

# Regularization Methods for the Stable Identification of Probabilistic Characteristics of Stochastic Structures



Vladimir Kulikov and Alexander Kulikov

**Abstract** This chapter covers the method of experimental data analysis and processing in cyber-physical systems for medical monitoring, control of manufacturing processes and management of industrial facilities. The suggested methods are used to develop mathematical models of dynamic systems with stochastic properties for managing complex structural subsystems of cyber-physical systems. The most important computational stage of the simulation is thereat the identification of multimodal (in general) densities of the random variable distribution. A matrix conditioning analysis is herein suggested with minimizing relevant functionals of the identification problem. For the method of identifying multimodal densities of random variable distribution a matrix condition analysis is suggested with minimizing the relevant functionals of the problem. It is shown that under ill-conditioning of the equivalent system of equations an algorithm for regularization of solutions is needed. The regularization of the basic method for identifying distribution densities based on the ridge regression-algorithm (RRA) is proposed and substantiated. The classical RRA is improved and modified for local regularization showing the advantage of the high-order unstable SLAEs over the classical Tikhonov method. The suggested regularization algorithms and programs are universal, applicable to the study of random structures in natural science, biomedicine, and computational mathematics.

**Keywords** Cyber-physical systems (CPS) · Parameter monitoring · Identification · Multimodal densities · Ill-conditioning of matrices · Ridge regression-algorithm · Minimization of functionals

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V. Kulikov (✉) · A. Kulikov  
Nizhny Novgorod State Technical University n. a. R. E. Alekseev, 24 Minin St., 603950 Nizhny  
Novgorod, Russia  
e-mail: [vb.kulikov@yandex.ru](mailto:vb.kulikov@yandex.ru)

A. Kulikov  
e-mail: [akulikov@nntu.ru](mailto:akulikov@nntu.ru)

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## 1 Statement of the Problem

This chapter is concerned with the study of a universal method for identifying distribution densities of stochastic characteristics and its modification under regularization conditions. Regularization algorithms and methods are universal and applicable to the study of complex structures with random properties (technology, medicine, biology).

Cyber-physical systems (CPS) are in this regard of particular interest including subsystems described by stochastic characteristics. Nonlinear dynamic properties of similar structures, their evolution in terms of random processes and stochastic variables manifest themselves as complex (non-Gaussian, multimodal) distributions to be subject to correct identification [1, 2]. Experimental information for this procedure is usually provided by various sensors including those of the so-called “intellectual nature”.

Such information on the law of characteristics distribution may further be used to simulate a mathematical stochastic model for a local control object of a CPS subsystem. The CPS global characteristics may also be identified during the control process by the proposed method just in near real-time for solving any system-wide problems. The considered approach at the level of algorithms and programs has a modular, universal character. It is easily integrated into existing cyber-physical systems. For example, it may be used to create an experimental-mathematical model of the human gastrointestinal tract functioning when analyzing EGEG signals [1], to develop systems for monitoring of critically important parameters of glass melting furnaces or vibration stability of aircraft engines during their testing and operation.

The considered methods for identification of distributions are being continuously evolved, improved. In particular, it is suggested to complete the method for identifying multimodal densities of random variable distribution [1–3] with a matrix conditioning analysis while minimizing basic functionals with algorithmic integration of a solution regularization module there into (in case of ill-conditioning of a problem).

As shown by computational experiments, some peculiarities in the singular spectrum of matrices of equations equivalent to minimized functionals may cause inadmissible distortions of solutions.

Any probable ill-conditioning of matrices may result in unstable and erroneous decisions making the procedure of restituting the random values distribution law to be incorrect. Such peculiarities include the cases when a rapid decrease in singular values to the level of  $10^{-12}$  and below is noted in the singular matrix spectrum. Furthermore, such instability may be caused by the assignment of an unreasonably large number of steps in minimizing the functional.

When regularizing problems of identifying the random values distribution laws, it is suggested to apply the classical RR-algorithm (epsilon-structuring).

The RR-algorithm is a version of the Tikhonov regularization method. In general, this is an algorithm for solving one-dimensional inverse problems based on the regularization method for Fredholm integral equations of the 1st kind.

The Tikhonov regularization method [4] consists in the reduction of an integral equation to a system of linear algebraic equations the solution thereof is sought under restriction to the solution norm value. The selection of the restriction value depending on the perturbation value is a major problem in the regularization method [5–12]. The desired solution for an integral equation is represented as a piecewise constant function, i.e. vector  $\varphi$ , which coordinates are values of function  $\varphi(t)$  at  $n$  points on the segment  $[a, b]$ .

Using the numerical integration formula the integral equation is replaced by the system of equations  $R\varphi \approx y$ , where  $R$  is a relevant matrix of size  $l \times n$ ,  $y$  is a vector composed of  $l$  independent measurements of the observed function. Many publications are devoted to solving unstable systems of algebraic equations with approximately specified right-hand sides; in particular, there should be noted [13–15].

Since the RR-algorithm (ridge regression-algorithm) is methodologically most developed as a stochastic regularization method (within the framework of a multidimensional linear regression problem), the choice of this regularization method as a more common one (as compared to the classical Tikhonov regularization algorithm) is regarded to be reasonable and correct [16].

In future chapters, there will also be studied some original and modified methods for the regularization of singular decompositions in solving ill-conditioned systems of linear equations taking into account the above features. These approaches are implemented in the form of algorithms and software (MATLAB) for the method of identifying multimodal densities of random variables distribution.

## 2 Method of Solving the Problem

So, when minimizing the functional, it is necessary to solve the system of equations under constraint conditions [17]  $\|\varphi\|^2 = \sum_{i=1}^n \varphi_i^2 \leq r^2$ , that is equivalent to minimizing the smoothing functional

$$M^\alpha(\varphi) = \|y - R\varphi\|^2 + \alpha \|\varphi\|^2,$$

where  $\alpha$  is the constraint-compliant regularization parameter (Lagrange multiplier). In terms of matrix operators, a regularized normal system is solved

$$(R^T R + \alpha E)\varphi = R^T y \tag{1}$$

The RR-algorithm consists of the following steps:

1.  $\varepsilon$ —net is introduced in the system solution space, which consists of the following vectors

$$V = \sum_{j=1}^n \frac{\varepsilon \mu_j}{\lambda_j} \psi_j$$

where  $\lambda_j$  and  $\psi_j$  are matrix eigenvalues and eigenvectors  $R^T R$ ,  $\mu_j$  are random integral values,  $\varepsilon$  is a scalar parameter assigning a step to  $\varepsilon$ -net.

2. With a fixed value of the parameter  $\alpha$ , the normal system (1) is solved,  $\varepsilon$ -net node is sought closest to the solution found for  $\varphi_\alpha$ .
3. Further, the quality of the  $\varphi_\alpha$  solution is assessed with fixed  $\alpha$ , which is composed of the following two constituents: the estimate of the mean risk functional value achieved on the vector  $V_\alpha$  (the closest node of  $\varepsilon$ -net) plus the estimate of a change in the value of the same function in the transition from  $\varphi_\alpha$  to  $V_\alpha$ . The final estimate [17] takes the form

$$J(\alpha) = \left[ \frac{\frac{1}{l} \|y - R V_\alpha\|^2}{1 - \sqrt{[k(\ln \frac{l}{k} + 1) - \ln \eta]/l}} \right]_\infty + \frac{1}{l} \|R(V_\alpha - \varphi_\alpha)\|^2,$$

where  $1 - \eta$  is the likelihood of this estimate validity,  $k$  is the number of linearly independent nodes of  $\varepsilon$ -net satisfying the condition  $\|V\| \leq \|\varphi_\alpha\|$ .

The regularization parameter value  $\alpha$  and the constraint valuer is determined by the minimization of the estimate of  $J(\alpha)$  for  $\alpha$  and  $\varepsilon$ , thereunder the resulting solution  $\varphi_\alpha$  is optimal for a specified experimental data volume.

It is important to note that the RR-algorithm plots for regression problems ridge estimates which are shifted but best with respect to the standard mean square deviation (with some constraints by the value of an input data error) than the least-squares method in the classical formulation [17]. These estimates are more stable than least-squares estimates since the reduction in error variance caused thereby is more than it is required for the compensation of offset entered.

The author's modification of this algorithm is suggested in this chapter using the MATLAB package, namely:

- the replacement of the algorithm for finding eigenvalues and eigenfunctions (implemented through the standard EIGEN procedure in the FORTRAN system) by the MATLAB package algorithm for computations by means of orthogonal similar transformations with a matrix in the upper Hessenberg form and using the QR-algorithm of Francis and Kublanovskaya;
- the replacement of the algorithm for solving the regularized SLAE (1) to find  $\varphi_\alpha$  with the transformation to a triangular form by the algorithm for system matrix pseudo-inversion using the SVD decomposition;
- the generalization of the classical RR-algorithm with the scalar parameter of global regularization to a local version (this is a major distinctive feature), then  $\alpha$  becomes a random vector of a relevant dimension ( $n$ ) with various components.

In the first two options, we get more economical and fast-acting algorithms to simplify the software design procedure and also have the possibility to control the stability of solutions.

In the latter case, a new original regularization option is suggested, when the found optimal value  $\alpha^*$  serves as a scale factor to specify  $n$  samples of a uniformly

distributed random variable on the segment  $[0, 1]$ . In this case at each step of the cycle, the arrangement of the random vector projections in descending order is performed and local regularization parameters are formed, the maximum component thereof is approximately equal to (but does not exceed)  $\alpha^*$ .

Further, this vector shall be substituted into (1) (where matrix “castling move” of  $\alpha$  and  $E$  has been made) to find a locally regularized solution for  $\varphi_\alpha^*$  and to calculate the empirical risk value on the resulting solution:

$$I_s = \frac{1}{l} \left\| y - R\varphi_\alpha^* \right\|^2. \tag{2}$$

The stochastically optimal solution of system (1) shall be finally determined by minimization (2). An approach associated with the simulation of disturbances and the analysis of the subsequent reaction of a structure or a system is widely used in computational practice. These methods are based on the classical Monte Carlo algorithms and their current modifications [18].

To verify the work of the RR-algorithm and regularization programs, the solutions of test SLAEs were performed with rectangular matrices of higher dimensionality. The maximum matrix size was  $(315 \times 190)$ . As a test, there was studied the integral equation solution using random-noise distorted measurements of the right-hand side [17].

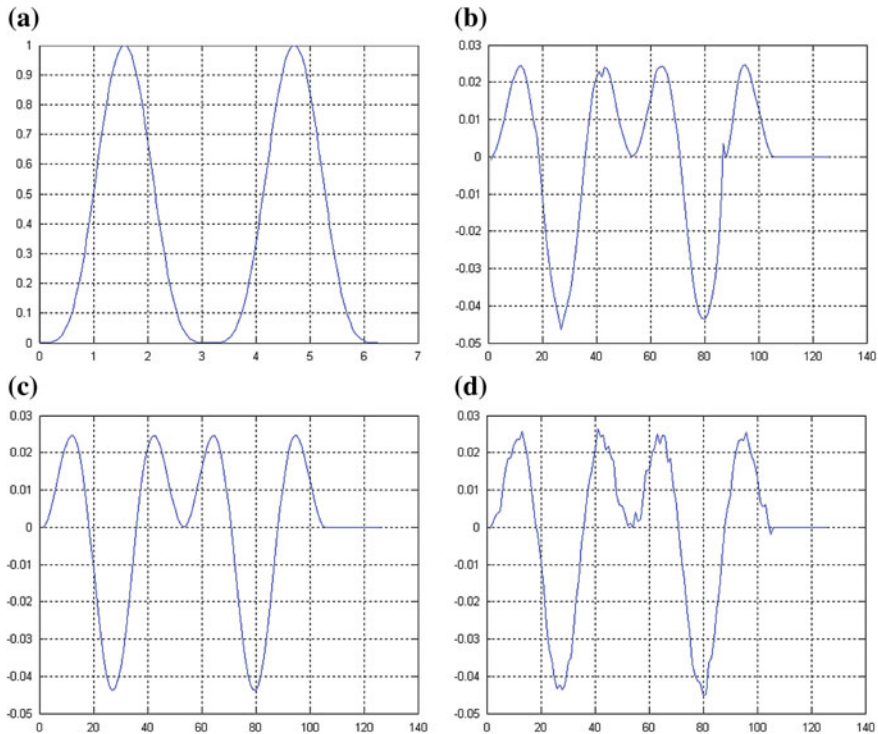
The integral equation algebraization reduces to a system with the number of equations  $M = 210$ , number of unknowns  $K = 126$ . Matrix elements were calculated by the following formula

$$\begin{aligned} A(I, J) &= [0.164 * (I - 1) - 0 * 328 * (J - 1)]_+; \\ I &= 1, \dots, 210; J = 1, \dots, 126; \\ [..]_+ &= \{x, x \geq 0; 0, x < 0\}. \end{aligned} \tag{3}$$

All non-zero matrix elements lie below the main “quasi-diagonal”, matrix A is extremely ill-conditioned,  $\text{rank}(A) = 105$ ,  $\text{cond}(A) = \text{Inf}$  (an infinitude in MATLAB). Some results of solutions of SLAEs with matrix A  $(210 \times 126)$  are shown in Fig. 1.

Note that for version (b) the optimal regularization parameter  $\alpha = 0.005$ , the discrepancy with the optimal regularization parameter is  $d = 4.2549e-005$ . In version (c) the perturbation level for each of six projections is  $\sim 7\%$ ,  $\alpha = 0.50$ ,  $d = 0.0025$ ; for (d)  $\alpha = 0.05$ ,  $d = 1.863e-004$ . The calculation time of a regularized solution for each version is no more than 1.3 s.

As we can see in the Fig. 1 in the test example the “exact” solution has a locally smooth but “impulse” form. The number of sign variations reaches six. Such problems are quite difficult for the correct solution recovery under conditions of right-side projection distortion [19–22]. The suggested algorithms demonstrate sufficiently high efficiency and speed.



**Fig. 1** Verification of the RR-algorithm for regularizing solutions of SLAEs with matrix  $A$  ( $210 \times 126$ ): **a** the graphic chart for projections of the right-side unperturbed vector  $Y$  on the segment  $[0, 2\pi]$ ; **b** the graphic chart for projections of the SLAEs solution in case of no  $Y$  perturbation; **c** the solution for deterministic distortion of six projections of  $Y$ ; **d** the solution for a random perturbation of all projections of  $Y$  (the normal interference distribution law with zero mean and m.s.d. equal to 0.001); on the x-axis for **(b–d)**—solution projections readings

### 3 Algorithms and Singularities of Problem Solution for RR-Algorithm Modification

The original regularization version, when the found optimal  $\alpha^*$  value serves as a large-scale factor in the formation of local regularization parameters, has passed testing on very complex examples.

Computational experiments in solving SLAEs with an approximately specified right sideshow that this algorithm is not always effective. The high algorithm accuracy is limited by the structure of the singular spectrum of SLAE matrices as well as by the conditioning number (not more than  $10^{12}$ ). Based on the accumulated experience the author suggests for complex problems a more perfect algorithm (in the general case of vectorial one) of RR-regularization.

The essence thereof is as follows. The stage is preserved when local regularization parameters are formed and their maximum component is approximately equal to

$\alpha^*$ . A situation may herewith occur when the “tail” of the regularization vector contains, just by chance, too small parameters. The procedure of “cutting off” these parameters finds the basis for a new algorithm. The randomness of the  $\alpha^*$  value is simultaneously taken into account, which is determined by the random nature of vector  $y$  of system  $R \varphi \approx y$  (measurement errors or a parametric uncertainty factor in the experiment).

To this end, the found optimal  $\alpha^*$  value enters the “stochastic cycle” (of 50–100 iterations) for multiple calculations of:

1. local regularization parameters (uniform distribution);
2. a solution of the relevant regularized SLAE;
3. finding the empirical risk value  $I_\sigma$ —formula (2);
4. determining a super-optimal vector of regularization parameters.

At each step of the cycle, firstly, a vector of local regularization parameters is calculated; secondly, to the  $\alpha^*$  value, a proportionally small random variable is added distributed according to the normal law with small variance and zero means. For example,  $\alpha^* = 0.500$ ,  $CL(i) = \alpha^* + 0.015 * randn$ . Where  $CL(i)$  is the  $i$ -th threshold value of regularization parameters,  $\sigma = 0.015$ —m.s.d. of perturbation. Further, all local regularization parameters smaller than  $CL(i)$  shall be replaced by this computed constant. The algorithm performs this operation at each step of the stochastic cycle. The selection of the optimal regularization vector occurs as before in minimizing the functional (2).

Thus, a stochastically stable and super-optimal solution is chosen: there are no too small incidental values of local parameters. The level of smallness in replaced parameters depends on the initial singular spectrum of a matrix. In fact, in the final local parameters there is a combination of the following two distributions and two versions:

- the uniform distribution for the “upper” parameters, when  $CL(i)$  is smaller than  $\alpha^*$  and the “Gaussian threshold” for the “lower” parameters, i.e.  $CL(i)$  has the normal distribution and determines the constant, which replaces small regularization parameters;
- when the random (Gaussian) value  $CL(i)$  is higher than  $\alpha^*$ , we have one global constant of the regularization parameter (the vector shifts to a super-optimal scalar).

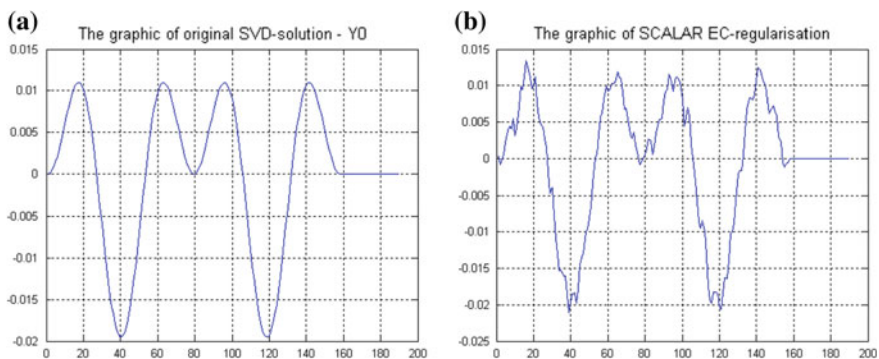
The new algorithm of the vector RR-regularization has passed multiple tests on a set of test problems of higher complexity, proved the high efficiency and computational accuracy for extremely ill-conditioned systems of equations. This algorithm is recommended for matrices with conditioning number  $\text{cond}(A) > 10^{12}$  at significantly higher levels of interference for the right side of the SLAE.

Many numerical results described below illustrate the new algorithm and its superiority as compared to the SLAE solution algorithm by the classical Tikhonov method.

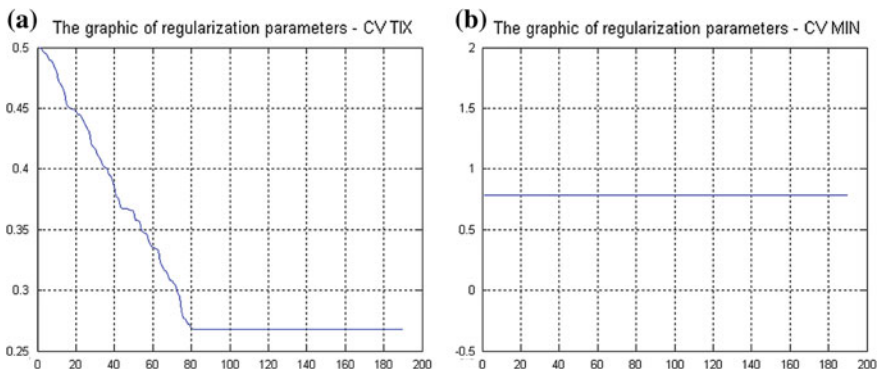
We describe now the “technology” and stages of the proposed super-optimal algorithm on the example of the above problem of solving an integral equation using random-interference distorted measurements on the right-hand side. The algorithm is implemented in MATLAB.

The complicated system  $Ax = Y$  is solved with the number of equations  $M = 315$  and number of unknowns  $K = 190$ . Matrix  $A$  elements are calculated by formula (3) with  $I = 1, \dots, 315; J = 1, \dots, 190$ . The right side, as before, is assigned by the expression  $Y = Y_0 = \sin^4(x/2)$ ,  $0 \leq x \leq 2\pi$ . Matrix  $A$  is extremely ill-conditioned,  $\text{rank}(A) = 157$ ,  $\text{cond}(A) = \text{Inf}$ .

Some results of solutions for SLAE with matrix  $A$  ( $315 \times 190$ ) are shown in Figs. 2, 3, 4, 5 and 6. The initial perturbation for  $Y$  is thereat an interference with a normal distribution law—zero mean and s.m.d. equal to 0.003 (i.e.  $Y = Y_0 + 0.003 \cdot \text{randn}$ ). The interference level is here three times higher than for the problem with  $A$  ( $210 \times 126$ ).

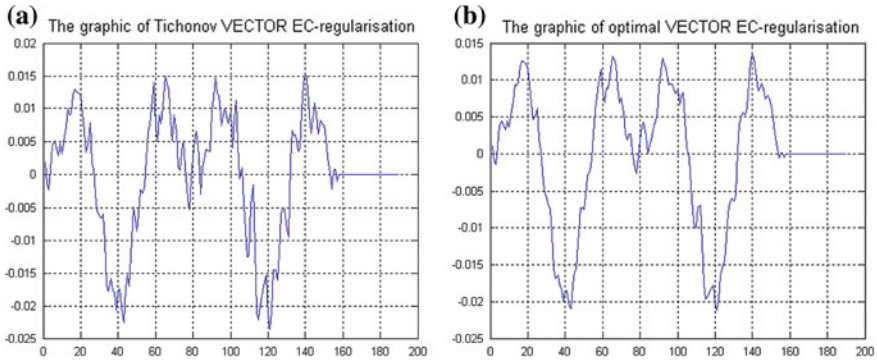


**Fig. 2** Verification of algorithms when solving SLAEs with matrix  $A$  ( $315 \times 190$ ): **a** the graphic chart of the SLAE solution by the SVD algorithm in case of no  $Y$  perturbation; **b** “scalar” regularized RR-solution with the initial perturbation of all  $Y$  projections; on the abscissa axis—readings of solution projections

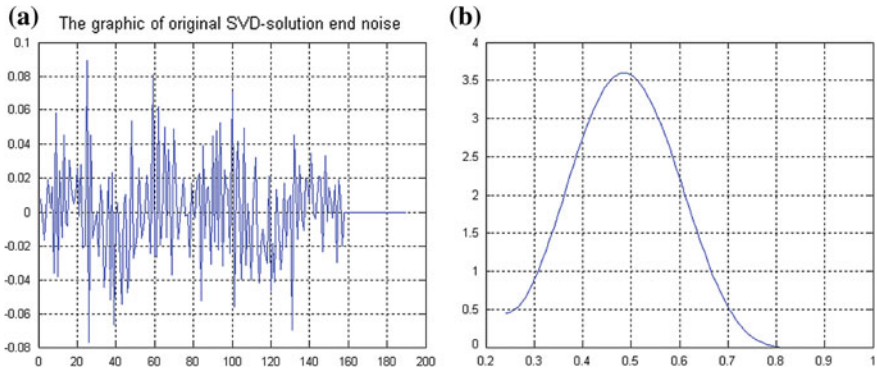


**Fig. 3** RR-algorithm for vector regularization of solutions of SLAEs with matrix  $A$  ( $315 \times 190$ ): **a** the graphic chart of regularized local parameters with the initial  $Y$  perturbation—the optimization in the cycle by the classical Tikhonov functional; **b** the graphic chart of the super-optimal regularization vector found by the minimum of the functional  $I_{\partial}$ ;  $CL_{OPT} = 0.687$





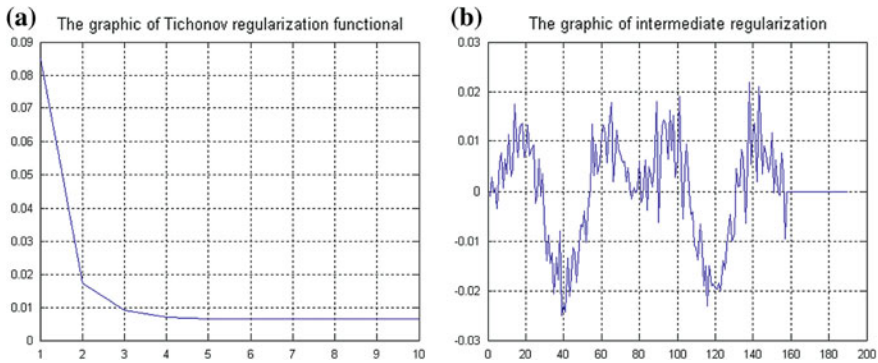
**Fig. 4** Regularized solutions of the modified RR-algorithm for SLAEs with matrix A ( $315 \times 190$ )—(test perturbation  $Y = Y_0 + 0.005 * \text{randn}$ ): **a** for local regularization parameters (Fig. 3a)—optimization in the stochastic cycle by the Tikhonov smoothing functional; **b** when the supra-optimal vector of regularization parameters (Fig. 3b) found on the minimum of the functional (f.2)



**Fig. 5** Verification of solutions of SLAEs with matrix A ( $315 \times 190$ ): **a** the graphic chart of the SLAEs solution by the standard SVD algorithm without regularization—the initial perturbation level of  $Y$ ; **b** the identified distribution density of  $CL$  values in a cycle of 100 iterations for the supra-optimal RR-regularization algorithm

Vectors of regularized parameters found as a result of optimizations (according to A. N. Tikhonov and the super-optimal RR-algorithm) are used for solutions of SLAEs with other perturbation levels, for example,  $Y = Y_0 + 0.005 * \text{randn}$ . In this case, the quality of the synthesized regularization algorithm is verified on random independent variations. It is assumed that the test interference levels may exceed the initial level.

We comment now on the results of a computational experiment, compare them to the method of obtaining normal pseudo-solutions of SLAE (the method of singular decompositions). Figure 2a represents such a solution for an exactly defined right part



**Fig. 6** Verification of the EC algorithm in solving SLAEs with matrix  $A$  ( $315 \times 190$ ): **a** the graphic chart for values of the Tikhonov functional when solving the SLAE—the initial perturbation level of  $Y$ ; **b** the graphic chart for the system solution at the minimum of the classical Tikhonov functional

of the test system. Due to the primary regularization of the singular decomposition, we have a smooth nearly ideal solution.

Figure 2b depicts a graph of a “scalar” regularized RR-solution for optimal  $\alpha^* = 0.500$ . Note that the initial  $\alpha$  value was assigned to be equal to 5.0; the final one to be equal to  $1.10^{-4}$ ; the scale multiplier was equal to 0.10.

Figures 3b and 4b illustrate the choice of the best regularization parameters and the super-optimal solution by minimizing the empirical risk functional using formula (2).

For example,—(Figs. 3a and 4a) show versions of choice for the classical Tikhonov smoothing functional.

With a specific interference level ( $0.003 * \text{randn}$ ) the optimal regularization vector shall be a particular case, which is a global parameter. For small interferences, the algorithm provides the limiting properties of the regularization principle.

Numerous tests show that the proposed super-optimal RR-algorithm surpasses the classical method.

Figure 5a shows the SLAE solution using the standard SVD algorithm (MATLAB) with the initial perturbation level of  $Y$ . The saw-tooth “spread” of solutions even with weak perturbations makes it impossible to use the SVD algorithm without regularization.

The method for identifying the laws of random variables distribution elaborated by the author of this chapter enables to restore the distribution density for CL values in an iterative cycle of 100 steps (Fig. 5b), thus, confirming the correctness of the suggested algorithm and its modifications.

Figure 6 provides the perception of what solution may be obtained if in the RR-algorithm the  $\varphi_\alpha$  solution quality and the Lagrange multiplier are assessed not by the functional  $J(\alpha)$  but by the classical Tikhonov smoothing functional [4]. The minimum of this function is either weakly expressed in the case of small values

of the regularization constant or there is an asymptotically slow decrease of the functional  $M^\alpha(\varphi) = \|y - R\varphi\|^2 + \alpha \|\varphi\|^2$ .

It is seen that the suggested versions of the RR-algorithm modifications surpass the classical methods. If necessary, the modified solutions of the RR-algorithm may be supplemented with a smoothing procedure of the arithmetic average of two adjacent values. The total calculation time of the results given is no more than 10 s.

Regularization software modules are built into the basic module for identifying random distribution densities in order to improve the operational reliability under conditions when it is a priori known that a complex structure is identified with many extremes of the multimodal distribution.

The elaborated algorithms are used in higher intricate applied problems. In particular, in restoring the distribution density of pore sizes in polymer membranes when studying the morphology of their surfaces by atomic force microscopy method (AFM) using the SPM-9700 scanning probe microscope (Shimadzu, Japan). Based on the proposed method, algorithms and programs, the results obtained confirm the multimodal density of the distribution of pore sizes and depth profiles.

The maximum scanning field of a microscope is an area of  $30 \times 30 \mu\text{m}$  in size. The characteristic geometric dimensions of polymer membranes measured by the AFM method are 3–10  $\mu\text{m}$ , the pore sizes are several orders smaller. The obtained results are stated in detail in the author's dissertation thesis.

In biomedicine, the considered method has shown high-resolution properties by the example of monitoring and stochastic analysis of EGEG signals from the actual clinical practice [1]. The identification of local signal sections has revealed the universal characteristics of fractional Brownian processes—the multimodal distribution of their parameters.

And multimodal stochastic characteristics contain information about the non-equilibrium, non-linear dynamics of the state of the body organs and systems. In this case, based on the density of local sections of the process there are calculated moment functions, entropy characteristics, the studied therapy process is monitored and expert health management systems are formed.

## 4 Results and Conclusions

The classical RR-regularization method is modified and implemented in the MATLAB package, evaluated in test problems of relatively high dimensionality (matrices of several hundred lines and columns).

It is shown that to obtain stable solutions with minimizing the basic functionals (at the stage of solving the SLAEs), the algorithm regularization is required.

The regularization of the basic method for identifying distribution densities based on the RR-algorithm was proposed and validated.

The classical RR-algorithm is developed within the framework of the original author's methods for vector regularization versions.

Computational experiments in solving SLAEs with matrices having a conditionality number of  $10^{12}$  or more confirmed the effectiveness of regularization algorithms.

The proposed approaches are important for the RR-algorithm development in local regularization under conditions of giving a priori information about the type of the identified distribution law and its structural features [23].

The scope of application for the developed regularization methods and programs covers flying object control systems (spacecraft, aeronautics), the regulation and control of complex technological processes, the monitoring of medical parameters, the analysis of operators of singular decompositions and multidimensional data arrays of computational mathematics [1–3].

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