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MODIFICATION OF THE SPECTRAL SENSITIVITY ANALYSIS METHOD IN PARAMETRIC SYNTHESIS PROBLEMS

The subject of the study is methods for analyzing the spectral sensitivity of parameters in parametric synthesis problems related to the reconstruction of medium characteristics from spectral data. **The aim** of the work is to develop a modification and investigate the applicability of the spectral sensitivity analysis method to improve the stability and identifiability of parameters in parametric synthesis problems. **To achieve this goal**, the following tasks were addressed: analysis of the causes of instability in parametric synthesis problems; investigation of approaches for evaluating spectral sensitivity of parameters; conducting numerical experiments to study the influence of parameters on the spectral response; and assessment of parameter informativeness using appropriate quantitative metrics. **The research methods** are based on the use of an analytical model of the spectral response, differential analysis of sensitivity functions, and numerical methods for computing integral characteristics and eigenvalues of the spectral sensitivity matrix. **The obtained results** demonstrate that the parameters have significantly different impacts on the spectral shape, which is confirmed both by the visual analysis of sensitivity functions and by numerical evaluation of their integral measures. It is established that the dominance of certain parameters leads to substantial differences in influence scales and results in the presence of poorly identifiable parameters. The spectrum of eigenvalues of the sensitivity matrix is analyzed, revealing features indicating the proximity of the problem to a degenerate case. Additionally, the condition number is evaluated, confirming the potential instability of the solution. It is concluded that spectral sensitivity analysis is an effective tool for preliminary assessment of parameter informativeness and can be used to improve the stability of parametric synthesis problems. The obtained **results** can be applied in the development of more complex spectral analysis models and in improving parameter identification methods.

Keywords: spectral sensitivity; parametric synthesis; parameter identifiability; problem stability; spectral analysis; numerical experiment; analytical model; parameter informativeness; information technologies.

1. Introduction

Parametric synthesis in spectroscopy is a key component of analyzing complex physical systems, in which the parameters of the medium are determined based on experimentally measured spectral characteristics. Such problems arise in various fields, including optics, materials science, laser diagnostics, and biomedical research, where spectral data serve as the primary source of information about the properties of the objects under study. Traditionally, parametric synthesis is formulated as the problem of minimizing the functional difference between the experimental and model spectra. However, in practice, such problems are often characterized by solution instability, which is caused by the limited nature of spectral data, the presence of noise, and the complex interdependence of model parameters. As a result, even small changes in the input data can lead to significant deviations in the recovered parameters, complicating their physical interpretation.

One of the key causes of instability is the non-uniform spectral sensitivity of the parameters, i.e., the varying degree of influence that individual parameters have on the shape of the spectrum within a given spectral

range. In cases where a change in a parameter has practically no effect on the spectral response, or can be compensated for by other parameters, the problem of their weak identifiability arises. This, in turn, leads to the degeneracy of the parametric synthesis problem and the emergence of non-physical or unstable estimates. In this regard, it is important to apply methods that allow for the analysis of the informativeness of spectral data regarding model parameters even before the stage of their numerical reconstruction. One such method is the spectral sensitivity analysis method, which is based on the study of changes in the spectral response as parameters vary. This method allows one to assess the contribution of each parameter to the formation of the spectrum, identify weakly sensitive or interdependent parameters, and determine the conditions under which the synthesis problem is well-posed.

This scientific article investigates the possibilities of applying the spectral sensitivity analysis method to improve the stability of parametric synthesis problems. The main focus is on evaluating the identifiability of parameters based on their influence on the spectral signal and the analysis of corresponding numerical characteristics. To illustrate the advantages, model

spectral dependencies are used, which clearly demonstrate the peculiarities of parameter behavior in cases of full and partial identifiability. The results obtained can be used for preliminary analysis of parametric synthesis problems, improving their robustness, and making a well-founded selection of parameters to be estimated, which creates the prerequisites for a more reliable application of numerical and neural network methods for processing spectroscopic data in practical problems. From the perspective of information technology, the modified method can be viewed as a component of the spectral data processing and decision support process in parametric synthesis problems. In particular, the analysis of spectral sensitivity enables the formation of informative features, the evaluation of the parametric space, and the selection of an effective configuration of parameters, which are characteristic tasks of modern information-analytical systems.

2. Literature Review and Problem Statement

The problems of parametric synthesis and parameter recovery based on spectral characteristics belong to the class of inverse problems, for which solutions are typically unstable, the formulation is ill-posed, and results are highly dependent on errors in the input data. Fundamental works on the theory of inverse problems have shown that even minor noise in spectral measurements can significantly affect the accuracy of parameter recovery, especially when there is strong correlation between them or the experimental data are insufficiently informative [1–3]. Furthermore, for complex multiparameter models, the problem is complicated by the limited amount of available information and the possibility of multiple close solutions [4].

Parameter identifiability analysis plays a crucial role in ensuring the correctness of parametric synthesis. In [5, 6], methods were developed based on the analysis of the profile likelihood function and the study of parametric dependencies, which allow for the determination of parameters that cannot be unambiguously estimated from the available data. However, most of these methods were developed primarily for biological or dynamic models, so when applied to spectroscopic problems with a large number of parameters, they often prove computationally complex.

The study [7] examines the relationship between spectral sensitivity and parameter identifiability in inverse uncertainty estimation problems. The authors

demonstrated that parameters with a weak influence on the spectral signal are significantly more difficult to recover correctly. A similar approach is used in [8], where the Fisher information matrix is applied to assess the informativeness of parameters. At the same time, such methods are primarily focused on statistical analysis of the model and do not always provide a sufficiently clear explanation of exactly how individual parameters influence the shape of the spectral dependence.

The problem of instability is particularly noticeable in modern spectroscopic problems, where spectral models are characterized by complex structures and a significant number of interrelated parameters. For example, in [9], a paper on photoacoustic tomography, the high sensitivity of the results to noise and prior model assumptions is emphasized. Similar difficulties are described in [10] for optical coherence tomography problems, where even high-quality spectral data do not guarantee the uniqueness of parameter recovery due to the possibility of multiple equivalent solutions.

A separate area of current research involves the use of neural network and hybrid methods for solving spectral parameter synthesis problems. In [11], a neural network model for analyzing diffuse reflection spectra is presented, which enables rapid parameter estimation. However, the authors note that the accuracy of such models depends significantly on the quality and representativeness of the training sample, and in cases of weak parameter identifiability, the effectiveness decreases noticeably. In [12], machine learning is applied with consideration of physical laws for spectral reconstruction; however, the problem of instability and insufficient informativeness of the parameters remains relevant. Thus, even modern neural network methods do not completely eliminate the problem of degeneracy in the parametric space, but only partially compensate for it due to the approximation properties of the models.

Regularization methods are traditionally used to stabilize solutions to inverse problems. In [13], a modern interpretation of Tikhonov regularization is presented as a tool for reducing the influence of noise and stabilizing ill-posed problems. However, regularization alone does not eliminate the problem of weak parameter informativeness. If the parameters have similar or nearly linearly dependent sensitivity functions, even regularized solutions may remain unstable or physically ambiguous.

In recent years, considerable attention has been paid to the use of automatic differentiation and methods based on partial differential equations in parametric

reconstruction problems. In [14], the effectiveness of automatic differentiation for the reconstruction of spectral functions is demonstrated, while in [15], the problem of parameter identifiability in PDE models is investigated. However, these methods focus primarily on the numerical aspect of solving problems and take into account, to a lesser extent, the preliminary analysis of parameter informativeness based on their spectral sensitivity.

In [16–18], methods for adaptive parametric synthesis and the creation of hybrid systems for analyzing the spectral characteristics of multilayer structures were developed. In particular, [16] considers the use of an adaptive informative subset of parameters to improve the stability of spectral synthesis. In the studies [17, 18], hybrid models of inverse analysis and the concept of a digital spectral twin of thin-film structures are presented. The obtained results confirm the promise of adaptive parameter space restriction; however, the issues of analyzing the spectral sensitivity of parameters and its impact on the degeneracy of the problem remain insufficiently studied.

Thus, the above analysis of current scientific works indicates that most existing methods of parametric synthesis are primarily focused on the numerical solution of inverse problems or the stabilization of results using regularization or machine learning. In contrast, insufficient attention is paid to the preliminary analysis of spectral sensitivity of parameters, which allows for the assessment of their informativeness and identifiability even before the synthesis stage. This is precisely why it is relevant to study methods of spectral sensitivity analysis to identify poorly informative parameters, evaluate the structure of the parametric space, and improve the stability of parametric synthesis problems.

3. Research Objectives and Tasks

The object of the study is the process of parametric synthesis of multilayer thin films.

The subject of the study is the information technology for analyzing the spectral sensitivity of parameters in parametric synthesis problems based on spectral data and the corresponding methods for evaluating their informativeness and identifiability.

The aim of the work is to develop a modified method for analyzing spectral sensitivity and to formalize the information technology for its application to improve the stability of solutions to parametric synthesis problems.

To achieve this goal, the following tasks must be solved:

Analyze the characteristics and causes of instability in parametric synthesis problems in spectroscopy and examine methods for analyzing the spectral sensitivity of parameters based on the differential characteristics of the spectral model.

Investigate the influence of spectral sensitivity on the identifiability of parameters and the correctness of their recovery, and develop a modified method for spectral sensitivity analysis.

Develop and formalize the structure of the information technology for spectral sensitivity analysis of parameters in parametric synthesis problems.

To conduct a numerical experiment to evaluate the behavior of parameters in cases of full and partial identifiability.

To analyze the possibility of using the results of spectral sensitivity analysis to improve the stability of parametric synthesis.

4. Materials and Methods

Research hypothesis, accepted assumptions, and simplifications. The hypothesis of the research conducted in this scientific work is that the use of a modified method for analyzing the spectral sensitivity of parameters, which includes the normalization of sensitivity functions and spectral analysis of the sensitivity matrix, makes it possible to improve the identifiability of parameters and the stability of parametric synthesis problems as early as the stage of their preliminary analysis.

A number of assumptions and simplifications are made in this work. The spectral response is a continuous and differentiable function of the parameters, while the parameters affect the spectrum independently or are weakly correlated in a local region. The study is conducted in a fixed spectral range with sufficient discretization, and the influence of noise in the data is not taken into account, which allows us to focus on the internal properties of the model. Another simplification is the use of a generalized analytical model of the spectrum instead of a complete physical model. A local (linear) approximation via sensitivity functions is considered, and continuous integral relations are replaced with their discrete counterparts. Additionally, normalization of sensitivity functions is applied to eliminate the influence of different parameter scales, which allows for a correct

comparison of their contributions to the formation of the spectral response.

Presentation of the main material

This paper presents a modified method for analyzing the spectral sensitivity of parameters in parametric synthesis problems. The method is based on classical methods of sensitivity analysis and parameter informativeness estimation, which are widely used in inverse modeling and spectroscopy problems [1, 19]. The developed modification involves the use of normalization of sensitivity functions, as well as spectral analysis of the sensitivity matrix to evaluate the stability of the synthesis problem.

The spectral response of the system is defined as a mapping

$$S = S(\lambda, p), \quad (1)$$

where λ is a spectral variable, and $\vec{p} = (p_1, p_2, \dots, p_N)$ is a parameter vector.

To investigate the influence of the parameters, the spectral sensitivity functions are defined as

$$\Phi_i(\lambda) = \frac{\partial S(\lambda, \vec{p})}{\partial p_i}. \quad (2)$$

To analyze sensitivity, the partial derivatives of the spectrum with respect to the parameters that determine the spectral sensitivity functions are considered. These functions characterize the change in the spectrum as the corresponding parameter varies and allow us to evaluate its contribution to the formation of the spectral signal. The integral estimate of the parameter's influence is determined as follows

$$I_i = \int_{\Lambda} \left| \frac{\partial S(\lambda, \vec{p})}{\partial p_i} \right|^2 d\lambda = \int_{\Lambda} \Phi_i^2(\lambda) d\lambda, \quad (3)$$

which characterizes the total contribution of the parameter to the formation of the spectrum.

To account for differences in scale, it is proposed to use normalized sensitivity functions

$$\Phi_i^n(\lambda) = \frac{\Phi_i(\lambda)}{\|\Phi_i(\lambda)\|}, \quad (4)$$

where $\|\Phi_i(\lambda)\|$ is the norm of the function, defined as the square root of the integral of the square of the sensitivity function over the spectral range:

$$\|\Phi_i\| = \sqrt{\int_{\Lambda} \Phi_i^2(\lambda) d\lambda}. \quad (5)$$

In addition, to analyze the interdependence of parameters, a spectral sensitivity matrix is formed using the formula:

$$M = [M_{ij}], \quad M_{ij} = \int_{\Lambda} \frac{\partial S}{\partial p_i} \frac{\partial S}{\partial p_j} d\lambda = \int_{\Lambda} \Phi_i(\lambda) \Phi_j(\lambda) d\lambda. \quad (6)$$

This matrix allows us to assess the linear independence of the parameters and determine the effective dimension of the parameter space. In the case where the rank of the matrix decreases, i.e.,

$$\text{rank}(M) < n, \quad (7)$$

the parametric synthesis problem becomes degenerate, leading to unstable solutions (n is the number of spectrally independent model parameters).

In normalized form, the matrix takes the form

$$M_{ij}^n = \int_{\Lambda} \Phi_i^n(\lambda) \Phi_j^n(\lambda) d\lambda. \quad (8)$$

To analyze the identifiability of the parameters, spectral decomposition is used

$$Mv_k = \lambda_k v_k, \quad (9)$$

where λ_k – eigenvalues, v_k – eigenvectors.

The condition number is defined as

$$k(M) = \lambda_{\max} / \lambda_{\min}. \quad (10)$$

The effective rank of the matrix is estimated using the following condition

$$r_{\text{eff}} = |\{\lambda_k : \lambda_k > \varepsilon\}|, \quad (11)$$

where ε is the threshold value.

To demonstrate the effectiveness of the modified method, a test analytical model of the spectrum

$$S(\lambda) = p_1 \cdot \exp\left(-\frac{\lambda - \lambda_0}{2\sigma^2}\right) + p_2(\lambda - \lambda_0) + p_3, \quad (12)$$

which reproduces the typical features of spectral dependencies (amplitude component, slope, offset).

For this test model, the corresponding sensitivity functions take the form:

$$\Phi_1(\lambda) = \exp\left(-\frac{\lambda - \lambda_0}{2\sigma^2}\right), \quad (13)$$

$$\Phi_2(\lambda) = \lambda - \lambda_0, \quad (14)$$

$$\Phi_3(\lambda) = 1. \quad (15)$$

A numerical experiment was conducted on synthetic data in the range $\lambda \in [400, 600]$. Sensitivity functions, integral indices I_i , the matrix M , and its eigenvalues were computed. The results showed that without normalization of the sensitivity functions, certain parameters dominate, leading to a loss of information from others. The developed modification, which includes normalization and analysis of the spectral characteristics

of the matrix, allows this effect to be eliminated, ensures a correct interpretation of the influence of parameters, and increases the stability of the parametric synthesis problem. Thus, the theoretical framework described above can be regarded as a modification of the spectral sensitivity analysis method, oriented toward practical application in spectroscopy and related fields.

For the practical implementation of the modified method, a discrete representation of spectral data is used. Let the spectral variable be given as a discrete set of values λ_k , $k = 1, \dots, N$. In this case, the integral relations (3), (5)–(8) are replaced by the corresponding discrete sums, which enables the numerical implementation of the algorithm. In particular, the integral sensitivity index is calculated as the sum of the squares of the values of the sensitivity function on a discrete grid, and the norm of the function is defined as the square root of this sum. This method allows one to transition from a continuous formulation of the problem to a computationally efficient discrete model without loss of information. The spectral sensitivity matrix in the discrete case is formed as a matrix of scalar products of discrete sensitivity vectors, which ensures convenient implementation in the form of matrix operations and allows for the effective use of standard numerical methods of linear algebra to find eigenvalues and estimate rank.

The numerical implementation was carried out using the Python programming language with standard scientific computing libraries. Sensitivity functions were computed analytically and numerically. To evaluate the properties of the problem, the eigenvalues of the matrix, its rank, and the diagonal elements of the inverse matrix were analyzed as indicators of the stability of parameter estimation. It is precisely this implementation that allows us to investigate the influence of spectral sensitivity on the stability of parametric synthesis, as well as to justify the feasibility of restricting the parametric space to parameters with a sufficient level of informativeness.

The developed modification can also be interpreted from the perspective of inverse modeling problems. In particular, the spectral sensitivity matrix is analogous to the sensitivity matrix or Jacobian used in least-squares methods. In this context, the analysis of its spectral characteristics allows one to assess the conditionedness of the problem and predict the behavior of numerical optimization methods. The algorithm for applying the method includes the following main steps: forming a spectral response model, computing spectral sensitivity

functions, normalizing the functions, constructing the sensitivity matrix, performing spectral analysis of the matrix, and evaluating integral indices, the condition number, and the effective rank. It is precisely this sequence of algorithmic steps that allows for a preliminary diagnosis of the parametric synthesis problem prior to the stage of solving the inverse problem.

The method modified by the author of this article can be used as a tool for the preliminary analysis of parametric synthesis problems. Its practical application involves the following sequence of steps: spectral sensitivity functions of the parameters are computed based on a given spectral response model, after which they are normalized to eliminate the influence of scales. Next, a spectral sensitivity matrix is formed and its eigenvalues are computed. In the final stage, integral sensitivity indices and the condition number are determined. Based on the obtained characteristics, the informativeness of the parameters is evaluated. Parameters with low integral sensitivity values or those corresponding to small eigenvalues of the matrix can be excluded or fixed to improve the stability of the problem. Additionally, the method can be integrated into optimization procedures as a preliminary stage of parameter selection. Thus, the method allows for a justified reduction in the dimensionality of the parameter space even before the numerical synthesis stage.

As a component of information technology, the modified method can be implemented as a sequence of computational procedures, including the processing of input spectral data, the construction of sensitivity functions, the formation of a matrix of characteristics, and their spectral analysis. It is precisely this structure that corresponds to the typical stages of information technology for data processing and can be integrated into spectral analysis software packages as a module for the preliminary diagnosis of parametric models.

The formalized structure of the information technology takes the form of an ordered set of components:

$$IT = \langle D, M, A, S, U, R \rangle, \quad (16)$$

where D is the input spectral data, M is the spectral response model, $A = \{A1, A2, A3\}$ is the set of procedures for calculating and analyzing spectral sensitivity functions, S is the parameter informativeness evaluation block, U – the decision-making block for their selection, R – the resulting parametric model. Figure 1 presents the developed scheme of the information technology for analyzing the spectral sensitivity of parameters.

This information technology implements a sequence of spectral data processing from the model-building stage to the evaluation of parameter informativeness and decision-making regarding their selection, which ensures an increase in the robustness of parametric synthesis tasks. The obtained characteristics are used to evaluate the informativeness of parameters and make decisions regarding their selection, which in turn

ensures an increase in the robustness of parametric synthesis tasks. It should be noted that the modified method can be implemented as a software module or framework that integrates into spectral analysis systems and provides automated assessment of parameter informativeness and support for decision-making regarding their selection.

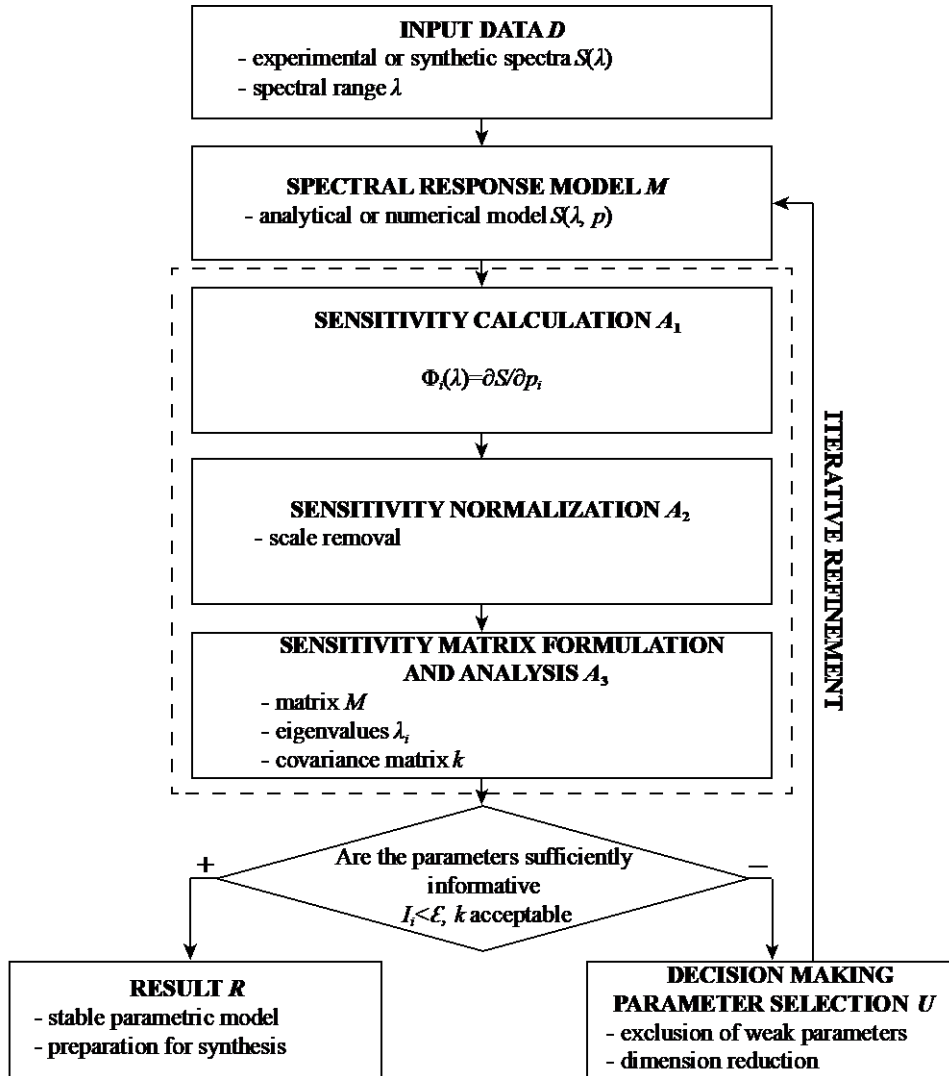


Fig. 1. Block diagram of the information technology for analyzing the spectral sensitivity of parameters

5. Research Results

To investigate the effect of spectral sensitivity on the stability of parametric synthesis, a numerical experiment was conducted based on the analytical spectral model described by formula (12). The use of synthetic data allows us to control the behavior of parameters, vary the conditions of identifiability, and clearly demonstrate the key properties of the problem

without the influence of experimental noise and errors. This model reproduces the generalized features of spectral dependencies characteristic of optical systems, in particular multilayer thin films, where the spectrum is formed as a result of interference and resonance effects. In particular, the localized spectral component models resonant transmission or reflection peaks, the linear trend accounts for background variations associated with the dispersion properties of the medium, and the

additive offset accounts for the baseline signal level. Furthermore, this choice of model is not intended to reproduce a specific physical structure but is used as a test bed for investigating general patterns of how parameters affect the spectral response, allowing us to focus on analyzing spectral sensitivity and parameter identifiability, which are universal characteristics of parametric synthesis problems.

The spectral dependence was defined as a superposition of three components: a localized resonant component (Gaussian peak), a linear trend, and an additive offset. Accordingly, these parameters have

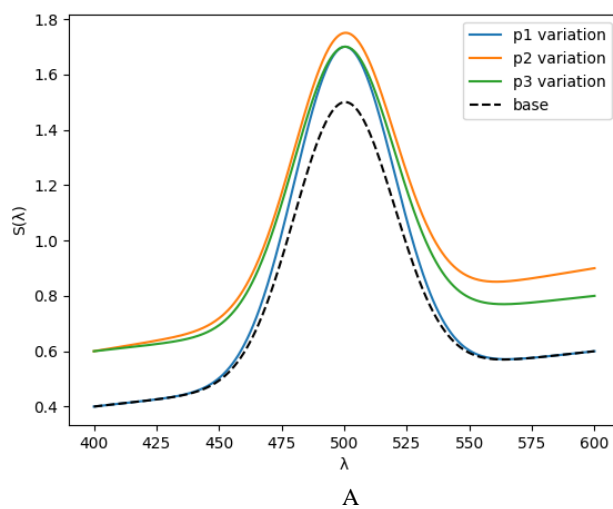


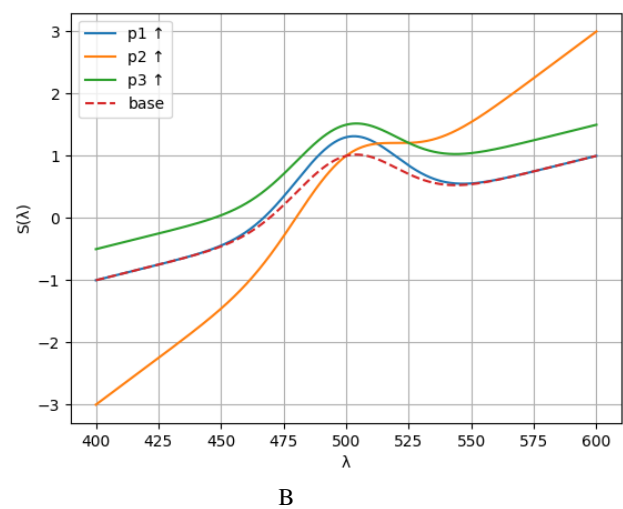
Fig. 2. The influence of parameters on the spectrum

Fig. 2A shows the effect of parameters on the spectral dependence in its original form. In this case, the slope parameter p_2 and the shift parameter p_3 are visually weak due to the use of an uncentered spectral variable and relatively small variations in the parameters. In Fig. 2B, the spectral variable is centered ($\lambda - \lambda_0$), and the parameter variations are increased, which allowed the effects to be clearly distinguished: parameter p_2 is responsible for the change in the spectral slope, while p_3 is responsible for its vertical shift.

Fig. 3A shows the spectral sensitivity functions on the original scale. Due to a significant difference in orders of magnitude, the linear function $\Phi_2(\lambda)$ dominates the others, with the result that $\Phi_1(\lambda)$ and $\Phi_3(\lambda)$ are virtually indistinguishable visually. The linear function $\Phi_2(\lambda)$ increases in the range of λ values (400–600) and significantly exceeds the other functions in magnitude. As a result, the localized function $\Phi_1(\lambda)$

different physical interpretations: parameter p_1 determines the amplitude of the spectral line, p_2 is responsible for the background slope, and p_3 for the overall signal level. A model constructed in this way allows for the investigation of both local and global effects in the spectrum.

Figures 2–4 show the results of a numerical experiment in two visualization variants: (A) – the initial representation without additional data processing, (B) – an improved representation that accounts for scaling and normalization to enhance the clarity of the results.



has a significantly smaller amplitude and visually "merges" with the axis, while the constant function $\Phi_3(\lambda)$ practically overlaps the lower part of the graph. Thus, all three functions are actually present, but their simultaneous display without normalization leads to a loss of visual distinctiveness.

Fig. 3B shows the normalized sensitivity functions, which allowed them to be brought to a comparable scale and clearly distinguished all three components: localized (Φ_1), linear (Φ_2), and constant (Φ_3).

Fig. 4A shows the eigenvalues of the spectral sensitivity matrix on a linear scale. In this case, a single dominant peak is observed, while the other values are practically imperceptible, creating the impression of degeneracy without a quantitative assessment. Fig. 4B uses a logarithmic scale, which allows us to visualize the entire spectrum of eigenvalues and assess their relative magnitudes. The rank of the matrix, which characterizes the effective dimension of the parametric space, is 3 in our case.

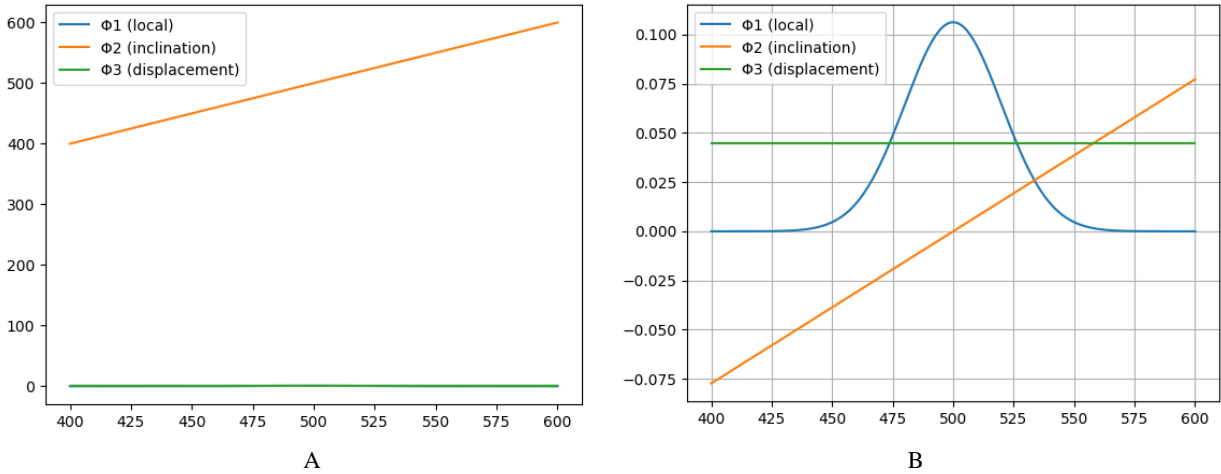


Fig. 3. Spectral sensitivity functions

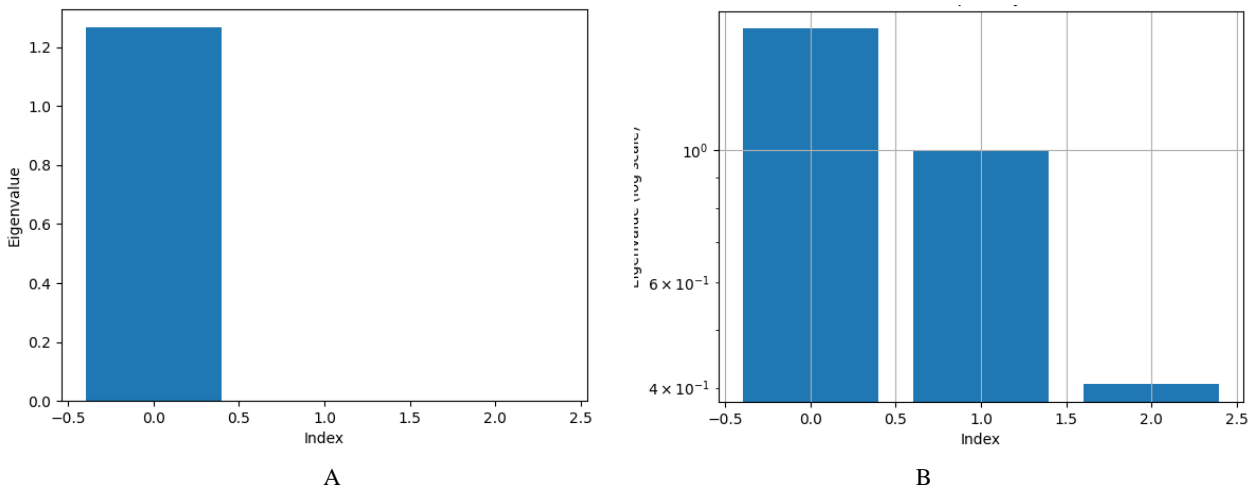


Fig. 4. Eigenvalues of the sensitivity matrix

The results shown in Figure 4 indicate a significant difference in the informativeness of the parameters: one direction in the parametric space is determined much better than the others. This situation is typical for problems with sensitivities of varying scales and can be interpreted as an approximation to a degenerate case. Smaller eigenvalues correspond to poorly identified parameters, which potentially leads to instability in their estimation.

Thus, the transition from option (A) to (B) makes it possible to eliminate the effects of dominance of individual components, increase the informativeness of the graphs, and ensure the correct interpretation of the results of spectral sensitivity analysis. Additionally, the obtained results confirm that spectral sensitivity analysis allows for the identification of parameters with varying levels of informativeness even before the synthesis problem is solved. Visualization of the sensitivity functions and the eigenvalue spectrum of the

matrix allows one to interpret the structure of the problem, explain the causes of instability, and justify the need to restrict the parameter space. Meanwhile, to improve visualization, it is advisable to use normalization of spectral sensitivity functions or plotting on a logarithmic scale, which will help avoid the dominance of individual components and allow for a more intuitive comparison of the parameters' contributions.

To quantitatively assess the contribution of parameters to the formation of the spectral response, integral indices of spectral sensitivity were calculated, defined as the integral of the square of the corresponding sensitivity functions, and which are $I_1 \approx 35.4$, $I_2 \approx 1.67 \times 10^5$, $I_3 \approx 200$. This confirms a significant difference in the magnitude of the parameters' influence on the spectral response, with the slope parameter (p_2) being dominant. Additionally, the condition number of the spectral sensitivity matrix M was determined,

which for the case under consideration is of the order of $10^3 - 10^4$, indicating the potential instability of the parametric synthesis problem. Furthermore, the effective rank of the spectral sensitivity matrix is estimated, defined as the number of significant (non-zero, taking into account the threshold value) eigenvalues. The result obtained demonstrates that the effective rank is smaller than the formal number of parameters, which indicates the presence of weakly identified parameters and confirms the problem's approximation to a degenerate case. The obtained estimates are consistent with the shape of the eigenvalue spectrum (Fig. 4) and confirm the presence of significant non-uniformity in the informativeness of the parameters.

6. Discussion of Results

The obtained results confirm the general provisions of the theory of inverse problems regarding their instability and dependence on data informativeness [1–3]. In the present study, this manifests itself through significant non-uniformity in the spectral sensitivity of the parameters, as seen in the form of the functions $\Phi_i(\lambda)$ (Fig. 3) and the integral indices I_i (Equation (3)). The dominance of certain parameters leads to a decrease in the identifiability of others, which is consistent with the conclusions regarding the possibility of the existence of close solutions [4]. Unlike identifiability analysis methods based on complex numerical procedures [5], the developed modification of the method allows for a visual assessment of parameter informativeness based on sensitivity functions (Equation (2)) and their normalization (Equations (4)–(5)), which in turn ensures better interpretability of results in spectral analysis problems. Analysis of the eigenvalue spectrum of the sensitivity matrix (Fig. 4) reveals the presence of dominant components, confirming the non-uniformity of the parameters' influence. A large value of the condition number $k(M)$ (Equation (9)) indicates the potential instability of the problem, which is consistent with the results of studies in spectroscopy [9]. Compared to methods based on statistical estimates, in particular the information matrix [8], the developed modification allows for the direct analysis of the contribution of parameters to the formation of the spectrum. Furthermore, unlike regularization methods [12], it also allows for the identification of the causes of instability even before the problem is solved. Thus, the results

obtained demonstrate that the modified spectral sensitivity analysis method is an effective tool for the preliminary assessment of parameter identifiability and can be used to improve the stability of parametric synthesis problems.

The scientific novelty of this work lies in the modification of the spectral sensitivity analysis method for evaluating parameter identifiability and improving the stability of parametric synthesis problems in spectroscopy, as well as in the development of a method for its implementation as an information technology that includes the stages of spectral data processing, sensitivity analysis, and decision support for parameter selection.

The uniqueness of the method lies in the combination of the simplicity of the analytical model with the possibility of quantitative analysis of parameter informativeness through sensitivity functions and the eigenvalue spectrum of the corresponding matrix, which ensures a clear interpretation of the problem's properties.

An important advantage of the developed modification is its invariance to parameter scales, achieved through the normalization of sensitivity functions. It is this invariance that allows avoiding the dominance of parameters with large derivative values and ensures a more accurate comparison of their effects. Despite its advantages, the developed method has a number of limitations that should be taken into account when applying it. First, the use of an analytical model of spectral response simplifies real physical processes, which may limit the accuracy of parameter estimation in complex systems. Second, the results of the spectral sensitivity analysis depend on the choice of the spectral variable range and discretization, which can affect the values of integral indices and the spectral characteristics of the sensitivity matrix. Third, the method is based on local analysis, since sensitivity functions are defined as derivatives with respect to parameters, which assumes small variations in parameters in the vicinity of the selected point. In the case of highly nonlinear dependencies, this can lead to a loss of adequacy in the estimates. Furthermore, while normalizing the sensitivity functions eliminates scaling effects, it may partially reduce information about the absolute contribution of the parameters. It should also be noted that the analysis of the spectral sensitivity matrix does not account for noise in the data, which is characteristic of real experimental conditions. In such cases, it is necessary to additionally account for the statistical characteristics of the measurements and apply

regularization methods. Thus, the modified method is suitable for use as a tool for preliminary analysis and diagnosis of parametric synthesis problems, with subsequent refinement of the results based on more complex models and experimental data.

The results obtained can be used as a basis for developing information technology for spectral data analysis, in which the modified method performs the functions of processing, evaluating, and selecting parameters, opening up opportunities for its integration into spectral analysis software systems and intelligent decision support systems. The results of spectral sensitivity analysis obtained in this work are of practical significance for parametric identification problems in complex physical systems. The modified method allows for the identification of poorly identified parameters and the assessment of the stability of computational procedures at the problem formulation stage, which is critically important for improving the reliability of numerical modeling. In an industrial context, the method can be applied in spectroscopic material analysis, optoelectronics, non-destructive testing, and thin-film research technologies, where it is necessary to estimate medium parameters based on experimental spectral data. Furthermore, the method is relevant for automated process monitoring systems, where ensuring the stability of synthesis algorithms in the presence of noise and limited data is crucial. Thus, the spectral sensitivity method can be integrated into modern information technologies as a tool for preliminary diagnosis of the correctness of parametric synthesis and for improving its computational stability.

7. Conclusions

This research investigates the influence of the spectral sensitivity of parameters on the stability of parametric synthesis problems in spectroscopy. It is shown that the non-uniformity of sensitivities is one of the main causes of instability and deterioration of parameter identifiability.

A modification of the method for analyzing parameter informativeness based on spectral sensitivity functions and their correlation matrix has been developed, which allows for the estimation of the effective dimension of the parametric space. A structure of an information technology for spectral sensitivity analysis has been developed and formalized, which ensures the evaluation of parameter informativeness and

can be used to improve the stability of parametric synthesis problems. The developed modification of the method has been implemented as a component of an information technology for spectral data processing and decision support in parametric synthesis problems.

Based on a numerical experiment using synthetic spectral data, it has been demonstrated that parameters have varying degrees of influence on the spectral response, as confirmed by the form of the sensitivity functions and the eigenvalue spectrum of the corresponding matrix. It has been established that the presence of dominant eigenvalues of the spectral sensitivity matrix indicates the proximity of the problem to a degenerate case and points to the presence of weakly identified parameters. It is shown that the use of normalization and scaling allows for increasing the informativeness of the visualization and ensuring the correct interpretation of the results of spectral sensitivity analysis.

Prospects for further research include extending the method to more complex physical models, in particular multilayer thin-film structures, integration with numerical methods (TMM, RCWA), and use within hybrid and neural network architectures for solving parametric synthesis problems in spectroscopy. Furthermore, the obtained results can be used for preliminary analysis of parametric synthesis problems, the justified selection of parameters, and improving the stability of numerical methods for their recovery.

Conflict of Interest

The authors declare that they have no conflict of interest, particularly of a financial, personal, authorial, or any other nature, that could influence the research or the results published in this article.

Funding

The research was conducted without financial support.

Data Availability

The manuscript has no associated data.

Use of Artificial Intelligence

The ChatGPT artificial intelligence model (version GPT-5.3, OpenAI) was used in the preparation of the

manuscript. AI tools were used exclusively during the auxiliary stages of work on the manuscript, specifically to check the grammar, spelling, and punctuation of individual text fragments; to perform automated checks of linguistic formatting without altering the scientific content; and to conduct a preliminary search and compile a list of potentially relevant scientific sources from the past 5 years.

All selected literature sources were additionally and meticulously verified by the authors using scientific databases and, where necessary, edited. Linguistic edits were also manually checked for compliance with scientific writing style.

No substantive part of the manuscript, including the abstract, introduction, methods and models, results and discussion, as well as conclusions, was created or generated using AI tools. All main provisions, research results, and their interpretation were obtained by the authors independently.

The results obtained using artificial intelligence tools were thoroughly verified by the authors. The use of AI did not affect the scientific content of the work, the reliability of the results, their interpretation, or the conclusions drawn.

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Received (Надійшла) 06.04.2026

Accepted for publication (Прийнята до друку) 15.05.2026

Publication date (Дата публікації) 29.05.2026

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ІНФОРМАЦІЙНА ТЕХНОЛОГІЯ АНАЛІЗУ СПЕКТРАЛЬНОЇ ЧУТЛИВОСТІ В ЗАДАЧАХ ПАРАМЕТРИЧНОГО СИНТЕЗУ

Предметом вивчення є інформаційна технологія аналізу спектральної чутливості параметрів у задачах параметричного синтезу за спектральними даними й відповідні методи оцінювання їх інформативності та ідентифікованості. **Мета дослідження** – розроблення модифікованого методу аналізу спектральної чутливості та формалізація інформаційної технології його застосування для підвищення стійкості розв’язків задач параметричного синтезу. Для досягнення поставленої мети розв’язано такі завдання: проаналізовано причини нестійкості задач параметричного синтезу; досліджено спосіб оцінювання спектральної чутливості параметрів; проведено чисельний експеримент для аналізу впливу параметрів на спектральний відгук; оцінено інформативність параметрів за допомогою відповідних кількісних показників. Крім того, сформовано й обґрунтовано структуру інформаційної технології аналізу спектральної чутливості, яка забезпечує послідовне опрацювання спектральних даних, оцінювання інформативності параметрів і підтримку прийняття рішень у задачах параметричного синтезу. **Методи дослідження** ґрунтуються на використанні аналітичної моделі спектрального відгуку, диференційного аналізу функцій чутливості та чисельних методів обчислення інтегральних характеристик і власних значень матриці спектральної чутливості. **Досягнуті результати** демонструють, що параметри мають суттєво різний вплив на форму спектра, що підтверджується як візуальним аналізом функцій чутливості, так і чисельними оцінками їх інтегральних показників. Встановлено, що домінування окремих параметрів призводить до значної різниці масштабів впливу й зумовлює появу слабо ідентифікованих параметрів. Проаналізовано спектр власних значень матриці спектральної чутливості, що дало змогу виявити ознаки наближення задачі до виродженого випадку. Додатково оцінено число обумовленості, яке підтверджує потенційну нестійкість розв’язків. **Висновки:** аналіз спектральної чутливості є ефективним інструментом попереднього оцінювання інформативності параметрів та може використовуватися для підвищення стійкості задач параметричного синтезу. Досягнуті результати можуть бути застосовані для побудови більш складних моделей спектрального аналізу та вдосконалення методів ідентифікації параметрів.

Ключові слова: спектральна чутливість; параметричний синтез; ідентифікованість параметрів; стійкість задач; спектральний аналіз; чисельний експеримент; аналітична модель; інформативність параметрів; інформаційні технології.

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