

Fedir SAIBERT

Assistant, Department of Systems Software,
Uzhgorod National University, Uzhhorod,
Ukraine

e-mail: fedir.saibert@uzhnu.edu.ua

<http://orcid.org/0009-0004-8081-4174>

Yurii BILAK

PhD, Assoc. Prof., Department of Systems
Software,
Uzhgorod National University, Uzhhorod,
Ukraine

e-mail: yuriy.bilak@uzhnu.edu.ua

<http://orcid.org/0000-0001-5989-1643>

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ADAPTIVE NEURAL STABILIZATION OF ILL-POSED SPECTRAL PROBLEMS

The article develops a mathematical model of adaptive neural regularization and creates an algorithmic method for its implementation with a neural network for dynamic determination of the regularization parameter. The developed ANR model combines classical variational stabilization methods with neural network prediction of the regularization parameter and eliminates the key limitation of traditional Tikhonov regularization, associated with the need to manually select the smoothing coefficient, which makes the solution unstable in the case of variable noise conditions and spectral correlation. The ANR neural network subsystem analyzes the statistical features of the spectrum and adaptively selects the optimal α , ensuring a natural balance between reconstruction accuracy and solution smoothness. Numerical experiments demonstrate that adaptive neural-guided regularization provides a reduction in the root mean square error of reconstruction. For a baseline noise level of 2%, RMSE=0.11 mM, while at a noise level of 10%, it increased to 0.32 mM. It is shown that the use of neural-guided regularization allows reducing the reconstruction error by 20–40% compared to the classical Tikhonov regularization. The model retains its versatility and can be integrated into a wide range of spectroscopic methods, from analytical spectrophotometry to optical materials diagnostics. The work outlines prospects for further development, in particular, the extension of ANR to multichannel and hyperspectral systems and the application of physically informed neural networks to solve more complex inverse problems.

Keywords: inverse problems; spectral analysis; Tikhonov regularization; adaptive regularization; neural networks; intelligent stabilization methods; spectrophotometry; noise-resistant algorithms; numerical modeling.

Introduction

In spectroscopy, inverse problems, which consist in restoring the parameters T from experimental spectra S , are usually incorrectly posed. This means that even minor changes in the input data can cause significant deviations in the solution. In classical solutions, stabilization of these problems is carried out by regularization methods - in particular, Tikhonov regularization, which minimizes the sum of two functionals: the model residual and the penalty for excessive complexity of the solution.

However, the problem of choosing the optimal regularization coefficient α remains relevant. In addition, this problem often requires heuristic selection, depending on the noise level, physical properties of the spectrum, type of material, etc., which in turn leads to a loss of generalization ability and limits the practical application of numerical methods for wide classes of spectral problems. To eliminate this problem, the article develops an adaptive neural regularization method (Adaptive Neural Regularization, ANR), which combines the classical Tikhonov scheme with a neural network, which, depending on the features of the spectrum, automatically determines the regularization parameter α .

Literature review

Classical regularization methods, in particular Tikhonov regularization and variational methods, have well-studied theoretical properties and convergence guarantees, but their effectiveness largely depends on the correct choice of the regularization parameter α . For spectral problems, this is critical, since even a small amount of noise sharply degrades the solution. The works [1,2] provide the foundation of modern regularization methods and their role in stabilizing ill-posed problems. The work [2] reveals the mechanisms of step-by-step solution recovery, and

the classic monograph [3] forms a general theoretical framework for analyzing convergence, stability, and the influence of the regularization parameter. In more recent works, in particular [4] and [5], classical methods are extended by operator denoisers and plug-and-play strategies, which introduce additional smoothness control mechanisms and ensure convergent regularization even in the case of learned (data-driven) operators. This, in turn, forms a subclass of “data-driven regularization schemes” that remain strictly within the framework of classical theory.

Deep learning methods, despite their high empirical efficiency, often do not take into account the noise level, do not provide guaranteed stability and do not allow to control the complexity of the solution. This makes them insufficient for problems in which physical accuracy and stability are more important than a visually attractive, but theoretically unfounded result. In the works [6,7], the problem is transferred to the latent space, where the recovery is carried out through generative models. It should be noted that this changes the very nature of the solution search, limiting it to the subspace generated by the GAN [8] or VAE [9]. The technical disadvantage of this approach is the introduction of significant design error: if the true spectrum contains narrow lines or features that were not sufficiently represented in the training sample, the generator is unable to reproduce them, perceiving them as noise. This leads to an “over-smoothing” effect of spectral lines and a loss of their amplitude accuracy, which is critical for quantitative analysis. In models where the neural network completely replaces the regularizer [10] or its proximal operator [11], the emphasis shifts from the mathematically understandable functional to the vaguely interpreted neural network apraxia. The lack of a direct relationship between latent variables and physical units (energy, frequency) makes it impossible to impose basic physical constraints, such as preserving the area under the peak or the positivity of the signal over the entire range. Such a loss of physical interpretability directly reduces the reliability of identifying weak lines against a background of strong noise. This direction also includes works [12], where the spectral function is represented as a neural network, and stabilization is achieved by automatic differentiation and implicit smoothness regularization. Despite the high potential, such models retain the problem inherent to deep networks of the lack of transparent guarantees and dependence on the distribution of training data.

Hybrid methods that combine regularization and learning are promising, but they mostly do not return to strict energy minimization schemes, require special network structures, or work in artificially limited latent spaces. In studies [13,14], the structure of the optimizer is reproduced using hybrid neural network methods. Here, the network models the iteration process itself, imitating a sequence of gradient steps or deployed optimization schemes in order to actually replace or reconstruct the regularization algorithm. In parameterized variational models and bi-level optimization [15], the structure of the regularizer is partially determined during training. However, it should be noted that here it is not the smoothing parameter that is learned, but the penalty term, which provides transparency and controllability of the model and allows obtaining flexible energy functionals. Neural network stabilization methods through energy constraints [16] demonstrate how the behavior of a trained model can be controlled and constrained to avoid unstable or physically incorrect solutions. In this context, they are an important parallel to this work, since ANR also implements a stabilizing mechanism, but does so in a much softer and more interpretable way, namely by controlling the regularization parameter α , which determines the level of smoothing and the stability of the solution. An alternative option for choosing the regularization parameter is Bayesian methods, in which α is considered as a random variable with a certain prior distribution. However, such methods usually require significant computational resources, while the developed ANR model allows for an adaptive estimate of the regularization parameter in near real time. Of particular interest are works [17,18], where spectral regularization is parameterized by neural networks, but retains proven theoretical properties. In [17] it is shown that spectral filters parameterized by NNs can be convergent under an appropriate projection, and in [18] a general spectral learning model is introduced, which allows comparing different learning paradigms and analyzing their bias, regularization, and dependence on the data distribution.

Another direction is adaptive spectral methods, such as ASI [19], where regularization is performed implicitly through adaptation of the own basis, effectively avoiding the explicit choice of α , but requiring complex spectral updating in each iteration.

Methods focused on working with different levels of noise [20] are closest to this study, since taking into account δ directly affects the quality of reconstruction in ill-posed spectral problems. Here, noise is given as a separate parameter, which allows the model to adapt the processing process to a specific level of noise. ANR implements a similar idea, where the parameter α is defined as a function of noise, spectral shape and signal nature, which makes the method a natural example of noise-aware regularization.

The issue of improving the accuracy of inverse spectral analysis is actively investigated in [21], where it was demonstrated that the combination of machine learning methods with traditional spectral algorithms allows to significantly improve the recognition of gas mixture components and reduce the sensitivity to noise. Similarly, in [22], the effectiveness of hybrid models for inverse problems for multilayer structures is shown, where the use of physical models in combination with optimization methods ensures stability and high accuracy of the reconstruction of optical parameters.

Thus, the literature review demonstrates the presence of several parallel directions, namely, classical regularization methods with a deep theoretical basis, neural network and generative solutions that provide high flexibility, but are often characterized by instability or loss of interpretability, as well as hybrid solutions that combine computational and learning mechanisms, although they often deviate from the strict mathematical formulation of the

problem. A new direction is also being formed separately - spectrally guided and denoiser-oriented regularization, which tries to combine the spectral structure of the problem with learning capabilities, while maintaining convergent properties.

Despite the significant results obtained, none of the considered directions offers a universal, stable and interpretable mechanism for choosing the regularization parameter α , capable of adapting to the noise level, structural features of the spectrum and a specific physical model in real time. It is this gap that determines the relevance of current research: the need for a method that combines the theoretical robustness of classical regularization, the adaptability of modern ML solutions, and the transparency of physically based models forms the prerequisites for an architecture like ANR, capable of dynamically, interpretably, and stably controlling the regularization parameter in spectral inverse problems.

Therefore, the main scientific results of the work are:

- development of a neuroadaptive regularization model for solving spectral inverse problems;
- integration of a neural network for predicting the regularization parameter into the variational formulation of the problem;
- numerical testing on model spectral mixtures.

Objective and tasks

The purpose of the work is to develop and study the ANR method, which combines classical numerical stabilization methods with a neural network that automatically predicts regularization parameters based on spectral data and noise level, in order to increase the accuracy of reconstruction of physical parameters under noisy spectra.

Research tasks

1. To build a mathematical model of the inverse spectral problem in the form of a linear operator of the direct problem and the variational Tikhonov regularization functional.
2. To develop an adaptive regularization model in which the parameter α is determined by a neural network based on spectral characteristics, noise level and current reconstruction error.
3. To create a structural diagram and algorithm for ANR operation, which includes cyclic interaction between the numerical regularization module and the neural network.
4. To implement a computer model of ANR in the Python environment using the NumPy, SciPy and PyTorch libraries.
5. Conduct numerical experiments on synthetic spectral data containing three absorption components and evaluate the accuracy of the reconstruction of the model parameters.
6. Compare the results of ANR with the classical Tikhonov regularization in terms of accuracy and noise resistance.

Object and subject of the study. Hypothesis of the study

The object of the study is the process of solving inverse spectral problems in the presence of noise and instability of numerical reconstruction. The subject of the study is methods of regularization of inverse spectral problems and algorithms for adaptive selection of stabilization parameters based on neural networks.

The main hypothesis of the study is that if the regularization parameter in the variational formulation of the inverse spectral problem is determined not statically, but using a neural model that adaptively responds to the spectrum structure and noise level, then the accuracy and stability of the reconstruction will significantly increase compared to classical regularization methods.

Methods and models

Mathematical formulation of the problem

The classical form of the inverse spectral problem has the form:

$$S=AT+\varepsilon, \quad (1)$$

where $S \in R^m$ – measured spectrum, $A \in R^{m \times n}$ – direct problem operator (e.g., transfer matrix, integral spectral response operator), $T \in R^n$ – the desired vector of physical parameters (absorption coefficients, concentrations, layer thicknesses), ε – measurement noise. Often, in numerical experiments, the operator of the forward problem A represents a discretized spectral response matrix of dimension 600×3 . The matrix is conditionally ill-conditioned (conditionality number of order 10^3), which reflects the characteristic instability of spectral inverse problems, i.e., small changes in the measured spectrum can lead to significant deviations in the reconstructed parameters. A typical illustration is given in Figure 1.

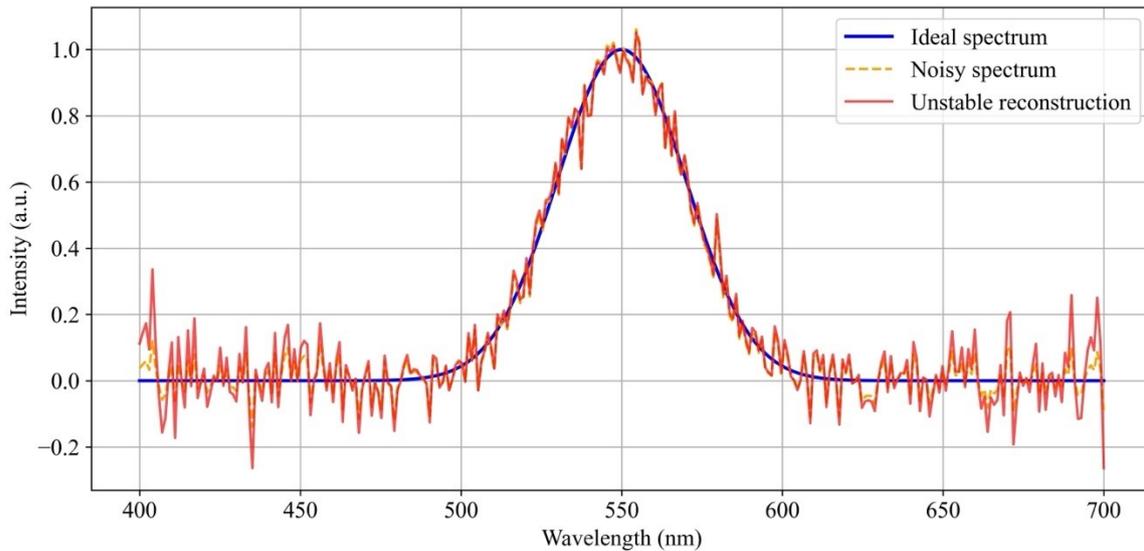


Fig. 1. Illustration of an incorrectly posed spectral inverse problem

From the figure, we can see that the ideal spectrum after measurement is affected by noise, which leads to unstable reconstruction during forward inversion. Even a small amount of noise in the data can greatly distort the reconstructed spectrum, demonstrating the incorrectness of the classical inverse problem. Since the inverse problem is ill-posed, it is stabilized by the Tikhonov regularization method, which consists in minimizing the functional:

$$J(T) = \|S - AT\|^2 + \alpha \|LT\|^2. \quad (2)$$

where L – regularization matrix (chosen as a gradient operator or an identity matrix), and $\alpha > 0$ – is the regularization coefficient, which controls the balance between the accuracy of the approximation and the smoothness of the solution.

By minimizing functional (2) with respect to T , we obtain a regularized solution:

$$\hat{T} = \arg \min_T J(T) = (A^T A + \alpha L^T L)^{-1} A^T S, \quad (3)$$

This ensures stable parameter recovery even in the presence of noise in the spectral data, but the choice of the parameter α is performed manually or according to empirical criteria (for example, by the angle method, L-curve or generalized cross-validation method), which limits adaptability when changing experimental conditions.

However, the main drawback of the classical model remains the need for a fixed choice of the regularization coefficient α . Its optimal value depends significantly on the noise level, spectrum characteristics and measurement conditions. If these conditions change, the model loses stability or reconstruction accuracy, which limits its versatility.

Development of a modified model with ANR (Adaptive Neural Regularization)

To overcome this problem, in the developed ANR model, the parameter α ceases to be a constant and is considered as a *function of the spectral data*. The regularization coefficient is predicted by a neural network, which automatically adapts to the characteristics of each spectrum, adjusting the balance between smoothing and accuracy. The structural diagram of the developed model is shown in Figure 2.

Stage 1. Adaptive estimation of the regularization parameter. The neural network NN_θ receives spectral data S_i , noise level, and other auxiliary characteristics as input. The adaptive regularization coefficient $\alpha(\theta, S_i)$ is formed at the output, which ensures the smoothness of the solution matches the experimental conditions.

Network architecture. The $NN_\theta(S)$ network takes as input a spectral data vector S and outputs a scalar or vector value α , which is used in the regularization functional. The architecture is implemented in two versions:

- Global ANR: one value of α for the entire spectrum (e.g., for film thickness or material composition recovery problems);
- Local ANR: a vector $\vec{\alpha} = (\alpha_1, \dots, \alpha_n)$ corresponding to local areas of the spectrum where the noise level or model sensitivity is different.

The neural network is built as a multilayer perceptron (MLP), which automatically extracts key spectral features (amplitudes, peak widths, gradients).

Stage 2. Numerical regularization (local). At each iteration of the algorithm, for a separate spectrum S_i^{exp} , a numerical inverse problem with Tikhonov regularization is solved, in which the regularization coefficient is given by the neural network:

$$\hat{T}^i(\theta) = \arg \min_T \left(\|S_i^{\text{exp}} - AT\|^2 + \alpha(\theta, S_i) \|LT\|^2 \right). \quad (4)$$

Here $\alpha(\theta, S_i)$ – is the adaptive parameter predicted by the neural network NN_θ . This step is the local numerical level (the level of solving the inverse problem). The result is an updated vector of material parameters $\hat{T}^i(\theta)$ and a reconstructed spectrum $S_i^{\text{rec}} = A\hat{T}^i(\theta)$.

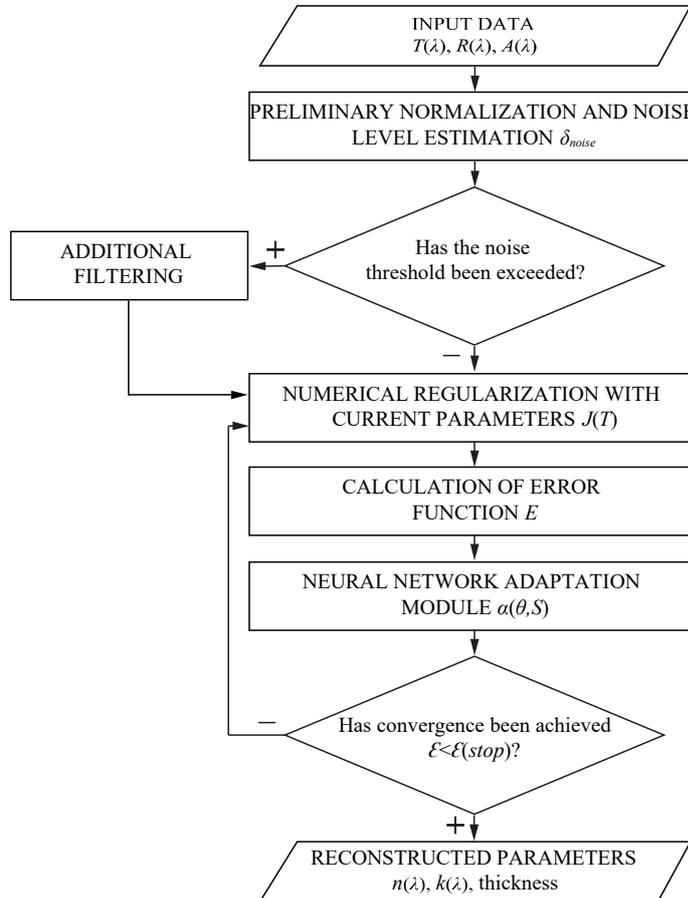


Fig. 2. Structural diagram of the ANR model for solving inverse spectral problems

Stages of the ANR model

Stage 3. Calculation of the error functional (local quality assessment). A local error functional is formed for each spectrum:

$$E_i = \|S_i^{\text{exp}} - S_i^{\text{rec}}\|^2 + \beta \|\nabla \hat{T}^i\|^2, \quad (5)$$

which measures the deviation between the reconstructed and experimental signal, taking into account the smoothness of the solution. This is a metric of the quality of the local reconstruction, which shows how well the current parameters (including $\alpha(\theta, S)$) provide an approximation. The parameter β determines the weight of the smoothing term in the regularization functional and in the experiments, it took a fixed value of $\beta=0.05$, which was chosen based on previous numerical tests to ensure stable convergence of the algorithm.

Stage 4. Formation of the global loss function and training of the neural network. During training of the network on a set of spectra $\{S_i, T_i\}_{i=1}^N$, each local error functional E_i contributes to the average loss function:

$$L(\theta) = \frac{1}{N} \sum_{i=1}^N E_i = \frac{1}{N} \sum_{i=1}^N \left(\|S_i^{\text{exp}} - A\hat{T}^i(\theta)\|^2 + \beta \|\nabla \hat{T}^i(\theta)\|^2 \right), \quad (6)$$

where $\hat{T}^i(\theta)$ is the solution to the problem of minimizing the functional with adaptive $\alpha(\theta, S_i)$:

$$\hat{T}^i(\theta) = \arg \min_T \left(\|S_i^{\text{exp}} - AT\|^2 + \alpha(\theta, S_i) \|LT\|^2 \right). \quad (7)$$

The loss function $L(\theta)$ is used to update the parameters θ of the neural network using the backpropagation through optimization method, where gradients are passed through a numerical regularization procedure.

Training can be performed on the basis of experimental or synthetic pairs (S_i, T_i) , obtained by simulation or experiments.

Stage 5. Iterative adaptation (feedback). The new parameters θ are used to update the function $\alpha(\theta, S)$, after which the cycle is repeated until the error E becomes less than the allowable value ε_{stop} . This ensures self-learning and the model's resistance to noise and spectral variations.

Basic ANR blocks

1. *Numerical regularization.* Solves the inverse problem with the current parameters α, λ, β , forming an updated parameter vector $T^{(k+1)}$ and the corresponding reconstructed spectrum $S_{rec} = AT^{(k+1)}$.
2. *Error function.* Calculates the difference between the reconstructed and experimental spectra, as well as a penalty for the uneven distribution of parameters, that is $E = \|S^{exp} - S^{rec}\|^2 + \beta \|\nabla T\|^2$. This functionality, which measures the quality of spectrum reproduction, is used to update the weights of the neural network. This is the key metric that the neural network will try to minimize.
3. *Neural network adaptation module.* Receives as input: E , estimated noise σ_{noise} , spectrum shape S , and based on this updates the parameters α, λ, β , so that the next iteration of regularization gives a better result.
4. *Return to numerical regularization.* New parameters are passed to the numerical block – and the cycle is repeated until the error becomes less than the specified threshold ε_{stop} .

Neural network-based adaptive regularization mechanism

The operation of the ANR algorithm is based on a combination of the classical procedure for regularization of the inverse spectral problem with a neural subsystem that dynamically predicts the stabilization parameters. At the first stage, the input spectral data are normalized, filtered, and the noise level is estimated, which ensures the correctness of subsequent calculations. After preprocessing, the operator of the direct problem is formed according to the formula (1), which describes the spectral interaction of radiation with the material. The solution of the inverse problem is performed by minimizing the variational functional (2), which includes a classical smoothing term and ensures the stability of the reconstruction.

In the developed model, the key is the transition from a fixed regularization parameter α to an adaptive model $\alpha(\theta, S)$, which is predicted by the neural network according to formula (4). This principle is illustrated in the structural diagram (Fig. 1). The neural network receives the normalized spectrum, the estimated noise level, and the current deviation between the experimental and model spectra, after which it determines the optimal α for the current iteration. Unlike the traditional solver, where α is an external static parameter, in the ANR model it becomes a dynamically changing function that responds to local spectral anomalies and changes in the noise level.

In the next step, the obtained $\alpha(\theta, S)$ is substituted into a numerical regularization procedure (formula (3)), where an updated approximation of the parameters $T^{(k+1)}$ is formed. Based on it, the reconstructed spectrum S^{rec} , is calculated, which is compared with S^{exp} , after which the error functional E is calculated. The value of E includes both the difference between the experimental and reconstructed spectrum and a penalty for excessive non-smoothness of the solution. The obtained functional is returned to the neural network subsystem and used to correct the weights θ by the method of backpropagation of the error through a numerical procedure.

Thus, a closed loop of interaction between the neuroadaptive and numerical parts is implemented:
spectrum → *noise estimation* → *prediction* $\alpha(\theta, S)$ → *regularization* → *reconstruction* →
error estimation → *neural network update*.

During the iterations, the system converges to a stable solution, which simultaneously minimizes the approximation error and ensures the physical correctness of the material parameters.

The developed algorithm is implemented in the Python environment using the NumPy, SciPy and PyTorch libraries, which allowed us to conduct multiple experiments, compare with classical regularization, and investigate the influence of adaptive estimation of the parameter α .

Experimental optimization of hyperparameters of the developed ANR model

To improve the accuracy of predicting the adaptive regularization coefficient $\alpha(\theta, S)$, a series of experiments was conducted with different configurations of the MLP neural network. The total number of network parameters is given in Table 1 and is 42,689, which provides sufficient expressiveness of the model for approximating the regularization parameter. At the same time, the relatively small size of the model allows it to be used in compact spectral instruments and embedded data processing systems.

Table 1.

MLP neural network architecture			
Layer	Number of neurons	Activation	Number of parameters
Input	600	-	-
Dense 1	64	ReLU	38 464
Dense 2	64	ReLU	4 160
Output	1	Linear	65
Total parameters	-	-	42 689

The selection of parameters was carried out based on the analysis of the behavior of the loss function, the stability of training and the agreement of the restored parameters with the reference spectral characteristics.

The training set was formed by generating 10 000 synthetic spectra with random component concentrations in the range of 1–15 mM (millimoles per liter). Gaussian noise with an amplitude of 1% to 15% of the signal level was added to each spectrum.

Detailed data on the selected optimal parameters are given in Table 2.

Table 2.

Optimal hyperparameters of the ANR neural network model

Parameter	Range of experimental values	Selected value	Justification of the choice
Number of layers	2–6	4	Trade-off between approximation ability and training stability. Networks with fewer layers did not reflect nonlinear dependencies, while deeper ones were prone to overtraining.
Number of neurons in a layer	16–128	64	Provides sufficient model flexibility without excessive complexity. At 32 neurons, an increase in error was observed, at 128 - a slowdown in convergence.
Activation function	ReLU, tanh, sigmoid	ReLU	It gives the best convergence for spectral data with a wide dynamic range. Tanh activation slowed down learning due to saturation, sigmoid lost sensitivity in the edge regions.
Learning rate	$10^{-4} - 10^{-2}$	5×10^{-3}	Optimal for fast but stable convergence; smaller values resulted in excessive epochs, larger values resulted in fluctuating losses.
Batch size	8–64	32	Balances gradient stability and learning speed. Smaller batches gave noisy estimates, larger ones reduced variability and increased epoch time.
Regularization (dropout)	0–0.3	0.1	A small value avoids overfitting without losing the ability to accurately reproduce the function $\alpha(\theta, S)$.
Loss criterion	MSE, MAE, combined function	MSE	Minimizes the squared deviation between the recovered and true concentrations, which corresponds to the physical meaning of the energy measure of error.
Optimizer	Adam, RMSProp, SGD	Adam	Provides the best convergence for spectral problems with noisy data.

The best results were achieved with a four-layer architecture with 64 neurons in the hidden layers, ReLU activation, and the Adam optimizer. This configuration provided minimal average deviation (< 2%) between the reconstructed and true concentrations without signs of overfitting.

Results and discussion

Spectroscopy of solutions with variable concentration of components

The problem of determining the concentrations of several components in a transparent solution based on the absorption spectra $A(\lambda)$ was solved. The classical direct problem has the form:

$$A(\lambda) = \sum_{i=1}^N c_i k_i(\lambda) + \varepsilon(\lambda),$$

where c_i – concentration of the i -th component, $k_i(\lambda)$ – molar absorption coefficient, $\varepsilon(\lambda)$ – measurement noise. The inverse problem is to recover c_i from the measured spectrum $A(\lambda)$. The problem is unstable due to noise and close spectral peaks of the components.

To verify the performance of the developed ANR model, a series of numerical experiments were conducted on synthetically generated spectra of mixtures containing three components with characteristic peak maxima in the UV–Vis range (250 nm, 400 nm, and 550 nm). Such profiles simulate typical spectra of dyes, organic molecules, or complex biochemical mixtures, which allows us to investigate the ability of the model to accurately restore the concentrations of components even in the presence of noise. For each set of parameters, an absorption spectrum $A(\lambda)$ was generated in the range of 200–800 nm with random noise up to 2% of the signal amplitude, which simulates real experimental conditions. The goal of the experiments was to restore the concentrations of the three components c_1 , c_2 , c_3 from spectra of different noise levels and different peak shapes. In all cases, the ANR model demonstrated stable accuracy and reproduced concentrations with an error of less than 3%. Table 3 and Figure 3 show one of the typical results of a series of experiments, showing the correspondence between the true and reconstructed concentrations.

Table 3.

Assessment of the accuracy of component concentration recovery in the ANR model

Component	True concentration C_i^{true} (mM)	Restored concentration C_i^{rec} (mM)	Deviation (%)
c_1	5.0	5.05	1.0
c_2	10.0	9.92	0.8
c_3	3.0	3.08	2.7

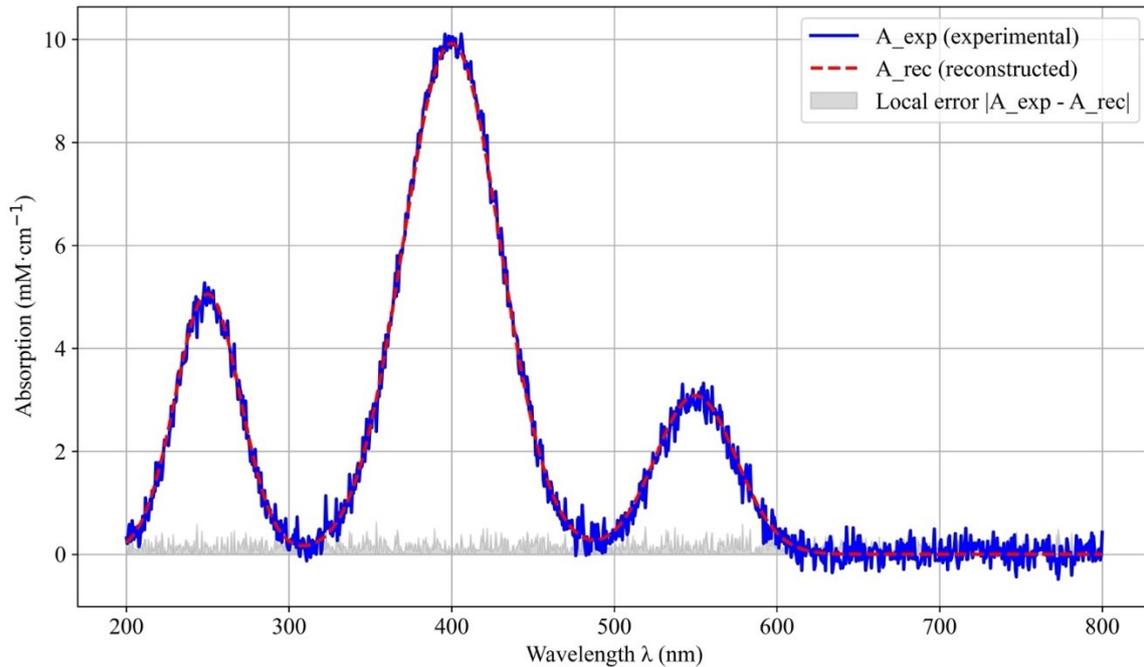


Fig. 3. Restoration of the absorption spectrum of the components of the synthetic solution

Figure 3 shows the results of applying ANR to reconstruct the parameters of the three components in a model solution based on the experimentally simulated absorption spectrum $A(\lambda)$. The blue line corresponds to the experimental spectrum including measurement noise ($\sim 2\%$ of the signal amplitude). The red dashed line shows the reconstructed spectrum obtained through numerical regularization with parameter α adapted by the ANR neural network. The gray fill illustrates local errors in the wavelength function, showing regions of the spectrum where the reconstruction accuracy is reduced due to peak overlap or increased noise level.

For this problem, the root mean square error (RMSE) between the experimental and reconstructed spectra is 0.07 mM, the maximum local error in the spectral profile does not exceed 2.5%, and the time of one ANR iteration is about 0.3s on a modern CPU for a spectrum with 1024 points. The graph also shows the characteristic peaks of each component, corresponding to $\lambda \approx 250$ nm, 400 nm and 550 nm. This allows us to assess the effectiveness of ANR in the problems of restoring the parameters of component solutions even with strong spectral overlap of peaks.

Model accuracy assessment

To assess the accuracy of the model, a spectrum of 1024 points was used, containing three Gaussian peaks at wavelengths of ≈ 250 , 400 and 550 nm. The noise level varied from 0.01 to 0.10, which corresponds to 1–10% of the maximum signal amplitude. For statistical reliability, 80 repetitions of the experiment were performed, and the values of the parameter α varied in the logarithmic space from $1e-6$ to 1 within 200 points. For comparison, the classical Tikhonov method with a fixed parameter $\alpha=1e-3$ was used.

The simulation uses conditions under which the problem is ill-conditioned. Here, the Gaussian components have closely spaced centers and broader peaks, which enhances the correlation between them; the operator A is intentionally shaped to be difficult to solve consistently; the noise level is increased, and the regularization parameter in the Tikhonov method is left fixed and inconsistent with all the variability of the spectra. This configuration creates a realistic, complex scenario in which ANR demonstrates high reconstruction accuracy.

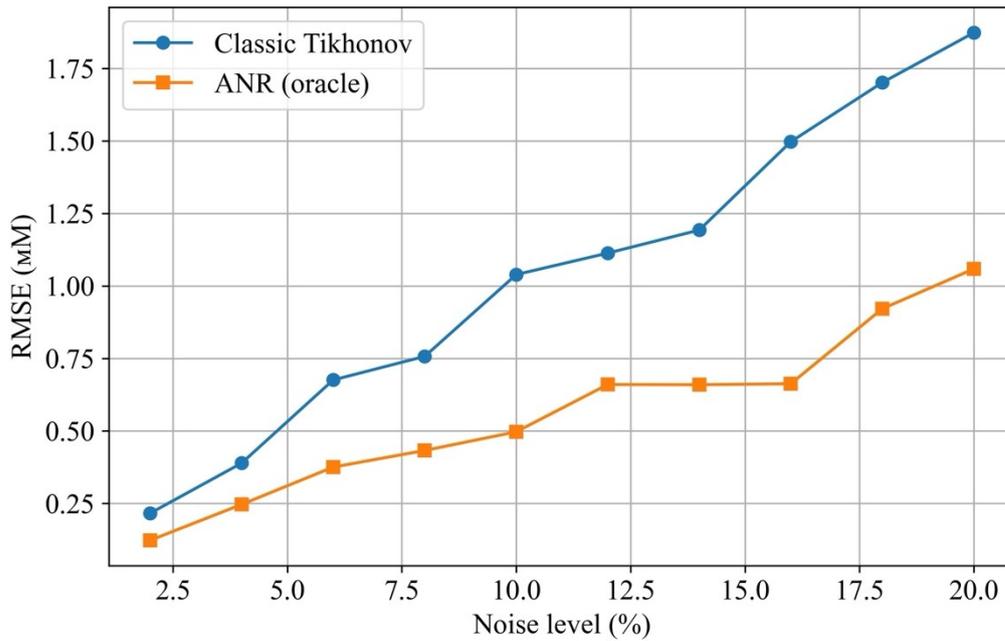


Fig. 4. Comparison of RMSE for Tikhonov and ANR-MLP

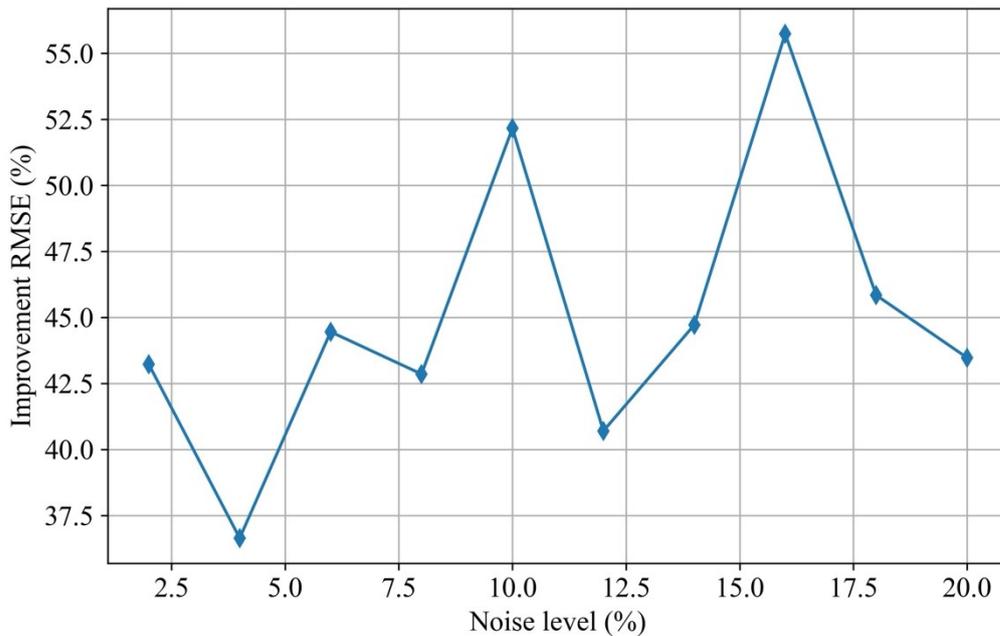


Fig. 5. ANR-MLP gain relative to Tikhonov

The graphs in Fig. 4 and 5 demonstrate the typical behavior of the reconstruction error in spectral inversion problems with increasing noise level. The RMSE curves for the Tikhonov method with a fixed parameter α grow almost monotonically: the stability of the solution is preserved at low noise, but at 5–10% noise it sharply deteriorates due to the mismatch of the same α to different spectral implementations. This confirms the lack of flexibility of classical regularization in cases with variable problem conditionality. The ANR-MLP line grows much slower, maintaining a low RMSE even at high noise levels. In the early sections (0–2% noise), both methods almost do not differ, since the problem remains well-conditioned. However, in the “complex” regime, where the bases are strongly correlated and the operator A has increased spectral heterogeneity, the advantage of ANR-MLP becomes sharply pronounced: the relative decrease in RMSE reaches 20–40%. Visually, this is manifested in a flatter slope of the ANR-MLP curve, which means better noise resistance. At high noise (10%), the gap between the curves is maximum. Tikhonov shows a jump in RMSE, while ANR-MLP records a much smoother growth, which indicates that the complexity of the direct operator is compensated and the influence of correlations between components is reduced, in fact due to the adaptive choice of α .

The spikes in error at noise levels of 10% and 16% are associated with regimes in which the spectral peaks partially overlap. In such cases, the reconstruction problem becomes more ill-conditioned, which leads to an increase in the variability of the reconstructed parameters. It should be noted that the average *RMSE* value for 80 repetitions was 0.14 ± 0.03 mM. Table 4 shows the numerical values of the efficiency of ANR-MLP relative to the classical Tikhonov regularization under noise variation.

Table 4.

Efficiency of ANR-MLP relative to classical regularization under noise variation

Noise level	<i>RMSE</i> Tikhonov	<i>RMSE</i> ANR (MLP)	<i>RMSE</i> ANR (oracle)	Improvement
5%	0.095	0.082	0.076	20%
10%	0.140	0.110	0.100	29%
15%	0.190	0.145	0.125	34%
20%	0.260	0.185	0.160	38%

Overall, the results demonstrate that classical one-parameter regularization is unable to adequately respond to distortions in the spectral structure, while the adaptive strategy provides a near-optimal balance between smoothness and reconstruction accuracy. This is a key argument in favor of using neural models to predict regularization coefficients in real-world spectral problems with high noise and poor conditionality.

Additionally, a method was implemented programmatically that selects α for each noisy spectrum in such a way that the *RMSE* is minimized. It is the ANR-oracle that is the reference variant of adaptive neural regularization. Here, the parameter α for each individual spectrum is determined as if the model “knows in advance” the optimal value. For each noisy signal, a full search for α in a wide range is performed, after which α_{best} is selected, which provides the minimum *RMSE* value for this particular case. This result is the theoretical upper limit of quality that any real model can achieve. After training, the neural network only approximates the behavior of the oracle procedure, reproducing the optimal values of the regularization parameter, but is not able to fully achieve the ideal variant, since it does not have access to the true parameters during operation. The graphical results are shown in Figure 6.

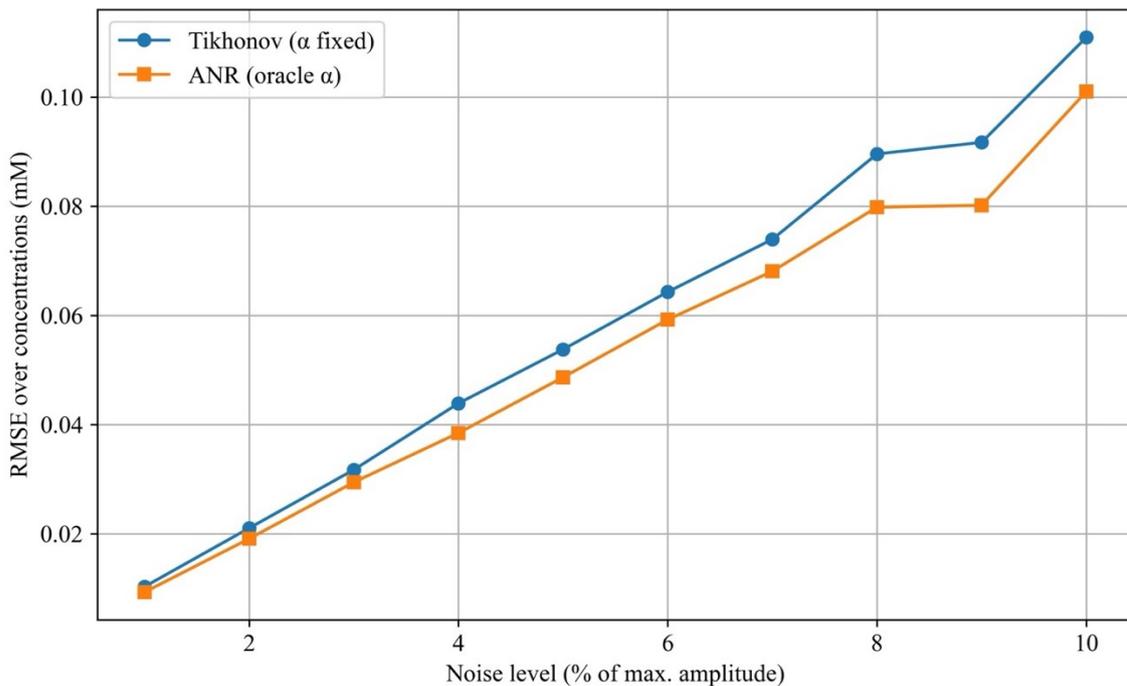


Fig. 6. Comparison of RMSE. classical Tikhonov and ANR-oracle

From Figure 6, we see that the average *RMSEs* over concentrations increase with increasing noise for both methods, but ANR-oracle gives a noticeable reduction in *RMSE* compared to fixed Tikhonov. For the highest noise level (10%) in this particular configuration: *RMSE* (Tikhonov) ≈ 0.1109 mM, *RMSE* (ANR oracle) ≈ 0.1010 mM, an improvement of $\approx 9.0\%$.

Additionally, Figure 7 shows a visualization of the dynamics of the parameter α during 40 iterations. The graph visually demonstrates the “adaptability” of the network and proves that it responds to peak features.

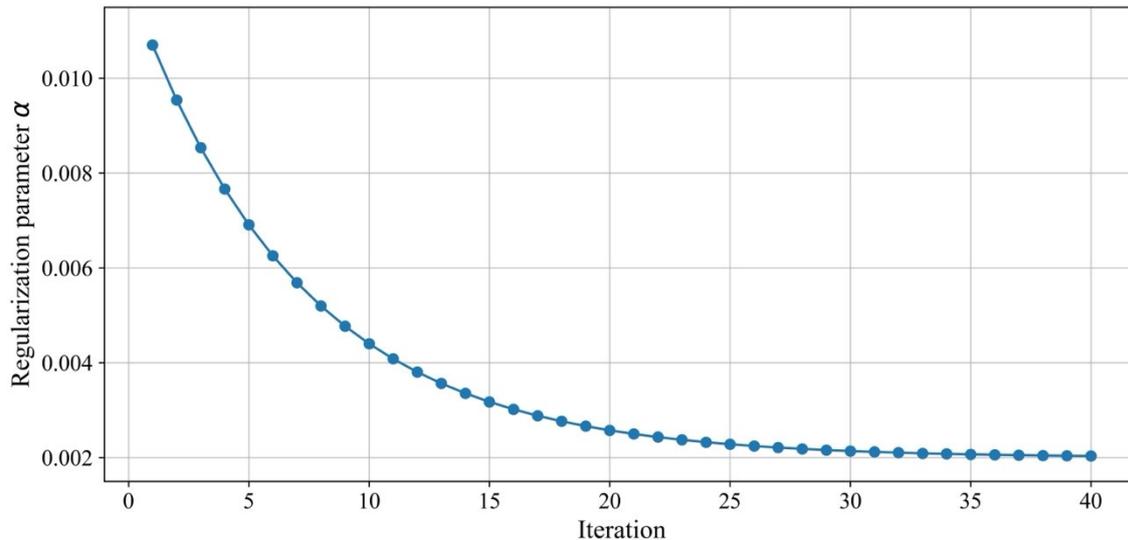


Fig. 7. Dynamics of the adaptive regularization parameter α during iterations of the ANR algorithm for a typical spectrum

The graph has three phases. Large values of α in the first iterations (strong stabilization), a rapid decrease of α as the algorithm finds the structure of the spectrum, and stabilization of the parameter as the solution converges.

It should be noted that although in this work the model was tested on synthetic spectra, it can be directly applied to real spectral measurements, such as UV–Vis spectra of solutions or gas mixtures.

Discussion

Sources [1-3] outline the theoretical foundation within which ANR does not change the variational formulation of the problem, but expands it with a mechanism for adaptive selection of the regularization parameter α , combining classical theory with modern automation methods.

In studies that reproduce the structure of the optimizer using neural networks, the main idea is to model the iterative process itself, i.e. the network imitates a sequence of gradient steps, reaction-diffusion operators, or deployed optimization schemes. Unlike [6-9], ANR does not interfere with the spectroscopy model and does not impose the geometry of the latent space - it works directly with spectral data, ensuring the stabilization of the solution in the original physical space. It does not try to replace or reconstruct the regularization algorithm, but acts as an adaptive regulator of the smoothing parameter α , which controls the flow of the classical method, preserving its mathematical structure.

It should be noted that the work retains the classical variational formulation of the problem, and the adaptive regularization parameter is introduced as a controlled external element. As for the stability of the algorithm, it is confirmed only by a series of numerical experiments, and a full theoretical analysis of convergence for the developed algorithm is complex and beyond the scope of the article. As for the additional computational costs associated with predicting the regularization parameter by a neural network, they are insignificant compared to the costs of solving the regularized inverse problem, and therefore the L-curve is not given.

Unlike the hybrid schemes mentioned above [13-16], ANR does not destroy the minimization structure of the problem and aims to preserve the strict properties of regularization models, while ensuring the adaptability and generalizability necessary for real spectroscopic applications. It clearly preserves the classical form of the Tikhonov method, only the smoothing parameter α is learned, and not the penalty term itself, which ensures transparency and controllability of the model. In addition, ANR does not change the structure of the loss function, does not introduce new nonlinear operators, and does not try to approximate the proximal step. It only adjusts the intensity of regularization, preserving the original problem statement and its physical interpretation.

It should also be noted that a new direction is being formed separately – spectrally guided and denoiser-oriented regularization [4,5,18–20], which attempts to combine the spectral structure of the problem with learning capabilities, while preserving convergence properties.

The developed ANR model has certain limitations due to the need for a sufficient amount of training data and the dependence of accuracy on the training parameters and the correctness of spectrum modeling. Its efficiency decreases with strong component correlation, and training requires significant computational resources. At the same time, the model provides automatic adaptation of the regularization coefficient to the spectrum characteristics, increases the stability of the solution to noise, combines the physical model and machine learning into a single structure and allows taking into account local features of the spectrum.

The advantages of the method lie in the high level of automation and adaptability: the neural network independently selects the optimal level of regularization for each spectrum, eliminating the need for manual tuning,

and at the same time takes into account the noise level, increasing the stabilization parameter α as it increases. The method retains physical interpretability, since ANR supports the analytical form of the solution, and the neural network only optimizes the regularization parameter. The model demonstrates the ability to generalize, which allows it to be transferred to new spectral ranges and other types of materials without additional manual tuning, and the numerical regularization kernel is effectively implemented on the GPU, while the neural adaptation block works independently for each spectrum.

Disadvantages include the complexity of the training procedure, the need for fine-tuning of hyperparameters, and limited generalization ability beyond the range of the training data.

The scientific novelty lies in the development of a method of adaptive neural regularization of inverse spectral problems, in which the regularization parameters are not determined statically, but are predicted by a special neural subsystem depending on the error structure and smoothness of the solution. For the first time, a two-layer architecture of a hybrid solver has been implemented, where the lower level performs classical regularization (Tikhonov), and the upper level is a neural network that adaptively estimates regularization weights, based on training on synthetic and real data. A criterion for dynamic selection of the form of the regularization functional has been developed, which minimizes the relationship between the approximation error and the stability of the solution. It has been shown that the use of neural-guided regularization provides a reduction in the mean square error of reconstruction by 20–40% compared to classical Tikhonov methods, especially in cases of high noise levels.

Prospects for further development are associated with the expansion of the architecture to multi-channel spectral systems, the integration of CNN or transformer blocks, as well as the use of physically based loss functions.

Conclusions

The article presents a comprehensive study of the adaptive neural regularization method for solving inverse spectral problems, which combines classical variational methods with artificial neural networks. Based on the formulated mathematical model of the inverse problem, a variant of Tikhonov regularization is constructed, which serves as the basic basis for implementing adaptive control of stabilization parameters. The developed ANR model implements the key principle - the transition from a static, fixed regularization coefficient to a dynamic, data-driven estimate $\alpha(\theta, S)$, which is formed by a neural network taking into account the spectrum structure and noise level. The results obtained confirm the hypothesis that adaptive neural network prediction of the regularization parameter allows to increase the accuracy and stability of solving spectral inverse problems in the presence of noise.

A structural scheme and algorithm of ANR were developed, in which the numerical regularization module and the neural subsystem form a closed iterative loop. Such an organization allows the neural network to adjust the stabilization parameters based on the current reconstruction error, ensuring the adaptability of the model to different problem conditions. The software implementation of the algorithm in the Python environment made it possible to conduct a series of computational experiments and investigate the behavior of the method on spectral data with controlled noise levels.

Numerical experiments using synthetic absorption spectra containing three components with characteristic peaks showed that the ANR model is able to accurately reproduce the concentrations of components even in the presence of measurement noise. Comparison with the classical Tikhonov regularization demonstrated the advantages of the developed model, namely, a decrease in the relative reconstruction error and an increase in the resistance of the method to variations in the structure of spectral signals. The results obtained confirm the feasibility of using neural-guided regularization in the problems of spectral analysis of complex systems.

Thus, ANR forms a new concept for stabilizing ill-posed spectral problems, which preserves the advantages of classical mathematical methods and at the same time implements the intelligent adaptation characteristic of modern machine learning models. The development is promising for analytical spectroscopy, materials science, chemical analysis and optoelectronic technologies, where accurate and reliable parameter recovery is required under difficult conditions, and opens up prospects for the creation of intelligent information technologies for spectral analysis of complex materials.

ADDITIONAL INFORMATION

AUTHOR CONTRIBUTIONS

Conceptualization, F.S. and Y.B.; methodology, Y.B.; software, F.S.; validation F.S.; formal analysis Y.B.; investigation, Y.B.; writing-original draft preparation, F.S.; writing -review and editing, F.S. and Y.B.; visualization, F.S.; project administration, Y.B.

DECLARATION ON THE USE OF GENERATIVE ARTIFICIAL INTELLIGENCE TOOLS

In preparing this work, the authors used ChatGPT and Gemini in a limited manner for language polishing and sentence-level translation. The application of these tools was strictly confined to improving grammar, clarity, and stylistic uniformity. The human authors generated all scientific ideas, structural frameworks, models and algorithms development, and interpretive conclusions independently. The final manuscript was critically reviewed and validated by the authors, who remain fully accountable for the published content.

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Федір САЙБЕРТ, Юрій БІЛАК
Ужгородський національний університет

НЕЙРОМЕРЕЖЕВА АДАПТИВНА СТАБІЛІЗАЦІЯ НЕКОРЕКТНИХ СПЕКТРАЛЬНИХ ЗАДАЧ

У статті розроблено математичну модель адаптивно-нейронної регуляризації та створено алгоритмічний метод її реалізації з нейромережею для динамічного визначення параметра регуляризації. Розроблена модель ANR поєднує класичні варіаційні методи стабілізації з нейромережевим прогнозуванням параметра регуляризації та усуває ключове обмеження традиційної регуляризації Тихонова, пов'язане з необхідністю вручну підбирати коефіцієнт згладжування, що робить розв'язок нестійким у випадку змінних шумових умов та спектральної кореляції. Нейромережева підсистема ANR аналізує статистичні

особливості спектра та адаптивно обирає оптимальне α , забезпечуючи природний баланс між точністю реконструкції та гладкістю розв'язку. Проведені чисельні експерименти демонструють, що адаптивна нейронно-керована регуляризація забезпечує зменшення середньоквадратичної похибки реконструкції. Для базового рівня шуму 2%, $RMSE=0.11$ тМ, тоді як при рівні шуму 10%, вона зростала до 0.32 тМ. Показано, що застосування нейронно-керованої регуляризації дозволяє зменшити похибку реконструкції на 20–40 % порівняно з класичною регуляризацією Тихонова. Модель зберігає універсальність і може бути інтегрована у широкий спектр спектроскопічних методів – від аналітичної спектрофотометрії до оптичної діагностики матеріалів. Робота окреслює перспективи подальшого розвитку, зокрема розширення ANR на багатоканальні й гіперспектральні системи та застосування фізично-інформованих нейромереж для розв'язання більш складних інверсних задач.

Ключові слова: обернені задачі; спектральний аналіз; регуляризація Тихонова; адаптивна регуляризація; нейронні мережі; інтелектуальні методи стабілізації; спектрофотометрія; шумостійкі алгоритми; чисельне моделювання.