

CRITERIA FOR A LINEAR STRUCTURE OF VARIANCE AND OBTAINING THE PROCESS FUNCTIONS FROM PRINCIPAL COMPONENTS

V. V. Gavrik

Ludwig-Gies-Str. 18, Cologne, 50769 Cologne, Germany; gavrik@metronet.de

ABSTRACT

The description of multivariate data with principal components allows most accurately to approximate a random function with a given number of expansion terms. The question is how to establish that the biorthogonal expansion is really finite in the physical sense and an experimental function is a random linear combination of several non-random functions over the instrumental error. Many situations are expected to result in the linear variance structure or be reducible to it on the base of physical considerations. Statistical criteria have been elaborated to detect the situations since a data variance could not be directly seen to possess the linear structure even in two-dimensional situations. Some analytical properties of principal components are shown to give reliable rotation criteria for calculation the informal process functions. The approach is illustrated with the variance-linearization and rotation transforms for large sets of experimental dependencies describing the leap-like changes in the yield of a chemical process at the atom-by-atom growth of catalyst nanoclusters. Facing the latest results on the neural algorithms of identification and decision-making, the approach appears to promise efficiently to decode the large arrays of data on the electrical activities of brain.

1. LINEAR STRUCTURE OF VARIANCE

The huge amounts of measured data on complex systems require efficient methods to reduce their dimensionality and efficiently to analyze them. The multivariate statistical analysis by the method of principal components is one of the most powerful means concisely to describe large families of similar experimental dependencies obtained at various test conditions [1, 2]. The experimental vectors, Y , can be considered as realizations of a random function, $y(t)$. They form overestimated rectangular matrices (r, n) if the number of tests, r , overcomes the number of ordinates, n . The variance of experimental vectors is commonly considered as consisting of 'physical' variance, which describes the processes under study, and an instrumental error, which can base a criterion to restrict the analysis with the information on the variability of process functions only.

The description by principal components is optimal in the sense of minimizing the mean-square deviation [3 - 5]. It bases on the biorthogonal Karhunen-Loève expansion that most accurately approximates a random function with a given number of expansion terms [6, 7]. Several terms of the generally infinite expansion that take into account a main portion of experimental variance, are frequently considered [4] as informal linear constituents and their properties are ascribed to some physical (chemical, physiological, etc.) processes assumed.

The infinite expansion can degenerate to a finite one if the experimental dependencies are actually the random linear combinations of several non-random functions, which do not depend on variables other than t in the realizations considered:

$$y(t) = \sum_{k=1}^l a_k \mathbf{j}_k(t), \quad (1)$$

$\mathbf{j}_k(t)$ are dissimilar non-random functions that describe l contributing physical processes and a_k are their random weights under given experimental conditions.

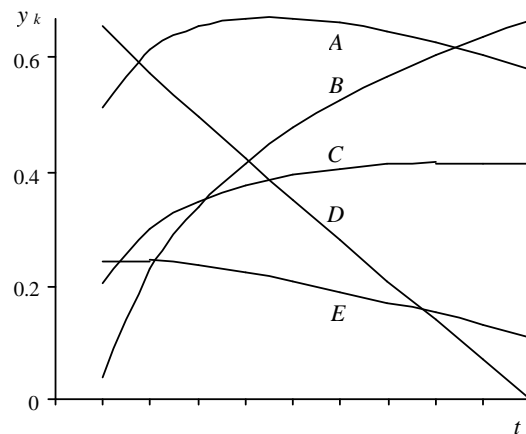


Figure 1. Linear combinations of basic curves 1 and 2 of Fig. 2. Weighting factors: 2, 1.6 (A); 2.5, 0 (B); 1.5, 0.6 (C); -0.25, 2.2 (D); and 0.3, 0.8 (E), respectively.

Owing to their mainly additive contributions and their linear growth with the process intensity, many of physical variables can be expected to result in such a linear structure of variance or be easily transformed to it (say, with taking a logarithm of a product of multiplicative variables). It would be advantageous to reduce a measured set of dependencies to situation (1) that offers obvious opportunities for a better understanding of the contributing physical processes [8, 9]. Unfortunately, one cannot directly see that the experimental dependencies possess such a linear structure of variance. When looking at curves A to E of Fig. 1, you can hardly suggest them to be the linear combinations of simple logarithmic (1) and linear (2) 'process' functions from Fig. 2. Therefore, a proper statistical criterion would be useful for independently to examine the linearity hypothesis.

A mathematical procedure has been developed to test (a) if the experimental dependencies really have the structure of Eq.(1) and (b) if they possess some analytical properties, which allow independently to calculate the process functions, $\mathbf{j}_k(t)$, from the principal components with using no arbitrary assumptions.

2. THE LINEARITY CRITERION

One of the most intriguing questions of the method is whether one could independently derive the process functions if basing on only analytical properties of principal components obtained.

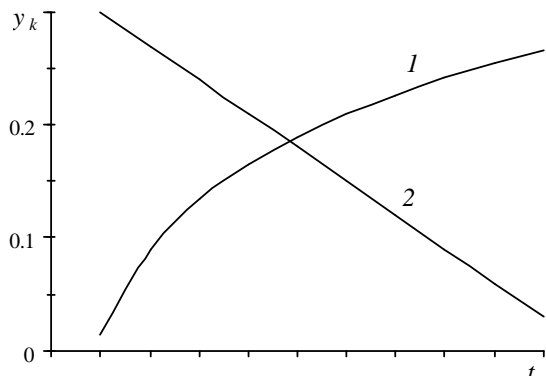


Figure 2. 'Process functions' whose linear combinations constitute the dependencies of Fig. 1.

The usual search for principal components (the first eigenvectors of covariation matrix) to describe the experimental dependencies within the accuracy of measurement is a numerical procedure to obtain the first terms of the Kahrnen-Loève expansion [6, 7] of random function $y(t)$, whose realizations $y^*(t)$ on the range $[T_1, T_2]$ are the experimental vectors, Y , obtained at different test conditions. For simplicity, assume them to have a zero mathematical expectation, $M[y(t)] = y_m(t) = 0$. If $y(t)$ is continuous on $[T_1, T_2]$ in the quadratic mean,

$$\lim_{t_1 \rightarrow t_2} M[|y(t_2) - y(t_1)|^2] = 0, \quad (2)$$

there is a convergent biorthogonal expansion,

$$y(t) = \sum_{j=1}^{\infty} b_j \mathbf{y}_j(t), \quad \lim_{n \rightarrow \infty} M[y(t) - \sum_{j=1}^n b_j \mathbf{y}_j(t)] = 0 \quad (3)$$

where $\mathbf{y}_j(t)$ are orthonormal:

$$\int_{T_2}^{T_1} \mathbf{y}_q(t) \mathbf{y}_s(t) dt = 0 \text{ at } q \neq s \text{ and } 1 \text{ at } q = s, \quad (4)$$

and the expansion factors,

$$b_j = \int_{T_2}^{T_1} y(t) \mathbf{y}_j(t) dt, \quad (5)$$

are non-correlated:

$$M[b_q b_s] = 0, \quad q \neq s. \quad (6)$$

It is necessary and sufficient that $\mathbf{y}_j(t)$ were eigenfunctions of the covariation function, $B[t, t_1]$, used as the kernel of the Fredholm homogeneous integral equation of the second kind [9, 10], and their spreads, $M[b_j^2]$, were its eigenvalues, λ_j :

$$\int_{T_2}^{T_1} B(t, t_1) \mathbf{y}_j(t_1) dt_1 = \lambda_j \mathbf{y}_j(t). \quad (7)$$

A given number of the expansion terms approximates the random function, $y(t)$, with the highest accuracy among other expansions, and a given accuracy would be attained with using the least number of expansion terms [4, 7, 11, 12].

For numerically to solve Eq. (7), its matrix representation is used [3, 13, 14]. For a sample of r vectors Y , each is a set of n ordinates of a test curve, consider biorthogonal vectors X_j , which approximate them most accurately at any $p = 1, 2, \dots, n$:

$$y_i = y_{im} + \sum_{j=1}^p b_j x_{ij}, \quad (8)$$

y_i , x_{ij} , and y_{im} are i -th coordinates of Y , X_j , and the mean vector, Y_m , respectively, at i -th abscissa; b_j is the weighting factor of j -th basis vector. The maximum likelihood estimates of X_j [4] will be the eigenvectors of the symmetric covariation matrix:

$$K(n, n) = U'U/(r-1), \quad (9)$$

$U(r, n)$ and $U'(n, r)$ are the centered matrix of experimental data and its transposition, respectively. The lines of U and columns of U' are $Y - Y_m$, the differences between an experimental curve and the mean curve. The transition from U to K is a variant of least-squares method permitting to avoid the error-caused incompatibilities in the simultaneous equations, overestimate their system by involving $r \gg n$ equations, and increase the sample representativity and accuracy of solution [15]. The equation,

$$(K - I_j E) X_j = 0, \quad (10)$$

E is the matrix unit, has n real roots only. The eigenvectors are orthogonal, $(X_q X_s) = 0$ at $q \neq s$, and usually normalized to unity, $(X_q X_q) = 1$. Their weights for i -th experimental curve are:

$$b_j = \sum_{i=1}^n (y_{is} - y_m) x_{ij}. \quad (11)$$

The eigenvalues λ_j obtained are positive and their sum, the spur of the matrix K , is equal to the whole variance of initial data:

$$Sp = \sum_{i=1}^n \lambda_j = \sum_{i=1}^n k_{ii} = \sum_{i=1}^n \sum_{s=1}^m (y_{is} - y_m)^2, \quad (12)$$

k_{ii} is the element of the principal diagonal of K . An eigenvalue is equal to the spread accounted for a respective eigenvector:

$$K = I_1 X_1' X_1 + I_2 X_2' X_2 + \dots + I_n X_n' X_n \quad (13)$$

where X_j' is transposition of X_j . It is common to number the eigenvectors in the order of decreasing eigenvalues λ_j .

If the experimental dependencies (1) had included no instrumental error, the kernel of Eq. (7) would have degenerated [11]. If the contributions of l 'process functions' are non-correlated even if in part, the number of the expansion terms is l . Since

$$B(t, t_1) = M[y(t)y(t_1)] = \sum_{k=1}^l \sum_{r=1}^l \mathbf{j}_k(t) \mathbf{j}_r(t_1) M[a_k a_r], \quad (14)$$

the left part of Eq. (7) is as follows:

$$\int_{T_2}^{T_1} \sum_{k=1}^l \sum_{r=1}^l M[a_k a_r] \mathbf{j}_k(t) \mathbf{j}_r(t_1) \mathbf{y}(t_1) dt_1 = \sum_{k=1}^l \sum_{r=1}^l M[a_k a_r] c'_{jk} \mathbf{j}_k(t)$$

where $c'_{jk} = \int_{T_2}^{T_1} \mathbf{j}_r(t_1) \mathbf{y}(t_1) dt_1$, and the eigenfunctions,

$$\mathbf{y}_j(t) = \sum_{k=1}^l h_k \mathbf{j}_k(t), \quad (15)$$

are connected by a linear transform with the equivalent basis of the constituent process functions:

$$\mathbf{j}_k(t) = \sum_{j=1}^l \mathbf{a}_{jk} \mathbf{y}_j(t). \quad (16)$$

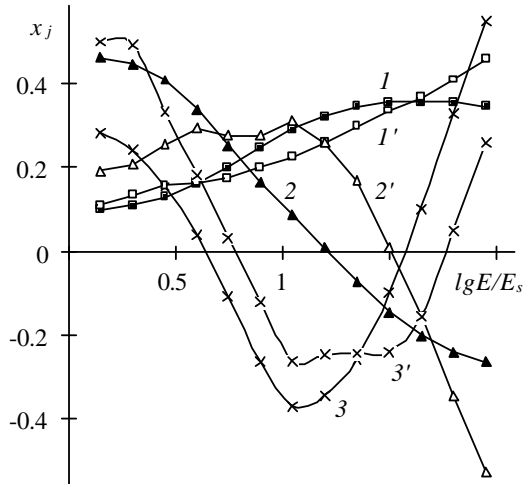


Figure 3 Principal components of $D(\log E/E_s)$ curves: various materials and development conditions (1, 2, 3); technological variability of a material (1', 2', 3').

The first l eigenvectors, capable of describing the experimental curves within their instrumental error, are called the *principal components*. If the experimental variance has a more complex structure than Eq. (1), the number of eigenfunctions will be theoretically infinite. Since an n -dimensional experimental vector is formally a random linear combination of n delta-functions [12], the maximum number of eigenvectors is restricted by n . Due to the optimal expansion properties, the description error,

$$\mathbf{s}_e = \sqrt{(1 - \sum_{j=1}^l \mathbf{I}_j / Sp) / (n - p)(r - 1)}, \quad (17)$$

tends to the instrumental error and the further $(n - p)$ eigenfunctions is commonly neglected.

In the physical case of Eq. (1), the extra $(n - l)$ eigenvectors are induced by the instrumental error. With no error, p is equal to l or may be in principle less than l . If the weights, a_k , of two process functions are proportional to each other in a sample, they cannot be distinguished and a principal component disappears. If two of the process functions, $\mathbf{j}_k(t)$, are similar, they also cannot be distinguished. For the process functions normalized to unity, the condition not to degenerate is:

$$\int_{T_2}^{T_1} \mathbf{j}_q(t) \mathbf{j}_s(t) dt < 1, \quad q \neq s. \quad (18)$$

The l principal components, X_j , of a sample of experimental curves can be transformed into the principal components, Z_u , of another sample with an orthogonal matrix, $G(l, l)$. Its elements,

$$g_{ju} = (X_j, Z_u) = \sum_{i=1}^n x_{ij} z_{iu}, \quad (19)$$

are correlation factors between respective elements of principal components and characterize redistribution of process weights, $M[a_k a_s]$. The instrumental error, \mathbf{s}_e , declines $G(l, l)$ from the orthogonal properties and the sums of g_{ju}^2 in any column or line of matrix G be less than unity by $\Delta_j \geq 0$. The description error of an element of X_j with vectors Z_u is as follows:

$$\mathbf{s}'_j = \sqrt{\frac{\Delta_j}{n-l}} = \frac{1}{\sqrt{n-l}} \sqrt{1 - \sum_{u=1}^l g_{ju}^2}. \quad (20)$$

What Δ_j should result from the instrumental error, \mathbf{s}_e ? Let the spread of an element of X_j be of the same order as the spread of the mean, Y_m , in a sample of r curves, $\mathbf{s}_j \approx \mathbf{s}_e / (r \mathbf{I}_j)^{1/2}$. Then the error of g_{ju} would be about:

$$\mathbf{s}_g^2 \approx \sum_{i=1}^n (z_{iu}^2 \mathbf{s}_j^2 + x_{ij}^2 \mathbf{s}_u^2) = \mathbf{s}_j^2 + \mathbf{s}_u^2 \approx \mathbf{s}_e^2 (\mathbf{I}_j^{-1} + \mathbf{I}_u^{-1}) / r \quad (21)$$

and the spread of the sums of g_{ju}^2 in any line or column of G :

$$\Delta_j \approx D[\sum_{u=1}^l g_{ju}^2] \approx 4 \sum_{u=1}^l g_{ju}^2 \mathbf{s}_g^2 = 4 \mathbf{s}_e^2 [p / \mathbf{I}_j + \sum_{u=1}^l g_{ju}^2 / \mathbf{I}_u] / m. \quad (22)$$

The relation was confirmed with using two artificial sets of functions (1) at $l = 3$ and the 'instrumental error' generated as normally distributed random numbers. The Δ_j values of transformation matrix practically coincided with those from Eq. (22).

3. THE ROTATION CRITERIA

If the experimental dependencies under study obey Eq.(1), some mathematical properties of the process functions, $\mathbf{j}_k(t)$, can be detected from its principal components. If within the range of t from T_1^* to T_2^* , every \mathbf{j}_k is a linear combination of a non-constant function, $\mathbf{j}^*(t)$, with a constant, c_k :

$$\mathbf{j}_k(t) = \mathbf{g} \mathbf{j}^*(t) + \mathbf{d} c_k, \quad (23)$$

\mathbf{g} and \mathbf{d} are their weights, there is a linear dependence between respective elements of any two principal components there:

$$\mathbf{y}_j(t) = \mathbf{a}_{ju} \mathbf{y}_u + \mathbf{b}_{ju}, \quad (24)$$

\mathbf{a}_{ju} is a factor, \mathbf{b}_{ju} is a constant. That can be proved with substitution of relations (23) into Eq. (15). Linear dependencies (24) between respective elements of principal components indicate that all the process functions are linear combinations of a constant with $\mathbf{j}^*(t)$. That can be shown with substituting Eqs. (24) into Eq. (16). In the simplest and most probable case, a process function is $\mathbf{j}^*(t)$ and the other $(l - 1)$ process functions are constants, $\mathbf{j}_k(t) = c_k$, within the t range from T_1^* to T_2^* .

Thus, if a dependence between the respective values of any two principal components is linear from T_1^* to T_2^* , all of $\mathbf{j}_k(t)$ but one are constants or all of them are linear combinations of a constant with common $\mathbf{j}^*(t)$. Also if:

- the respective values of any two principal components are proportional to each other, all of $\mathbf{j}_k(t)$ differ by only a factor or all of them but one, $\mathbf{j}^*(t)$, turn into zero there;
- every principal component takes constant values, all of the process functions are constants, $\mathbf{j}_k(t) = c_k$, there.

In the first case, the straight portion or its prolongation goes through the origin of coordinates, and in the second case, the entire $[T_1^*, T_2^*]$ gathers together practically into a point. It can be expected to find extra indicative correspondences between the analytical properties of principal component and respective process functions. If the properties are expressed in at least l points, Eq. (16) gives l simultaneous linear equations with l unknown factors, \mathbf{a}_{jk} , and the entire process functions, $\mathbf{j}_k(t)$, can be calculated as linear rotations of principal components. An equation follows from the normalization condition of process functions

that are determined up to a factor like the principal components themselves. After \mathbf{a}_{jk} are obtained, the rest of a process function can be calculated with using Eq. (16).

If a process function has a constant weight in all the sample dependencies, it will be lost with the mean, y_{im} , subtracted. If the analytical properties of process functions not the data statistics as such are of interest, it can sometimes be advantageous to use the symmetric matrix B of initial moments instead of K for no principal component to be lost.

4. A PRACTICAL EXAMPLE

4.1 A Process and Its Linear Variance

Consider, for example, the dependencies of optical density, D , of photographic image on the logarithm of light exposure, E :

$$D = D_{max} f(\log E/E_s) = D_{max} f(\log E - \log E_s). \quad (25)$$

The optical densities are additive physical characteristics as the logarithms of multiplicative transmission factors. The varying light sensitivity, $1/E_s$, as a non-linear contribution to the experimental variance can be excluded from consideration by a shift of experimental curves along the $\log E$ axis [1, 8, 9, 16, 17]. The dependencies were also known to contain a linear component bound with the 'fog', D_o , that developed without light exposure and added a 'reversal' curve to exposed fields:

$$D = D_{max} f(\log E/E_s) + D_o [1 - p f_o(\log E/E_s)], \quad p \ll 1. \quad (26)$$

The residual variance of the shifted $D(\log E/E_s)$ dependencies was usually by one to two orders of magnitude larger than the instrumental error and its structure remained unclear.

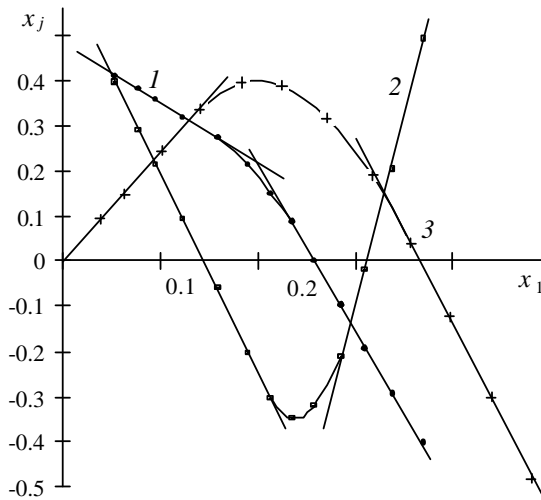


Figure 4. Dependencies of elements of second (1) and third principal components (2) on the elements of the first one at $D \log E = 1.8$. Curve 3 is obtained at $D_o = 0$.

The number of principal components was $p = 7$ for the dependencies of various silver bromide materials considered with no shift along the $\log E$ axis. It decreased to 4 after the curves were shifted so that their E_s formally coincided [16, 17]. So the three extra principal components were produced by the formal expansion of the non-linear component of variance caused by different

light sensitivities. After the log-exposure range was decreased from 2.4 to 1.8, the number of principal components became 3. It remained the same also for a single photographic material considered within a typical technological instability of its development conditions (the primed numbers on Fig. 3) [8].

Subtraction of D_o (or using the curves with $D_o = 0$) or numerical differentiation of $D(\log E/E_s)$ with respect to $\log E$ eliminated a principal component. That confirmed a constant D_o additively to enter Eq.(26) and the non-constant fog contribution, $f_o(\log E/E_s)$, to consist of the same constituents as the light dependence itself since not to increase the dimensionality of the variance [8].

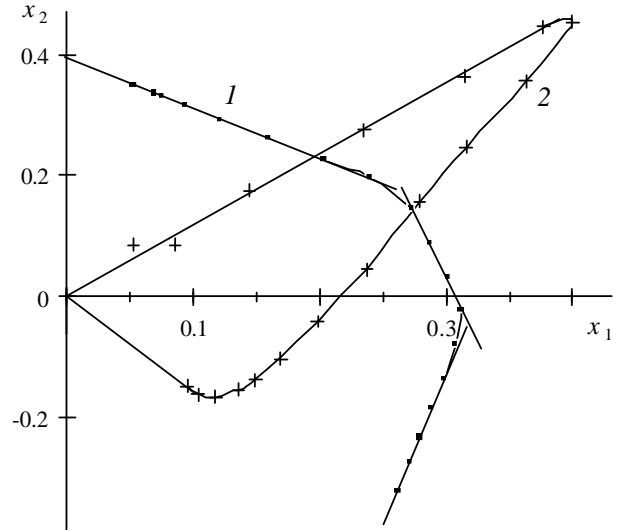


Figure 5. Dependencies of elements of second principal component on the elements of first principal component, $D \log E = 2.4$: 1 - $D(\log E/E_s)$, 2 - derivatives $D'(\log E/E_s)$ with respect to $\log E$.

To test the linearity of the residual variance, we considered two sets of $D(\log E/E_s)$ curves that strongly differed in the weights of constituent process functions. A set of 68 curves represented various photographic materials at various development conditions and another set of 22 curves represented only the technological variability of a single photographic material whose curves were absent in the first set [8]. The principal components (Fig. 3) of the samples strongly differed but their transformation matrix declined from the orthogonal properties within the experimental error. The sums of its elements squared in a line or column differed from unity by 0.001, 0.01, and 0.015 for the first, second, and third principal components, respectively. The differences did not overcome their values estimated with using Eq. (22): 0.001 for the first and about 0.025 for the second and third principal components. That proved the $D(\log E/E_s)$ dependencies to possess the linear structure of experimental variance described by Eq.(1). They were further examined to meet the intrinsic analytical criteria, which would enable the calculations of underlying process functions.

4.2 The Rotation of Principal Components

The dependencies of respective elements of any pair of principal components had two characteristic linear portions [8, 9] within the log-exposure range of 1.8 (Fig. 4). When the mutual dependencies of principal components indicated an initial constant value range (curves 1 and 2), a zero range was indicated after D_0 was absent or subtracted (curve 3). This meant initial zero ranges for all the process functions there except for the non-zero constant of fog. Within the log-exposure range of 2.4, three linear regions were regularly observed (curve 1, Fig. 5). Those in the initial part and likely the end part of the experimental curves were obviously directed to the origin of coordinates if the derivatives of experimental curves were considered (curve 2).

The dependencies showed that the initial portion of a D -log E curve was formed by the fog constant, D_0 , while all the other process functions but one (function II) reduced to zero. In a middle part of $D(\log E/E_s)$ curves, all the process functions but one (function III) were constants and function IV took zero values. Within the end portion, all the process functions but function IV were non-zero constants. Since the straight portions were expressed in $s > l$ points, we obtained $s > l$ simultaneous equations and solved them with respect to the l unknown factors, a_{jk} .

4.3 The Constituent Processes

The weighting factors, a_{jk} , substituted into Eq.(16), allowed us to calculate the additive constituents II, III, and IV of the experimental variance of $D(\log E/E_s)$ curves (Fig. 6). One more process curve was the constant bound with the fog.

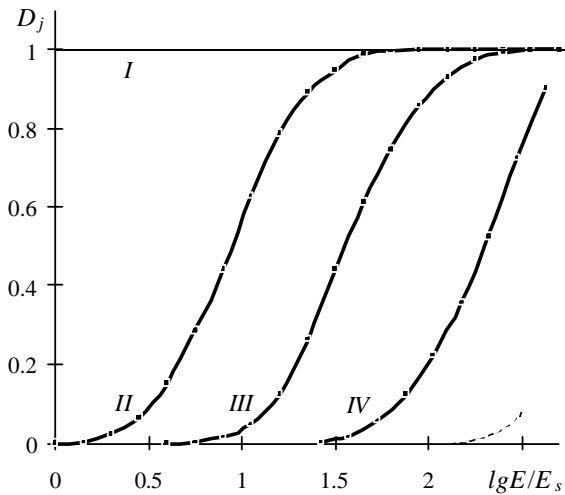


Figure 6. The process functions describing the leap-like increases in the development rate with the atom-by-atom growth of latent image centers with light exposure.

The S -shaped process functions, being apart from one another at almost identical distances along the $\log E$ axis, were confirmed further in direct experiments (Fig. 7) [18]. They could be most obviously seen on the graphs of the first derivative D' of experimental dependencies with respect to $\log E$ where each of the S -shaped dependencies turned into a bell-shaped curve. Further studies detected up to seven regular components within the log-

exposure range of about 5.5 [19]. At fast penetration of developer solution into a gelatin layer, the efficient number of the S -shaped process functions grew with decreasing rate of silver reduction in a silver bromide microcrystal [18].

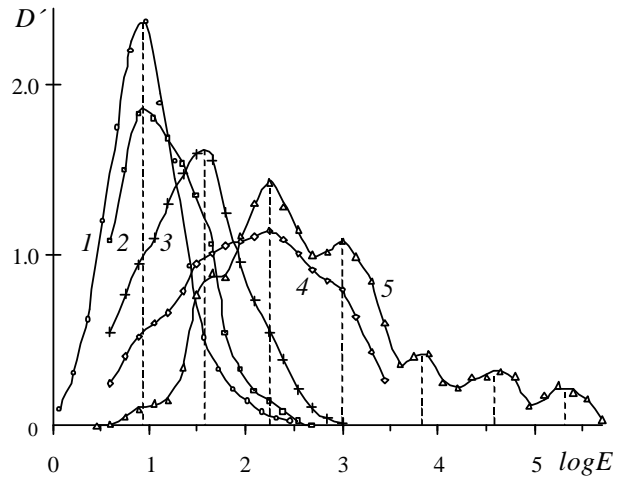


Figure 7. Derivatives of D -log E dependencies of a photographic film with respect to $\log E$. The rate of silver reduction in a silver bromide microcrystal decreases with increasing curve number.

Mathematical simulation of photolytic growth of silver nanoclusters has shown the same almost identical log-exposure increments to produce subsequent single-atomic increases in the size of the largest silver nanoclusters at a silver halide microcrystal [9, 19, 20]. The regular S -shaped constituents turned out to be regular leaps in the developed silver mass with the atom-by-atom growth of the catalytic nanoparticles of photographic latent image (the smallest active particle was known to contain four atoms) with increasing light exposure. The silver particles turned out to occur in two more catalytic states that differed in the spaces along the $\log E$ axis [9, 20 - 23]: (a) at another silver salt that, unlike silver bromide, had no crystal lattice correspondences to them, and (b) after deprived of contact to any initial light-sensitive salt before development. In the first case, the $\Delta \log E$ spaces were half as large, and in the second case twice as large as above. Another example was the optical and chemical components of the modulation transfer function of the recording media [17, 24].

5. VARIANCE LINEARITY OCCURRENCE

The variance linearity is not rare. The weights of physical processes are dominated by energetics or concentration contributions that are mostly linear and additive even if the single-process functions themselves could be very complex. A threshold variability component of light sensitivity, a psychophysical perceptibility, etc. in a physical or biological system can be removed with a shift transform as it was shown above. A data variability, based on probabilistic interactions (as in the cases of multi-particle absorption of radiation, multi-stage signal transmission, etc.),

frequently results in a multiplicative structure variance, which is reduced to the additivity with a logarithmic transform.

The latter case is also relevant to the neural algorithms of identifying subject or situation features and binding them to make a decision how to react. The latest results have demonstrated a multiplicative moiety of the neural 'tolerance functions', which can be derived from a simple feed-back process that compares a variable input with a memorized feature statistics [9, 25 - 27]. The multiplicative structure of variance and the characteristic constancies of the single-feature tolerance functions [28 - 30] appear to be the necessary prerequisites for an efficient decoding of the large sets of the EEG, ERG, MfRI, etc. recordings.

6. SUMMARY

A statistical procedure is proposed to test if the principal components calculated are not simply the first formal terms of an infinite expansion to describe experimental dependencies close to the measurement accuracy but really indicate a number of physical processes contributing to the data variance observed.

Analytical criteria are proposed and tested that allow independently to calculate the functions separately describing the contributing physical processes, basing on intrinsic analytical properties of the principal components of large sets of experimental dependencies with the linear structure of variance above.

The examination and linearization of variance structure have been demonstrated for a complex photochemical system. Its process functions calculated were confirmed and physically identified in further decisive experiments. Substantial opportunities were noted efficiently to apply the procedures above to the analysis of electrical brain activities in the course of feature identification, binding, and decision-making processes.

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