Methodology for Solving High-dimensional Multi-Parameter Inverse Problems of Indirect Measurements

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***Abstract*—Inverse problems (IP) of indirect measurements are a class of IP encountered in most modern nature science experiments. Unfortunately, they are characterized by a number of properties making them hard to solve: they may be ill-posed or even incorrect, non-linear, and often they are characterized by high dimension by input and/or by output. As such, IP of indirect measurements require special methods to solve them. One of the classes of such methods are methods of machine learning (ML), which however possess special properties which should be taken into account when using them. In this paper, the authors suggest an outline of a special methodology, which can become the base for a standard scenario for processing data of indirect measurement IP with ML methods. The main notions underlying this methodology are also described and explained.**

Keywords—inverse problems, indirect measurements, machine learning, optical spectroscopy, exploration geophysics

I. Introduction

The times when a scientist had an opportunity to measure directly the quantities he was interested in, seem to be gone forever. Nearly every nature science experiment nowadays provides indirect measurements – scientists measure the quantities they are able to measure, and then they have to solve the problem of restoration of the quantities they are interested in from those measured in experiment. Nearly the same often refers to computational science or computational experiment – the results of such computations most often require a method of transfer to the desired quantities.

From the mathematical point of view, the studied object implements the direct function $Y=F(X)$ performing transfer from the studied quantities – *parameters* X (which are primary) to those measured or calculated during real or computational experiment – the *observed values* Y (which are secondary). This means that a scientist performing real experiment or calculation of the direct function encounters a problem of the inverse transfer, i.e., the problem of estimation or approximation of the inverse function $X=F^{-1}(Y)$ – an inverse problem (IP). Such problems require special methods to solve them.

The problem is that IP possess specific properties [1]. They may be ill-posed or even incorrect, and IP of indirect measurements are often non-linear, they often have high dimension by input and/or by output. For this reason, elaboration of a special methodology for solving high-dimensional multi-parameter IP of indirect measurements may be useful for a wide range of scientists who encounter such problems, and it was the goal of the present study. The study is based on the large experience of the authors in solving IP of the considered type from two problem domains: exploration geophysics (EG) [2] and optical spectroscopy (OS) [3].

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II. General Approaches to Solution of Inverse Problems with Machine Learning Methods

There are two in principle different general approaches to the solution of IP of the considered type with ML methods, and one intermediate approach. This classification was first introduced in [4, 5].

A. Model-based Approach

Here we assume that an adequate model of the direct function $Y=F(X)$ is available. Such model may be an analytical formula or a result of computational solution of the direct problem. This means that we can obtain training, validation, and test sets with necessary representativity to build ML models to approximate the inverse function $X=F^{-1}(Y)$ with necessary precision. However, the obtained solution of the IP will be only as adequate as the initial model of the direct function.

An example of the class of IP where the model-based approach is effectively used are the IP of exploration geophysics – e.g., gravimetry, magnetometry and magnetotelluric sounding [6-8].

B. Experiment-based Approach

The opposite situation is when no adequate model of the direct function is available, but when we have an array of patterns *(X, Y)* describing the object of the study, obtained in experiment. In this case, the relevancy of the patterns is ensured by the experiment (to the extent of the experimental error) – contrary to the model-based approach, no special notions or *a priori* information are used to obtain the data. However, in many cases the amount of data within the experiment-based approach may be insufficient to provide the necessary representativity of the datasets necessary to use the ML methods, thus making reduction of the input dimensionality of the problem nearly obligatory.

An example of the class of IP where the experiment-based approach is effectively used are the IP of spectroscopy, especially optical spectroscopy of liquid objects where no analytical or computational solution of the direct problem are available – optical or IR absorption spectroscopy, Raman spectroscopy, fluorescence spectroscopy [9-11].

C. Qusi-Model Approach

This intermediate approach has to be used in the worst case when neither an adequate model of the direct function, nor a large enough amount of the experimental data are available. Then the only way out is the following: attempt to construct a so-called quasi-model of the direct function based on the small amount of the experimental data that is available. Usually, such model is a statistically based one, or an approximation one, in contrast to a substantial subject area informed model used within the model-based approach. The quasi-model can be also used to provide the necessary amount of data, with necessary representativity. However, the IP solution obtained within the quasi-model approach can be only as adequate as the quasi-model is.

It is interesting to note, that since this classification was first introduced in 2002 [4, 5], the authors of this study had only a few examples of relatively successful application of the quasi-model approach. Usually transfer from the experiment-based approach to the quasi-model approach did not lead to any improvement in the IP solution quality, independent on the method that was used to build the quasi-model to solve the direct problem: different kinds of interpolation or various ML methods. It was only in 2021 [12], 2022 [13], and 2023 [14] when we have demonstrated that use of variational autoencoders (VAE) as quasi-models can yield stable positive effect: when the experimental dataset was expanded by the artificial data generated by VAE built on the experimental data, the error of the solution of an IP of optical spectroscopy was substantially reduced.

III. Types of Integration

The main emphasis in the developed methodology is on the integration of three types – the integration of data, algorithms and physical methods.

The grounds for using integration are as follows.

Integration of data by cross-validation or other types of bagging allows one to take into account variability of data in an optimal way, especially in the case when the amount of data available is relatively small.

Integration of algorithms by ensembling using algorithms differing from each other is based on the fact that errors of different algorithms are uncorrelated. In this situation, combining the answers of various algorithms within an ensemble allow the algorithms to partly compensate the errors of each other.

Both above types of integration are well known, and they are often used to solve any type of problems with ML, not only the IP.

Less trivial is the integration of physical methods (IPM). It is based on the fact that when used to determine the same set of IP parameters, various physical methods may bring different information. Their joint use may allow one to utilize all this information simultaneously.

However, there is a possible shortcoming in using the IPM for high-dimensional IP. Direct combining of the physical methods by simultaneous use of their data leads to a several-fold increase in the input dimension of the problem, thus significantly worsening the ratio between the number of patterns and the number of input features, which may be critical for many types of ML methods (e.g., for neural networks). So, this situation increases the requirements for reduction of the input dimensionality of the problem.

As a result, IPM is not always effective. Previous studies of the authors demonstrated that IPM is effective when the results provided by the combined methods separately are comparable [8, 15]. If one method gives much smaller IP solution error than the other one, then the "strong" method alone may outperform the results of IPM [16, 17].

IV. Methods of Reduction of the Dimensionality of a Problem

For the high-dimensional multi-parameter IP, both types of dimensionality reduction should be discussed – by input and by output.

Methods of input dimensionality reduction may be divided into two main groups: feature selection and feature extraction methods. Among the main merits of feature selection is the opportunity of analysis of the selected most significant features from the point of view of the subject area of the problem. Such analysis may provide the scientist with additional information about the studied object.

Feature selection method are in their turn usually divided into three large groups: filter methods, wrapper methods, and embedded methods.

Filter methods are based on comparison of relevance of input features in respect to a specific output feature separately, one by one; the relevance is usually estimated with the help of statistical methods (e.g., correlation). Possible multicollinearity of the input features (that may be also estimated by cross-correlation of the features) may require to be taken into account separately [18].

Wrapper methods are based on repeated solution of the studied problem on various subsets of the input features – e.g. by gradual adding or by gradual discarding them.

Finally, embedded methods are based on the solution of the studied problem with an ML method with subsequent analysis of the method coefficients (e.g. neural network weight analysis or analysis of regression coefficients).

A more detailed description of feature selection methods may be found elsewhere [19].

Feature extraction methods provide transfer of the input data into another feature space using some transformation of the features (e.g., principal component analysis, Fourier or wavelet decomposition). Such methods allow only indirect analysis of importance of initial features, but they are usually able to provide a greater reduction in the input dimensionality of the problem.

As for the output dimensionality of the multi-parameter IP, there are also several ways to deal with it. Here we may distinguish autonomous, group/simultaneous, and sequential determination of parameters [20].

The simplest and most obvious way to solve an N-parameter IP is by solving N separate single-parameter IPs. In this case, each of the N partial problems is simpler, but we have to solve N problems instead of one and in this way, we do not take into account possible interconnections among the output features.

The opposite approach is to try solving the multi-parameter IP "as is", using muti-output ML methods. Such methods may take into account the interconnections among the output features, but they rapidly degrade with increasing number of the outputs.

An intermediate way is to use the so-called group determination of parameters. In this case, parameters are combined into groups with simultaneous determination of the values of the parameters within each group; the groups are processed separately. The efficiency of this approach depends on the grouping – it is most effective if the parameters within each group have similar dependences on the output features, or at least they depend on mostly coinciding sets of the input features [20, 21].

Finally, the sequential determination of parameters may be effective if the parameters differ much in the quality of the IP solution in the autonomous determination mode. In this case we may start with determination of the parameters that are determined best, followed by determination of other parameters using the values of the parameters already determined as additional input features [22]. This approach is the one most difficult to implement.

It should be also noted that, according to our previous studies, simultaneous use of group and sequential determination of parameters is ineffective [23].

V. Formulation of the Methodology

We will present here the main provisions of the formulated methodology. The solution of high-dimensional nonlinear IP of indirect measurements using ML methods consists of the following main stages.

Stage 0. Carry out planning of experimental measurements (in case of implementation of the experiment-based or quasi-model approaches) or model calculations of the direct problem (DP) (in case of implementation of the model-based approach). When planning, it is necessary to take into account the possibility of implementing the integration of physical methods (IPM), for which it will be necessary to plan experimental studies or calculations with the formulation of associated IP with a common set of determined parameters for various physical methods.

Stage 1. In accordance with the plan developed at Stage 0, carry out experimental measurements or calculations of the direct problem, as a result of which a basic data set will be obtained to determine the desired parameters by solving the IP. Maximize the number of patterns in the base set as much as possible. If necessary, use the generation of additional data within the framework of the quasi-model approach.

Stage 2. Analyze the data in the base set. Evaluate the number and relationship of the parameters to be determined. Make an initial decision about the need and ways to reduce the output dimension of the data.

Stage 3. Evaluate the input dimension of the data. Make an initial decision about the types of lowering the input dimension of data (meaningful selection of input features, adaptive selection of input features, transformation of the space of input features (feature extraction)) and about their methods. Perform the reduction of the dimension of the input data.

Stage 4. Evaluate the ratio of the number of patterns and the number of input features in the transformed feature space, as well as the variability of the data. Make an initial decision on the need to use integration of data – cross-validation and other types of bagging.

Stage 5. Evaluate the arsenal of ML methods available for use, implementing various ways to solve the problem, primarily methods of approximating the inverse function. Make an initial decision about which of these methods and in what order will be used.

Stage 6. Build the basic solutions of the desired IP based on individual ML methods, in the autonomous determination mode, based on the data of each physical method separately. In the future, these basic solutions will be used as reference solutions. If possible, select the optimal values of the algorithm parameters using the grid search method.

Stage 7. Consider the possibilities and available ways of integrating algorithms, primarily the construction of homogeneous and weighted ensembles and stacking. Implement the integration of algorithms and compare its results with reference ones.

Stage 8. Implement, if possible, the integration of physical methods. Compare the results with the reference ones.

Stage 9. Evaluate the effectiveness of the approaches used in the process of solving the problem. If necessary, make changes to the initial decisions made earlier in stages 2-5 and repeat the work, starting from the corresponding stage.

The sequence of actions is repeated until the desired result is achieved or until the available resources for solving the problem are exhausted.

Some stages of the described methodology can be omitted depending on the specifics of the task being solved, as well as on the available resources.

Conclusion

This study presents an integrated methodology for solving high-dimensional multi-parameter inverse problems of indirect measurements. This methodology may be used as a checklist by a researcher starting to solve an inverse problem of the specified type.

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