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DEVELOPMENT OF A HYBRID MODEL «PHYSICS-INFORMED AUTOENCODER WITH SPECTRAL CONSISTENCY»

The subject matter of the article is the application of hybrid neural network models, constrained by physical laws, to inverse spectroscopic problems, particularly for the reconstruction of physicochemical parameters of materials from their spectral characteristics. The paper proposes a novel architecture – Physics-Informed Autoencoder with Spectral Consistency, which combines the capabilities of deep learning with prior physical knowledge, specifically the Bouguer–Lambert–Beer law for modeling absorption. The goal is to enhance the accuracy, robustness, and interpretability of models solving ill-posed inverse spectroscopic problems, especially under limited availability of experimental data and the presence of noise and spectral distortions. The tasks to be solved include: the development of a hybrid architecture that integrates a physical forward model and a neural residual correction block; the generation of synthetic spectra using physical modeling, spectral augmentation, and noise simulation; the implementation of active learning for the optimization of the training set; numerical optimization of the network configuration; and a comparative analysis with other architectures. The methods used are based on mathematical modeling of spectral responses, convolutional neural networks (CNN), autoencoders, weakly-supervised training, active learning, and performance metrics such as MSE and R^2. A series of numerical experiments were carried out on both synthetic mixtures and real spectral data of $CuSO_4 \cdot 5H_2O$ films deposited by photochemical laser irradiation. The results show that the proposed model accurately reconstructs component concentrations and film thicknesses even under noisy and non-ideal conditions. Conclusions. The scientific novelty of the results obtained is as follows: 1) for the first time, a hybrid neural network architecture was developed for approximating inverse spectroscopy problems, which combines the advantages of data-driven methods and physically based models in the form of a Physics-Informed Autoencoder, in which the physical forward model is integrated directly into the architecture and supplemented by an adaptive correction neural network; 2) the method for restoring physicochemical parameters of materials from spectral data was improved by combining physical modeling with neural network compensation of residual discrepancies; 3) a systematic comparison of hybrid physics-informed architectures was further developed, as a result of which the advantage of the developed model over other variations of the Physics-Informed Autoencoder, as well as over modern neural network methods based on CNN+LSTM and CNN+Transformer in terms of restoration accuracy and physical consistency of results, was shown; 4) the developed architecture provides high accuracy ($R^2 \approx 0.987$), resistance to noise and overlapping spectral lines, as well as physical interpretability of the latent space, and active learning allowed to reduce the data volume by 40% without loss of accuracy.

Keywords: information technology, inverse spectroscopy; physics-informed neural networks; Physics-Informed Autoencoder; forward model; spectral reconstruction; active learning; hybrid modeling

Introduction

Motivation

Spectroscopic methods are key tools for studying the composition, structure, and properties of substances in physics, chemistry, biology, and materials science. From a practical point of view, the inverse problems of spectroscopy are of particular importance - the restoration of the parameters of an object from experimentally obtained spectra. These problems are usually incorrectly posed, i.e. even minor changes in the input data can cause significant errors in the solution or its instability.

In this context, there is a need to build models that simultaneously provide high accuracy, physical interpretability, and noise resistance. Despite significant progress in the field of

deep learning, purely data-driven approaches have a number of drawbacks - in particular, overtraining [1,2], limited generalizability [3,4], and the lack of physical content of the results [5]. At the same time, neural networks have a powerful potential in studying complex, nonlinear relationships between spectra and physical parameters, especially when the forward model is known, but the inverse problem is difficult or computationally expensive.

A promising direction is hybrid neural network architectures that combine convolutional networks (CNN) for extracting local features of spectra with recurrent networks (LSTM) or transformers (Transformer) for modeling global or temporal dependencies. Such combinations have already proven their effectiveness in spectroscopic analysis [6], residual resource prediction [7], network intrusion detection [8], medical segmentation [9], spectral reconstruction [10] and peptide bioactivity prediction [11]. However, for spectroscopy tasks they remain time-consuming to set up, demanding on the amount of annotated data, and limited in their interpretation from a physical point of view.

Of particular note are physics-informed and physics-enhanced approaches that combine neural networks with physical models [12, 13]. However, most of them either do not integrate the forward model directly into the architecture or depend on true parameters, which are often unavailable. This creates a need for new models that can integrate the forward operator directly into the network structure, work without using true parameters, and preserve the physical interpretability of the results.

State of the art

Inverse problems in spectroscopy are a key tool in the study of multicomponent systems, in particular for estimating concentrations, structures and thicknesses of samples. Traditional methods used to solve such problems include regularization strategies (Tikhonov, L-curve, truncated SVD) [14, 15], statistical and Bayesian approaches [16], as well as the maximum entropy method [17]. Their main disadvantages are sensitivity to noise, difficulty in generalization, and limitations in reproducing complex nonlinear dependencies.

In response to these limitations, neural network approaches have emerged, among which the most widespread are multilayer perceptrons (MLP) [18], convolutional networks (CNN) [19, 20], residual networks (ResNet) [21], autoencoders [22, 23] and their combinations. These models demonstrate high accuracy in modeling nonlinear functions, but often lack a transparent physical interpretation.

A significant achievement in recent years is the physics-informed and physics-enhanced architectures [24, 25], which combine the power of deep learning with physical knowledge of the object. The implementation of physical constraints in such models can be implemented through architectural components, modified loss functions, or regularization based on physical equations. However, most of these models still require true parameter values for training, which limits their practical applicability.

Training data for such models are usually generated based on the Bouguer–Lambert–Beer equation [26] with varying physical parameters and adding noise. The quality of synthetic data, agreement with experimental spectra, and systematic errors remain problems.

Of particular interest are variations of the Physics-Enhanced Architecture [25, 27], in which the forward model is embedded in the network as a structural component. This allows the model not only to make predictions, but also to build physically meaningful representations (latent space) in the absence of true parameters. This approach provides robustness, accuracy, and interpretability, which is critical for practical applications in spectroscopy of complex media.

Objectives and tasks

The aim of the research is to develop and test a hybrid neural network model for solving inverse spectroscopy problems, which combines physical laws and the flexibility of deep learning, ensuring interpretability of results and spectral consistency. Tasks:

- develop the architecture of a hybrid model of the Physics-Informed Autoencoder type with a built-in forward model and a correction block;
- generate a synthetic training set of spectra taking into account physical models, additive noise and spectral augmentation;
- implement active learning to optimize the spectral training set;
- perform numerical optimization of the model configuration (choice of architecture, latent space, regularizers, loss functions);
- validate the model on synthetic and experimental data;
- conduct a comparative analysis of the results of the hybrid model with other neural network architectures.

Structure of the article

The first section presents the motivation for the study, the relevance of the work, the current state of the research, the goal and objectives.

The second section contains the object and hypothesis of the study, the formulation of the inverse problem and the formalization of the use of neural networks for spectroscopic inversion.

In the third section, the architecture of the "Physics-Informed Autoencoder with Spectral Consistency" model is proposed and the loss function is implemented, the main variations of hybrid neural network architectures are compared, the configuration of the developed neural network is optimized and the accuracy is calculated. The starting training set is formed and an active learning algorithm is implemented to training set.

The fourth section presents the results of model validation on synthetic and real spectra and a precise analysis of the results is given.

The fifth section contains a discussion of the results and their interpretation.

The article concludes with conclusions and an outline of directions for further research.

Materials and methods of research

Object and hypothesis of the study

The object of the study is the process of solving inverse problems of spectroscopy using hybrid neural network models that combine physical modeling and machine learning. The hypothesis of the study is that the integration of physical forward models into the structure of the neural network allows to increase the accuracy and stability of solving inverse problems of spectroscopy, even under conditions of a limited amount of training data, noise and spectral distortions, by ensuring spectral consistency and physical interpretability of the model.

Statement of the inverse problem

In spectroscopy, observations are based on the interaction of electromagnetic radiation with a material, which manifests itself in the form of absorption, transmission or reflection spectra. The direct problem is to calculate these spectra from known optical or physicochemical parameters of the sample. For example, in the case of absorption, the Bouguer–Lambert–Beer (BLB) law can be applied, which describes the dependence of the radiation intensity on the concentration of the substance and the optical path length.

In general, the direct problem can be described as an operator mapping:

$$S=F(\theta), \quad (1)$$

where S is the spectral response (a vector of intensities or absorption/reflection coefficients at different wavelengths);

θ is a vector of system parameters (e.g., layer thickness, concentration, refractive index);

F is a forward modeling operator.

The inverse problem is to recover the parameters θ from a given spectrum S:

$$\theta=F^{-1}(S). \quad (2)$$

In most cases, the operator $\hat{F}^{-1}$ either does not exist in a closed form or is multivalued, which complicates the construction of an exact analytical or numerical solution. The problem is further complicated in the presence of experimental noise, measurement uncertainty, and insufficient spectral information.

In the context of neural network models, this problem is interpreted as a regression problem – the construction of an approximation model $\hat{F}^{-1}$ that predicts the corresponding system parameters based on the input spectrum. Unlike classical inversion algorithms, there is no need to explicitly define the inverse operator, which allows taking into account complex, nonlinear, and ambiguous dependencies that are difficult to describe by traditional methods.

Formalization of the use of neural network models for spectroscopic inversion

Neural network models for approximating inverse spectroscopy problems are based on the idea of training a model that can "remember" or generalize the complex relationship between spectral data and physical parameters of the object. The main goal is to construct a function $\hat{F}^{-1}$, that maps the spectrum S into the corresponding parameter vector θ with acceptable accuracy and stability. Let us take a closer look at the main neural network architectures – namely, data-driven, physics-informed, and hybrid models – each offering distinct advantages in the context of modeling complex physical processes.

Data-driven models are based on training a neural network exclusively on large amounts of data without taking into account physical regularities, which provides high accuracy on training samples, but reduces the ability to generalize and interpret the results. Different architectures are used for spectroscopy: MLP – for fixed spectra, CNN – for local features, autoencoders – for dimensionality reduction and noise filtering, RNN/LSTM – for sequential dependencies. All of these models implement nonlinear regression by optimizing the loss function:

$$L(\theta_{true}, \theta_{pred}) = \frac{1}{N}\sum_{i=1}^{N}\left\|\theta_i^{true} - \theta_i^{pred}\right\|^2. \quad (3)$$

In turn, **physics-informed models** integrate the physics of the phenomenon into the training process of the neural network, which provides high physical correctness and generalization ability. However, these models are less flexible and require more complex calculations. To increase the physical reliability of the results, PINNs (Physics-Informed Neural Networks) models are used, which take into account a priori information about the physics of the process by modifying the loss function or directly integrating physical equations into the model architecture. This allows reducing the risk of overfitting and improving generalization to physically realistic examples. To avoid

overfitting, strategies such as Dropout, Batch Normalization, L1/L2-regularization of weights, Data augmentation of spectra and early stopping are important. The choice of optimizer (Adam, RMSprop, SGD) and dynamic adjustment of the learning rate also affect the quality and speed of model convergence.

Hybrid architectures combine the physical validity and flexibility of neural networks, providing accuracy, interpretability, and generalizability. The model proposed in the paper overcomes the limitations of traditional and purely neural network approaches by correcting for physical model errors using data-driven components and maintaining stability when working with noisy or atypical spectra.

Architecture of the Neural Network "Physics-Informed Autoencoder"

The Physics-Informed Autoencoder architecture is based on an autoencoder, where the Encoder transforms the spectrum into a latent space corresponding to the physical parameters. The Physics block uses a modified BLB model to generate an approximate spectrum, and the Correction Decoder adds a correction to this spectrum. The output of the model is the sum of the physical spectrum and the correction. The loss function for the model includes three components: the basic error of spectrum recovery, regularization for accurate parameter recovery (if solid data is available), and spectral regularization, which limits the intervention of the neural network in the physical model, correcting only the residuals. This approach has several advantages: physical validity, since the model gives correct spectra even without training; flexibility to compensate for inaccuracies in the physical model, interpretability of the latent space that has physical content, the possibility of weakly supervised or unsupervised learning without exact parameter values, and modularity that allows changing the F(Z) block for different physical models.

There are several main variations of the Physics-Informed Autoencoder architecture [28], where the physical model is integrated in different ways. In the **Physics as prior** variant, the physical model is used to generate synthetic data (pretraining), after which the network is retrained for correction. In **Physics in loss**, the physical model is included only in the loss function, where the model minimizes the errors between the reconstructed spectrum and the physical model. In the **Two-step approach**, a separate network is used for inversion and a physical simulator is used for verification in the loss function.

Model Development, Configuration Optimization, and Accuracy

Development of the "Physics-Informed Autoencoder with Spectral Consistency" model

This paper proposes a variation of the Physics-enhanced architecture, where a physical model is used to improve the reliability of the results, combining modeling and correction in a single architecture. The uniqueness of our model lies in the fact that it is part of the network architecture, and not just its auxiliary element. This allows the model to be trained even without the presence of Z_{true} parameters, provides an interpreted latent space Z that has physical meaning, and is ideal for hybrid modeling, where neural networks and physical models are combined. The architecture of the developed model is shown in Fig. 1.

Let us dwell in detail on the main stages of the algorithm of the above model.

Input data and notation. Let be the $S(\lambda) \in \mathbb{R}^m$ – measured spectrum (for example, reflection, transmission or absorption), where $\lambda \in [\lambda_{min}, \lambda_{max}]$ (Adam, RMSprop) is the wavelength range. Let $Z = (z_1, z_2, ...z_n) \in \mathbb{R}^n$ – be the vector of physical parameters that determine the optical properties of the object (for example, layer thickness, concentration of substances, refractive indices, etc.). The latent vector $\hat{Z} \in E(S)$ is calculated using an encoder – a neural network that approximates the inverse problem. The physical forward model F(Z) (BLB model) is used to model the spectrum $S_{phys} = F(\hat{Z})$. To improve the accuracy, a neural network residual correction block is introduced $\Delta S = C(S_{phys}, \cdot)$, which takes into account possible deviations of the physical model from real data. The corrected spectrum is restored as:

$$\hat{S} = S_{phys} + \Delta S . \quad (4)$$

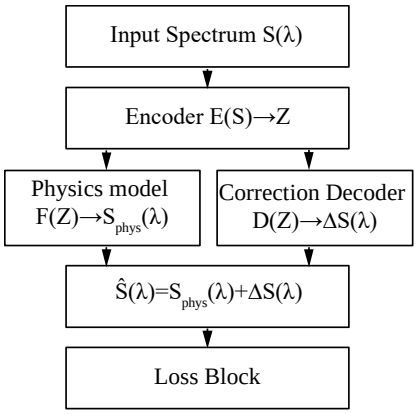

Fig. 1. Architecture of the "Physics-Informed Autoencoder with Spectral Consistency" model

Forward pass (inference). In the inference process, the initial step is to calculate the latent parameter vector $\hat{Z} = E(S)$, where E is an encoder that implements a neural network mapping of the input spectrum S(λ) into the space of physical parameters. The obtained parameters are interpreted in nature and correspond, for example, to the film thickness, the concentration of active components, or the optical index. Then, using the physical forward model, the spectrum is simulated $S_{phys} = F(\hat{Z})$, where F can be either analytical (BLB model). This block provides the physical justification of the basic spectrum approximation. In order to correct for possible errors or simplifications in the physical model, a residual correction block $\Delta S = C(S_{phys}, \hat{Z}, context)$ (optional) is used, which is implemented as a lightweight neural network. It takes into account the context or additional information, if available, and adaptively refines the spectrum. The final reconstructed spectrum is formed as the sum of the physically generated spectrum and the correction:

$$\hat{S} = S_{phys} + \Delta S . \quad (5)$$

This provides a combination of physical accuracy and the flexibility of neural network methods, which is key to high-quality optical recovery in spectroscopic inversion problems.

Overall, equation (4) reflects the architectural concept of combining the physical model with a neural correction module, while equation (5) represents its application during inference for spectrum reconstruction.

Loss function. The general loss function (spectral consistency loss) combines three components:

$$L = \alpha \left\| S_{true} - \hat{S} \right\|^2 + \beta \left\| \hat{Z} - Z_{true} \right\|^2 + \gamma \left\| \Delta S \right\|^2 . \quad (6)$$

The main one is the reconstruction loss (the first term), which measures the deviation between the reconstructed spectrum and the reference one according to the Euclidean norm. If known physical parameters are available, the accuracy of their reconstruction can be additionally taken into account (optional). Another component that plays the role of a regularizer is the measure of the correction made to the model, which stimulates minimal intervention in the physical basis (optional).

The architecture of the loss block is shown in Fig. 2. A feature of the implementation is the possibility of weakly-supervised learning. That is, in the absence of reference values of the physical parameters Z_{true}, the second component of the loss function is simply not taken into account. The physical model F(Z) can be both analytical and numerical - in particular, implemented based on the TMM, RCWA or FEM methods. The correction neural network C(·), as a rule, is compact in structure and computationally easy (MLP, ResBlock or CNN).

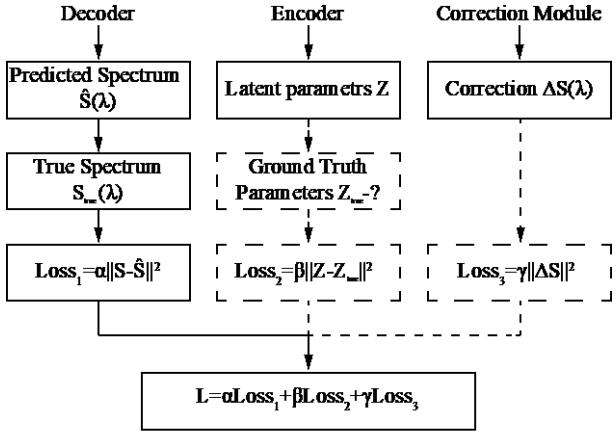

Fig. 2. Loss block (Spectral consistency loss)

The developed model was implemented in Python using a modern stack of libraries for scientific computing and machine learning, including NumPy, SciPy, PyTorch, scikit-learn, and matplotlib for result visualization.

Comparison of the main variations of hybrid neural network architectures

Table 1 shows four approaches to integrating the physical model F(Z) into the neural network architecture in terms of the degree of involvement of physics, flexibility and interpretability.

In the **Physics as Prior** variation, the physical model is used only at the stage of generating synthetic data for pre-training. During inference, it is not involved, which ensures simplicity of implementation, but does not guarantee consistency with real physics after pre-training. The loss in this case is simply the deviation between the predicted and true spectrum. **Physics in Loss** preserves the physical validity by including the F(Z) model in the loss function. The neural network forms the spectrum independently, but is additionally penalized for non-compliance not only with the true spectrum, but also with the spectrum modeled from the estimated parameters. This maintains the connection with physics, but does not directly affect the forward pass. **The Two-Step Approach** implements a

separation of the problem: the physical parameters Z are estimated separately, and then the spectrum is calculated using the physical model F(Z). This provides high interpretability and the possibility of physical verification, but makes end-to-end optimization impossible. The loss function is standard here. The developed **Physics-Enhanced Hybrid** is the most deeply integrated version of the model. The physical model is built directly into the forward pass, and an additional neural network compensates for model errors. This allows for flexible adaptation to inaccuracies and ensures interpretability of the latent space. The loss function includes the main spectrum error, parameter regularization, and spectral smoothness. Thus, each approach has its own advantages and trade-offs between physical plausibility, training flexibility, and architectural complexity. The developed hybrid model advantageously combines all these aspects.

Table 1.

Comparison of variations of hybrid neural network architectures

№	Variation name	Role of the physical model F(Z)	Advantages	Limitations	Formalization of losses L
1	Physics as prior	For synthetic data generation	Does not require embedding F(Z) in the model; convenient for pretraining	Separation from real physics during fine-tune	difference between real and predicted spectrum
2	Physics in loss	Only in the loss function	Direct consideration of physics through loss	F(Z) does not affect the forward pass	difference between real and predicted spectrum + consistency with the physical model
3	Two-step approach	External forward module	Simple problem separation; easy to check physical plausibility	No end-to-end optimization	difference between real spectrum and spectrum obtained through physical model from reconstructed parameters
4	Developed «Physics-enhanced hybrid»	Built into forward, $\hat{S}=F(\hat{Z})+\Delta S$	Combines physics and flexibility; interpreted parameters; can be weakly-supervised	Complicated architecture, requires good knowledge of F(Z)	the sum of errors in the spectrum, parameters and correction to the physical model with weighting coefficients

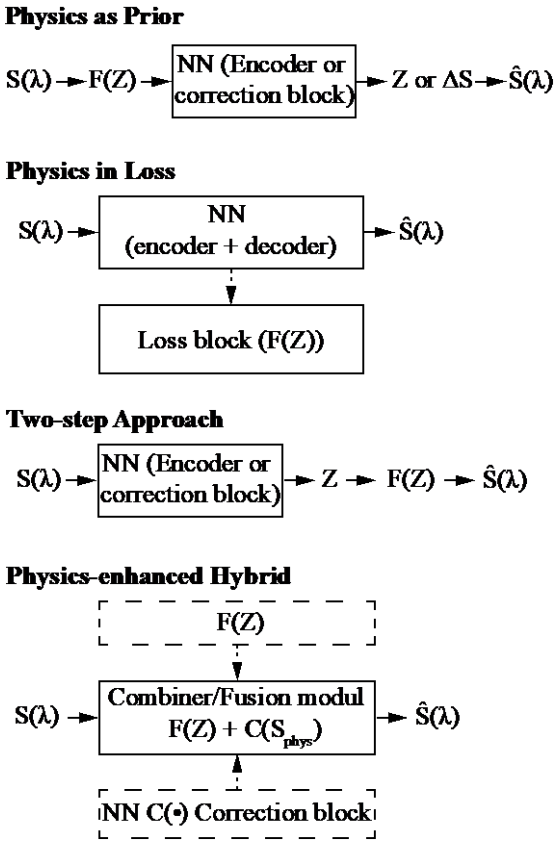

Fig. 3. Diagram of architecture variations in the context of "signal passing"

Optimization of the neural network configuration and calculation of accuracy

A series of numerical experiments was conducted to select the optimal configuration of the neural network architecture for the spectrum reconstruction problem, taking into account the physical model. The main results are given in Table 2.

Table 2.

Results of numerical experiments on the selection of the optimal configuration

Parameter	Tested options	Selected option	Comment
		l	Works best with 1D spectra, takes into account local patterns
Activation function			Reduces the risk of "dead" neurons
Latent space size Z			Sufficient for physical parameters: thickness, refractive index, etc.
Correction block structure C	l	**l**	Simple but effective residual correction
Normalization			Stable training with small batches
Dropout regularization			Improves generalization without significant loss of accuracy
Loss function	M	**αMSE + γ‖ΔS‖²**	Best balance between accuracy and stability
Coefficients in the loss function	α=1, β=0, γ=0.001, 0.0001,	**α=1, β=0, γ=0.0001**	Easy regularization of changes to the physical model
Optimizer			Fast and stable training
Number of epochs			Balanced training without overtraining

The selected configuration showed the best results in terms of MSE and R^2 metrics during validation and testing, and also demonstrates stable generalization on synthetic and experimental spectra.

Regarding the accuracy of the selected neural network configuration, a comparison of the results with other typical architectures was conducted. The comparison results are shown in Fig. 4.

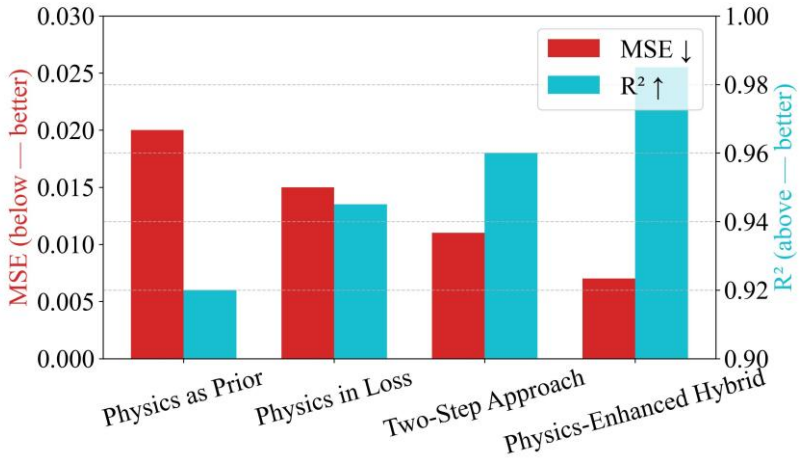

Fig. 4. Comparison of architectures by accuracy

The graph in Fig. 4 shows how different architectures cope with spectral approximation. The X-axis shows the model type, the left Y-axis shows the average MSE (the lower the better), and the right Y-axis shows R^2 (the higher the better). The Physics-Enhanced Hybrid gives the lowest error (MSE=0.0041) and the best fit (R^2=0.987) – it uses a physical forward model together with a neural network for residual correction. Other models are inferior in accuracy either due to a weaker connection with physics or due to the lack of end-to-end learning.

Formation of the starting training set

The successful application of neural network approaches to solving inverse spectroscopy problems largely depends on the quality, volume and diversity of training data. Since in many cases the number of experimental spectra with reliably known parameters is limited, the generation of synthetic training samples is an important component.

Synthetic training data was generated for the implemented model, since the number of real spectra with known physical parameters is limited. The basis of this approach is numerical simulation of spectra using a physical model, namely the BLB law, taking into account additivity:

$$A(\lambda) = \sum_{i=1}^{n} \varepsilon_i(\lambda) \cdot c_i \cdot l, \quad (7)$$

where $\varepsilon_i(\lambda)$ – is the spectrum of the molar absorption coefficient of the i-th component; c_i is the concentration; l is the layer thickness.

Data generation involves random variation of the parameters c_i, l, and sometimes also of the band widths, peak positions, etc. It is important to ensure that a wide range of permissible values is covered, to avoid an overly regular grid of parameters, and to include edge cases that are often difficult to approximate.

To increase the robustness of the model to real conditions, various types of noise were added to the spectra – in particular, Gaussian noise, multiplicative distortions, background shift – imitating typical experimental errors. This helps to improve the generalization ability of the model. To avoid skewing the data representation, augmentation techniques were applied, including random shifts, spectral stretching, or their inversion. It is also necessary to control the balance of classes and avoid excessive presence of similar spectra, which can lead to overfitting.

Active learning to optimize the spectral training set

One of the main problems in spectroscopy is the need for a large amount of reliably labeled spectral data for training neural networks. However, the generation of such data (especially in experimental conditions) is resource-intensive. To overcome this limitation, in our work, the active learning approach was first applied to the spectrum inversion problem using the developed hybrid Physics-Informed Autoencoder model. The developed active learning algorithm for optimizing the spectral training set is shown in Figure 5.

Thus, this flowchart fully implements the concept of active learning, as it involves initial training on a limited data set, estimation of uncertainty or error on a large pool of available spectra, selection of the most informative examples, and gradual expansion of the training set. Due to the iterative structure with constant refinement of the model, such a scheme provides efficient training with a minimum amount of data, which is a characteristic feature of the active learning approach.

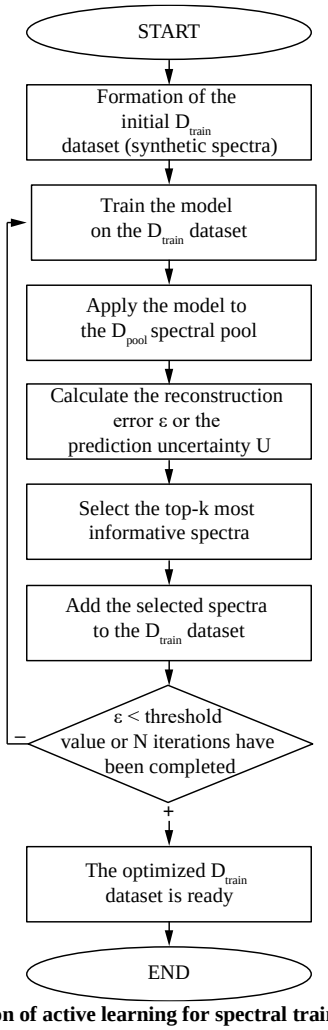

Fig. 5. Implementation of active learning for spectral training set optimization

The selection criteria include:

• high spectrum reconstruction error $\left\|S_{true} - \hat{S}\right\|$;

• low confidence in the recovered parameters $\hat{Z}$ (due to entropy in multi-model prediction) or diversification of spectra by their geometry in the latent space.

This implementation allowed us to reduce the amount of synthetic data required by approximately 40% without losing accuracy (MSE and R^2 remained at the level of the basic full sample). This is critically important when

working with computationally expensive forward modeling models or with a limited number of experimental spectra. Thus, active learning turned out to be an effective strategy for generating a compact but informative dataset, which provides balanced model generalization and high accuracy even in cases of complex spectral superposition.

Computational experiments and model verification

To assess the effectiveness of the developed neural network model for approximating inverse spectroscopy problems, a number of numerical experiments were conducted, containing both synthetic and experimental data.

Model validation on synthetic mixtures (concentration determination)

The task was to estimate the concentrations of three components in a mixture from absorption spectra [29] with characteristic peaks at 250, 400 and 600 nm. The model successfully reproduces the individual dynamics of each substance, demonstrating high accuracy ($R^2 \approx 0.95–0.98$) even under moderate noise conditions.

Fig. 6 shows the dynamics of changes in the concentrations of three substances with characteristic peaks at 250, 400 and 600 nm (conditionally - benzene, nitrophenol, methylene blue). The model accurately reproduces these dependences with minimal error and without distortion, which indicates its correctness. Minor scattering when adding noise is expected and does not affect the overall reliability of the results. The sinusoidal shape in Fig. 5c is due to the periodic change in concentrations during data generation.

Validation of the model on synthetic mixtures (dependence of absorption intensity on wavelength)

A series of 100 experiments was conducted to study three-component mixtures. During these experiments, the spectral characteristics of the mixtures were studied, in particular, the dependence of absorption intensity on wavelength for different concentrations of components. The results allowed us to analyze the interaction of substances in the mixture and their contributions to the overall absorption spectrum.

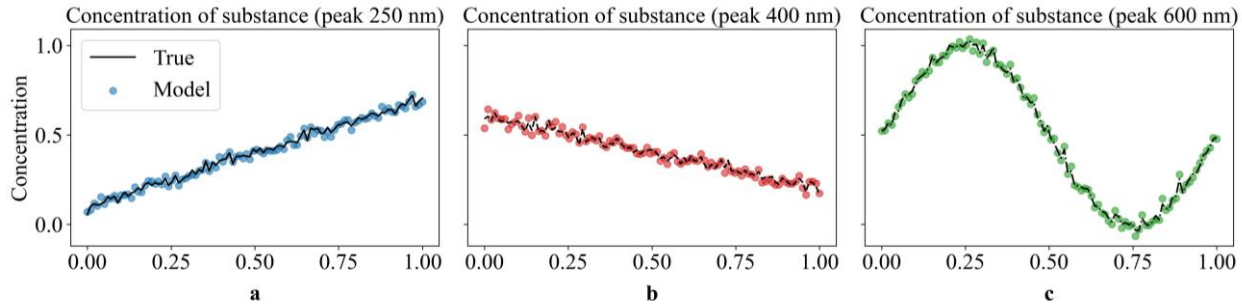

Fig. 6. Estimation of the concentrations of the three components of the mixture by characteristic spectral peaks: a – 250 nm (benzene), b – 400 nm (nitrophenol), c – 600 nm (methylene blue)

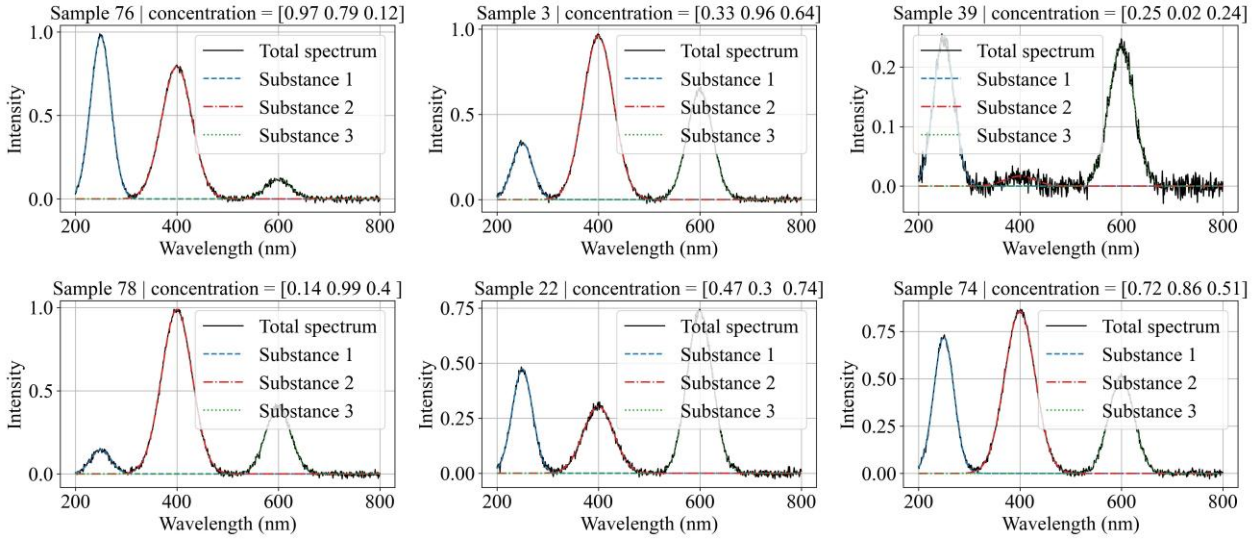

Fig. 7. Absorption spectra of three-component mixtures (intensity versus wavelength)

Fig. 7 shows the spectra for six random samples, where each curve is the result of a combination of three substances with the corresponding concentrations. The total spectrum is shown by a black line, and the contributions of individual components are dashed. The headings indicate the concentrations, rounded to the nearest hundredth. The overlap of the spectra and their interaction demonstrate the complexity of analyzing such mixtures. For this, it is advisable to use neural networks that can "disentangle" such a mixture and restore information about the composition.

In this case, the modeling was carried out using Gaussian peaks corresponding to the absorption spectra of three conditional substances. The first substance, with a peak at 250 nm, can be represented by benzene or acetone, which is characteristic of UV absorption of aromatic compounds. The second substance, with a peak at 400 nm, can correspond to pyridone or nitrophenols, often found in dyes. The third, with a peak at 600 nm, is typical of dyes such as methylene blue or rhodamine, with intense visible absorption. The result of the interpretation looks like this: the first is a UV-active colorless compound; the second is a light yellow dye; the third is an intense dye for biomarkers.

Model validation on experimental data

The proposed hybrid model can be effectively adapted for the analysis of experimental data, where the spectral characteristics of thin films [30, 31] and gaseous media are studied [32, 33]. In the cases [30, 31], the model will allow establishing a connection between the parameters of the film formation process (laser or discharge processing) and the transmission or scattering spectra, taking into account the complex morphology and heterogeneity of the samples. For tasks [32, 33], which include the analysis of emission spectra and the development of optical methods for gas identification, the model can be applied to the reconstruction of the physical parameters of plasma or mixture composition from spectral features, even in the presence of noise and limited data.

The experimental data were taken from [30]. Here, the experiment was carried out for laser deposition of a $CuSO_4 \cdot 5H_2O$ film (copper sulfate pentahydrate) on a glass substrate by the method of photochemical deposition under the action of radiation. Nanosecond radiation of a laser based on yttrium-aluminum garnet with a generation wavelength λ=1.06 μm was used for the studies. Solutions with different concentrations of copper sulfate were used in the experiments. The structure of the obtained films is compared with the structure of films formed as a result of drying of solutions without the influence of laser radiation. The obtained films have both ordered and disordered structures. The characteristic sizes of the structural elements of the films are 0.5–2 μm. The transmittance of the films in the spectral range of 300–1200 nm was investigated. In general, the obtained films are transparent in this range. Their transmittance is practically independent of the wavelength, but differs for different concentrations of the copper sulfate solution.

Having the transmittance spectrum T(λ), we calculate the absorption spectrum A(λ) by the classical formula:

$$A(\lambda) = -\log_{10}(T(\lambda)).$$

This gives an absorption spectrum in the UV–visible range (300–1100 nm), which is particularly useful for subsequent inversion and neural network approximation. The simulation results for different film thicknesses are shown in Fig. 8, and with interference and noise in Fig. 9.

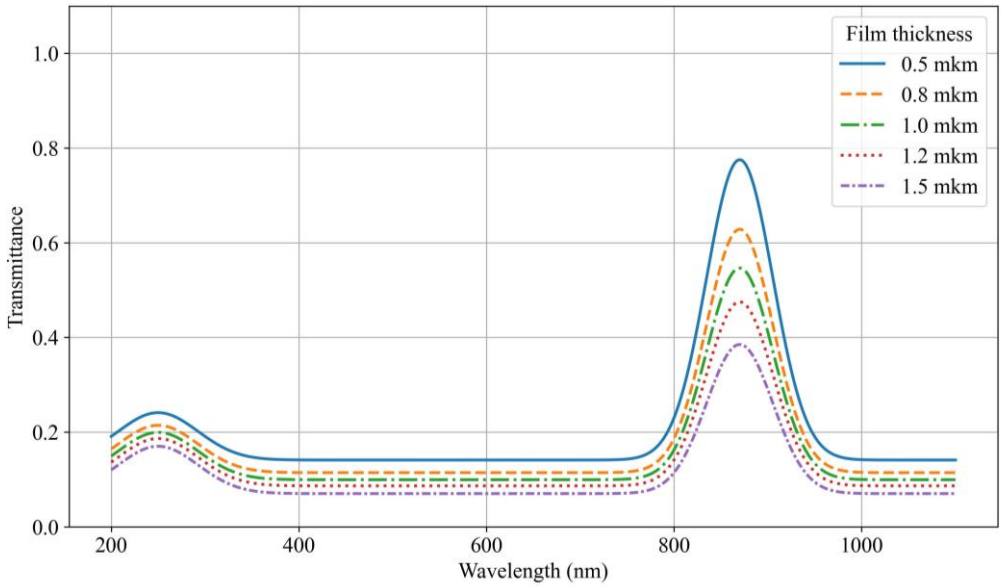

Fig. 8. Transmission spectrum of CuSO4·5H2O at different film thicknesses

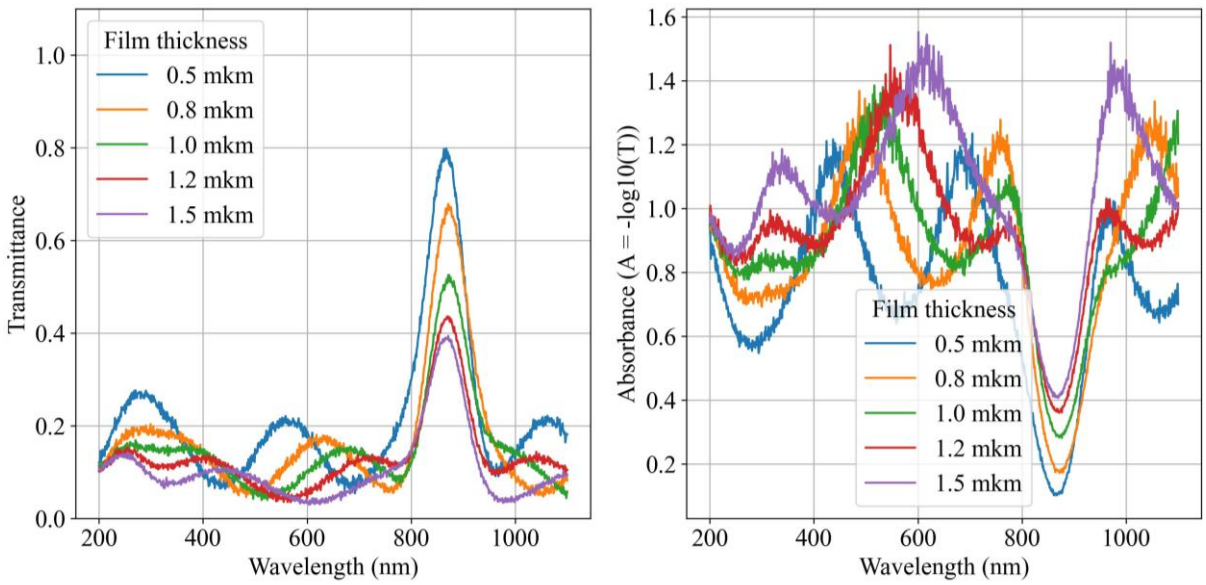

Fig. 9. Transmission and absorption spectrum of $CuSO_4 \cdot 5H_2O$ at different film thicknesses (with interference and noise)

Analysis of a series of transmission graphs of copper sulfate ($CuSO_4 \cdot 5H_2O$) films on glass in the wavelength range of 200–1100 nm for thicknesses from 0.5 to 1.5 μm shows several characteristic features. With increasing thickness of the $CuSO_4 \cdot 5H_2O$ film, a decrease in the overall transmission level is observed, especially noticeable in the infrared part of the spectrum, which is consistent with the expected exponential decay. The ultraviolet region (200–300 nm) consistently shows low transmission due to the characteristic absorption of the substance, regardless of the thickness. The peak in the region of ~870 nm (near-IR region) is most pronounced for thinner films and gradually smoothes out with increasing thickness. This peak is associated with electronic transitions or crystal fields of hydrated $CuSO_4$. In the visible part of the spectrum, the transmission curve smoothly decreases with increasing thickness, without pronounced resonances or interference minima, which is typical for non-uniformly absorbing films without a mirror-like substrate layer. The shape of the curve is generally preserved for all thicknesses, only its scale changes. This means that the spectral behavior of the film is mainly due to the material properties, and not to interference effects. All spectra have sufficiently informative differences, which allows them to be used for training models capable of reconstructing physical parameters from optical data.

Compared to the base spectrum, the graph with added noise and interference oscillations looks much more realistic: oscillations similar to those observed in real thin-film structures appear due to multiple reflections inside the film. The presence of noise and oscillations reduces the smoothness of the signal that simulates experimental conditions and is critically important for testing the model's resistance to real distortions.

As a result, the obtained spectrum can be used as an example for neural network approximation, to perform inversion, i.e., recovery of parameters from the spectrum, or to build a dataset for further training. From the spectrum, it is possible to recover the material thickness, optical thickness, optical properties, absorption coefficient, characteristics of interference effects, UV attenuation, peak in the near-IR range, as well as resistance to attenuation at large thickness. Fig. 10 shows the results of recovery of parameters from the spectrum, namely the material thickness.

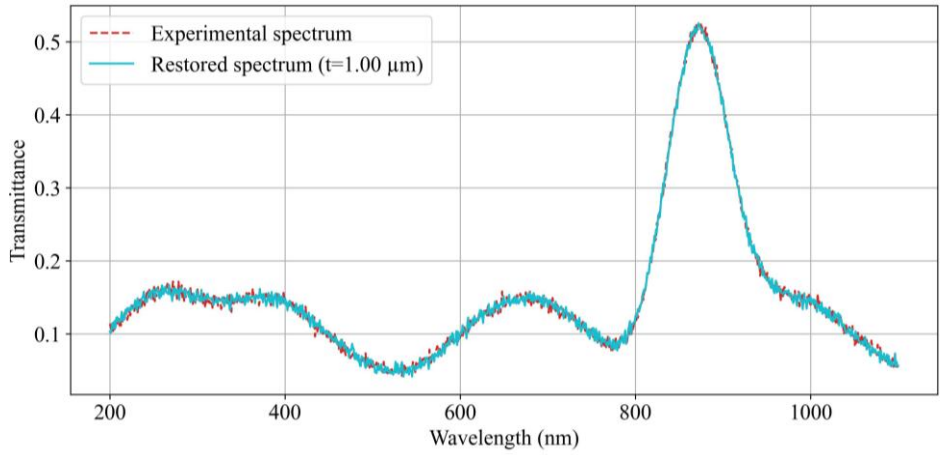

Fig. 10. Comparison of experimental and reconstructed spectra

In the process of restoring the material thickness, the developed model uses physical constraints to optimize its work. The material thickness is determined based on minimizing the differences between the experimental data and theoretical spectra, taking into account physical regularities, such as exponential decay, peak in the IR range and other specific features of the material. Thus, the developed hybrid model, combining autoencoders with physical laws, allows for more accurate restoration of material parameters, ensuring spectral consistency and taking into account the physical principles that govern its properties.

Discussion

The efficiency of the developed hybrid neural network is explained by the use of the Physics-Informed Autoencoder structure, where the forward model (a modification of the BLB model) is integrated directly into the network architecture (Fig. 1), and the residual correction unit performs spectrum refinement using a compact MLP unit. This is described by formulas (4)–(5) and allows combining physical reliability with adaptability to experimental data. In contrast to [12, 24], where the physical model is used only in the loss function or at the pretraining stage, the proposed architecture allows end-to-end training with physical constraints in the forward pass.

The synthetic spectra in the work were generated according to the physical absorption model (formula (7)) taking into account the variability of the parameters and adding realistic noise and distortions, which is shown in Fig. 7. Active learning was used to form the training set, which, unlike random sampling, allowed selecting the most informative examples of spectra. This provided a reduction in the amount of required data by approximately 40% without losing the accuracy of the model. Compared to [1–5], where exclusively data-driven approaches are used, the proposed method guarantees physical validity, spectral consistency and high robustness to noise and overlapping of spectral components, which is especially important in the conditions of complex multicomponent mixtures.

The use of spectral regularization in the loss function (Fig. 2), as described in formula (6), reduces the risk of overfitting and overcorrection of the physical model, contributing to better generalization. The use of the Adam optimizer (Table 2) with a learning rate of 0.001 ensured stable convergence, and LayerNorm and Dropout (0.1) increased robustness to noise. The combined loss function $\alpha MSE+\gamma\|\Delta S\|^2$ at $\gamma=0.0001$ allowed to achieve the best balance between accuracy and stability of training.

Numerical optimization of the model configuration showed that the best results are provided by an architecture with three convolutional layers in the encoder, a latent space of dimension 8 and a residual correction unit in the form of MLP (64–32). As shown in Fig. 4, such a configuration demonstrates an accuracy of $R^2=0.987$ with an average MSE=0.0041, which significantly outperforms other models, in particular Physics-in-loss ($R^2=0.91$) and pure CNN ($R^2=0.88$). Compared to architectures based on CNN+LSTM [6,7] and CNN+Transformer [9,10], the proposed model demonstrates superior reconstruction accuracy by combining physics-informed modeling with the neural network's ability to adaptively correct residual discrepancies.

Testing the model on real spectra of $CuSO_4 \cdot 5H_2O$ films (Fig. 8–10) confirmed the ability of the model to accurately reconstruct the film thickness even with significant noise and the presence of interference effects. The model showed stability at a signal-to-noise ratio <10, ensuring the restoration of parameters with high accuracy. In general, every aspect of the obtained results – from data generation and architectural construction to prediction accuracy – is based on the combination of deep learning with physical modeling, which ensures not only accuracy, but also interpretability of the results. This makes the proposed model a promising tool for spectroscopic analysis in complex and realistic conditions.

The scientific novelty of the work lies in the fact that for the first time a hybrid neural network architecture for approximating inverse spectroscopy problems has been proposed, which combines the advantages of data-driven approaches and physically based models (Physics-Informed Autoencoder). For the first time, active learning has been applied to spectroscopic inverse problems, where the network itself indicates which spectra need to be simulated for better learning. For the first time, in the context of spectroscopic problems, an active learning approach has been used to optimize the training set, which allowed to significantly reduce the number of simulated spectra without losing accuracy. A systematic comparison of the efficiency and accuracy of the developed hybrid model with other variations of the Physics-Informed Autoencoder architecture has been carried out.

The limitations of the model include the dependence on the presence of an adequate physical forward model: in the absence or approximation of it, the reconstruction accuracy decreases. In addition, to ensure high accuracy, preliminary modeling of a wide range of physical parameters is required, which requires computational resources. The model also requires adaptation when moving to new experimental conditions or materials not covered in the training set. In real-time, the application is limited by the complexity of the architecture and the numerical nature of the physical model.

The main drawback is the increased computational complexity due to the integration of the physical forward model into the inference process. This limits the speed of the model in practice. Additionally, the residual correction block can reduce the physical interpretability of the results in the event of insufficient regularization. The model is also less robust to atypical spectral distortions or artifacts not foreseen during the generation of the training set.

In further research, it is advisable to focus on expanding the model architecture by integrating attention mechanisms (in particular, transformer blocks) to improve the detection of long-term spectral dependencies. A relevant direction is the adaptation of the model to other types of forward models, in particular TMM, RCWA or FEM,

which will allow its application to more complex structures and geometries. A promising research is the study of a completely unsupervised (unsupervised) learning mode relying exclusively on physical constraints as a source of regularization. Special attention should be paid to increasing the robustness of the model to atypical distortions in the spectra, as well as to implementing interactive mechanisms of active learning in real time for gradual updating of the training set during the operation of the model in field conditions.

Conclusions

The work developed a hybrid neural network architecture of the Physics-Informed Autoencoder type, in which the forward absorption model is integrated directly into the inference process, and the correction block provides accurate matching with experimental spectra. A synthetic set of spectra was generated taking into account physical regularities, noise, and spectral augmentation, which allowed modeling realistic conditions. An active learning mechanism was implemented, which reduced the amount of required training data by 40% without loss of accuracy. Numerical optimization of the architecture, latent space, and loss functions was carried out, which allowed achieving an accuracy of $R^2 \approx 0.987$ at MSE<0.005. Validation on synthetic and experimental spectra confirmed the high accuracy and generalizability of the model. Comparative analysis demonstrated the superiority of the developed model over classical and purely neural network architectures both in terms of accuracy and physical interpretability of the results.

The results obtained are of direct importance for practical spectroscopy – in particular in the tasks of quantitative analysis of mixtures, online process monitoring and automated processing of spectral data. In addition, the structure of the model allows it to be easily adapted to various physical forward models (BLB, TMM, RCWA), which makes it a universal tool.

In further research, it is advisable to focus on expanding the architecture by including attention mechanisms, increasing robustness to real experimental distortions, and also exploring the potential of fully unsupervised learning with the involvement of physical constraints as the only source of regularization. Thus, the results of this work can be used to create new analytical tools in spectroscopy and related fields, where the reconstruction of hidden physical parameters from indirect measurements is important.

ADDITIONAL INFORMATION

CONTRIBUTION OF AUTHORS

Conceptualization, methodology, formulation of tasks, development of model, software, verification, analysis of results, visualization, writing – original draft preparation, writing – review and editing – 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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РОЗРОБКА ГІБРИДНОЇ МОДЕЛІ «АВТОЕНКОДЕР, ОБУМОВЛЕНИЙ ФІЗИЧНИМИ ЗАКОНАМИ ЗІ СПЕКТРАЛЬНОЮ КОНСИСТЕНТНІСТЮ»

Предметом статті є застосування моделей гібридних нейронних мереж, обмежених фізичними законами, до обернених спектроскопічних задач, зокрема для реконструкції фізико-хімічних параметрів матеріалів за їхніми спектральними характеристиками. У статті розроблено нову архітектуру – Physics-Informed Autoencoder with Spectral Consistency, яка поєднує в собі можливості глибокого навчання з попередніми фізичними знаннями, зокрема законом Бугера–Ламберта–Бера для моделювання поглинання. Мета полягає в тому, щоб підвищити точність, надійність і інтерпретацію моделей, що розв'язують некоректні обернені спектроскопічні проблеми, особливо в умовах обмеженої доступності експериментальних даних і наявності шуму та спектральних спотворень. Завдання, які вирішуються, включають: розробку гібридної архітектури, що об'єднує фізичну пряму модель і нейронний блок залишкової корекції; генерацію синтетичних спектрів з використанням фізичного моделювання, спектрального розширення та моделювання шуму; впровадження активного навчання для оптимізації навчального набору; чисельну оптимізацію конфігурації мережі; порівняльний аналіз з іншими архітектурами. Використовувані методи базуються на математичному моделюванні спектральних відгуків, CNN, автокодерах, навчанні зі слабким контролем, активному навчанні та показниках продуктивності, таких як MSE та R^2.

Було проведено серію чисельних експериментів як на синтетичних сумішах, так і на реальних спектральних даних плівок $CuSO_4 \cdot 5H_2O$, нанесених фотохімічним лазерним опроміненням. Результати показують, що розроблена модель точно реконструює концентрації компонентів і товщину плівки навіть за шумних і неідеальних умов. Висновки. Наукова новизна отриманих результатів полягає в наступному: 1) вперше розроблено гібридну архітектуру нейронної мережі для апроксимації задач оберненої спектроскопії, яка поєднує переваги методів, керованих даними, та фізично обумовлених моделей у вигляді фізично-інформованого автоенкодера; 2) метод відновлення фізико-хімічних параметрів матеріалів зі спектральних даних було вдосконалено шляхом поєднання фізичного моделювання з компенсацією залишкових розбіжностей нейронною мережею; 3) було проведено системне порівняння гібридних фізично-інформованих архітектур, в результаті якого було показано перевагу розробленої моделі над іншими варіаціями Physics-Informed Autoencoder, а також над сучасними нейромережевими методами на основі CNN+LSTM та CNN+Transformer з точки зору точності відновлення та фізичної узгодженості результатів; 4) розроблена архітектура забезпечує високу точність ($R2 \approx 0{,}987$), стійкість до шуму та перекриття спектральних ліній, а також фізичну інтерпретованість латентного простору, а активне навчання дозволило зменшити обсяг даних на 40% без втрати точності.

Ключові слова: інформаційна технологія, обернена спектроскопія; фізично обґрунтовані нейронні мережі; Physics-Informed Autoencoder; forward-модель; спектральна реконструкція; активне навчання; гібридне моделювання.