НАУЧНО-ТЕХНИЧЕСКИЙ ВЕСТНИК ИНФОРМАЦИОННЫХ ТЕХНОЛОГИЙ, МЕХАНИКИ И ОПТИКИ
ноябрь–декабрь 2015 Том 15 № 6 ISSN 2226-1494 http://ntv.ifmo.ru/
SCIENTIFIC AND TECHNICAL JOURNAL OF INFORMATION TECHNOLOGIES, MECHANICS AND OPTICS
November–December 2015 Vol. 15 No 6 ISSN 2226-1494 http://ntv.ifmo.ru/en
УНИВЕРСИТЕТ ИТМО

METHOD OF TRAINING EXAMPLES IN SOLVING INVERSE ILL-POSED PROBLEMS OF SPECTROSCOPY

V.S. Sizikov[a], A.V. Stepanov[b]

[a] ITMO University, Saint Petersburg, 197101, Russian Federation
[b] Vernadsky Crimean Federal University, Simferopol, 95342, Russian Federation
Corresponding author: sizikov2000@mail.ru

Article info
Received 20.09.15, accepted 12.10.15
doi:10.17586/2226-1494-2015-15-6-1147-1154
Article in English
For citation: Sizikov V.S., Stepanov A.V. Method of training examples in solving inverse ill-posed problems of spectroscopy. *Scientific and Technical Journal of Information Technologies, Mechanics and Optics*, 2015, vol. 15, no. 6, pp. 1147–1154.

Abstract
Subject of Study. The paper deals with further development of the method of computational experiments for solving ill-posed problems, e.g., the inverse spectroscopy problem. This method produces an effective (nonoverstated) estimate for solution error of the first-kind equation. **Method of Research.** An equation is solved by the Tikhonov regularization method. We have obtained nonoverstated estimate for solution error and a new principle for choosing the regularization parameter on the basis of the truncating singular number spectrum of an operator. It is proposed to estimate the truncation magnitude by results of solving model (training, learning) examples close to an initial example (problem). This method takes into account an additional information about the solution. **Main Results.** We have derived a new, more accurate estimate for regularized solution error using the truncation parameter g. Ways for determining g according to the results of solving model examples are proposed. The method of modeling or training is applied to solving the inverse spectroscopy problem (restoration of a fine spectrum structure by solving integral equation on the basis of an experimental spectrum and the spread function of a spectral device). The method makes it possible to resolve close lines and select weak lines. **Practical Relevance.** The proposed method can be used to restore smoothed and noisy spectra, in other words, to enhance the resolution of spectral devices by mathematical and computer processing of experimental spectra.

Keywords
ill-posed problems, Tikhonov regularization, solution error, method of training examples, inverse problem of spectroscopy, integral equation, spread function of spectral device, measured spectrum, training spectra, restored spectrum.

Acknowledgements
This work was supported by the Russian Foundation for Basic Research (RFBR), grant №13-08-00442.

СПОСОБ ОБУЧАЮЩИХ ПРИМЕРОВ В РЕШЕНИИ ОБРАТНЫХ НЕКОРРЕКТНЫХ ЗАДАЧ СПЕКТРОСКОПИИ

В.С. Сизиков[a], А.В. Степанов[b]

[a] Университет ИТМО, Санкт-Петербург, 197101, Российская Федерация
[b] Крымский федеральный университет им. В.И. Вернадского, Симферополь, 95342, Российская Федерация
Адрес для переписки: sizikov2000@mail.ru

Информация о статье
Поступила в редакцию 20.09.15, принята к печати 12.10.15
doi:10.17586/2226-1494-2015-15-6-1147-1154
Язык статьи – английский
Ссылка для цитирования: Сизиков В.С., Степанов А.В. Способ обучающих примеров в решении обратных некорректных задач спектроскопии // Научно-технический вестник информационных технологий, механики и оптики. 2015. Т. 15. № 6. С. 1147–1154.

Аннотация
Предмет исследования. Дано дальнейшее развитие способа вычислительных экспериментов решения некорректных задач, например, обратной задачи спектроскопии. Этот способ позволяет получить эффективную (незавышенную) оценку погрешности решения уравнения первого рода. **Метод.** Уравнение решается методом регуляризации Тихонова. Получены незавышенная оценка погрешности решения и новый способ выбора параметра регуляризации на основе использования усечения спектра сингулярных чисел оператора. Величину усечения предлагается оценивать по результатам решения модельных или обучающих примеров, «близких» исходному примеру (задаче). Данный способ учитывает дополнительную информацию о решении. **Основной результат.** Выведена новая, более точная оценка погрешности регуляризованного решения с использованием параметра усечения g. Предложены способы определения g по результатам решения модельных примеров. Способ моделирования или обучения применен к решению обратной задачи спектроскопии (восстановлению тонкой структуры спектра путем решения

интегрального уравнения на основе экспериментального спектра и аппаратной функции спектрального прибора). Способ позволил разрешить близкие линии и выделить слабые линии. **Практическая значимость.** Предложенная методика может быть использована для восстановления заглаженных и зашумленных спектров, другими словами, для повышения разрешающей способности спектральных приборов путем математической и компьютерной обработки экспериментальных спектров.

Ключевые слова: некорректные задачи, метод регуляризации Тихонова, погрешность решения, способ обучающих примеров, обратная задача спектроскопии, интегральное уравнение, аппаратная функция спектрального прибора, измеренный спектр, обучающие спектры, восстановленный спектр.

Благодарности. Работа выполнена при поддержке РФФИ (грант № 13-08-00442).

Introduction

As is well known [1–4], it is practically impossible to obtain an effective (nonoverstated) error estimate for solution of ill-posed problem, e.g., the inverse spectroscopy problem without an additional (a priori) information about the solution. In this paper, we develop an adaptive method of computational experiments for estimating the solution error and choosing the regularization parameter α in solving ill-posed problems by the Tikhonov regularization method. The method is also known as: the technique of model, standard, learning, training examples, the way of the pseudoinverse operator [1–8]. This method takes into account an additional (a priori) information about the desired solution (an estimate of the number of maxima, their abscissas and ordinates, etc.) and, in this respect, resembles the methods such as the Tikhonov α-regularization with constraints on the solution [9], solution on a compact [4, 9], the methods of descriptive regularization [10], also taking into account a priori information on the solution (nonnegativity, monotonicity, convexity, parameters of extrema, etc.). However, the specific implementation of the method of computational experiments differs from these methods.

This method has been earlier developed and applied to signal processing [1–3], image restoration [5, 6] and spectroscopy [5–8]. In this paper, we propose its modification and application to the inverse problem of spectroscopy.

Basic relations

Consider an operator equation of the first kind

$$Ay = f, \quad y \in Y, \quad f \in F, \tag{1}$$

where y is desired, and f is given elements of Hilbert spaces Y and F; A is a linear bounded operator from Y into F. The operator A is not expected to be continuously invertible, i.e. the problem of solving equation (1) is ill-posed. However, for the exact f we assume that equation (1) is solvable.

The problem is to find an element $y \in Y$ with minimal norm, which supplies the minimum value for the discrepancy $\| Ay - f \|_F$ and which is the pseudosolution, in particular, the normal solution [4, 9, 11].

In the zero-order Tikhonov regularization method [4, 9, 11, 12], giving one of the most effective ways for obtaining pseudosolutions, instead of (1) the equation

$$(\alpha E + \tilde{B})\, y_\alpha = \tilde{A}^* \tilde{f}, \tag{2}$$

is solved, where

$$\tilde{A} = A + \Delta A, \quad \tilde{f} = f + \Delta f, \quad y_\alpha = y + \Delta y_\alpha, \tag{3}$$

moreover, A, f and y are the exact operator and elements; $\tilde{A}$, $\tilde{f}$ and y_α are their practical values; ΔA, Δf and Δy_α are their errors; $\alpha > 0$ is the regularization parameter; $\tilde{B} = \tilde{A}^* \tilde{A}$; E is the unit operator.

Estimate of solution error. Consider the question of estimating the error Δy_α of the regularized solution y_α and choosing the regularization parameter α.

It is known [13] that it is almost impossible to obtain an effective (nonoverstated) estimate of the error Δy_α without using additional (a priori) information on the solution. In this paper, we propose to use the results of solving "close" model (learning) examples as additional information. Taking into account the ratio $\tilde{A}^* A y = \tilde{A}^* f$, which follows from (1), as well as the ratios (2) and (3), we obtain

$$(\alpha E + \tilde{B})\, \Delta y_\alpha = -(\alpha E + \tilde{A}^* \Delta A) y + \tilde{A}^* \Delta f$$

or

$$\Delta y_\alpha = (\alpha E + \tilde{B})^{-1} \tilde{A}^* (\Delta f - \Delta A\, y) - \alpha (\alpha E + \tilde{B})^{-1} y,$$

from where we find the following estimates in the norm of absolute and relative errors of the regularized solution

$$\| \Delta y_\alpha \| \le \| (\alpha E + \tilde{B})^{-1} \tilde{A}^* \| \cdot (\| \Delta f \| + \| \Delta A \| \cdot \| y \|) + \alpha \, \| (\alpha E + \tilde{B})^{-1} \| \cdot \| y \|,$$

$$\frac{\| \Delta y_\alpha \|}{\| y \|} \le \| (\alpha E + \tilde{B})^{-1} \tilde{A}^* \| \cdot \left(\frac{\| \Delta f \|}{\| y \|} + \| \Delta A \| \right) + \alpha \| (\alpha E + \tilde{B})^{-1} \| . \quad (4)$$

Taking into account that $\| A \| \cdot \| y \| \ge \| f \|$ or $1/\| y \| \le \| A \| / \| f \|$, we obtain the estimate (4) for the relative error of the regularized solution in the form

$$\sigma_{\text{rel}}(\alpha) \equiv \frac{\| \Delta y_\alpha \|}{\| y \|} \le \| (\alpha E + \tilde{B})^{-1} \tilde{A}^* \| \cdot \| A \| (\delta_{\text{rel}} + \xi_{\text{rel}}) + \alpha \| (\alpha E + \tilde{B})^{-1} \| , \quad (5)$$

where

$$\delta_{\text{rel}} = \frac{\| \Delta f \|}{\| f \|}, \qquad \xi_{\text{rel}} = \frac{\| \Delta A \|}{\| A \|}$$

are the relative errors of the right-hand side f and operator A. The right-hand side of (5) is the upper envelope of the true relative error $\sigma_{\text{rel}}(\alpha)$. The first summand in the right-hand side of (5) is due to the errors of data, while the second summand is determined by regularization. In (5), we have (cf. [14–17]): $\| (\alpha E + \tilde{B})^{-1} \tilde{A}^* \| \le 1/(2\sqrt{\alpha})$, and norm $\| (\alpha E + \tilde{B})^{-1} \|$ can be expressed through minimum singular number μ of symmetric positively determined operator $\alpha E + \tilde{B}$:

$$\| (\alpha E + \tilde{B})^{-1} \| = 1/\mu_{\min}(\alpha E + \tilde{B}) = 1/(\alpha + \mu_{\min}(\tilde{B})) .$$

We obtain (cf. [14–17]):

$$\sigma_{\text{rel}}(\alpha) \equiv \frac{\| \Delta y_\alpha \|}{\| y \|} \le \frac{\| \tilde{A} \|}{2\sqrt{\alpha}} \eta + \frac{\alpha}{\alpha + \mu_{\min}(\tilde{B})}, \quad (6)$$

where $\eta = \delta_{\text{rel}} + \xi_{\text{rel}}$.

However, in practice, estimate (6) (as well as (5)) may give a significant overstatement for $\sigma_{\text{rel}}(\alpha)$, since, in case of ill-conditioned and ill-posed problems, $\mu_{\min}(\tilde{B})$ is close or equal to zero and then (when $\mu_{\min}(\tilde{B}) = 0$)

$$\sigma_{\text{rel}}(\alpha) \equiv \frac{\| \Delta y_\alpha \|}{\| y \|} \le \frac{\| \tilde{A} \|}{2\sqrt{\alpha}} \eta + 1 . \quad (7)$$

The estimate (7) is not only overstated, but not having the minimum with respect to α.

To obtain more effective estimate of $\sigma_{\text{rel}}(\alpha)$ we use the concept of the pseudoinverse operator having enclosed in it, however, a sense somewhat different from the pseudo-inverse Moore–Penrose matrix A^+ which gives the solution $y = A^+ f$ [4, 12, 18] and from the regularized operator $(\alpha E + \tilde{B})^{-1} \tilde{A}^*$ which gives the solution $y_\alpha = (\alpha E + \tilde{B})^{-1} \tilde{A}^* f$. The point is that A^+ corresponds to the case $\alpha \to 0$, $\mu_{\min}(\tilde{B}) \ne 0$, while regularization is dealing with a finite value of $\alpha > 0$ and $\mu_{\min}(\tilde{B}) \approx 0$, which leads to an overstatement of $\sigma_{\text{rel}}(\alpha)$ in both cases.

In order to bring the estimate $\sigma_{\text{rel}}(\alpha)$ nearer to the true estimate of $\sigma_{\text{rel}}(\alpha)$, we *truncate* the spectrum of the operator (matrix in the discrete case) $\tilde{B}$ from below, namely, instead of $\mu_{\min}(\tilde{B})$ we use a value $g > \mu_{\min}(\tilde{B})$ and write (6) in the form

$$\sigma_{\text{rel}}(\alpha) \equiv \frac{\| \Delta y_\alpha \|}{\| y \|} \le \varepsilon(\alpha) , \quad (8)$$

where

$$\varepsilon(\alpha) = \frac{\| \tilde{A} \|}{2\sqrt{\alpha}} \eta + \frac{\alpha}{\alpha + g} . \quad (9)$$

It was shown in [1, 2, 4] that the function $\varepsilon(\alpha)$, according to (9), has a (unique) minimum under the condition

$$\frac{\| \tilde{A} \|}{\sqrt{g}} \eta < \frac{3\sqrt{3}}{4} \approx 1.30 . \quad (10)$$

From the condition $\varepsilon'(\alpha) = 0$, we obtain the equation for α (cf. [2, 4])

$$\alpha = \left(\frac{\| \tilde{A} \| \eta}{4g} \right)^{2/3} (\alpha + g)^{4/3} . \quad (11)$$

As shown in [2], in this case $\varepsilon''(\alpha) > 0$, i.e. (11) corresponds to the minimum of the function $\varepsilon(\alpha)$.

According to relations (8) and (9), a relative error estimate $\| \Delta y_\alpha \| / \| y \|$ of regularized solution y_α depends on $\tilde{A}$ and η (more exactly, on the product $\| \tilde{A} \| \eta$). Therefore, if we solve a few examples (e.g., a few spectra are being processed) with the same $\tilde{A}$ and η (spread function and noise), then their error estimates (9) will be identical and nonoverstated (in function of α). It follows that when solving some original example P (i.e. when processing $\tilde{f}_P$) with unknown solution (spectrum) y_P, one can use the results of solving other (model, training) example Q with known (given) exact solution (spectrum) y_Q, with the same $\tilde{A}$ and η as in example P. Furthermore, when solving example Q, one can calculate the function $\sigma_{\text{rel}}(\alpha)_Q = \| \Delta y_{\alpha Q} \| / \| y_Q \|$ and, based on this function, find $\alpha_{\text{opt}\,Q}$ (optimal value of α, at which $\sigma_{\text{rel}}(\alpha)_Q = \min\limits_{\alpha}$). This value $\alpha_{\text{opt}\,Q}$ can be used for solving the original example (spectrum) P.

Estimate of parameter g**.** Furthermore, it is necessary to determine the parameter g, which comes into (9). An estimate of g can be obtained *graphically*, namely, by fitting such value of g, at which envelope $\varepsilon(\alpha)$ contacts curve (or a set of curves) $\sigma_{\text{rel}}(\alpha)_Q$. The value of α corresponding to the contact point we denote as α_g.

Determining g can also be performed *analytically*. Equating $\sigma_{\text{rel}}(\alpha)$ and $\varepsilon(\alpha)$, as well as taking into account the condition $\varepsilon'(\alpha) = 0$, we obtain two equations for two unknowns α and g:

$$\left.\begin{aligned} &\frac{\| \tilde{A} \|}{2\sqrt{\alpha}} \eta + \frac{\alpha}{\alpha + g} = \sigma_{\text{rel}}(\alpha), \\ &\alpha = F(\alpha), \end{aligned}\right\} \tag{12}$$

where, according to (11),

$$F(\alpha) = \chi \left(\alpha + g \right)^{4/3}, \quad \chi = \left(\frac{\| \tilde{A} \| \eta}{4g} \right)^{2/3}. \tag{13}$$

Here, $\sigma_{\text{rel}}(\alpha)$ is the calculated upper curve from a set of curves $\sigma_{\text{rel}}(\alpha)_Q = \| \Delta y_{\alpha Q} \| / \| y_Q \|$. The first equation in (12) is the condition of contact of $\varepsilon(\alpha)$ (according to (9)) and $\sigma_{\text{rel}}(\alpha)$, whereas the second equation is the minimum condition of function $\varepsilon(\alpha)$, i.e. $\varepsilon'(\alpha) = 0$ at the contact point. The first equation can be resolved relatively to g:

$$g = \alpha \cdot \left[\left(\sigma_{\text{rel}}(\alpha) - \frac{\| \tilde{A} \| \eta}{2\sqrt{\alpha}} \right)^{-1} - 1 \right].$$

Then, obtained system of two equations can be solved by iterations:

$$\alpha_0 = \chi, \quad \alpha_i = \chi_{i-1} \left(\alpha_{i-1} + g_{i-1} \right)^{4/3}, \quad \chi_{i-1} = \left(\frac{\| \tilde{A} \| \eta}{4 g_{i-1}} \right)^{2/3},$$

$$g_i = \alpha_i \cdot \left[\left(\sigma_{\text{rel}}(\alpha_i) - \frac{\| \tilde{A} \| \eta}{2\sqrt{\alpha_i}} \right)^{-1} - 1 \right], \quad i = 1, 2, 3 \ldots$$

This iterative process for α converges to some $\alpha = \alpha_g$, since $|F'(\alpha)| < 1$, as follows from (13).

However, since the function $\sigma_{\text{rel}}(\alpha)$ is given in tabular form, it is more convenient to solve the problem *graphically* displaying onto a computer monitor the curves $\sigma_{\text{rel}}(\alpha)$ and $\varepsilon(\alpha)$ at different g. To enhance the efficiency of this method when working out a model example Q (or several examples) it is necessary to use an additional information about the original example (spectrum) P, namely, an estimate of the number of maxima (spectral lines) in the desired solution (spectrum) y_P, ratios of their intensities, values of its abscissa (wavelengths or frequencies), the type of kernel (SF), etc. Such information will be helpful to choose more "successfully" the regularization parameter α and estimate the error of solving the examples (spectra) Q and P.

The modeling method generates a *regularizing algorithm* (RA), since when $\eta \to 0$, $\alpha = o(\eta^2)$ and finite $\| \tilde{A} \|$ and g, we have for original and model examples according to (8) and (9) (cf. [2, 4]):

$$\sigma_{\text{rel}}(\alpha) \equiv \frac{\| \Delta y_\alpha \|}{\| y \|} \to 0,$$

i.e. at zero errors of initial data, the solution y_α turns into the exact solution (normal pseudosolution).

Remark 1. Although the method of modeling (training, learning) requires a lot of preliminary work on drawing up and solving the model (training) examples, it is very effective in cases when it is required to solve a significant number of "close" examples (to resolve signals for a number of times, to restore several similar spectra in the inverse spectroscopy problem, etc.). Moreover, this method gives the possibility to explore practical potentials of the used method and algorithm applied to a particular problem on a number of training examples (to obtain the real solution error, the possibility of restoring the fine solution structure, etc.).

Remark 2. The objection can arise that, because of the ill-posedness of a problem, even small differences of the model problem (example, spectrum) from the original one can lead to significant differences of the regularization parameter α, the relative solution error $\| \Delta y_\alpha \| / \| y \|$, etc. However, firstly, the problem is solved by a stable regularization method and it is the conditionally well-posed (by Tikhonov), and secondly, relations (8) and (9) show that the error estimates for solutions $\| \Delta y_\alpha \| / \| y \|$ are the same for the original and model examples under the condition of identity of $\| \tilde{A} \| \eta$.

An example from spectroscopy

Let us illustrate the foregoing method of modeling (training, learning) by an example from the inverse spectroscopy problem (cf. [8]). The problem is to restore a spectrum via solving the Fredholm integral equation of the first kind (an ill-posed problem)

$$Ay \equiv \int_a^b K(\lambda,\lambda')\, y(\lambda')\, d\lambda' = f(\lambda), \qquad c \le \lambda \le d\ , \tag{14}$$

where $K(\lambda,\lambda')$ is the spread function of a spectral device, $y(\lambda)$ is the true (desired) spectrum, $f(\lambda)$ is the measured (experimental) spectrum, λ is the wavelength, $[a,b]$ are the limits for desired spectrum, $[c,d]$ are the limits for measured spectrum.

We assume that, instead of exact f and K, we have $\tilde{f}$ and $\tilde{K}$ such that $\| \tilde{f} - f \| \le \delta$, $\| \tilde{A} - A \| \le \xi$. Equation (14) is solved by the Tikhonov regularization method according to (2), where $A^* = A^T$.

At first, we consider the *original example P* with known measured noisy spectrum $\tilde{f}(\lambda)$ (Fig. 1) on a uniform grid $\lambda = \lambda_{\min}, \lambda_{\min} + h, \ldots, \lambda_{\max}$, where $\lambda_{\min} = c = 450$ nm, $\lambda_{\max} = d = 650$ nm, $h = \Delta\lambda = \text{const} = 1$ nm is the discretization step, and $n = (\lambda_{\max} - \lambda_{\min})/h = 200$ is the number of discretization steps in λ.

It is assumed that the spread function (SF) $K = K(\lambda,\lambda')$ of spectral device has a variable width, i.e. it is nondifference. As it is known [8, 19], the SF width $\omega(\lambda)$ at level of 0.5 is proportional to wavelength λ. Therefore, we assume $\omega(\lambda) = q\lambda$, where $q = 0.015$. This corresponds to $\omega(c) = \omega(450 \text{ nm}) = 6.75$ nm, $\omega(485 \text{ nm}) = 7.275$ nm, $\omega(620 \text{ nm}) = 9.3$ nm, and $\omega(d) = \omega(650 \text{ nm}) = 9.75$ nm.

We use the dispersion SF

$$K(\lambda,\lambda') = \frac{\omega(\lambda)/2\pi}{(\lambda-\lambda')^2 + [\omega(\lambda)/2]^2}\ . \tag{15}$$

It is shown in [8] that SF of this type gives one of the most accurate restorations of a spectrum. To characterize the SF, along with the width $\omega(\lambda)$ at a level of 0.5, one may also use the integral SF width $W(\lambda)$ (the ratio of the SF area to its height)

$$W(\lambda) = \int_{-\infty}^{\infty} K(\lambda,\lambda')\, d\lambda' \Big/ K(\lambda,\lambda)\ .$$

For a dispersion SF, we have: $W(\lambda) = (\pi/2)\,\omega(\lambda) \approx 1.571\,\omega(\lambda)$.

Figure 1 shows the SF $K(\lambda,\lambda')$ (17) at $\lambda = 485$ and 620 nm.

Analysis of Fig. 1 shows that the true (unknown) spectrum has, most likely, two close lines in the vicinity of $\lambda \approx 525$ nm and near $\lambda \approx 620$ nm, but they are poorly resolved in the measured spectrum $f(\lambda)$. Moreover, there is an indication that there is one weak line at $\lambda \approx 507$ nm, as well as at $\lambda \approx 543$ nm in true spectrum $y(\lambda)$. Thus, everything indicates that there are at least nine spectral lines in the spectrum $y(\lambda)$, although the number of lines in the measured spectrum $f(\lambda)$ is fewer (6 or 7).

In connection with this, the second (model, training) example *Q* "close" to the original *P* was modeled. The true spectrum of example *Q* contains 9 as well as 8 and 10 spectral lines in the form of Gaussian (cf. [3, 8]), i.e. several examples *Q* were modeled.

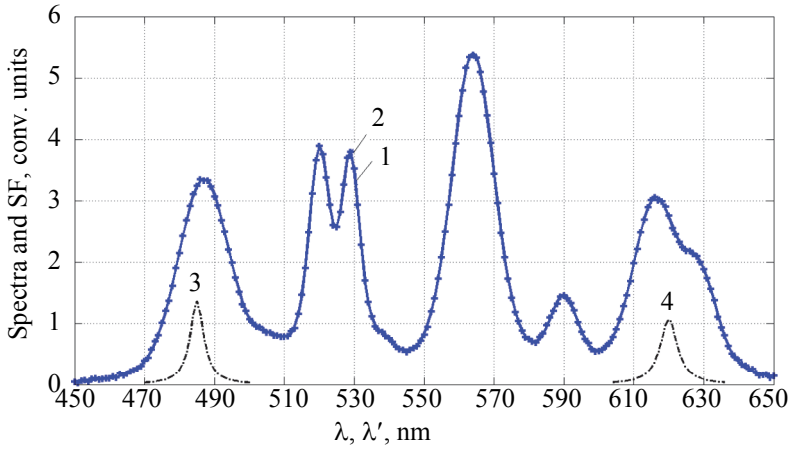

Fig. 1. Example *P*. 1 – exact spectrum $f(\lambda)$; 2 – noisy spectrum $\tilde{f}(\lambda)$ and two cross-sections of SF: 3 – $10K(485,\lambda')$ and 4 – $10K(620,\lambda')$ (conventional units)

The measured spectra $f_Q(\lambda)$ in examples Q were numerically calculated by formula

$$f_Q(\lambda) = \int_a^b K(\lambda,\lambda')\, y_Q(\lambda')\, d\lambda', \quad c \le x \le d\ .$$

Furthermore, $a = 460$ nm, $b = 640$ nm.

The measurement errors δ of the spectrum $f_P(\lambda)$ were estimated at about 1%, which corresponds to the standard deviation (SD) ≈ 0.02. Therefore, the values of $f_Q(\lambda)$ were noisy by random errors with SD from 0.01 to 0.04, which corresponds to $\delta_{\text{rel}} \approx 0.5-2\%$ (because the value δ_{rel} is known inexactly). The SF in example Q was taken in the form (15), moreover (since the SD is also known inexactly), $w(\lambda)$ was taken to be $w(\lambda) = q(1+\zeta)\lambda$, where $\zeta \in [-0.02, 0.04]$, which corresponds to $\xi_{\text{rel}} \approx 0-4\%$.

Further, the "close" model examples Q were solved by the quadrature method with Tikhonov regularization via solving equation (2) at SF (15) for several values of the regularization parameter α. The dependence of the relative error of regularized solutions $y_\alpha(\lambda) = y_{\alpha Q}(\lambda)$ was calculated with respect to exact solutions $y(\lambda) = y_Q(\lambda)$:

$$\sigma_{\text{rel}}(\alpha) = \frac{\| y_\alpha(\lambda) - y(\lambda) \|}{\| y(\lambda) \|}\ .$$

Figure 2 shows dependences $\sigma_{\text{rel}}(\alpha)_Q$ for series of "close" model examples and for several values of errors $\delta_{\text{rel}} = \delta/\| f \|$ and $\xi_{\text{rel}} = \xi/\| A \|$ (the region between the curves 1 and 2). Note that the curve 3 in the modeling method is supposed to be unknown; it is given for illustration only.

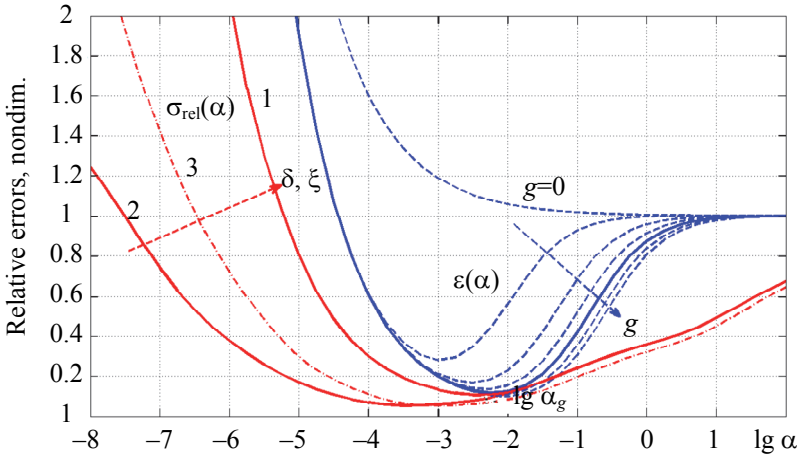

Fig. 2. Relative errors $\sigma_{\text{rel}}(\alpha)$ for examples Q (1 and 2 – the boundaries above and below, 3 – $\sigma_{\text{rel}}(\alpha)_P$) and envelope curves $\varepsilon(\alpha)$ for several values of parameter *g* (non-dimensional)

Figure 2 shows also several envelopes $\varepsilon(\alpha)$ according to (9) at $\| \tilde{A} \| = \| A \| = 0.843$ and $\eta = \delta_{\text{rel}} + \xi_{\text{rel}} = 2 \cdot 10^{-2}$ for several values g from 0 to 0.1. We choose such value g at which the condition (10) is satisfied and one of the curves $\varepsilon(\alpha)$ contacts the set of curves $\sigma_{\text{rel}}(\alpha)$, namely, $g = 0.045$. This corresponds to regularization parameter $\alpha = \alpha_g = 10^{-2.2}$. It is seen from Fig. 2 that, despite the scatter of curves $\sigma_{\text{rel}}(\alpha)$ and $\varepsilon(\alpha)$, the value of g and, as a consequence, α are estimated reliably.

Figure 3 shows solution (restored spectrum) at $\alpha_g = 10^{-2.2}$, $\sigma_{\text{rel}}(\alpha_g) = 0.073 = 7.3\%$. We can see that the spectrum is restored accurately: close lines are resolved and weak lines are separated.

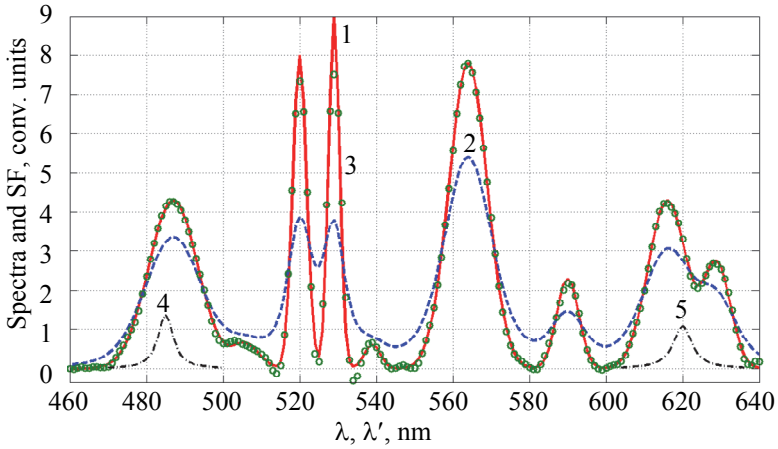

Fig. 3. Example *P*. 1 – true spectrum $y_P(\lambda)$; 2 – measured spectrum $f_P(\lambda)$; 3 – restored spectrum $y_{\alpha P}(\lambda)$ at $\alpha = \alpha_g = 10^{-2.2}$ and two cross-sections of SF: 4 – $10K(485,\lambda')$ and 5 – $10K(620,\lambda')$ (conventional units)

Remark 3. Although we assume in the modeling method that the exact spectrum (solution) $y(\lambda)$ is unknown in original example *P*, we adduce the exact spectrum $y_P(\lambda)$ (Fig. 3) to demonstrate the potential possibilities of a technique. However, the spectrum $y_P(\lambda)$ is not used for choosing α_g.

Conclusion

There are a number of ways for choosing the regularization parameter α and estimating error $\| \Delta y_\alpha \|$ for regularized solution y_α. We should note the discrepancy principle [18], the generalized discrepancy principle [9], the modified discrepancy principle (the Raus–Gfrerer rule) [20], the cross-validation method [21], the L-curve criterion [22], the local regularizing algorithm [23], the new criterion of a posteriori choosing [15], the adaptive specialized generalized discrepancy principle [13], the new version of a posteriori choosing [16, 17], etc.

The errors δ and ξ (as well as sourcewise representability of the solution) are usually used in these methods as the additional information about the solution. As a result, the regularization parameter α at finite δ and ξ is chosen reliably (but with some overstatement in comparison with α_{opt}). Furthermore, the solution error $\| \Delta y_\alpha \|$ is obtained mainly in the form of asymptotic estimates, and the estimate $\| \Delta y_\alpha \|$ at finite δ and ξ is usually obtained with a large overstatement (see. Fig. 2, the curve $g = 0$).

We have developed a method of model (training, learning) examples, that gives the possibility to choose α and, most importantly, to obtain nonoverstated error estimate $\| \Delta y_\alpha \|$ (see Fig. 2, the contact of curves $\sigma_{\text{rel}}(\alpha)$ and $\varepsilon(\alpha)$ at $\alpha = \alpha_g$, as well as Fig. 3, the curve $y_{\alpha P}(\lambda)$). The method of modeling or training has been applied to solving the inverse spectroscopy problem (restoration of a fine spectrum structure by solving an integral equation with the use of an experimental spectrum and the spread function of a spectral device). The method has enabled to resolve close lines and to select weak lines. The proposed technique can be used for restoration of smoothed and noisy spectra, i.e. for enhancement of the resolving power of spectral devices by mathematical and computer processing of experimental spectra.

References

1. Sizikov V.S. Application of modelling for solution of ill-posed problems // Electronic Modeling. 1981. N 6. P. 3–8 (in Russian).
2. Sizikov V.S. Generalized method for measurement data reduction. I. Processing of tonal (narrow-band) signals // Electronic Modeling. 1992. V. 13. N 4. P. 618–633.

3. Sizikov V.S. Generalized measurement reduction method. III. Results of numerical simulation // Electronic Modeling. 1993. V. 13. N 6. P. 1023–1035.
4. Verlan' A.F., Sizikov V.S. Integral Equations: Methods, Algorithms, Programs. Kiev: Nauk. Dumka, 1986. 544 p. (in Russian).
5. Sizikov V.S. Inverse Applied Problems and MatLab. St. Petersburg: Lan' Publ., 2011. 256 p. (in Russian).
6. Sizikov V.S. Integral Equations and MatLab in Tomography, Iconics, and Spectroscopy Problems. St. Petersburg-Saarbrücken: LAP, 2011. 252 p. (in Russian).
7. Verlan' A.F., Sizikov V.S., Mosentsova L.V. Method of computation experiments for solving integral equations in the inverse spectroscopy problem // Electronic Modeling. 2011. V. 33. N 2. P. 3–12 (in Russian).
8. Sizikov V.S., Krivykh A.V. Reconstruction of continuous spectra by the regularization method using model spectra // Optics and Spectroscopy. 2014. V. 117. N 6. P. 1010–1017. doi: 10.1134/S0030400X14110162
9. Tikhonov A.N., Goncharsky A.V., Stepanov V.V., Yagola, A.G. Numerical Methods for the Solution of Ill-Posed Problems. Dordrecht: Kluwer, 1995. 232 p.
10. Voskoboinikov Yu.E., Preobrazhenskii N.G., Sedel'nikov A.I. Mathematical Processing of Experiment in Molecular Gas Dynamics. Novosibirsk: Nauka, 1984. 240 p. (in Russian).
11. Engl H.W., Hanke M., Neubauer A. Regularization of Inverse Problems. Dordrecht: Kluwer, 1996. 328 p.
12. Petrov Yu.P., Sizikov V.S. Well-Posed, Ill-posed, and Intermediate Problems with Applications. Leiden-Boston: VSP, 2005. 234 p.
13. Leonov A.S., Yagola A.G. Adaptive optimal algorithms for ill-posed problems with sourcewise represented solutions // Computational Mathematics and Mathematical Physics. 2001. V. 41. N 6. P. 807–824.
14. Bakushinsky A., Goncharsky A. Ill-Posed Problems: Theory and Applications. Dordrecht: Kluwer, 1994. 268 p.
15. Kojdecki M.A. New criterion of regularization parameter choice in Tikhonov's method // Biuletyn WAT (Biul. Mil. Univ. Technol.). 2000. V. 49. N 1(569). P. 47–126.
16. Sizikov V.S. On discrepancy principles in solving ill-posed problems // Computational Mathematics and Mathematical Physics. 2003. V. 43. N 9. P. 1241–1259.
17. Sizikov V.S. Further development of the new version of a posteriori choosing regularization parameter in ill-posed problems // International Journal of Artificial Intelligence. 2015. V. 13. N 1. P. 184–199.
18. Morozov V.A. Methods for Solving Incorrectly Posed Problems. New York: Springer, 1984. 240 p.
19. Starkov V.N. Constructive Methods of Computational Physics in Interpretation Problems. Kiev: Nauk. Dumka, 2002. 264 p. (in Russian).
20. Gfrerer H. An a posteriori parameter choice for ordinary and iterated Tikhonov regularization of ill-posed problems leading to optimal convergence rates // Mathematics of Computation. 1987. V. 49. N 180. P. 507–522.
21. Golub G.H., Heath M., Wahba G. Generalized cross-validation as a method for choosing a good ridge parameter // Technometrics. 1979. V. 21. N 2. P. 215–222.
22. Hansen P.C., O'Leary D.P. The use of the L-curve in the regularization of discrete ill-posed problems // SIAM Journal of Scientific Computing. 1993. V. 14. N 6. P. 1487–1503.
23. Voskoboinikov Yu.E., Mukhina I.N. Local regularizing algorithm for high-contrast image and signal restoration // Optoelectronics, Instrumentation and Data Processing. 2000. N 3. P. 41–48.

Valery S. Sizikov – D.Sc., Professor, Professor, ITMO University, Saint Petersburg, 197101, Russian Federation, sizikov2000@mail.ru

Andrey V. Stepanov – D.Sc., Professor, Head of Chair, Vernadsky Crimean Federal University, Simferopol, 95342, Russian Federation, abc17101@yandex.ua

Сизиков Валерий Сергеевич – доктор технических наук, профессор, профессор, Университет ИТМО, Санкт-Петербург, 197101, Российская Федерация, sizikov2000@mail.ru

Степанов Андрей Валерьевич – доктор технических наук, профессор, заведующий кафедрой, Крымский федеральный университет им. В.И. Вернадского, Симферополь, 95342, Российская Федерация, abc17101@yandex.ua