education. According to Babarykin, since chemistry and biology (disciplines about life) were excluded from obligatory subjects at school in Latvia, people have become too credulous, unable to evaluate independently the expediency of many important things influencing their lives.

In any case, this is an alarming signal, which demands a critical analysis of the adequacy of the educational materials, the methods of teaching and research and other components of any educational practice.

But the most important, our educational programmes are structured in the way that perpetuates the myth that knowledge exists in separate compartments, as if there were no relationships between physics, chemistry, biology; between language and literature, and art, and history, and in so doing, encourages a similar compartmentalization of the mind. At the same time, the main problem area mentioned concerns the link between theoretical knowledge and students' envisioning their utilitarian value.

To fuels students' interest as citizens so that they would be curious about the state of current knowledge and new technologies regardless of their major subject, a project was initiated as an educational supplement featuring the reflections of the general public on nanotechnologies. Our mission had a focus on preparing students to follow the evolution of knowledge and technologies, to be active citizens today and speak knowingly on questions dealing with quality of life on earth and within society.

A group of the first-year students (concurrently with a general nanoeducation course) investigated public concerns about nanotechnology in their project work (Fig. 7).

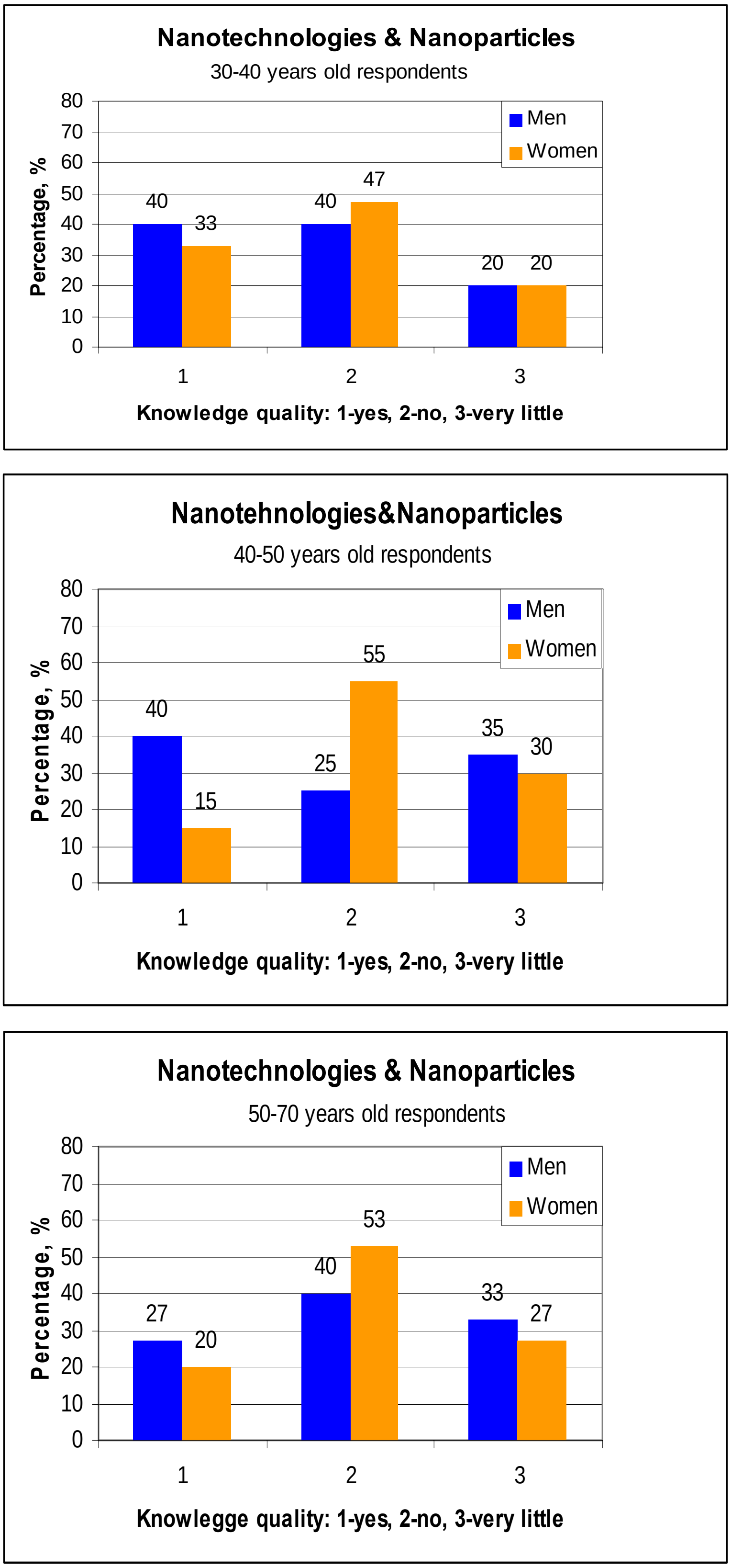



*Figure 7.* Latvian citizen awareness of nanotechnologies in various age groups

Normally, survey-based research on the public understanding of science and technologies is performed by social scientists, who are sometimes – and sometimes not – well-informed about the field of science and technical activities in question, but who are not themselves knowledge producers within the field.

The nanotechnology students' surveys represent a direct link between the producers and the (potential) users of nano-knowledge. Another result of their learning process was the development of a strong commitment to engaging in dialogue with lay citizens. By fostering their hybrid imagination, the students developed a kind of 'scientific citizenship', which simultaneously embraces scientific competence and social responsibility.

## Conclusions

The European context is a stage for developing new relationships, new ideas, new discoveries and new people. It is the stage for European-wide educational and scientific exchange and success for those individuals who can engage their intellectual and emotional potentials in scientific research and development, talents for openness and flexibility in order to exchange innovative thoughts, ideas, approaches and strategies.

This research is not attempting to solve the problem. The intent is to highlight the possibilities available through systemic, integral education to shape up and manage students' intellectual potential development, which offers a powerful philosophical, theoretical and practical approach to educating new generation specialists capable of providing the solutions to many long-standing medical, social and environmental problems. These ideas are all leading to what is termed 'disruptive' solutions, when the old ways of making things are completely overtaken and discarded. New solutions demand new ways of thinking.

The new paradigm of the contemporary technologically advanced society brings to the agenda a new paradigm of higher education. This new paradigm envisages that higher education practitioners become pluriskilled, transdisciplinary mediators promoting constructive solutions to innovative unprecedented problems of the day.

Problems are international and exist beyond our times. To speak out is to show commitment to our environment and to our colleagues, to begin to work towards peace, cooperation, the development of human activities, and for good and healthy life for our generation and the ones to follow.

Learning to move with the times, understanding the fundamental knowledge of our day, learning how to share in the governance of our society, and showing solidarity – these are the components of learning how to live together as humans as well as the broad guidelines in citizenship education.

The basis of any reflection, whether personal or social, rests on an enlightened and critical intellect. Given its ubiquitous nature, nanotechnology is an essential component of the citizenship education. It motivates the young adult to shape his thought process, to favour opportunities that refine his critical judgment and allow him to look upon the society of which he is a full member with a clear and constructive eye. He will then be ready to play his role as a citizen and contribute to the ongoing growth and wellbeing of his community.

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# CUMULATIVE INDEX

## *COMPUTER MODELLING and NEW TECHNOLOGIES, volume 15, No. 1, 2011*

## *(Abstracts)*



The capability of a multitude of parallel electroactive nanostructures in a given substrate to show collective interactions has been examined. Specifically, we consider here electroactive nanostructures as well as (a) electrolyte-filled current spike-emitting latent ion tracks in thin polymer foils and (b) metal cluster-filled etched ion tracks in the TEMPOS structures (i.e. in thin SiO2 layers on Si substrates). Whereas the electroactive nanostructures are usually operated in the first case by application of a sinusoidal voltage at low frequency to trigger the current spike emission, TEMPOS structures are usually operated by applying a constant voltage to them.

An electroactive nanostructure can influence the performance of neighbouring nanostructures by modifying the entrance or exit potentials (or both) of the latter one, via lateral charge exchange through the common front or backside conductors or contacts. For the two cases considered here, this leads to two different effects:

(a) The collective interaction of many current spike-emitting latent tracks in electrolytic ambient leads to pulse-locked synchronization as predicted by Neural Network theory;

(b) In TEMPOS structures with etched tracks in SiO2 on Si, with metal nanocluster coverage of both the oxide layer and the track walls, with at least two contacts on the oxide surface and one on the Si substrate, and with the insulator/semiconductor interface exhibiting two extreme states of resistivity (a high and a low Ohmic one), the collective track interaction can induce negative differential resistances.

This is the consequence of a chain reaction triggered by spontaneous opening of previously closed (or closing of previously open) neighbored tracks. Periodic repetition of such opening/closing processes leads to self-pulsating devices. It is suggested to modify these interacting track systems further, to develop more sophisticated, yet unknown electronic devices. Combined with the known possibilities of physical/chemical/biological sensing and logic decision-making of track-based structures, a challenging new field of unconventional solid and liquid electronic devices based on collective interactions appears to emerge.

**Keywords:** *electroactive nanostructures, ion track electronics, physical/chemical/biological sensing*



This work is devoted to theoretical study of electron transfer (ET) processes between molecular pair of organic π-conjugated luminophores: tyrosine-tryptophan complex. Therefore, the rate of intermolecular ET is evaluated according to Fermi golden rule. Calculations are done using semi-empirical ZINDO approximation method, which is suitable for UV/Visible absorbance spectra calculation.

**Keywords:** *Organic luminophores, electron transfer, electronic states, Fermi golden rule*



The considerable quantity of publications about significant opportunities statistical and free-of-charge R environment makes pay to it the most steadfast attention. In the present work the review of the user opportunities of language and R environment is done. An explanation of the structure of the environment and detailed elaboration of some opportunities will allow the user to get more deeply and more quickly skills of work in environment R. From the other side, the basic applicability of R environment is reduced to realization of classical and modern statistical methods. The problem of construction nonlinear regression dependencies of dependent variable Y on independent variable X remains topical. On an example of this class of problems we show the opportunities of the language means of R environment for their solution. In the work the so-called nuclear construction tools of nonlinear regresses are discussed, their comparison with usual estimations of a method of the least squares is done. For realization of such nuclear estimations modern means of environment R, which are reduced to an opportunity of a choice at a program level the so-called "width of a window" – bandwidths, which allows receiving nuclear regression estimation in the "best" image, are used.

**Keywords:** *R environment, regression analysis, nuclear estimations*

**V. Dreimanis.** Methodology of Risk Determination Based on Multi- Criteria Risk Analysis as a Part of Logistical Leadership, *Computer Modelling and New Technologies*, vol. 15, No 1, 2011, pp. 36–48.

Logistical Leadership defines that the purposeful and well-founded evaluation of conditions might take place before any decision has been made. It is particularly important in case of handling security elements of the state, society or infrastructure. It has to be underlined that the meaning of infrastructure security has changed and has to be understood as much broader spectrum of interdependent branches, starting from the raw material, transportation and energy producing elements and finishing with providing telematic monitoring, banking or state governing element functionality. The cornerstone of decision making in such environment is the exploration of the risks and the consequences as well as the necessity of taking into consideration all possible risks even before any element has been created. Methodology is the way of combining theoretical and practical measures with the aim to create a systematic approach for achieving the set goal or for accomplishing the given tasks. Methodology renders practical recommendations how to answer the following questions: 1) what to do for practical solving the problem? 2) how to perform these practical activities? 3) how to evaluate the process and its credibility? and 4) how to analyze the results?

By specifying the tasks of such methodology and concentrating attention on the problems in safety and security areas, the detailed answers to the above mentioned questions have been given through an overview of a scientific research called "Substantiation of the decision making process on the basis of multi-criteria risk analysis with the aim of solving defence related tasks" (AZPC – 02/01-2009; ISBN 9984-625-23-0). Therefore the presented methodology defines only the sequence of the activities to be performed as well as renders the procedural references for the risks determination in the safety and security areas on the basis of experts' conclusions, although taking into account that the methodology can, under equal conditions, be used by any decision-maker who personally can undertake an expert responsibility.

The methodology could be eventually divided into three main parts:

1. Problem formulation
2. Assembling a group of experts
3. Identification, analysis and evaluation of risks

The concluding part, namely the development of the proposals for the decision making on the basis of the safest alternative, hasn't been considered as a dependent part of the methodology, but is (has to be) the product of its utilization.

**Keywords:** *logistic management, decision making, risk management, methodology of risk determination*

**Y.-R. Kalnins, I. Pakalnite.** Singular Value Decomposition of Images with the Simple Elements, *Computer Modelling and New Technologies*, vol. 15, No 1, 2011, pp. 49–54.

Simple image elements are analyzed by singular value method. Analytical results for a few matrix forms are received. Nonequivalence of image diagonal and parallel elements is shown. Division into sub-blocks method is used in order to eliminate noise in the case of diagonal clustering.

**Keywords:** *singular value decomposition, matrix, eigenvectors*

**T. Lobanova-Shunina, Yu. N. Shunin.** Nanothinking as an Essential Component of Scientific Competence and Social Responsibility in the 21st Century Society, *Computer Modelling and New Technologies*, vol. 15, No 1, 2011, pp. 55–64.

Around the world, the pace, complexity and social significance of technological changes are increasing. Striking developments in such areas as computer and communications technology, biotechnology and nanotechnology are finding applications and producing far-reaching effects in all

spheres of business, government, society and the environment. However, the far-reaching social consequences are often not understood until after new technologies become entrenched. Historically this has resulted in important lost opportunities, significant social and environmental costs and channeling societal development down long-term unhealthy paths. Knowing how to live together healthily, safely, and humanely in society is certainly a worthwhile cause. It is also a real challenge for those who educate young citizens of today. This paper outlines how nanotechnology education can be considered to be a fundamental discipline of the 21$^{st}$ century educational systems for supporting the development of responsible citizenship, since it touches the most significant areas of the well-being of every citizen – health, safety and security, and the environment – which occupy a privileged position in all cultures and all considerations. Citizenship education does not rest on the acquisition of explicitly theoretical knowledge. Rather, it targets the development of civic behaviour in all inhabitants of a given territory (one they identify with) and ultimately throughout the entire world.

**Keywords:** *Nanothinking, nanoeducation, nanomanagement, nanochallenges, nanorisks*

# COMPUTER MODELLING and NEW TECHNOLOGIES, 15.sējums, Nr. 1, 2011 (Anotācijas)

**D. Finkls, A. Kivs, D. Fuks, G. Munozs H., S. A. Kruzs, V. R. Fārners, K. Hops.** Jonu Celiņa Elektronikas Kopējā Mijiedarbiba, *Computer Modelling and New Technologies,* 15.sēj., Nr.1, 2011, 7.–18. lpp.

Darbā tiek izskatītas paralēlu elektroaktīvu nanostruktūru daudzuma iespējas noteiktā substrātā, lai parādītu kopēju mijiedarbību. Īpaši, autori šeit pievēršas elektroaktīvām nanostruktūrām, kā arī (a) elektrolītu piepildītu tekošu smaili-izstarojošu latentu jonu celiņiem plānās polimēra plēvēs un (b) metāla kopu-piepildītiem iegravētiem jonu celiņiem TEMPOS struktūrās (t.i., plāni SiO2 slāņi uz Si pamatnēm). Tā kā elektroaktīvas nanostruktūras parasti darbojas pirmajā gadījumā, piemērojot sinusoidālu spriegumu zemā frekvencē, lai izraisītu tekošo smailes emisiju, TEMPOS struktūras parasti darbojas, uz tām pielietojot konstantu spriegumu.

Elektroaktīvas nanostruktūras var ietekmēt blakusesošo nanostruktūru veiktspēju, mainot pēdējās ieejas vai izejas potenciālus (vai abus), caur vispusīgu lādiņa apmaiņu, izmantojot kopējos priekšējos vai aizmugurējos vadus vai kontaktus. Diviem gadījumiem, kas tiek šeit izskatīti, tas virza uz diviem dažādiem efektiem:

(a) daudzu tekošu smaili-izstarojošu latentu celiņu kolektīvas mijiedarbības elektrolītiskajā vidē noved pie pulsa-bloķētas sinhronizācijas, kā tas tika paredzēts Neironu Tīkla teorijā;

(b) TEMPOS struktūrās ar iegravētiem celiņiem SiO2 saturā, rēķinot uz Si, ar metāla nanoklastera segumu gan oksīda slānim, gan celiņa sienām, ar vismaz diviem kontaktiem uz oksīda virsmas un vienu uz Si pamatnes, un ar izolatoru/pusvadītāju interfeisu, uzrādot divus galējos pretestības stāvokļus (augstu un zemu Omisko), kopējā celiņu mijiedarbība var izraisīt negatīvu starpību pretestību.

Tā ir ķēdes reakcijas konsekvence.

**Atslēgvārdi:** *elektroaktīva nanostruktūra, jonu celiņu elektronika, fizikāla/ķīmiska/bioloģiska zondēšana*

**N. Galikova, M. Kelminskas, A. Gruodis, L. M. Balevičius.** Tirozīna-triptofāna komplekss: starpmolekulārā elektronu pārraide, izmantojot kvantuma ķīmijas pieeju, *Computer Modelling and New Technologies,* 15.sēj., Nr.1, 2011, 19.–23. lpp.

Šis darbs tiek veltīts elektronu pārraides procesu teorētiskai izpētei starp organisku π-konjugētu luminoforu molekulāriem pāriem: tirozīna-triptofāna komplekss. Tādēļ starpmolekulārā ET likme tiek vērtēta pēc Fermī zelta likuma. Aprēķini tiek veikti, izmantojot daļēji empīrisku ZINDO aproksimācijas metodi, kas ir piemērota UV / Redzamās absorbcijas spektra aprēķinam.

**Atslēgvārdi:** *organisks luminofors, elektronu pārraide, elektroniski stāvokļi, Fermī zelta likums*

**A. Krivčenkovs, V. Ļumkis.** Regresiju atkarību uzbūve 'R' vidē, *Computer Modelling and New Technologies,* 15.sēj., Nr.1, 2011, 24.–35. lpp.

Nozīmīgs publikāciju daudzums par svarīgām iespējām statistiskajā un bezmaksas 'R' vidē liek pievērst visstingrāko uzmanību. Dotajā darbā tiek veikts lietotāja valodas un 'R' vides iespēju pārskats. Vides struktūras izskaidrojums un dažu iespēju detalizēta izstrāde atļaus lietotājam iegūt darba padziļinātas prasmes 'R' vidē. No citas puses pamata 'R' vides pielietojums tiek reducēts uz klasisko un mūsdienu statistisko metožu realizāciju. Nelineāras regresijas atkarības no atkarīgā mainīgā Y neatkarīgā mainīgā X uzbūves problēma joprojām ir aktuāla. Par piemēru par šīs grupas problēmām, mēs parādīsim valodas līdzekļu iespējas 'R' vidē to risinājumam. Darbā t.s. nelineāru regresu kodola celtniecības instrumenti tiek apspriesti, to salīdzinājums ar parastiem vērtējumiem par mazāko kvadrātu metodi tiek veikts dotajā darbā.

**Atslēgvārdi:** *'R' vide, regresijas analīze, kodola izvērtēšana*

**V. Dreimanis.** Riska lēmumu metodika, balstīta uz daudzkritēriju riska analīzi kā daļu no loģistikas vadības, *Computer Modelling and New Technologies*, 15.sēj., Nr.1, 2011, 36.–48. lpp.

Loģistiskā līderība nosaka, ka mērķtiecīga un pamatota novērtējuma nosacījumi varētu notikt pirms jebkura lēmuma pieņemšanas. Tas ir īpaši svarīgi valsts, sabiedrības vai infrastruktūras drošības elementu apstrādes gadījumā. Ir jāpasvītro, ka infrastruktūras drošības nozīme ir mainījusies un tā ir jāsaprot kā daudz plašāks spektrs savstarpēji atkarīgām nozarēm, sākot jau ar izejmateriāliem, pārvadājumiem un enerģijas ražošanas elementiem un beidzot ar telemātikas monitoringa nodrošināšanu, banku vai valsts reglamentējošo elementu funkcionalitāti. Lēmumu pieņemšanas stūrakmens šādā vidē ir risku un konsekvenču izpēte, kā arī nepieciešamība ņemt vērā visus iespējamos riskus pat pirms jebkura elementa radīšanas. Metodoloģija ir veids kā apvienot teorētisko un praktiskos līdzekļus, ar meŗķi radīt sistēmisku pieeju, lai sasniegtu nosprausto mērķi, vai arī , lai pabeigtu dotos uzdevumus.

Metodoloģiju var iedalīt trijās galvenajāas daļās:

1. Problēmas formulēšana
2. Ekspertu grupas izveide.
3. Risku identifikācija, analīze un izvērtēšana.

**Atslēgvārdi:** *loģistiskā vadība, lēmumu pieņemšana, riska vadība, riska metodoloģija*

**J.-R. Kalniņš, I. Pakalnīte.** Singulārā tēlu vērtību dekompozīcija ar vienkāršiem elementiem, *Computer Modelling and New Technologies*, 15.sēj., Nr.1, 2011, 49.–54. lpp.

Rakstā tiek analizēti vienkārši tēlu elementi ar singulāro vērtību metodi. Tiek sasniegti analītiskie rezultāti dažām matricu formām. Tēlu diagonālo un paralēlo elementu ne-ekvivalence tiek parādīta. Tiek pielietota sadales metode apakšblokos, lai novērstu troksni diagonālā klasteringa gadījumā.

**Atslēgvārdi:** *singulārā vērtību dekompozīcija, matrica, eigen-vektors*

**T. Lobanova-Šuņina, J. N. Šuņins**. Nanodomāšana kā būtisks zinātniskās kompetences un sociālās atbildības komponents 21.gadsimta sabiedrībā, *Computer Modelling and New Technologies*, 15.sēj., Nr.1, 2011, 55.–64. lpp.

Visā pasaulē temps, kompleksums un tehnoloģisko pārmaiņu sociālā nozīme pieaug. Pārsteidzoša attīstība tādās jomās kā kompjūteru un komunikāciju tehnoloģija, biotehnoloģija un nanotehnoloģija rod pielietojumus un rada tālejošus efektus visās biznesa, valdības, sabiedrības un vides sfērās. Lai gan tālejošās sociālās konsekvences bieži vien nav saprotamas, kamēr jaunās tehnoloģijas nekļūst ieviestas. Vēsturiski tas ir bijis par iemeslu daudzām svarīgām zaudētām iespējām, nozīmīgām sociālām un vides izmaksām un, novirzot sabiedrības attīstībai paredzētos neveselīgos ilgtermiņa virzienus. Zinot, kā dzīvot kopā veselīgi, droši un cilvēcīgi sabiedrībā, tas patiešām ir to vērts. Tas arī ir īsts izaicinājums visiem tiem, kas izglīto jaunatni šodien.

Šis raksts uzsver, ka izglītošana nanotehnoloģijā var tikt uzskatīta kā fundamentāla disciplīna 21. gadsimta izglītības sistēmā.

**Atslēgvārdi:** *nanodomāšana, nanoizglītošana, nanovadība , nanoizaicinājumi, nanoriski*

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