

A. M. Sokolov\*

*Institute for Nuclear Research, National Academy of Sciences of Ukraine, Kyiv, Ukraine*

\*Corresponding author: [amsklv@i.ua](mailto:amsklv@i.ua)

**SPECTRUM DECONVOLUTION: THE INDICATOR FOR THE BALANCE REGION AND REGULARIZATION PARAMETER CHOICE BY THE +S-CURVE METHOD<sup>1</sup>**

When solving the problem of spectrum deconvolution, i.e., the problem of eliminating the distorting influence of equipment during the registration of experimental spectrometric data, the choice of the regularization parameter (RP) in the commonly used regularization method is important. In the article, a tool (indicator) for determining the region of favorable values of the RP is proposed. The indicator shows the range of values of the RP for which a balance is observed between the size of a regularized solution and its fit to the given data. The graphical form of the balance range indicator (+S-curve) is convenient for comparing different RP choice methods. In the article own version of RP choice based on the +S-curve is proposed. The new approach is compared with popular RP choice methods such as the discrepancy principle and the L-curve method.

*Keywords:* spectrum deconvolution, Tikhonov regularization method, regularization parameter, discrepancy principle, L-curve method.

**1. Introduction**

Taking into account the distorting influence of equipment when recording experimental data leads to the solution of the Fredholm integral equation of the first kind:

$$\int_a^b K(t,s)x(s)ds = y_\delta(t), \quad t \in [c,d],$$

(in operator form  $Kx = y_\delta$ ), (1)

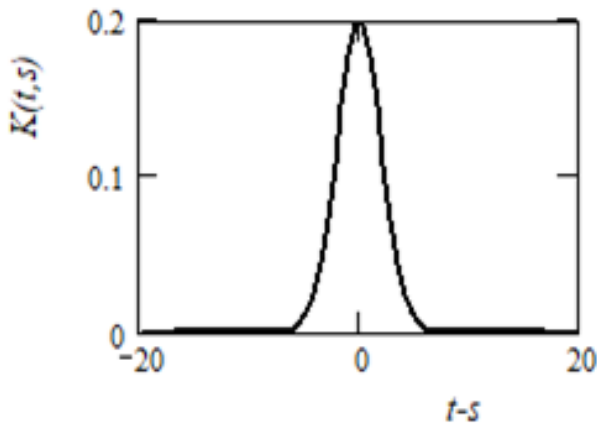


Fig. 1. Instrumental function  $K(t-s)$ .

where  $x(s)$  is the initial dependence of interest to us (undistorted spectrum),  $y_\delta(t)$  – is the obtained dependence as a result of recording the spectrum by the equipment (the recorded spectrum),  $\delta$  – is the level of its error ( $\|y - y_\delta\| \leq \delta$ ),  $K(t, s)$  is the instrumental function assumed to be given. For example, let the response function  $K(t, s) \equiv K(t - s)$  have the form as shown in Fig. 1. Then the input signal  $x(s)$  upon registration will turn into the corresponding output signal  $y_\delta(t)$  as shown in Fig. 2.

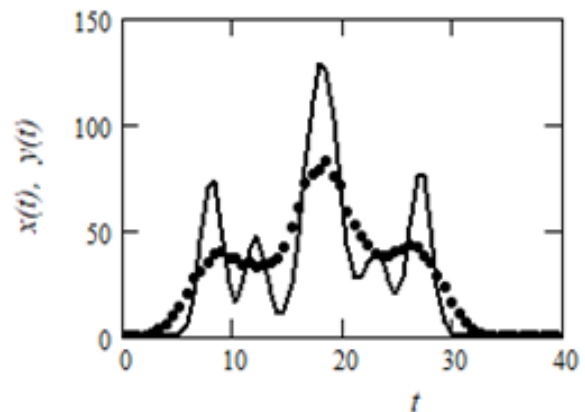


Fig. 2. Input signal  $x(t)$  (—) and output signal  $y_\delta(t)$  (.....).

The solution of Eq. (1) is strongly affected by the error in the right-hand side. Therefore, in Tikhonov’s regularization method [1, 2], Eq. (1) is replaced by a problem of minimizing the smoothing functional:

$$x_\alpha = \arg \min_x \left( \|Kx - y_\delta\|_{L_2}^2 + \alpha (\|x\|_{L_2}^2 + \|x'\|_{L_2}^2) \right). \quad (2)$$

The solution to problem (2), i.e., the function  $x_\alpha$ , depends on the regularization parameter (RP)  $\alpha$ , which balances the requirements for the parts of the functional in (2).

It is important to choose the correct (or successful) value of parameter  $\alpha$ . About a dozen of the methods already proposed have become quite popular [3]. Research into the problem of a RP

© The Author(s), 2026

Published by INR of NAS of Ukraine as an open access article under the CC BY-NC 4.0 license

<sup>1</sup> Presented at the XXXII Annual Scientific Conference of the Institute for Nuclear Research of the National Academy of Sciences of Ukraine, Kyiv, May 26–30, 2025.

choosing is continued. In this situation, it is useful to have a tool (indicator) that allows us to indicate the entire region of potentially favorable values of the RP. The balance region indicator will allow us to compare different methods of selecting a RP by the position of the proposed values in this region. In addition, it will be possible to construct our own version of selecting a RP within this area.

**2. Analysis of the components of Tikhonov’s functional**

Let us introduce parametric functionals (functions of the parameter  $\alpha$ ):

$$\rho(\alpha) = \|Kx_\alpha - y_\delta\|_{L_2} \text{ and}$$

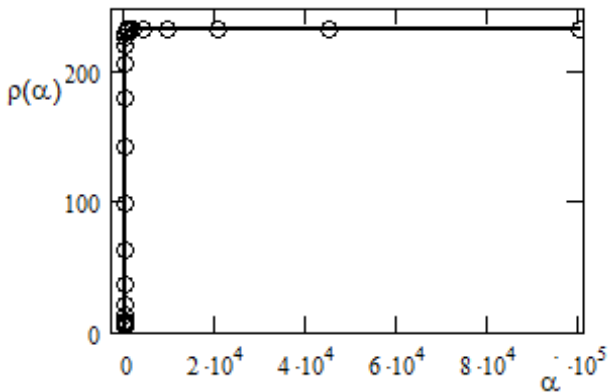


Fig. 3. Residual function  $\rho(\alpha)$  (normal scale).

The grid with respect to the argument  $\alpha$  is taken in the form  $\alpha_k = 10^{p_0 + \Delta k}$ ,  $p_0 = -12$ ,  $\Delta = 17/50$ ,  $k = 0, \dots, 50$ . The circles (dots) on the graphs represent the values of the corresponding grid functions. The dots are very unevenly distributed, grouped near the origin and near the inflection point of the graph. In Figs. 3 and 4, it is evident that the change in the magnitude of the dependencies under consideration occurs in a narrow region of small values of RP. At the same time, a large range of change in the values is observed. Therefore, usually, when depicting these functions on a graph, a logarithmic scale is used on both axes. The graphs of dependencies  $\rho(\alpha)$  and  $\gamma(\alpha)$  will change and will look like in Fig. 5.

Applying a logarithmic scale to the  $\alpha$  axis effectively means that we have moved to a new variable  $p$ , which is related to  $\alpha$  by the ratio  $\alpha(p) = 10^p$  or, in other words,  $p = \log_{10}(\alpha)$ . The transition to a logarithmic scale on the ordinate axis for  $\rho$  or  $\gamma$  means replacing a variable of the form  $\rho_{new} = \log_{10}(\rho_{old})$  and  $\gamma_{new} = \log_{10}(\gamma_{old})$ . When we made such a change of variables, we moved from functions  $\rho(\alpha)$  and  $\gamma(\alpha)$  to functions  $r(p)$  and  $g(p)$ :

$$r(p) = \log_{10} \|A \cdot x_{\alpha(p)} - y_\delta\|,$$

$$\gamma(\alpha) = \|x_\alpha\|_{W_2'} \equiv \left( \|x_\alpha\|_{L_2}^2 + \|x'_\alpha\|_{L_2}^2 \right)^{1/2}. \quad (3)$$

Their basic properties are well studied [2]. Both functions are strictly monotone. The function  $\rho(\alpha)$  (the discrepancy (or residual) of Eq. (1) on  $x_\alpha$ ) increases, the norm of the regularized solution  $\gamma(\alpha)$  decreases. Let us see how the properties of these functions manifest themselves in a specific case. Figs. 3 and 4 show the behavior of the functions for the case of an integral operator with a kernel as in Fig. 1, with a model input signal and with the right-hand side as in Fig. 2.

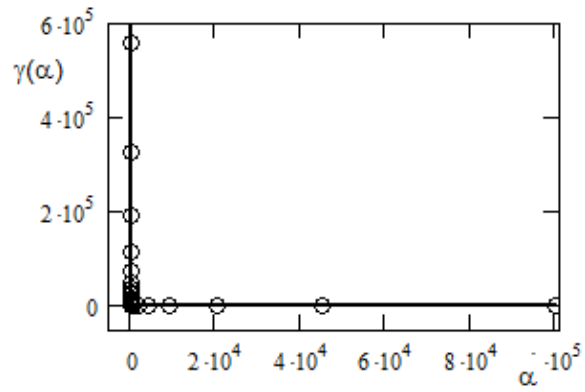


Fig. 4. Norm function  $\gamma(\alpha)$  (normal scale).

$$g(p) = \log_{10} \|x_{\alpha(p)}\|. \quad (4)$$

In Fig. 5, the values are given after this change of variables. Note that the functions  $r(p)$  and  $g(p)$  inherit the property of monotonicity.

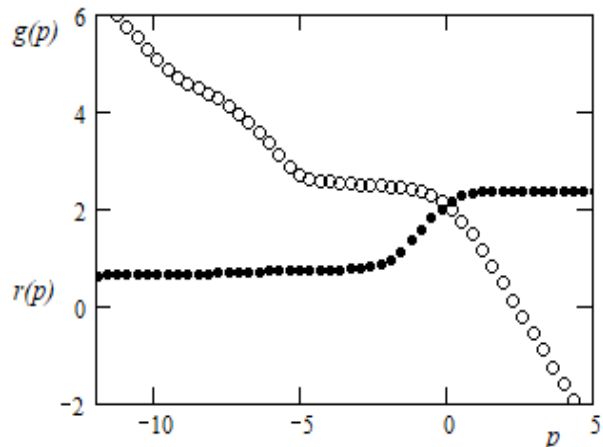


Fig. 5. The residual ( $r(p)$  ...) and the norm ( $g(p)$  ...) functions, given after the change of variables, coincide with the residual  $\rho(\alpha)$  and the norm  $\gamma(\alpha)$  in the log-log scale.

Note that it is more convenient to carry out calculations in formulas (3) and in problem (2), dealing with functions of the variable  $p$ , i.e., with the functions  $r(p)$  and  $g(p)$ .

Since the parameters  $p$  and  $\alpha$  are one-to-one related, the results obtained for the variable  $p$  are easy to interpret for the parameter  $\alpha$ .

### 3. Stage of RP choice

Methods for selecting the RP can be divided into two groups. The first, which assumes a known level  $\delta$  of error in the data, includes, for example, selection based on the discrepancy principle (selection based on the condition: the discrepancy of Eq. (1) on the regularized solution is the same as on the exact solution, i.e., equal to  $\delta$ ).

The criterion for selecting a RP based on the discrepancy principle [2] is based on the dependence  $p(\alpha)$  and is reduced to the equation

$$\rho(\alpha) = \tau\delta, \tau \approx 1. \quad (r(p) = \log(\delta)). \quad (5)$$

The solution of Eq. (5) corresponds to the intersection point of the graph of the function  $r(p)$  and the line at the level of  $\log(\delta)$  (Fig. 6).

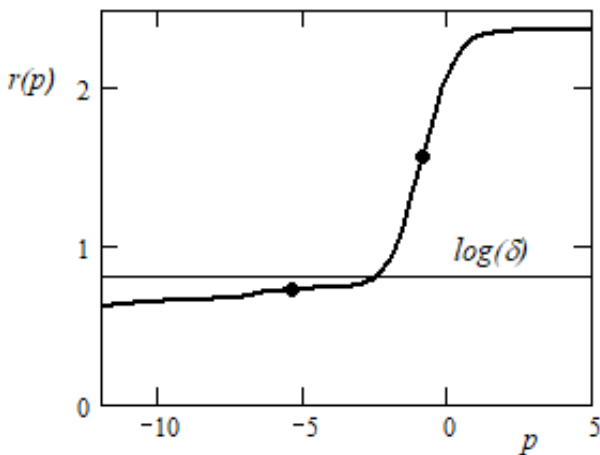


Fig. 6. Choice of RP by the residual principle.

Under certain natural conditions and taking into account the monotonicity of the function  $\rho(\alpha)$ , the solution to Eq. (5) exists and is unique.

The level of error is not always known exactly and can be specified only approximately. In this case, for small values of  $\delta$ , the intersection point of the straight line and the graph of the function  $r(p)$  will be determined with a large error, and the transition from  $\delta$  to  $\log(\delta)$  itself can increase the uncertainty in the position of the straight line.

*Criterion of RP selection by the L-curve.* The L-curve method [4, 5] of selecting the RP, attractive for its graphical clarity, belongs to the group of methods that do not use information about the level and nature of the error in the data.

Let us take the function  $g(p)$  of the log of the norm of the regularized solution, the graph of which is shown in Fig. 5, and make another change of variable  $p = p(r)$ , using the fact that the residual

function  $r(p)$  is strictly increasing and can be inverted. Thus, we obtain a complex function of the norm from the residual:  $g(r) = g(p(r))$ . In this case, the graph of the norm is transformed and takes the form shown in Fig. 7.

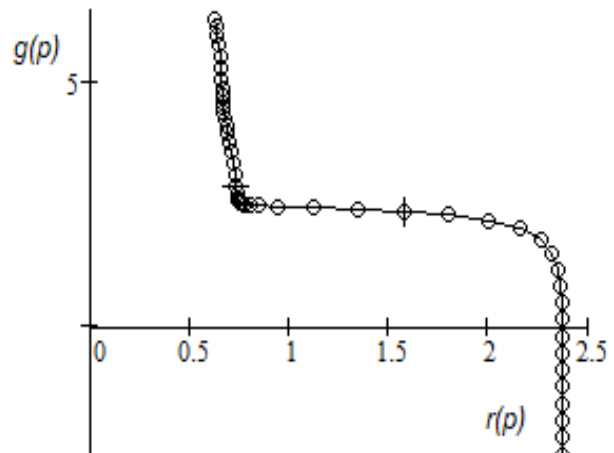


Fig. 7. Typical shape of the L-curve, which is given in parametric form and can be interpreted as a function of the residual norm in log-log scale.

The curve obtained from the curve of the norm graph in Fig. 5 retains a certain similarity with it. We see that the left part of the curve in Fig. 5 has shrunk into a narrow section in Fig. 7, from an inclined one, it has become almost vertical. The middle part has stretched into a large section, close to horizontal. The right part has shrunk into an almost vertical section.

The curve obtained from the norm graph in Fig. 5 is the L-curve (see Fig. 7). It usually has a characteristic bend, a “corner”, when the almost vertical part of the curve turns into an almost horizontal section. This corner corresponds to those values of the parameter  $p$  (and, accordingly, the parameter  $\alpha$ ), for which the section of small values of the discrepancy ends and its noticeable growth begins.

The L-curve criterion suggests choosing a value of the RP corresponding to the corner of the L-curve. Note that in this case, it will be necessary to search for a point representing the angle of the L-curve among a group of points that are compressed and almost overlapping each other in the region of the angle.

### 4. Balance region indicator and +S-curve approach for choosing a RP

In addition to choosing a specific value of the RP, it would be desirable to explore the entire region of favorable values of the RP and thereby obtain the ability to compare different methods of choosing the RP by the position of the proposed RP values within this region of favorable values. We will use the norm function of the regularized solution to identify

the balance condition. To do this, we compare the values of the function  $\gamma(\alpha)$  for two different values of the RP, for example, for  $\alpha$  and  $q \cdot \alpha$ , where  $q > 1$ . It is convenient to take the parameter  $q = 10$ , i.e., change  $\alpha$  by one order. As an indicator, we take the ratio

$$G(\alpha) = \frac{\gamma(\alpha)}{\gamma(q \cdot \alpha)}. \quad (6)$$

From the strict monotonicity of a decreasing function  $\gamma(\alpha)$  it follows that  $G(\alpha) > 1$ . Moreover, it turns out  $G(\alpha) \rightarrow q (\alpha \rightarrow \infty)$ . In the balance area, the graph of the function  $G(\alpha)$ , with a logarithmic scale for  $\alpha$ , has a well-defined, wide minimum, where the values of  $G(\alpha)$  are close to 1. If we move to the variable  $p$  in formula (6), we will get the same graph with a normal scale for  $p$ . The formula for the indicator  $G(p)$ , with such a transition, will take the form  $G(p) = \gamma(\alpha(p)) / \gamma(\alpha(p + \lg(q)))$ .

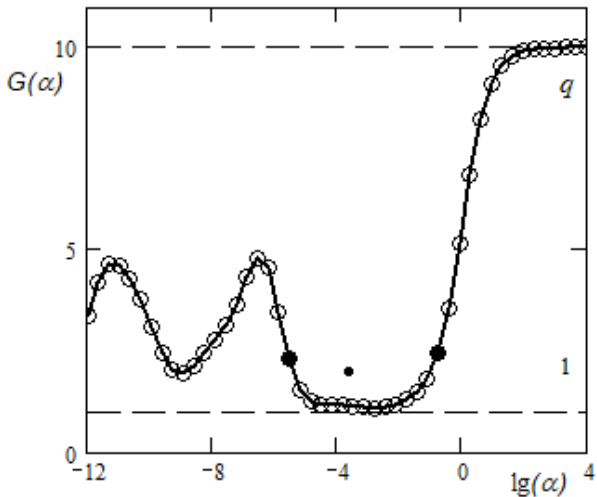


Fig. 8. Balance area indicator (+S-curve) in graphical form. Filled circles indicate the boundaries of the balance area.

The minimum of the  $G(\alpha)$  region corresponds to the balance region for the RP in (2). With an

increase in the parameter  $\alpha$ , the function increases, approaching the value  $q$ . Therefore, the right side of the graph  $G(\alpha)$  has a characteristic S-shaped form (Fig. 8).

We will define the boundaries of the flat minimum area using another parameter,  $w = 2$ . To do this, we will find two values  $pl$  and  $pr$  of the parameter  $p$ , where the function  $G(p)$  will exceed the value  $w$  when moving from the minimum point to the left or right. Thus, the balance region indicator has two main parameters:  $q$  and  $w$ .

Now we can take a new look at the proposed options for choosing the RP. For example, we can specify the boundaries of the balance area when choosing the RP based on the residual principle and the L-curve method. In Figs. 6 and 7, the points corresponding to the boundaries of the balance area are highlighted.

It is possible to propose a numerical characteristic for a qualitative assessment of the values  $pr$  of the RP proposed by different methods. The evaluation coefficient  $Cpr(pr)$  for the parameter  $pr$  shows the position of the  $pr$  within the boundaries of the balance region. The corresponding formula is:

$$Cpr(pr) = (pr - \text{left border}) / (\text{right border} - \text{left border}). \quad (7)$$

*Criterion +S-curve.* Using the balance area indicator, we can propose an option for choosing the RP within the balance area, namely:

$$RP = (\text{left border}) + Cpr(+S\text{-curve}) \times (\text{right border} - \text{left border}),$$

$$Cpr(+S\text{curve}) = 0.4. \quad (8)$$

The position of the RP value proposed in the +S-curve method is shown in Fig. 8. The results of applying the regularization method for the RP values selected according to different criteria are shown in Fig. 9.

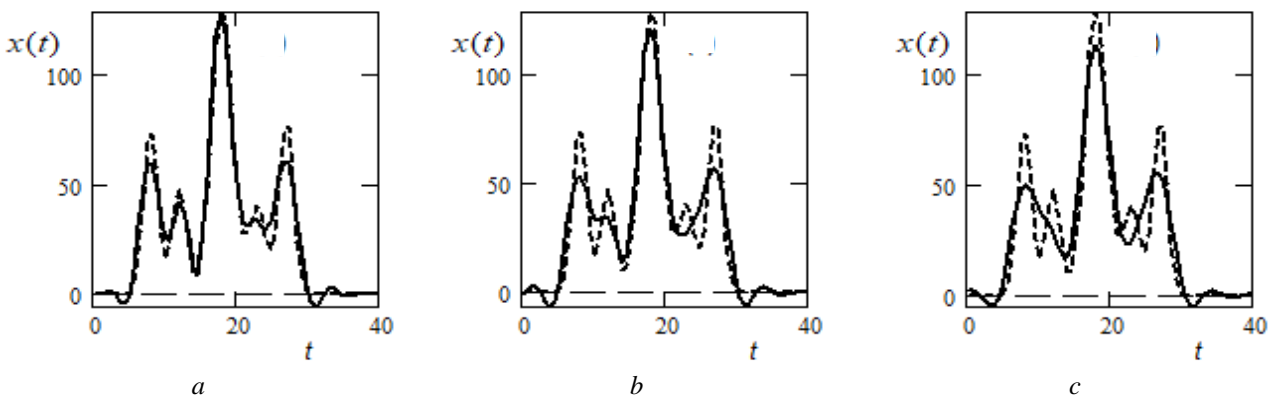


Fig. 9. Reconstructed input spectrum for the RP selected using the +S-curve (a), L-curve (b), and residual principle (c) methods. The exact input signal is shown as a dashed line.

The balance indicator can be a useful tool for comparing different criteria for selecting a RP. It provides a generalized view of the choice of a RP. For example, one can mark the value of the proposed RP values against the  $+S$ -curve and evaluate their position in the balance area relative to each other and relate to the boundaries of the balance area (Fig. 10).

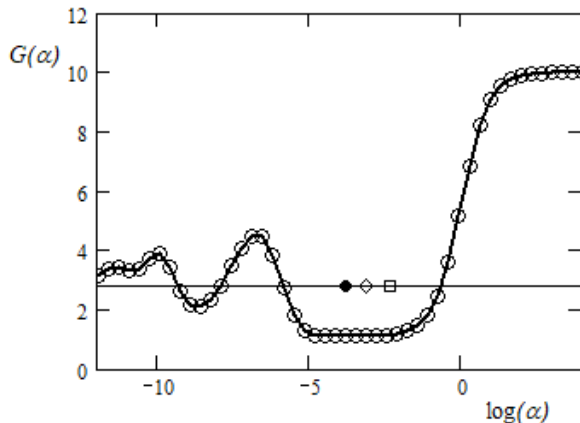


Fig. 10. The flat minimum of the  $+S$ -curve indicates the balance area. The RP values selected by the  $+S$ -curve method (point),  $L$ -curve (diamond) and by the residual principle (square) are marked on the axis.

For a specific variant in model calculations, the results of which are shown in Fig. 10, the proposed values of RP correspond to the coefficient  $Crp(+S\text{-curve}) = 0.4$ ,  $Crp(L\text{-curve}) = 0.53$ ,  $Crp(Descripency) = 0.69$ .

The  $+S$ -curve method has a certain similarity with other methods, which are also built on the basis of the properties and behavior of the function  $\gamma(\alpha)$  (the norm of the regularized solution as a function of the parameter  $\alpha$ ). For example, the choice of the RP in the Simple-L-ratio method [6] approximately corresponds to the choice of  $\alpha$  for which the minimum

of the function  $G(\alpha)$  is achieved. A similar result is obtained when choosing a quasi-optimal RP value [1]. Each of these methods indicates a specific RP value in the range of  $\alpha$  values where the norm of the regularized solution  $\gamma(\alpha)$  relatively slowly changes with  $\alpha$ . This range is clearly visible in Fig. 5 when we move to the log scale by  $\alpha$ , i.e. to the variable  $p$ . In fact, in the methods mentioned above, this is exactly the transition that is implied (scheme is  $\alpha \cdot \partial/\partial\alpha = \partial/\partial(\ln(\alpha)) = \partial/\partial p$ ). The  $+S$ -curve indicator highlights precisely this range.

## 5. Conclusion

A method (indicator) is proposed for determining the range of values of the RP for which the residual of Eq. (1) on the regularized solution and the norm of the regularized solution are in relative balance.

The graphical form of the balance area indicator is the  $+S$ -curve, which has a characteristic appearance. The  $+S$ -curve contains a section of a flat minimum, almost reaching 1, and a section of growth up to the limit value  $q$ , similar in shape to the letter  $S$ .

The RP values proposed by different methods are conveniently compared by their position within the boundaries of the balance area.

A variant of the selection of RP using  $+S$ -curve for a given value of coefficient  $Crp(pr)$  is proposed. The recommended value is  $Crp(+S\text{-curve}) = 0.4$ .

The proposed option for choosing RP is compared with the choice based on the residual principle and the  $L$ -curve method. In model calculations, the relation  $Crp(+S\text{-curve}) < Crp(L\text{-curve}) < Crp(Descripency)$  is usually satisfied. Therefore, in many cases, when RP is selected using the  $+S$ -curve method, it is possible to restore finer details of the input signal.

## REFERENCES

1. A.N. Tikhonov, V.Ya. Arsenin. *Methods for Solving Ill-Posed Problems*. 2nd ed. (Moskva: Nauka, 1979) 285 p. (Rus)
2. V.A. Morozov. *Regular Methods for Solving Ill-Posed Problems* (Moskva: Moscow State University Press, 1974) 359 p. (Rus)
3. F. Bauer, M.A. Lukas. Comparing parameter choice methods for regularization of ill-posed problems. *Math. Comput. Simul.* 81(9) (2011) 1795.
4. P.C. Hansen. The L-curve and its use in the numerical treatment of inverse problems. In: P.R. Johnston (Ed.). *Computational Inverse Problems in Electrocardiography* (Great Britain, Southampton, WIT Press, 2001) p. 119. Не має посилання в тексті.
5. P.C. Hansen, D.P. O'Leary. The use of the L-curve in the regularization of discrete ill-posed problems. *SIAM J. Sci. Comput.* 14(6) (1993) 1487.
6. S. Kindermann, K. Raik. A simplified L-curve method as error estimator. *Electron. Trans. Numer. Anal.* 53 (2020) 217.

**О. М. Соколов\****Інститут ядерних досліджень НАН України, Київ, Україна*\*Відповідальний автор: [amsklv@i.ua](mailto:amsklv@i.ua)**ЗАДАЧА ДЕКОНВОЛЮЦІЇ СПЕКТРА: ІНДИКАТОР ОБЛАСТІ БАЛАНСУ  
ТА ВИБІР ПАРАМЕТРА РЕГУЛЯРИЗАЦІЇ ЗА МЕТОДОМ +S-КРИВОЇ**

Під час розв'язання задачі деконволюції спектра, тобто задачі усунення спотворюючого впливу обладнання під час реєстрації експериментальних спектрометричних даних, важливим є вибір параметра регуляризації (ПР) у звичайному використуваному методі регуляризації. У статті пропонується засіб (індикатор) для визначення області сприятливих значень ПР. Цей індикатор вказує область значень ПР, за яких забезпечується відносний баланс вимог для регуляризованого рішення. Графічна форма індикатора області балансу (+S-крива) зручна для порівняння різних методів вибору ПР. У статті запропоновано свій варіант вибору ПР на основі +S-кривої. Проведено його порівняння з популярними методами вибору ПР за принципом нев'язки та за методом L-кривої.

*Ключові слова:* деконволюція спектра, метод регуляризації Тихонова, параметр регуляризації, принцип нев'язки, метод L-кривої.

Надійшла / Received 10.09.2025