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Aim and Scope

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Contents

Editorial

Kulyabov, D. S., Korolkova, A. V., Sevastianov, L. A., Rybakov, Y. P. Typesetting tables 235

Computer science

Khachumov, M. V., Emelyanova, Y. G., Khachumov, V. M. Construction and modeling of the operation of elements of computing technology on fast neurons 242

Modeling and simulation

Lapshenkova, L. O., Malykh, M. D., Matyukhina, E. N. On the algebraic properties of difference approximations of Hamiltonian systems 260

Vasilyeva, I. I., Druzhinina, O. V., Masina, O. N., Demidova, A. V. Analysis of the stochastic model "prey–migration area–predator–superpredator" 272

Belicheva, D. M., Demidova, E. A., Shtepa, K. A., Gevorkyan, M. N., Korolkova, A. V., Kulyabov, D. S. Using NeuralPDE.jl to solve differential equations 284

Physics and astronomy

Rybakov, Y. P. Dark matter hypothesis and new possibilities of the Skyrme–Faddeev chiral model 299

Letter to the editor

Egorova, M. A., Egorov, A. A. Research of hieroglyphic signs using audiovisual digital analysis methods 309

Shchetinin, E. Y., Velieva, T. R., Yurgina, L. A., Demidova, A. V., Sevastianov, L. A. Methods for developing and implementing large language models in healthcare: challenges and prospects in Russia 327

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Editorial

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Typesetting tables

Dmitry S. Kulyabov[1, 2], Anna V. Korolkova[1], Leonid A. Sevastianov[1, 2], Yuri P. Rybakov[1]

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Abstract. Recommendations are provided for the typesetting of tabular material in the journal in order to standardize its appearance.

Key words and phrases: table, table typesetting, LaTeX

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1. General recommendations for table typesetting

Tables are used to organize and visually present data in a structured format. They should contain clearly defined and comparable data, logically distributed across columns and rows.

- Rows contain different objects or records.
- Columns represent parameters or characteristics (e.g., numeric values, text).

It's important that the data is consistent within columns and well-structured for easy comprehension.

The table's appearance should be legible: clearly delineated columns and rows, column headings, and, if necessary, dividing lines. Tables shouldn't be cluttered: too many columns or rows make the table difficult to read.

1.1. Recommendations

- Avoid using excessively long text in cells—it reduces readability.
- Align data logically: text should generally be left-aligned, and numbers should be right-aligned or centered.
- Column headings should be informative but short.
- Avoid unnecessary borders and lines.

2. Typesetting of tables in LaTeX

LaTeX table layout tools are well-documented in the literature [1].

We'll give a brief overview of the LaTeX packages used for table typesetting (see Table 1).

You can refer to the CTAN (Comprehensive TeX Archive Network) category: https://ctan.org/topic/table.

Table 1

Using LaTeX packages for typesetting tables

Package	Features	When to Use
`tabular`	Basic syntax, minimal settings	Simple tables
`array`	Extended columns (p, m, b)	Tables with text
`tabularx`	Automatic width adaptation	Long tables
`booktabs`	Professional lines	Scientific publications
`tabularray`	Full control through key parameters	Complex layouts, templates

2.1. List of packages

2.1.1. Array package

- CTAN: https://ctan.org/pkg/array.
- Allows you to define new column styles.
- Can be used with other packages to extend their functionality.

2.1.2. Tabularx package

- CTAN: https://ctan.org/pkg/tabularx.
- Extension to the tabular package.
- Allows the creation of columns with automatically balanced widths.
- Introduces an additional column type, `X`.
- Creates a paragraph-like column whose width automatically expands to fill the declared environment width.

2.1.3. Tabulary package

- CTAN: https://ctan.org/pkg/tabulary.
- Similar to *tabularx*.
- Uses the full width of the table as an argument.
- Uses the `L`, `C`, `R`, and `J` column types for variable-width columns.
- Unlike `X` columns in *tabularx*, the width of each column is weighted according to the natural width of the widest cell in the column.

2.1.4. Longtable package

- CTAN: https://ctan.org/pkg/longtable.
- Allows you to create tables that continue onto the next page.
- Columns on consecutive pages have the same width.
- Unlike *supertabular*, it modifies the output procedure and therefore will not work in a multicolumn environment.

2.1.5. Booktabs package

- CTAN: https://ctan.org/pkg/booktabs.
- Open tables with extra spaces between rows.
- Longtable compatible.

2.1.6. Tabularray package

- CTAN: https://ctan.org/pkg/tabularray.
- Repository: https://github.com/lvjr/tabularray.
- Written in LaTeX3.
- Directly uses LaTeX3 functions to parse tables.
- Separates table content and style.
- Table style can be completely specified using keys.
- This package is recommended for typesetting tables.

3. Using the tabularray package

3.1. Features of the tabularray package

Keyword syntax is used. Tables are configured using keyword parameters in the `tblr` environment, making the code more readable:

```
\begin{tblr}{
  colspec = {rX},
  colsep = 8mm,
  hlines = {2pt, white},
  row{odd} = {azure8},
  row{even} = {gray8},
}
```

Flexible column and row settings:

- Dynamic alignment: automatic column width detection with manual adjustment.
- Color and formatting: built-in commands for cell shading and font changes:

```
\SetCell{bg=green9} Yes & \SetCell{bg=red8} No
```

- Support for complex structures.
- Macro expansion: Allows the use of complex structures within tables, including dynamic data.
- Integration with `booktabs`: Compatible with professional table styling via the `booktabs` package.

3.2. Basic principles of table construction

Use `colspec` to define column types:

```
\begin{tblr}{colspec={X[l] X[c] X[r]}}
```

- `X[l]`: Left-aligned column with automatic width.
- `c`, `r`: Centered and right-aligned, respectively.

Appearance settings:

- Horizontal lines: `hlines`, `hline{1}={blue, dashed}`.
- Vertical lines: `vlines`, `vline{1,4}={3pt}`.
- Cell background color: **`\SetCell`**`{bg=green9}`.

3.3. Integration with the booktab package

It makes sense to use the expressiveness of `tabularray` in `booktabs` (see Table 2).

3.3.1. Loading the booktabs library

Add the following command to the document's preamble:

`\UseTblrLibrary``{booktabs}`

- This enables compatibility with `booktabs`, allowing its commands to be used within the `tblr` environment.
- For multi-page tables, use the `longtblr` environment with the same style settings.
- Avoid vertical lines—they are contrary to professional design principles.
- Adjust the line thickness using the `rule thickness` parameter to closely match the `booktabs` style.

3.3.2. Basic elements of booktabs style

Commands for horizontal lines:

- **`\toprule`** — top line;
- **`\midrule`** — middle line;
- **`\bottomrule`** — bottom line.

Example setup:

Example of using booktabs

```
\begin{tblr}{
colspec = {ccc},
hline = {white}, % Disable standard horizontal lines
vlines = {0pt}, % Disable vertical lines (they are not present in the booktabs style)
}
\toprule
Header 1 & Header 2 & Header 3 \\
\midrule
Data 1 & Data 2 & Data 3 \\
\bottomrule
\end{tblr}
```

Header 1	Header 2	Header 3
Data 1	Data 2	Data 3

3.3.3. Example of a complete table

Let's give an example of a complete table set:

Table 2

Comparing tabularray with booktabs

Function	**tabularray**	**booktabs**
Syntax	Key parameters in the `tblr` environment	Traditional syntax `tabular`
Lines	**`\toprule`**, **`\midrule`**, **`\bottomrule`**	Same commands
Vertical lines	Not recommended	Disabled by default
Multipage tables	`longtblr` environment	`longtable` package

Example of a table in the booktabs style

```
\begin{tblr}{
colspec = {X[l] X[r] X[c]},
hline = {white},
vlines = {0pt},
row{1} = {font=\bfseries}, % Bold for headings
}
\toprule
Parameter & Value & Unit \\
\midrule
Length & 10.5 & m \\
Width & 2.3 & cm \\
Height & 5.1 & mm \\
\bottomrule
\end{tblr}
```

Parameter	**Value**	**Unit**
Length	10.5	m
Width	2.3	cm
Height	5.1	mm

3.4. Integration with the siunitx package

Loading:

```
\UseTblrLibrary{siunitx}
```

Add:

- key `si` for column type `Q`;
- column type `S` (like sugar for `Q` columns, centered by default).

Let's align it with the decimal point:

Align with the decimal point

```
\begin{tblr}{
  hlines, vlines,
  colspec =
   ↪ {Q[si={table-format=3.2},c]
   ↪ Q[si={table-format=3.2},c]},
  row{1} = {guard}
  }
  Head  & Head \\
  111 & 111 \\
  2.1 & 2.2 \\
  33.11 & 33.22 \\
\end{tblr}
```

Head	Head
111	111
2.1	2.2
33.11	33.22

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Набор таблиц

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Ключевые слова: таблицы, набор таблиц, LaTeX

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Construction and modeling of the operation of elements of computing technology on fast neurons

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Abstract. The article is devoted to the construction of fast neurons and neural networks for the implementation of two complete logical bases and modeling of computing devices on their basis. The main idea is to form a fast activation function based on semi-parabolas and its variations that have effective computational support. The constructed activation functions meet the basic requirements that allow configuring logical circuits using the backpropagation method. The main result is obtaining complete logical bases that open the way to constructing arbitrary logical functions. Models of such elements as a trigger, a half adder, and an adder, which form the basis of various specific computing devices, are presented and tested. It is shown that the new activation functions allow obtaining fast solutions with a slight decrease in quality compared to reference outputs. To standardize the outputs, it is proposed to combine the constructed circuits with a unit jump activation function.

Key words and phrases: new activation functions, parabola, full logical basis, element models, performance, experimental studies

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1. Introduction

The need to increase the speed of artificial neural networks (ANN) containing a huge number of neurons leads to the construction of "fast neurons", which is achieved by a special implementation of activation functions [1–3] and their hardware implementation. This has led to the expansion of research in the field of creating and studying new activation functions and their practical use. Currently, great efforts are aimed at accelerating the operation of activation functions for the construction of "fast" neurons and neural networks based on them. A comparison of various typical activation functions (AFs) in the ANN is performed in the works [4–6]. The issues of searching for methods to reduce the computational complexity of implementing AFs are discussed in [7–9].

Of interest is the creation of elements of computer technology (CT) using complete logical bases (complete systems of logical functions). These are, for example, ∧, ∨, ¬ (conjunction, disjunction, negation); ∧, ¬ (conjunction, negation); ∨, ¬ (disjunction, negation). The devices are implemented by covering them with neurons and neural networks. Interest in this approach is not weakening and is currently growing with the increasing interest in artificial intelligence technologies. It is worth noting the emergence of a class of specialized processors that serve to accelerate the work of neurons and the training algorithms of ANNs as a whole [10].

In this paper, we propose to implement typical elements of the VT on "fast" neurons obtained by replacing known activation functions with new functions that are characterized by a higher implementation speed. Previously, the authors proposed a new activation function called the s-parabola, created a complete logical basis and algorithms for setting up such neurons and neural networks [11, 12].

In this paper, the main focus is on the construction of fast neurons using new activation functions s-parabola, Sparabola-ReLU and ReLU-Sparabola, which are combinations of parabolas and linear functions. Based on them, fast VT elements are proposed: "XOR", trigger, half adder, adder.

Structure of the article

In section 2. Materials and Methods in paragraph 2.1. The basic requirements for activation functions are presented. Section 2.2. Standard and new activation functions propose new functions that can be used in ANNs configured using the backpropagation method. The settings and quality parameters of neurons that form the logical bases "AND"–"OR"–"NOT" and the bases "AND-NOT", "OR-NOT" are shown. The settings are linked to the basic neuron schemes (one neuron, two neurons, constructor) for configuring activation functions.

In section 3. Results in paragraph 3.1. show the settings of the activation functions on the logical basis "AND"–"OR"–"NOT" by the method of back propagation of the error. In relation to the basic circuits of neuron connection, comparative estimates of the speed of tuning and implementation of functions are given. Similar studies are performed in section 3.2. for tuning activation functions to the logical bases "AND-NOT", "OR-NOT". To expand the studies in section 3.3., new activation functions are additionally tuned to the XOR function. Section 3.4. considers the construction of VT elements on logical bases. The results of covering the circuits of the RS trigger of the half adder and adder with logical elements on neurons and the "XOR" function are shown.

In section 4. Discussion discusses the obtained results in comparison with the state of the world level of development of the subject area. The prospects of the proposed approach are associated with the use of fast activation functions in multilayer and convolutional ANNs. It is noted that significant acceleration can be achieved by switching to hardware implementation of activation functions in the form of bit-parallel circuits and the use of CORDIC family algorithms.

In section 5. Conclusion summarizes the results obtained and provides suggestions for further research development.

2. The materials and methods

2.1. Basic requirements for activation functions. Complete logical basis on traditional and fast neurons

The requirements for activation functions are quite contradictory, but at the same time, the following features can be highlighted.

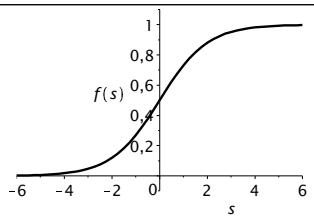
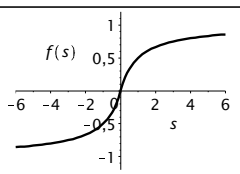
1. If neural networks are trained using the backpropagation method using the gradient descent process, then the layers in the model and the activation functions must be differentiable. Some activation functions, for example, linear or hyperbolic tangent, are differentiable over the entire range of admissible values.
2. The requirements for the activation function of an ANN are determined by a special theorem on completeness [13], according to which the function must be twice differentiable and continuous. The derivative of the activation function must be defined on the entire abscissa axis. To be used in a neuron, the function must be monotonically increasing or decreasing, have parameters that can be adjusted during the training process.
3. It is desirable that the output of the activation function be symmetrical with respect to zero, so that the gradients do not shift in a certain direction. Such a case corresponds, for example, to the sigmoid rational.
4. For logical problems, the excitation values of the output layer neurons must belong to the range [0, 1]. This corresponds, for example, to the sigmoid function and the unit jump (step function). However, the unit jump function does not meet the requirements of differentiability. It is not differentiable at point 0, and its derivative is 0 at all other points. Gradient descent methods do not work for such a function. This can create problems with training, since the numerical gradients calculated near the point where the derivative does not exist may be incorrect.
5. Since activation functions must be calculated repeatedly in deep networks, their calculation must be inexpensive in computational terms. This fact requires a revision of the implementation methods and, possibly, the creation of new functions, which we will call fast-acting.

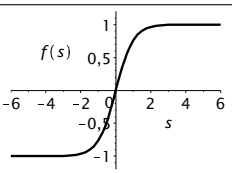
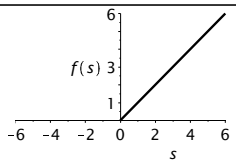
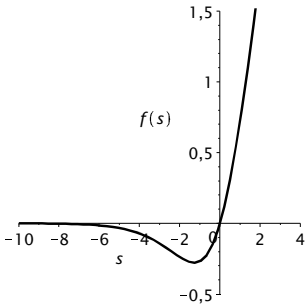
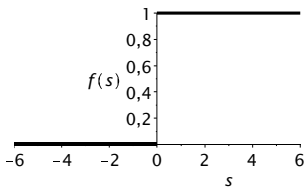
2.2. Typical and new activation functions

Table 1 presents activation functions that have found wide application in neural networks.

Table 1

Typical activation functions

Name	Formula	Schedule
Sigmoid	$f(s) = \frac{1}{1 + e^{-\alpha s}}$	
Sigmoid-rational function	$f(s) = \frac{s}{1 + \lvert s \rvert}$	

Hyperbolic tangent	$f(s) = \frac{e^{2s} - 1}{e^{2s} + 1}$	
ReLU	$f(s) = max(0, s)$	
SiLu	$f(s) = \frac{s}{1 + e^{-s}}$	
Single jump	$f(s) = \begin{cases} 1 & \text{if } s > 0 \\ 0 & \text{if } s \leq 0 \end{cases}$	

The approach proposed in this paper is based on the idea.

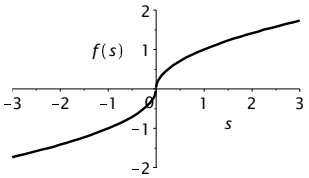
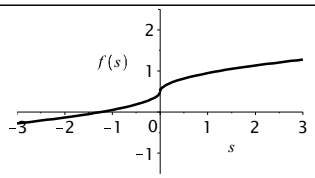
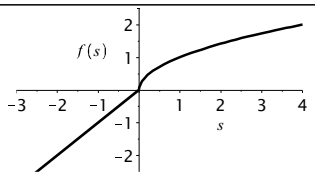
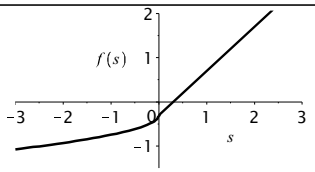
1. Construction of fast neuron models based on the activation function of the "s-parabola" type and their application in individual ANNs and classifier committees. The "s-parabola" function has a structure in which the upper part (the first quarter) is the upper branch of the parabola, and the lower part is a mirror image of the lower part of the parabola relative to the ordinate axis (the third quarter). The graph and formula of the proposed activation function are presented in Table 2 .
2. Combining different types of activation functions to achieve an effective solution to the problem.

The prospects and advantage of the s-parabola are associated with the simplicity of calculating the function, which ensures the speed of implementation. The s-parabola can be used as an activation function of the ANN, since it satisfies the established requirements of twice differentiability. A similar function can be used in multilayer direct propagation ANNs to solve problems of recognizing rigid objects and predicting time processes.

Table 2 presents some new neuronal activation functions.

Table 2

New activation functions: s-parabola and its variations

Name	Formula	Parameters	Schedule
S-parabola	$f(s)=\begin{cases}\beta+\sqrt{2ps} & \text{if } s>0\\ \beta-\sqrt{2ps} & \text{if } s\le 0\end{cases}$	$p=\frac{1}{3}$ $\beta=0.0$	
S-parabola	$f(s)=\begin{cases}\beta+\sqrt{2ps} & \text{if } s>0\\ \beta-\sqrt{-2ps} & \text{if } s\le 0\end{cases}$	$p=0.1$ $\beta=0.5$	
ReLU-Sparabola	$f(s)=\begin{cases}\beta+\sqrt{2ps} & \text{if } s>0\\ s+\beta & \text{if } s\le 0\end{cases}$	$p=0.5$ $\beta=0.01$	
Sparabola-ReLU	$f(s)=\begin{cases}s+\beta & \text{if } s>0\\ \beta-\sqrt{-2ps} & \text{if } s\le 0\end{cases}$	$p=0.1$ $\beta=-0.3$	

Let us consider the construction of a complete logical basis on fast neurons. The implementation of the functions “AND”, “OR”, “NOT”, “AND–NOT”, “OR–NOT” is carried out on the basis of basic circuits with one and two neurons Table 3 .

2.3. Performance evaluation of activation functions

Let n be the bit depth of the numbers being processed, then we can estimate the complexity of executing the activation functions (Table 3).

Table 3

Activation functions sorted in order of decreasing complexity

Function	Computational complexity	Rating (for $n=8$)
SiLu	$n^2((\log n)^2+\log n+1)+n$	840
Sigmoid	$n^2(1+(\log n)^2+\log n)$	832
Hyperbolic tangent	$n^2((\log n)^2+\log n)+2n+1$	785

Sigmoid-rational	$n(1 + n \log n)$	200
S-parabola	$2n^2$	128
ReLU-Sparabola	$n, n + 2n^2$	(8, 136), average 72
Sparabola-ReLU	$n + 2n^2, n$	(136, 8), average 72
ReLU	$n + 1$	9

For ReLU-Sparabola, Sparabola-ReLU the complexity of the implementation depends on which part of the function is executed (left or right).

2.4. Structural diagrams of neurons and their constructs

Variants of neuron schemes are presented in Fig. 1.

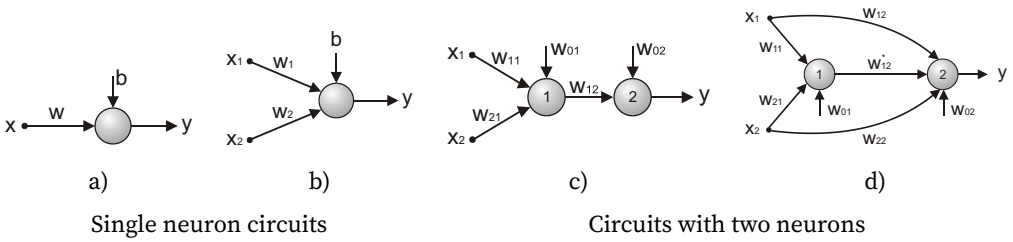


Figure 1. Basic neuron schemes for setting up activation functions

3. Results

The activation functions are configured using the backpropagation method for the logical functions “OR”, “AND”, “NOT” (Table 4-6).

The calculation of speed characteristics was performed on a personal computer with the following parameters: processor: Intel Core i5-6600K @ 3.50 GHz; RAM: 32 GB.

3.1. Activation function settings on the logical basis “AND”–“OR”–“NOT”

Table 4

Comparative characteristics of the setting for the “OR” function on one neuron

Characteristics of training	S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
Starting weights	$w_1 = 1, w_2 = 1, b = -0.5$			
Setup results	$w_1 = 1.385$, $w_2 = 1.351$, $b = -0.516$	$w_1 = 4.963$, $w_2 = 5.071$, $b = 3.812$	$w_1 = 0.475$, $w_2 = 0.483$, $b = -0.004$	$w_1 = 15.685$, $w_2 = 15.712$, $b = -6.967$
p	0.1	0.1	2.0	—
β	0.5	-0.5	0.25	—

α	—	—	—	0.5
Average deviation	0.124	0.189	0.181	0.009
Training time, ms	648	7307	27072	1483
Time to implement 10000000 data table cycles, ms	621	645	578	1040

Table 5

Comparative characteristics of the setting for the “AND” function on one neuron

Characteristics of training	S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
Starting weights	$w_1 = 1, w_2 = 1, b = -1.5$			
Setup results	$w_1 = 1.268$, $w_2 = 1.359$, $b = -1.756$	$w_1 = 0.516$, $w_2 = 0.405$, $b = 0.098$	$w_1 = 0.874$, $w_2 = 0.874$, $b = -0.514$	$w_1 = 16.338$, $w_2 = 16.338$, $b = -24.899$
p	0.1	1.75	0.1	—
β	0.5	-1.0	-0.3	—
α	—	—	—	0.5
Average deviation	0.123	0.274	0.098	0.010
Training time, ms	5942	602	34332	3159
Time to implement 10000000 data table cycles, ms	621	636	562	1053

Table 6

Comparative characteristics of the setting for the “NOT” function on one neuron

Characteristics of training	S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
Starting weights	$w = -1, b = 0$			
Setup results	$w = -3.994$, $b = 6.246$	$w = -3.993$, $b = 6.246$	$w = -0.999$, $b = 0.999$	$w = -18.328$, $b = 8.688$
p	0.5	0.5	0.5	—
β	-1.5	-1.5	0	—
α	—	—	—	0.5
Average deviation	0.001	0.001	0.0001	0.010
Training time, ms	219	218	218	2719
Time to implement 10000000 data table cycles, ms	220	219	183	2843

3.2. Settings of activation functions for logical bases “AND-NOT”, “OR-NOT”

Table 7–12 presents the results of the implementation of the alternative full basis “AND-NOT” and “OR-NOT” using one and two neurons.

Table 7

Characteristics of the setting for the “AND-NOT” function on one neuron

Characteristics of training	S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
Starting weights	—	$w_1 = 1, w_2 = 1, b = -1.5$		
Setup results	$w_1 = -1.040$, $w_2 = -1.035$, $b = 0.515$	$w_1 = -0.585$, $w_2 = -0.546$, $b = 1.871$	$w_1 = -0.510$, $w_2 = -0.562$, $b = 3.177$	$w_1 = -16.373$, $w_2 = -16.405$, $b = 24.852$
p	0.9	1	4	—
β	1.75	-0.75	-2	—
α	—	—	—	0.5
Average deviation	0.286	0.186	0.220	0.010
Training time, ms	1198	5064	8801	3223
Time to implement 10000000 data table cycles, ms	692	655	581	1043

Table 8

Characteristics of setting for the “AND-NOT” function on two neurons (Fig. 1(d))

Characteristics of training	S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
Starting weights	$w_{11} = -7, w_{21} = -7, w_{12} = -7, w_{22} = -4, w_{12}^* = -11$ $w_{01} = -2.6, w_{02} = 10$			—
Setup results	$w_{11} = -13.998$, $w_{21} = -12.525$, $w_{12} = -1.530$, $w_{22} = -1.461$, $w_{12}^* = -0.326$, $w_{01} = 1.289$, $w_{02} = 1.353$	$w_{11} = -6.892$, $w_{21} = -6.691$, $w_{12} = 0.364$, $w_{22} = 0.341$, $w_{12}^* = 0.193$, $w_{01} = 7.415$, $w_{02} = 0.469$	$w_{11} = -12.926$, $w_{21} = -12.057$, $w_{12} = -1.470$, $w_{22} = -1.431$, $w_{12}^* = -0.297$, $w_{01} = 1.583$, $w_{02} = 1.463$	$w_{11} = -0.073$, $w_{21} = -0.593$, $w_{12} = -4.991$, $w_{22} = -4.559$, $w_{12}^* = 3.812$, $w_{01} = 0.559$, $w_{02} = 5.303$
p	0.5	0.5	0.5	—
β	0.01	0.01	0.01	—
α	—	—	—	1.0
Average deviation	0.009	0.006	0.009	0.039
Training time, ms	538	450	506	10311
Time to implement 10000000 data table cycles, ms	39200	32600	36700	4303800

Table 9

Results of the implementation of the “AND-NOT” function on two neurons (Fig. 1(c))

x_1	x_2	y			
		S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
0	0	1.072	1.310	1.621	0.987
1	1	0.107	0.142	0.066	0.010
0	1	0.818	0.722	0.940	0.985
1	0	0.844	0.593	0.940	0.985

Table 10

Comparative characteristics of setting for the “OR-NOT” function on one neuron

Characteristics of training	S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
Starting weights	—	$w_1 = 1, w_2 = 1,$ $b = -0.5$	—	$w_1 = 1, w_2 = 1,$ $b = -0.5$
Setup results	$w_1 = -0.135,$ $w_2 = -0.135,$ $b = 0.158$	$w_1 = -0.325,$ $w_2 = -0.420,$ $b = 0.870$	$w_1 = -0.448,$ $w_2 = -0.515,$ $b = 1.583$	$w_1 = -16.226,$ $w_2 = -16.238,$ $b = 7.139$
p	4.0	2.0	3.0	—
β	-0.25	-1.0	-0.75	—
α	—	—	—	0.5
Average deviation	0.296	0.231	0.215	0.010
Training time, ms	5800	2232	6155	1597
Time to implement 10000000 data table cycles, ms	647	677	614	1120

Table 11

Characteristics of setting for the “OR-NOT” function on two neurons (Fig. 1(d))

Characteristics of training	S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
Starting weights	$w_{11} = -7, w_{21} = -7, w_{12} = -7, w_{22} = -4, w_{12}{}^* = -11$ $w_{01} = -2.6, w_{02} = 10$			—
Setup results	$w_{11} = -12.977,$ $w_{21} = -12.665,$ $w_{12} = 0.511,$ $w_{22} = 0.496,$ $w_{12}{}^* = 0.327,$ $w_{01} = 1.307,$ $w_{02} = 0.603$	$w_{11} = -6.932,$ $w_{21} = -6.747,$ $w_{12} = -1.395,$ $w_{22} = -1.375,$ $w_{12}{}^* = -0.204,$ $w_{01} = 7.709,$ $w_{02} = 1.558$	$w_{11} = -12.441,$ $w_{21} = -12.075,$ $w_{12} = 0.466,$ $w_{22} = 0.449,$ $w_{12}{}^* = 0.301,$ $w_{01} = 1.530,$ $w_{02} = 0.526$	$w_{11} = 0.508,$ $w_{21} = 0.536,$ $w_{12} = -9.564,$ $w_{22} = -9.557,$ $w_{12}{}^* = -0.360,$ $w_{01} = -0.464,$ $w_{02} = 3.900$
p	0.5	0.5	0.5	—
β	0.01	0.01	0.01	—
α	—	—	—	0.5
Average deviation	0.010	0.007	0.010	0.037
Training time, ms	377	819	279	18819
Time to implement 10000000 data table cycles, ms	1536	1488	1456	2512

Table 12

Results of the implementation of the "OR-NOT" function on two neurons (Fig. 1(c))

x_1	x_2	y			
		S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
0	0	0.852	0.681	0.874	0.983
1	1	-0.240	-0.236	-0.452	0.008
0	1	0.178	0.209	0.271	0.009
1	0	0.107	0.218	0.279	0.009

The tables show that when implementing a logical basis on two neurons using parabolic activation functions, the tuning results exceed the results of implementation on a sigmoid in accuracy and speed. Sigmoid is worst tuned to the "AND-NOT" function. When implemented on one neuron, sigmoid works more accurately, although slower.

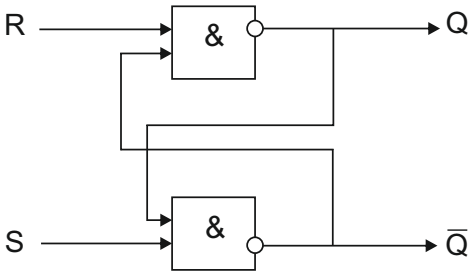
3.3. Tuning neurons to the "XOR" function

To expand the research, new activation functions were additionally configured using the backpropagation method on the "XOR" function using the ANN constructed according to the scheme in Fig. 1(d). The results are shown in Table 13.

Table 13

Characteristics of setting for the "XOR" function on two neurons (Fig. 1(d))

Characteristics of training	S-parabola	ReLU-Sparabola	Sparabola-ReLU	Sigmoid
Starting weights	$w_{11} = -7$, $w_{21} = -7$, $w_{12} = -7$, $w_{22} = -4$, $w_{12}^* = -11$ $w_{01} = -2.6$, $w_{02} = 10$			
Setup results	$w_{11} = -14.176$, $w_{21} = -13.494$, $w_{12} = -2.025$, $w_{22} = -1.963$, $w_{12}^* = -0.633$, $w_{01} = 1.375$, $w_{02} = 0.748$	$w_{11} = -6.872$, $w_{21} = -6.686$, $w_{12} = 1.733$, $w_{22} = 1.691$, $w_{12}^* = 0.392$, $w_{01} = 7.547$, $w_{02} = -1.079$	$w_{11} = -13.496$, $w_{21} = -12.694$, $w_{12} = -1.946$, $w_{22} = -1.876$, $w_{12}^* = -0.586$, $w_{01} = 1.557$, $w_{02} = 0.918$	$w_{11} = -6.999$, $w_{21} = -6.999$, $w_{12} = -6.275$, $w_{22} = -6.154$, $w_{12}^* = -14.208$, $w_{01} = 2.613$, $w_{02} = 9.382$
p	0.5	0.5	0.5	—
β	0.01	0.01	0.01	—
α	—	—	—	1.0
Average deviation	0.009	0.010	0.008	0.035
Training time, ms	603	542	550	23681
Time to implement 10000000 data table cycles, ms	1944	1511	1474	2489

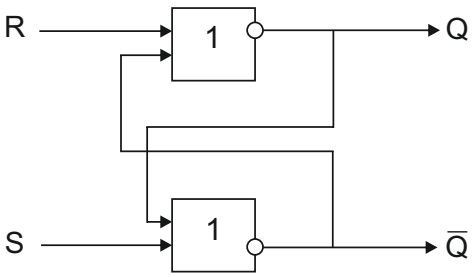


a) RS trigger on “AND-NOT” logic circuits

R	S	Q	$\overline{Q}$	Comment
0	0	1	1	Prohibition
0	1	1	0	Record “1”
1	0	0	1	Record “0”
1	1	×	×	Storage

b) Truth table

Figure 2. Trigger on “AND-NOT” elements



a) RS trigger on “OR-NOT” logic circuits

R	S	Q	$\overline{Q}$	Comment
0	0	×	×	Storage
0	1	1	0	Record “1”
1	0	0	1	Record “0”
1	1	0	0	Prohibition

b) Truth table

Figure 3. Trigger on “OR-NOT” elements

It is evident that the main trends identified in the compilation of logical bases are also preserved in the implementation of a more complex “XOR” function, which is widely used in computer elements.

3.4. Construction of CD elements on logical bases

The CD circuits are implemented by covering them with neurons and neural networks configured on the logical bases “AND”–“OR”–“NOT”, “AND-NOT”, “OR-NOT” or with the sequential formation of more complex elements. Fig. 2 and Fig. 3 show the results of such coverage of the RS-trigger circuits with logical elements on the neurons “AND-NOT” and “OR-NOT”.

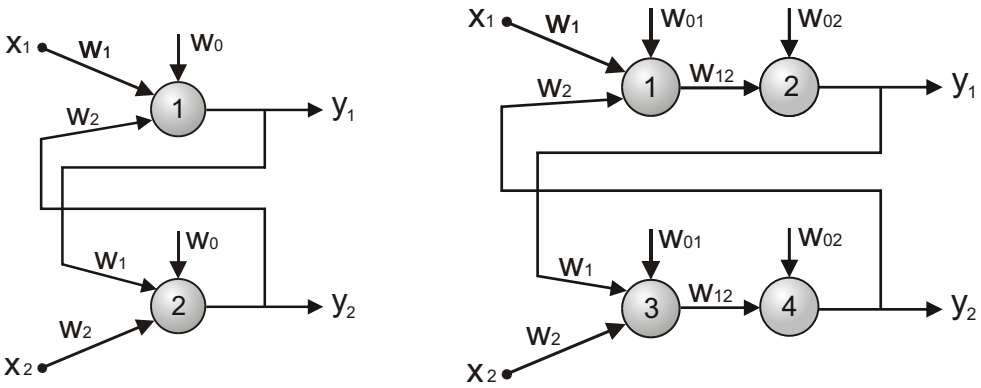
Fig. 4a shows the circuit diagrams of some basic elements of the CD, implemented in the logical basis of “OR-NOT”, and Fig. 4b shows with the addition of the “single jump” element.

Fig. 5a shows the implementation of the RS trigger on two “AND-NOT” neurons, and Fig. 5b adds a “single jump” type element to the outputs, which allows us to obtain clear values of “1” and “0” at the outputs.

The results of the RS-trigger simulation are presented in Tables 16-17.

Let us consider the construction of a neural network for the implementation of a half adder. A single-bit adder (half adder), designated as SM/2, does not have an input carry, since it is the least significant bit of a multi-bit adder. A half adder can be built on the basis of XOR logic circuits and the AND circuit (Fig. 6-7). The logic of SM/2 operation is determined by the truth table.

Based on two half adders and an “OR” circuit, a full one-bit adder SM can be constructed as shown in Fig.8-9.



a) using the outputs of "AND-NOT" neurons

b) adding neurons with the activation function "single jump"

Figure 4. RS trigger in which the "AND-NOT" element is implemented on one neuron

Table 14

Results of the RS trigger operation, in which the "AND-NOT" element is implemented on one neuron

x_1	x_2	y_1	y_2
0	0	Prohibition	
1	1	Storage	
0	1	2.713	-0.702
1	0	0.074	2.638

Table 15

Results of the RS trigger operation, in which the "AND-NOT" element is implemented on one neuron with the addition of neurons with the "single jump" activation function

x_1	x_2	y_1	y_2
0	0	Prohibition	
1	1	Storage	
0	1	1	0
1	0	0	1

Table 16

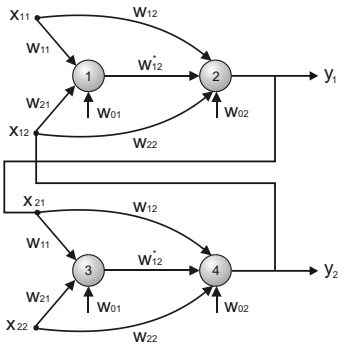
Results of the RS trigger operation, in which the "AND-NOT" element is implemented on two neurons

x_1	x_2	y_1	y_2
0	0	Prohibition	
1	1	Storage	
0	1	0.999	-0.059
1	0	-0.061	0.992

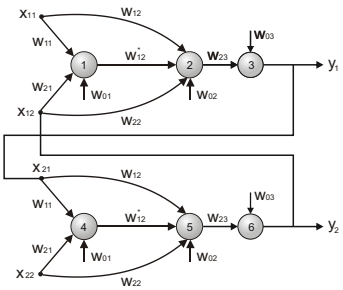
Table 17

Results of the RS trigger operation, in which the "AND-NOT" element is implemented on two neurons with the addition of neurons with the "single jump" activation function

x_1	x_2	y_1	y_2
0	0	Prohibition	
1	1	Storage	
0	1	1	0
1	0	0	1

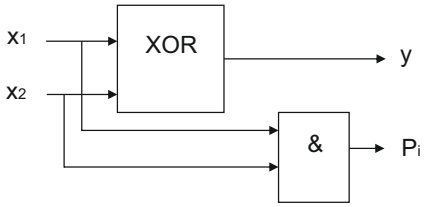


a) using “AND-NOT” neuron outputs



b) adding neurons with the activation function “single jump”

Figure 5. RS trigger in which the “AND-NOT” element is implemented on two neurons

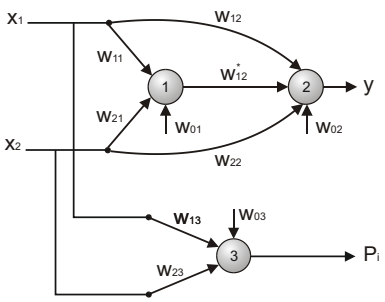


a) Half adder circuit (SM/2)

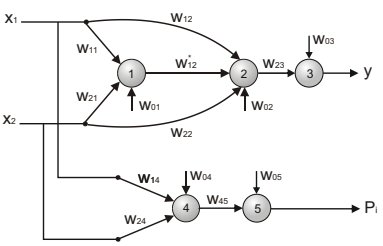
x_1	x_2	y	P_i
0	0	0	0
0	1	1	0
1	0	1	0
1	1	0	1

b) Truth table

Figure 6. Logical diagram of the half adder (SM/2)

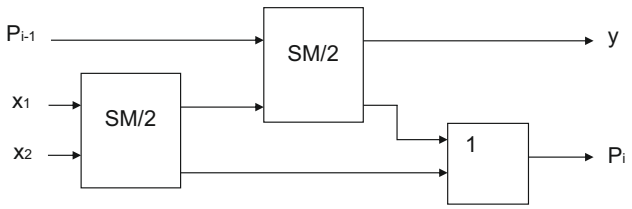


a) base model



b) model with additional neurons (with the “single jump” function)

Figure 7. Models of a half-adder (SM/2) on neurons



a) Full single-bit adder (SM)

x_1	x_2	P_{i-1}	y	P_i
0	0	0	0	0
0	0	1	1	0
0	1	1	0	1
1	0	0	1	0
1	0	1	0	1
1	1	0	0	1
1	1	1	1	1

b) SM operation logic

Figure 8. Logic diagram of the sub adder (SM)

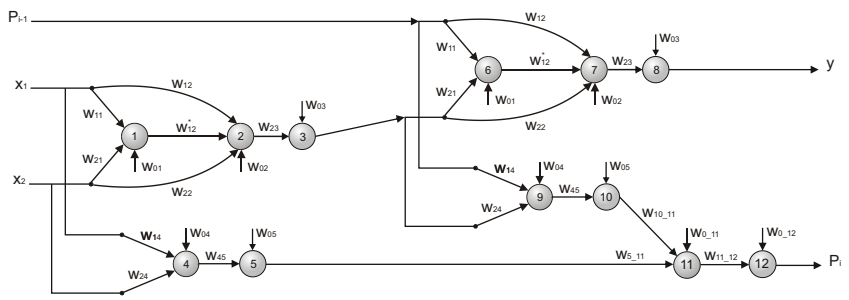


Figure 9. Model of a full adder (SM) on neurons

4. Discussion

Comparison of the obtained results with existing works in the field of implementation of activation functions shows that of interest is not only the decomposition of a complex activation function, for example, a sigmoid, into simpler functions in order to speed up its implementation [1, 2], but also a direct replacement of the function with other functions, for example, an s-parabola and its variations, which allow a more efficient implementation in time. In this case, the effect of acceleration is ensured by several times with some loss in the accuracy of the implementation of thresholds [0,1]. Undoubtedly, of interest is also some slight complication of the VT schemes due to the addition of neurons with the traditional single-jump function to the final cascades, as shown in paragraph 3.4.

Another aspect of acceleration is related to the efficient hardware implementation of activation functions. The special organization of “fast” neurons and neural networks is the subject of, for example, the works [14–16].

Great hopes are placed on bit-parallel circuits for calculating functions included in activation functions. We note a series of works aimed at increasing the speed of solving various problems of comparison, establishing correspondence between streams and performing arithmetic operations on bit vectors, including simultaneous processing of matrix columns [17–20].

In this case, the expected success is associated with the transition to CORDIC algorithms [21–23], which allow regulating the speed and accuracy of calculations. This direction will be developed in subsequent works by the authors.

5. Conclusions

Summing up, we can recapitulate.

1. The composition of activation functions based on the parabola has been expanded, including S-parabola, ReLU-Sparabola and Sparabola-ReLU.
2. Activation functions have been constructed that implement complete logical bases “OR-AND-NOT” and “AND-NOT, OR-NOT” on neurons and neural networks with new activation functions. Compared to implementations based on the “Sigmoid” function, in the general case, the implementation is accelerated by 1.6-1.8 times with a small possible loss in accuracy and setup time. Setup time is not a decisive factor here, since after setup, the neurons are further used without changing the established coefficients, which are fixed.
3. Typical elements of computing equipment have been implemented on them: triggers, half adders, adders.
4. It is planned to implement the s-parabola activation function in multilayer ANNs, including convolutional neural networks of the YOLO class. 5. The possibilities and applications of new activation functions in convolutional neural networks will be investigated.
5. To speed up the calculation of activation functions, bit-parallel calculation schemes will be proposed using the CORDIC family of algorithms.

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Построение и моделирование работы элементов вычислительной техники на быстрых нейронах

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Аннотация. Статья посвящена построению быстрых нейронов и нейронных сетей для реализации двух полных логических базисов и моделирования на их основе устройств вычислительной техники. Основная идея заключается в формировании быстрой функции активации на основе полупарабол и её вариаций, имеющих эффективную вычислительную поддержку. Построенные функции активации отвечают основным требованиям, позволяющим настраивать логические схемы методом обратного распространения ошибки. Основным результатом является получение полных логических базисов, открывающих путь к построению произвольных логических функций. Представлены и протестированы модели таких элементов как триггер, полусумматор, сумматор, составляющих основу различных конкретных вычислительных устройств. Показано, что новые функции активации позволяют получать быстрые решения при небольшом снижении качества по сравнению с эталонными выходами. Для стандартизации выходов предлагается комбинировать построенные схемы с функцией активации типа единичный скачок.

Ключевые слова: новые функции активации, парабола, полный логический базис, модели элементов, быстродействие, экспериментальные исследования

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On the algebraic properties of difference approximations of Hamiltonian systems

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Abstract. In this paper, we examine difference approximations for dynamic systems characterized by polynomial Hamiltonians, specifically focusing on cases where these approximations establish birational correspondences between the initial and final states of the system. Difference approximations are commonly used numerical methods for simulating the evolution of complex systems, and when applied to Hamiltonian dynamics, they present unique algebraic properties due to the polynomial structure of the Hamiltonian. Our approach involves analyzing the conditions under which these approximations preserve key features of the Hamiltonian system, such as energy conservation and phase-space volume preservation. By investigating the algebraic structure of the birational mappings induced by these approximations, we aim to provide insights into the stability and accuracy of numerical simulations in identifying the true behavior of Hamiltonian systems. The results offer a framework for designing efficient and accurate numerical schemes that retain essential properties of polynomial Hamiltonian systems over time.

Key words and phrases: Hamiltonian system, Kahan method, birational map, Appelroth quadratization

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1. Introduction

In the realm of computational mathematics, the precise simulation of complex dynamical systems is paramount for enhancing scientists' understanding of both natural and engineered phenomena. Hamiltonian described systems have many applications across diverse fields, including astrophysics, quantum mechanics, and both mechanical and electrical engineering.

One of the most fundamental models in celestial mechanics and theoretical physics is Hamiltonian equations of motion system. These systems delineate the evolution of mechanical and physical phenomena over time and are essential for comprehending the behavior of a wide range of physical systems: from simple pendulums to intricate planetary orbits. In numerous instances, the Hamiltonian of these systems is represented as a polynomial or algebraic function of canonical variables $(q_1, ..., q_n)$ and momenta $(p_1, ..., p_n)$. The way these equations are structured helps to keep important quantities like energy and momentum constant, it ensures that the obtained solutions are consistent with physical principles and empirical data [1].

One of the main numerical study problem lies in the development of difference approximations that accurately capture the qualitative behavior of the system. Traditional methods, such as the widely utilized Runge-Kutta schemes, provide high accuracy but may fail to conserve certain geometric properties intrinsic to Hamiltonian systems, including phase-space volume and symplectic structure[2]. Over extended timescales, these numerical methods can lead to significant deviations in the system's trajectory from its true path, particularly in chaotic or highly sensitive regimes [3]. The concept of "ordered chaos" finds profound resonance in both natural systems and technological applications, often analyzed through the lens of Hamiltonian mechanics. In nature, Hamiltonian systems describe the evolution of dynamic systems like planetary motion or fluid dynamics, where apparent chaos emerges from deterministic laws. Similarly, in technology, Hamiltonian principles underlie optimization in quantum computing and energy conservation in algorithms, demonstrating structured complexity. Whether modeling weather patterns or designing artificial intelligence systems, ordered chaos reveals how intricate behaviors can arise from foundational rules, bridging the gap between unpredictability and order in both realms. Consequently, alternative approaches that preserve the qualitative integrity of Hamiltonian dynamics are worth developing [4, 5].

2. Numerical approaches

In recent years, researchers have turned their attention to symplectic integration methods, specifically designed to preserve the symplectic structure of Hamiltonian flows [6]. These methods aim to conserve quantities such as energy and phase-space volume, providing a more faithful representation of the true motion of the system [7]. However, symplectic methods are often insufficient to fully capture the complexity of polynomial Hamiltonian systems, which may exhibit rich and diverse behaviors, including chaotic trajectories and resonance phenomena [8, 9]. Chaotic dynamics are utilized in optimization algorithms, particularly in exploring large, complex solution spaces. The unpredictable yet deterministic nature of chaotic trajectories helps avoid becoming stuck in local minima, improving the efficiency of finding global solutions in systems like neural networks, genetic algorithms, and quantum computation.

The study presented here focuses on difference approximations for Hamiltonian systems with polynomial Hamiltonians, a subset that includes many physically significant cases. We explore the idea of birational correspondences, wherein each step of the approximation represents a rational transformation between the initial and final states of the system [10]. This approach allows for exact preservation of certain structural properties and often leads to more accurate long-term simulations than traditional methods.

The finite difference method proposes replacing the system of differential equations

$$\frac{dx_i}{dt} = f_i(x_1, \dots, x_n), \quad i = 1, \dots, n,$$

or, for short,

$$\frac{d\mathfrak{x}}{dt} = \mathfrak{f}(\mathfrak{x}), \tag{1}$$

with a system of algebraic equations

$$g_i(\mathfrak{x}, \hat{\mathfrak{x}}, \Delta t) = 0, \quad i = 1, \dots, n, \tag{2}$$

relating the value $\mathfrak{x}$ of the solution at some moment in time t with the value $\hat{\mathfrak{x}}$ of the solution at the moment in time $t + \Delta t$.

The system of the algebraic equation (2) itself will be called a difference scheme for a system of the differential equation (1).

Discrete models are essential in connecting analytical solutions with numerical simulations in dynamical systems, particularly for Hamiltonian systems with polynomial Hamiltonians. Kahan's method is notable for preserving energy integrals and approximating elliptic oscillators, while symplectic schemes, like the midpoint method, ensure energy conservation in quadratic Hamiltonians, facilitating closed trajectories. Appelroth's quadratization technique simplifies complex systems by transforming polynomial right-hand sides into quadratic forms [11, 12]. Geometric integrators are designed to maintain the analytical properties of the original systems, ensuring qualitative behaviors are preserved. Additionally, combining Appelroth's quadratization with Kahan's method enhances the analytic properties of difference approximations for higher-genus curves. Together, these discrete models provide effective tools for simulating dynamical systems and deepen the understanding of the interplay between algebraic structures and physical phenomena.

In mechanics the quantity dt has often been treated as a finite increment, and it was implied that Newton's equations were actually difference equations [13].

For example, the explicit Euler scheme

$$\hat{\vec{x}} - \vec{x} = \vec{f}(\vec{x})dt$$

for linear oscillator preserves the energy $H = x^2 + y^2$ only at $dt \to 0$.

The problem is that classical difference schemes (explicit Runge-Kutta schemes) are not rich in algebraic properties. We do describe properties of discrete models by looking back at continuous models.

Kahan's method is intrinsically linked to the development of discrete models for dynamical systems, particularly in the context of Hamiltonian mechanics. Discrete models serve as numerical approximations of continuous systems, allowing for the simulation of complex dynamics over time. Kahan's discretization specifically addresses the challenges associated with preserving the geometric and analytical properties of Hamiltonian systems when transitioning from continuous to discrete representations [14, 15]. The method is designed to preserve the energy integral, which is crucial for maintaining the qualitative behavior of the system over time. In the context of a Hamiltonian system, the energy integral can be expressed as:

$$H(p, q) = C,$$

where C is a constant representing the total energy of the system. Kahan's method allows for the discretization of the Hamiltonian equations, leading to a difference scheme that can be written in the form of a quadrature:

$$\Delta u = \int_{x_n}^{x_{n+1}} v\, dq,$$

where $v\, dq$ represents an elliptic integral of the first kind. This formulation ensures that the points of the approximate solution lie on an elliptic curve, thus inheriting the geometric properties of the original Hamiltonian system.

Moreover, Kahan's discretization approximates the solution by defining a birational transformation on the integral curve $H(p, q) = C$, which does not extend to a birational transformation of the entire phase space pq. This method allows for the correction of the integral curve while preserving its genus, enabling the simulation of an elliptic oscillator. Although the symplectic structure is not preserved exactly in case of the methods or conditions of the system fail to respect the intrinsic geometric properties of Hamiltonian dynamic, it is inherited to a significant extent, making Kahan's method a powerful tool for imitating the dynamics of systems governed by cubic Hamiltonians [16].

In 1990s, the concept of geometric integrators was introduced, marking a significant advancement in the numerical analysis of differential equations. These integrators are designed to construct numerical schemes that preserve specific algebraic and geometric properties intrinsic to the original continuous model. It leads to maintaining the qualitative features of the dynamical system, such as symplectic structure, conservation laws, and invariants, which are often lost in traditional numerical methods. This approach enhances the fidelity of simulations and ensures that the long-term behavior of the system is accurately represented, thereby providing a robust framework for the analysis of complex dynamical phenomena.

Due to the following expression

$$\hat{\mathfrak{x}} - \mathfrak{x} = \tilde{\mathfrak{f}}\left(\frac{\hat{\mathfrak{x}} + \mathfrak{x}}{2}\right)\Delta t \tag{3}$$

we can outline that it is t-symmetric and symplectic. Also, (3) preserves quadratic integrals (Cooper's theorem).

The midpoint scheme is a numerical method used for solving ordinary differential equations (ODEs), particularly in the context of Hamiltonian systems. It is a type of symplectic integrator, which means it is designed to preserve the geometric properties of the original continuous system, such as energy conservation and symplectic structure.

3. Quadratic Hamiltonian

A quadratic Hamiltonian refers to a Hamiltonian function that is a quadratic polynomial in the phase space variables, typically the coordinates q and momenta p. In mathematical terms, a quadratic Hamiltonian can be expressed in the form:

$$H(p, q) = \frac{1}{2m}p^2 + \frac{1}{2}kq^2,$$

where m is the mass of the particle, k is a constant related to the spring constant in the case of harmonic oscillators, p is the momentum, and q is the position.

Quadratic Hamiltonians are significant in classical mechanics because they describe simple harmonic motion, such as that of a mass on a spring or a pendulum for small angles. The dynamics of systems with quadratic Hamiltonians can be analyzed using symplectic integrators, which preserve the structure of Hamiltonian mechanics, ensuring that energy is conserved over time. This makes them particularly useful in numerical simulations, as they provide accurate representations of the system's behavior [17].

The midpoint scheme perfectly imitates a Hamiltonian system

$$\frac{dx}{dt} = \frac{\partial H}{\partial y}, \quad \frac{dy}{dt} = -\frac{\partial H}{\partial x} \tag{4}$$

with a quadratic Hamiltonian H, for example, a harmonic oscillator with Hamiltonian $H = x^2 + y^2$.

- According to Cooper's theorem, the energy integral is preserved exactly on the scheme, and the approximate solution itself is a sequence of points $\mathfrak{x}_n = (x_n, y_n)$ of the circle $x^2 + y^2 = C$.
- Each step of the approximate solution is a rotation by an angle

$$\Delta u = \int\limits_{\mathfrak{x}_n}^{\mathfrak{x}_{n+1}} \frac{dx}{\sqrt{C - x^2}},$$

which does not depend on n.

4. Cubic Hamiltonian

Cubic Hamiltonians extend Hamiltonian mechanics beyond quadratic forms, expressed as:

$$H(p,q) = \frac{1}{3}aq^3 + \frac{1}{2}bp^2 + c,$$

with constants a, b, and c. The cubic term introduces nonlinear dynamics, potentially leading to chaotic behavior. It provides insight into complex transitions, enhances the realism of models, and enables the study of phenomena that cannot be explained by linear systems. Traditional symplectic integrators may struggle with these complexities, but methods like Kahan's discretization effectively approximate these systems, preserving integral properties and simulating relationships between initial and final states. This enhances numerical accuracy and provides greater insight into cubic Hamiltonian systems in both theoretical and applied contexts.

In the 1990s, it was anticipated that preserving a symplectic structure would enable the imitation of a continuous model in the nonlinear case. The midpoint scheme is a symplectic Runge-Kutta scheme, i.e.

$$d\hat{x} \wedge d\hat{y} = dx \wedge dy.$$

However, now the energy integral is not conserved, but is inherited in a very tricky formulation.

Theorem 1 (J. M. Sanz-Serna and M.P. Calvo, 1994). *For any $k \in \mathbb{N}$, there exists a polynomial $H_k(x, ydt)$ such that*

$$H_k \text{ goes to } H \text{ at } dt \text{ to } 0,$$
$$H_k(\hat{x}, \hat{y}, dt) = H_k(x, y, dt) + O(dt^k).$$

Thus, in computer experiments, it seems that approximate solution lies on closed curve $H_k(x, y) = c$ at sufficiently large k.

Let's get back to Kahan's method. Kahan's method for Hamiltonian systems:

1. Geometric properties of Kahan's method restricted to quadratic vector fields.
2. For the systems with cubic hamiltonian, Kahan's method conserved the modified Hamiltonian

$$H + \frac{dt}{3}\nabla H^T \left(E - \frac{dt}{2}\frac{\partial \vec{f}}{\partial \vec{x}}\right)^{-1} \vec{f}.$$

3. For the systems with cubic Hamiltonian, Kahan's method preserves the measure

$$\frac{dx_1 \wedge dx_2 \cdots \wedge dx_n}{\det\left(E - \frac{dt}{2}\frac{\partial \vec{f}}{\partial \vec{x}}\right)}.$$

Kahan's scheme perfectly imitates a Hamiltonian system with a cubic Hamiltonian H, for example, an elliptic $\wp$-oscillator.

1. According to 1st Celledoni's theorem, the symplectic structure is inherited, i.e.

$$d\hat{x} \wedge d\hat{y} = (1 + O(dt))dx \wedge dy.$$

2. According to 2nd Celledoni's theorem, the energy integral is inherited, thus the approximate solution itself is a sequence of points $\mathfrak{x}_n = (x_n, y_n)$ of an elliptic curve $f(x, y, dt) = c$.

Consider more closely the narrowing of Cremona map to the invariant curve $f(x, y, dt) = c$. Using constructions from Picard's theorem, it follows that the difference scheme can be again represented using quadrature

$$\int_{\check{x}}^{\hat{x}} v(x, y, dt)dx = \Delta u(dt),$$

where vdx_1 is an elliptic integral of the 1st kind on invariant curve and, of course,

$$vdx \to \frac{dx}{H_y} \quad (\text{at } dt \to 0).$$

5. Polinomial Hamiltonian

If the Hamiltonian is a polynomial of degree $r > 3$, then the exact solution to the continuous model lies on an algebraic curve

$$H(x, y) = c,$$

whose genus is greater than 1. Thus the quadrature

$$\int \frac{dx}{H_y(x, y)} = t + C$$

on the curve H is Abelian integral of the 1st kind.

The integral cannot be inverted, and the functions $x(t), y(t)$ (Jacobi problem). Formally, our method is suitable only for dynamical systems with quadratic right-hand sides, as the nonlinearity introduced by higher-order terms complicates the inversion process and the analytic behavior of the solutions. For more general systems, alternative methods, such as perturbation techniques or numerical approaches, are required to obtain meaningful results.

Theorem 2 (Appelroth, 1902). *Any dynamical system with polynomial right-side can be rewritten as dynamical systems with quadratic right-side in new variables.*

In the 21st century, the process of reducing a dynamical system characterized by a greater number of new variables than initial variables n to one with a quadratic right-hand side is termed quadratization. The method developed by Appelroth in the early 20th century facilitates this transformation specifically for systems with polynomial right-hand sides, thereby enabling the application of symplectic Runge-Kutta schemes, which preserve integrals of the system, though not all properties of the original formulation may be retained. Consequently, any polynomial Hamiltonian system can be effectively integrated using a reversible scheme that consists of two key steps: first, the quadratization as proposed by Appelroth, followed by the discretization method established by Kahan [18].

Although Newton's equations must define a one-to-one correspondence between the initial and final positions of a dynamical system, these equations do not actually define a one-to-one correspondence between the initial and final states of the system [10]. We can impose violently this property on the difference scheme. Currently, there are several implementations of quadratization algorythm [19]: Qbee by A. Bychkov and BioCham by M. Hemery et al. The example was produced via Sage using Qbee library made by Bychkov [20]. For more information, visit the https://github.com/AndreyBychkov/QBee repository on GitHub.

Example 1. Let's figure out how the following system can be solved:

$$\begin{cases} \dot{x}_1 = x^2, \\ \dot{x}_2 = x^4. \end{cases}$$

Consider the system with Hamiltonian of this system is

$$H = \frac{{x_1}^3}{3} - \frac{{x_2}^5}{5}.$$

The solution is described by the quadrature

$$\int \frac{dx_2}{\sqrt[2/3]{\frac{3}{5}x_2^5 + 3C}} = t + C'.$$

The particular solution of the system (4) with the initial conditions $x_1 = x_2 = 1$ at $t = 0$ has a branching point $t \approx 0.52$.

In the process of solving the given system of equations, we utilized Sage along with the Qbee library made by Bychkov. We started by defining the system, where the first equation is $\dot{x}_1 = x^2$ and the second equation is $\dot{x}_2 = x^4$.

```
x1, x2 = functions("x1, x2")
system = [
    (x1, eval("x2**4")),
    (x2, eval("x1**2"))
]
res = quadratize(system)
```

Using the capabilities of the Qbee library, we proceeded to perform the necessary calculations. The main problem we faced with was the Qbee output difference in comparison with Cremona in Sage which, in turn, is used to find the approximate solution of the system.

After quadratization implemented by Bychkov and restructured by us we've got the following system:

$$\begin{cases} \dot{x_1} = w_0 \cdot x_2, \\ \dot{x_2} = {x_1}^2, \\ \dot{w_0} = 2 \cdot w_1 \cdot x_1, \\ \dot{w_1} = {w_0}^2 + 2 \cdot w_2 \cdot x_2, \\ \dot{w_2} = 3 \cdot {w_1}^2, \end{cases}$$

which can be rewritten into the following form to be solved using Cremona in Sage:

```
['x1', 'x2', 'w0', 'w1', 'w2']
['w0*x2', 'x1**2', '3*w1*x1', 'w0**2 + 2*w2*x2', '3*w1**2']
```

The following problem is solved in the field of real numbers:

```
a1,a2,a3,a4,a5=1
pr2 = Initial_problem([eval(dn) for dn in derivative_names],
[eval(ed) for ed in equations_derivatives],
                      [a1,a2,a3,a4,a5], 0.6)
sol2=cremona_scheme(pr2, N=100, field=RR)
```

The approximate solution passes through the branch point as a pole. Before the branch point the exact and approximate solutions coincide. After this point the exact solution in imaginary, but the approximate is real.

The integral that connect old and additional variables is not preserved by reversible schemes.

Before the branch point the expression

$$w_0 = x_2^3$$

is equal to 0 on exact solution and is small on approximate solution, but its value at the branch point is very large (about 10^{29}).

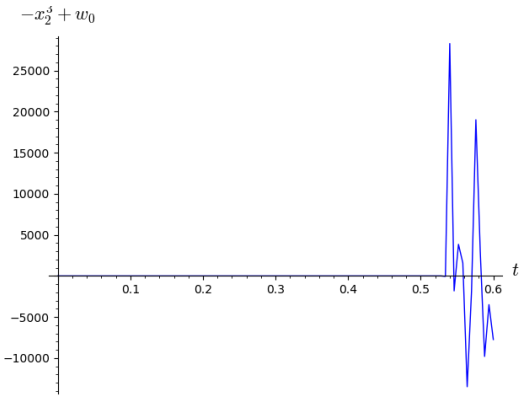

Figure 1. Approximate solution $-{x_2}^3 + w_0$ on t dependency

The appropriateness of applying the combined Appelroth-Kahan approach to natural phenomena depends on which properties of these phenomena are important for research and which can be sacrificed [21].

This approach is good if the one-to-one correspondence between the initial and final positions of the system is most important [22].

6. Discussion

The design of difference schemes that accurately replicate systems with polynomial Hamiltonians involves a complex interplay between algebraic properties and physical principles. A critical question arises regarding whether the correspondence between initial and final positions should be one-to-one, particularly in Hamiltonian dynamics, where preserving certain properties is vital for model integrity [23].

Historically, the quadrature ($\int \frac{dq}{H_p} = t$) has been fundamental in understanding Hamiltonian dynamics. However, it is known that this representation fails to express (q) as a single-valued analytic function of (t) when the genus of the curve defined by ($H(p,q) = C$) exceeds 1, underscoring the complexities of nonlinear systems and the challenges in simulating their behavior.

Our exploration reveals that while traditional symplectic methods, such as the midpoint scheme, effectively preserve energy in quadratic Hamiltonians, they may not extend this preservation to systems with cubic or higher-order Hamiltonians. This raises questions about whether preserving symplecticity guarantees that numerical solutions accurately reflect the system's dynamics [24].

Introducing additional variables, as seen in the many-body problem, presents a potential solution. Reformulating the system to include distances and reciprocal distances allows for a new set of differential equations that, despite losing Hamiltonian structure, preserve classical integrals of motion [25]. This approach highlights the importance of integrals in governing dynamical behavior and suggests that focusing on these may yield more accurate numerical approximations.

Furthermore, combining methods from Appelroth and Kahan offers a promising avenue for approximating solutions to polynomial Hamiltonian systems. Utilizing Cremona transformations can simplify the analytic properties of difference approximations compared to the original Hamiltonian model, raising the question of whether these simplified models are superior to their continuous counterparts [26].

Ultimately, the design of difference schemes transcends technical challenges, raising important questions about the nature of dynamical systems. The delicate balance between preserving essential properties and achieving computational feasibility significantly impacts the fidelity of numerical solutions.

7. Conclusion

In conclusion, investigating difference approximations for Hamiltonian systems necessitates further exploration of the governing principles. As we refine our understanding, we must consider both algebraic and physical implications of our numerical methods. The pursuit of accurate simulations of dynamical systems continues, with insights from this research contributing to advancements in theoretical and applied mathematics.

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Об алгебраических свойствах разностных приближений гамильтоновых систем

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Аннотация. В этой работе мы рассмотрим разностные аппроксимации динамических систем с полиномиальными гамильтонианами, в частности, сосредоточив внимание на случаях, когда эти аппроксимации устанавливают бирациональные соответствия между начальным и конечным состояниями системы. Разностные аппроксимации обычно используются численными методами для моделирования эволюции сложных систем, и при применении к гамильтоновой динамике они обладают уникальными алгебраическими свойствами, обсулолвленными полиномиальной структуры гамильтона. Наш подход включает анализ условий, при которых эти аппроксимации сохраняют ключевые черты гамильтоновой системы, такие как сохранение энергии и сохранение фазово-пространственного объёма. Исследуя алгебраическую структуру бирациональных отображений, вызванных этими приближениями, мы стремимся дать представление об устойчивости и точности численного моделирования в сравнении с поведением исходных гамильтоновых систем. Представленные результаты направлены на разработку эффективных и точных числовых схем, которые сохраняют существенные свойства полиномиальных гамильтоновых систем с течением времени.

Ключевые слова: Гамильтонова система, метод Кагана, бирациональное отображение, квадратизация Аппельрота

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Analysis of the stochastic model “prey–migration area–predator–superpredator”

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Abstract. Current research areas of dynamic migration and population models include the analysis of trajectory dynamics and solving parametric optimization problems using computer methods. In this paper we consider the population model “prey–migration area–predator–superpredator”, which is given by a system of four differential equations. The model takes into account trophic interactions, intraspecific and interspecific competition, as well as migration of the prey to the refuge. Using differential evolution parameters are found that ensure the coexistence of populations of prey, predator and superpredator, respectively, in the main habitat and the existence of a population of prey in a refuge. The transition to stochastic variants of the model based on additive noise, multiplicative noise and the method of constructing self-consistent models is performed. To describe the structure of the stochastic model the Fokker–Planck equations are used and a transition to a system of equations in the Langevin form is performed. Numerical solution of stochastic systems of differential equations is implemented by the Euler–Maruyama method. Computer experiments are conducted using a Python software package, and trajectories for deterministic and stochastic cases are constructed. A comparative analysis of deterministic model and corresponding stochastic models is carried out. The results can be used in solving problems of mathematical modeling of biological, ecological, physical, chemical and demographic processes.

Key words and phrases: system of differential equations; migration flows; stochastization; method of constructing self-consistent models; differential evolution

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1. Introduction

Among the key directions in the study of dynamic population models with migration flows one can highlight the investigation of trajectory dynamics and the development of computational methods for analyzing these models. The construction and study of deterministic and stochastic models of population dynamics taking into account trophic interactions between species and competition or considering species competition and migration flows are addressed, in particular, in [1–10]. In [1] a modification of the "predator–prey" model is proposed accounting for competition among predators for additional food. In [2] a "predator–prey" model is studied where the prey is characterized by an additive Allee effect and controlled migration flows are considered for the predator. In [6] a four-dimensional dynamic model with two migration habitats is proposed corresponding to the predator and prey respectively.

In [3] several types of three-dimensional models are considered, including species competition and trophic interactions of the "prey–predator–superpredator" type taking into account the possibility of prey infection by viral diseases. Complex trophic interactions with predator and superpredator saturation effects according to Holling are studied in [4]. For each considered model equilibrium states are obtained, trajectory dynamics are investigated and phase portraits are constructed. In most of the proposed models with trophic interactions, migration flows of populations are not taken into account, therefore, studying the impact of prey migration to refuges presents scientific interest. In [5] a distributed three-dimensional system of partial differential equations of the "prey–predator–superpredator" type is considered based on the reaction-diffusion equation which accounts for various factors of population growth and mortality as well as migration flows between habitats. However there arises a need to construct similar models based on systems of ordinary differential equations.

Stochastic population models represent significant theoretical and applied interest. Models with trophic interactions in the stochastic case is insufficiently studied. In [7] the impact of environmental fluctuations on a "prey–predator" model with a stage-structured prey population is investigated, a stochastic analysis of the model is carried out and conditions for stochastic stability are derived. In [8] the dynamical behavior of a "prey–predator" system is studied where both the prey and predator exhibit herd behavior. The stochastization of the model is performed by adding Gaussian white noise to the prey reproduction rates and the predator extinction rates.

One of the effective methods of stochastization is the method of constructing self-consistent stochastic models proposed in [11–15]. In [16] a stochastic model is obtained using an original software package that includes calculations of the interaction scheme, drift vector and diffusion matrix. In [9, 10] a "two competitors–two migration areas" model is considered which takes into account intraspecific and interspecific competition in two populations as well as bidirectional migration of both populations. The transition to the stochastic case for this model is carried out based on the method of constructing self-consistent one-step models.

Heuristic methods of parametric optimization inspired by nature are applied to study dynamic models [17]. In particular, [18] describes the differential evolution algorithm for numerical optimization. Differential evolution is based on the genetic annealing algorithm and is applied to real-valued input data. In [19] the results of development a software package for optimizing the parameters of population dynamic models are presented. The model "two competitors–one migration area" is considered which takes into account interspecific competition and bidirectional uneven migration of the first population to a refuge. Using differential evolution, a set of parameters satisfying the specified conditions for the coexistence of two species in the main habitat and the survival of the migrating specie in the refuge is found.

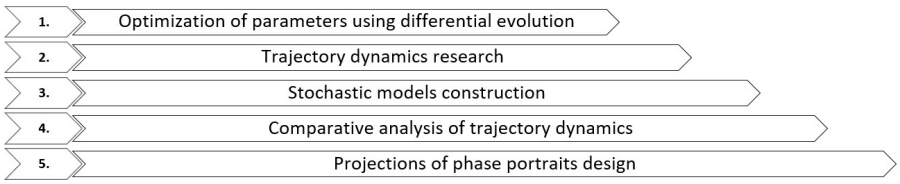

Figure 1. Stages of the algorithm for model (1) research

This paper is devoted to the study of a four-dimensional population model of the "prey–migration area–predator–superpredator" type which takes into account complex trophic interactions as well as prey migration to a refuge. In Section 2 the construction of the "prey–migration area–predator–superpredator" model with bidirectional species migration is considered. A search for model parameters is conducted using an evolutionary algorithm. The deterministic four-dimensional model is studied and projections of phase portraits are constructed. In Section 3 stochastic models of the "prey–migration area–predator–superpredator" type are developed taking into account the addition of additive and multiplicative noises as well as random migration coefficients. In this section stochastization is also performed using the method of constructing self-consistent stochastic models. The results of computational experiments are presented and an interpretation of these results is provided including a comparison of the stochastic models with the deterministic model. As a software tool for investigating the models a program complex developed in Python using the numpy, sympy, and scipy libraries is utilized. Section 4 presents a discussion of the results.

2. Description of the deterministic model and search for optimal parameters

We propose a description of a four-dimensional dynamic model that takes into account trophic interactions and prey migration based on a system of differential equations of the form

$$\begin{aligned}
\dot{x}_1 &= a_1 x_1 - p_{11} x_1^2 - q_{13} x_1 x_3 - q_{14} x_1 x_4 + \beta x_2 - \gamma x_1, \\
\dot{x}_2 &= a_2 x_2 - p_{22} x_2^2 - \beta x_2 + \gamma x_1, \\
\dot{x}_3 &= -c_3 x_3 - p_{33} x_3^2 - q_{34} x_3 x_4 + d_{13} x_1 x_3, \\
\dot{x}_4 &= -c_4 x_4 - p_{44} x_4^2 + d_{34} x_3 x_4 + d_{14} x_1 x_4,
\end{aligned} \tag{1}$$

where x_1 is the population density of prey in the main habitat, x_2 is the population density of prey in the refuge, x_3 is the population density of predator, x_4 is the population density of superpredator; a_i ($i = 1, 2$) are the natural growth rate coefficients of prey in the main habitat (a_1) and in the refuge (a_2); q_{13} is the interaction coefficient between prey in the main habitat and predator, q_{14} is the interaction coefficient between prey in the main habitat and superpredator; p_{ii} ($i = 1, 2, 3, 4$) are the intraspecific competition coefficients; q_{34} is the interaction coefficient between predator and superpredator; c_i ($i = 3, 4$) are the natural loss rate coefficients of predator (c_3) and superpredator (c_4); d_{13} is the growth coefficient of predator due to consumption of prey in the main habitat; d_{14} is the growth coefficient of superpredator due to consumption of prey in the main habitat; d_{34} is the growth coefficient of superpredator due to consumption of predator; β is the migration coefficient of prey from the main habitat to the refuge, γ is the migration coefficient of prey from the refuge to the main habitat.

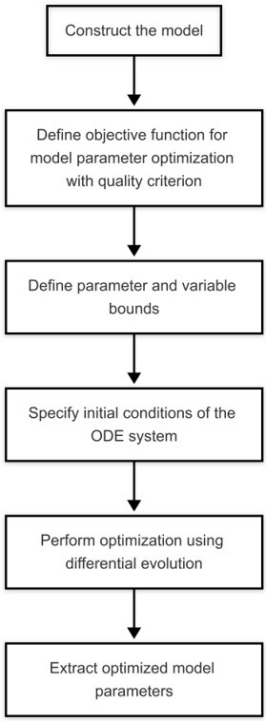

Figure 2. Stages of applying the differential evolution algorithm for parameters search

Figure 1 presents the stages of the algorithm for model (1) research in the form of a diagram.

For the four-dimensional system (1) an optimization search method is applied to find a parameter set that ensures the coexistence of prey, predator and superpredator in the main habitat as well as the survival of the species in the migration area. A computational experiment is conducted to adjust the parameters of model (1) considering the given initial conditions $(x_1(0), x_2(0), x_3(0), x_4(0)) = (3.0, 2.0, 1.0, 0.5)$. The optimization search for the parameter set is based on differential evolution taking into account a special choice of quality criterion consistent with ecological sense [19].

The algorithm of the modified differential evolution implements the minimization of a numerical criterion characterizing the deviation from the specified equilibrium state of differential equations system (1). The minimization criterion has the form

$$\frac{1}{n(s_1 - s_0)} \sum_{i=s_0}^{s_1} \|x_i - S^*\| \to \min, \tag{2}$$

where n is the number of trajectories considering different initial conditions, s_1 is the index of the last step of the ODE trajectory calculation algorithm, s_0 is the index of the initial step of the ODE trajectory calculation algorithm, x_i is the phase vector of the system at the i-th step.

The parameter search algorithm developed with consideration of criterion (2) allows for the identification of parameter sets under which model (1) exhibits a transition to stationary regimes. In particular the following set of parameters is obtained: $a_1 = 20.00$, $a_2 = 20.00$, $p_{11} = 4.00$, $p_{22} = 2.00$, $q_{13} = 0.30$, $q_{14} = 0.30$, $q_{34} = 0.38$, $\beta = 0.50$, $\gamma = 0.10$, $c_3 = 7.74$, $p_{33} = 0.12$, $c_4 = 0.10$, $p_{44} = 4.80$, $d_{13} = 4.36$, $d_{14} = 3.06$, $d_{34} = 3.76$. Using the identified parameter set a positive equilibrium state is obtained: $x_1 = 3.31$, $x_2 = 9.77$, $x_3 = 14.08$, $x_4 = 13.09$. The performed verification of the model based on the numerical solution of the differential equations system demonstrated that the solutions are close to the identified positive equilibrium state.

3. Stochastization of the model and comparative analysis of the deterministic model with stochastic variants

We proceed to the stochastic models corresponding to system (1), taking into account the introduction of additive and multiplicative noises. The stochastic differential equation (SDE) in the form of the Langevin equation has the following form:

$$dx = a(x,t)dt + b(x,t)dW, \tag{3}$$

where $x \in R^4$ is the system state function, $W \in R^4$ is the standard Brownian motion described by a random Wiener process, and $a(x,t)$ is the right-hand side of the differential equations system (1) presented in vector form. The matrix $b(x,t)$ in (3) is defined depending on the type of random noise. For SDE with additive noise, $b(x,t)$ is the identity matrix of size 4×4. For SDE with multiplicative noise in the trivial case we have

$$b(x,t) = \begin{pmatrix} \sigma x_1 & 0 & 0 & 0 \\ 0 & \sigma x_2 & 0 & 0 \\ 0 & 0 & \sigma x_3 & 0 \\ 0 & 0 & 0 & \sigma x_4 \end{pmatrix},$$

where σ is the noise intensity parameter.

When stochastization is based on additive and multiplicative noise the random processes do not follow from the internal structure of the model. Next we consider a stochastic model that incorporates multipliers containing a random Wiener process applied to migration rates

$$\begin{aligned} \dot{x}_1 &= a_1 x_1 - p_{11}x_1^2 - q_{13}x_1x_3 - q_{14}x_1x_4 + \sigma_1 W x_2 - \sigma_2 W x_1, \\ \dot{x}_2 &= a_2 x_2 - p_{22}x_2^2 - \sigma_1 W x_2 + \sigma_2 W x_1, \\ \dot{x}_3 &= -c_3 x_3 - p_{33}x_3^2 - q_{34}x_3x_4 + d_{13}x_1x_3, \\ \dot{x}_4 &= -c_4 x_4 - p_{44}x_4^2 + d_{34}x_3x_4 + d_{14}x_1x_4, \end{aligned} \tag{4}$$

where σ_1, σ_2 are the noise intensities, and W is the Wiener process. Thus, system (4) accounts for the random nature of the migration parameters.

In the computer program developed in Python within the Jupyter Notebook environment the solution of the SDE is implemented using the Euler–Maruyama method [14]. The essence of this method is in the discretization of time and the step-by-step approximate computation of the SDE solution taking into account both the deterministic and stochastic components.

Figure 3 shows the trajectories of model (1) and the trajectories of the corresponding stochastic models. The trajectories are obtained using the identified set of parameters and the specified initial conditions. Each of the four plots depicts the dynamics of the corresponding phase variable.

The results of the analysis of the system (1) trajectories and its stochastic variants presented in Fig. 3 show the coexistence of prey, predator and superpredator species as well as the survival of the species in the refuge. The introduction of additive noise has a minor effect on the behavior of the model. Adding a random process to the migration parameters significantly affects not only the population density of prey that can migrate to the refuge but also the population densities of predator and superpredator in the main habitat. The solution trajectories of the stochastic differential equations system reach a stationary regime. Fig. 4 shows the projections of phase portraits onto the planes (x_1, x_2) and (x_1, x_4) respectively.

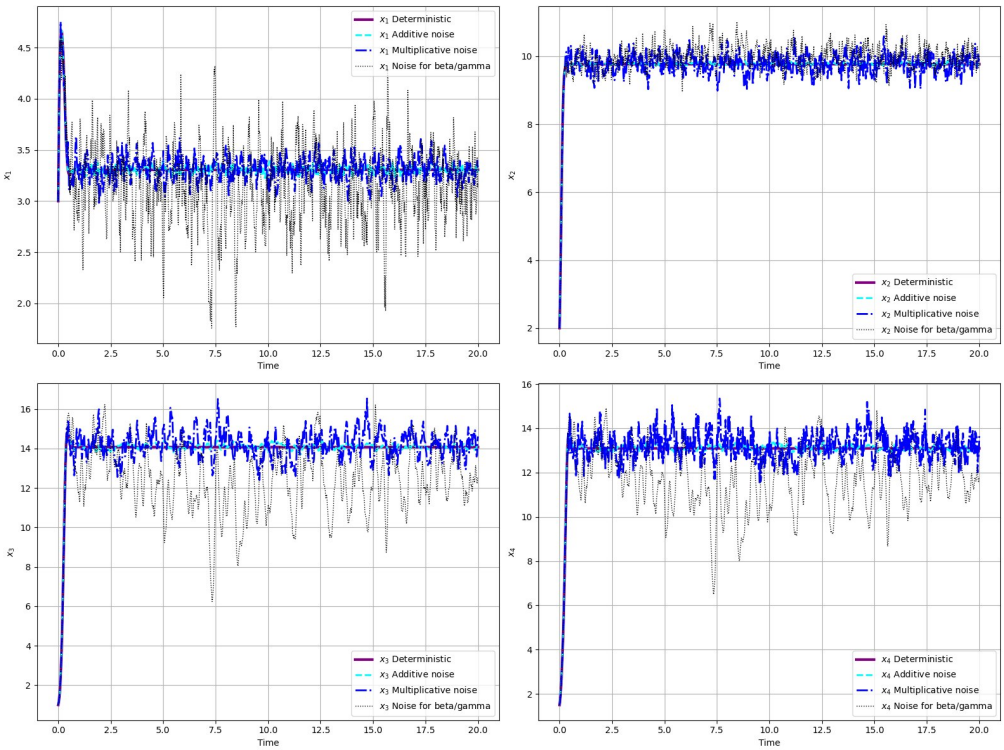

Figure 3. Trajectories of model (1) and the corresponding stochastic models

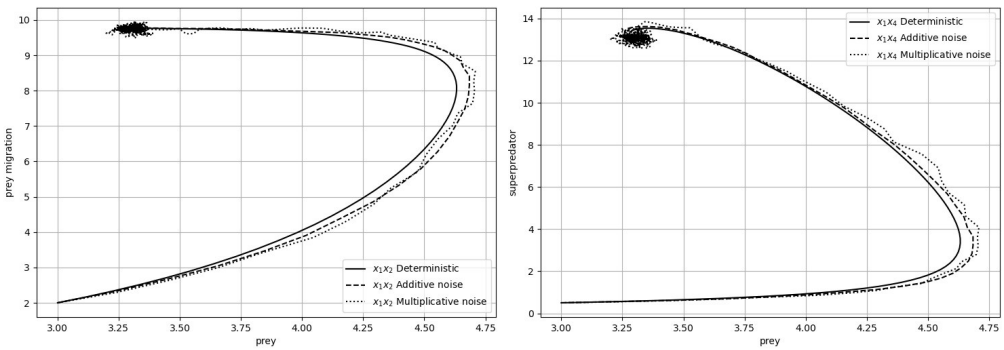

Figure 4. Projections of phase portraits onto the planes (x_1, x_2) and (x_1, x_4)

Projections of phase portraits are constructed which provide a geometric representation of the trajectories of the dynamical system for the specified set of parameters. The equilibrium state has the character of a stable node. The trajectories in the deterministic case and in the stochastic cases exhibit similar behavior.

We also consider the stochastization of model (1) based on the method of constructing self-consistent models [11–15]. This method involves deriving a stochastic differential equation with

consistent stochastic and deterministic parts. The specified stochastic differential equation is obtained through mathematical transformations from an interaction scheme which is a symbolic representation of all possible interactions within the system. In this paper the stochastic model is obtained using a software package developed in Python, the description of which is provided in [16].

As input data the software package uses a description of the interactions occurring in the system. One of the outputs of the software package is the interaction scheme which is represented using the Jupyter interactive interface. The following interaction scheme corresponds to system (1)

$$
\begin{gathered}
x_1 \xrightarrow{a_1} 2x_1, \quad x_2 \xrightarrow{a_1} 2x_2, \\
x_3 \xrightarrow{c_3} 0, \quad x_4 \xrightarrow{c_4} 0, \\
2x_1 \xrightarrow{p_{11}} x_1, \quad 2x_2 \xrightarrow{p_{22}} x_2, \quad 2x_3 \xrightarrow{p_{33}} x_3, \quad 2x_4 \xrightarrow{p_{44}} x_4, \\
x_1 + x_3 \xrightarrow{q_{13}} x_3, \quad x_1 + x_4 \xrightarrow{q_{14}} q_{14}x_4, \quad x_3 + x_4 \xrightarrow{q_34} x_4, \\
x_1 + x_3 \xrightarrow{d_{13}} x_1 + 2x_3, \quad x_1 + x_4 \xrightarrow{d_{14}} x_1 + 2x_4, \quad x_3 + x_4 \xrightarrow{d_{34}} x_3 + 2x_4, \\
x_1 \xrightarrow{\gamma} x_2, \quad x_2 \xrightarrow{\beta} x_1.
\end{gathered}
$$

The coefficients of the Fokker–Planck equation are as follows:

$$
A = \begin{bmatrix}
a_1x_1 - p_{11}x_1^2 - q_{13}x_1x_3 - q_{14}x_1x_4 + \beta x_2 - \gamma x_1, \\
a_2x_2 - p_{22}x_2^2 - \beta x_2 + \gamma x_1, \\
-c_3x_3 - p_{33}x_3^2 - q_{34}x_3x_4 + d_{13}x_1x_3, \\
-c_4x_4 - p_{44}x_4^2 + d_{34}x_3x_4 + d_{14}x_1x_4,
\end{bmatrix},
$$

$$
B = \begin{bmatrix}
B_{11} & -\beta x_2 - \gamma x_1 & 0 & 0 \\
-\beta x_2 - \gamma x_1 & B_{22} & 0 & 0 \\
0 & 0 & B_{33} & 0 \\
0 & 0 & 0 & B_{44}
\end{bmatrix},
$$

where $B_{11} = a_1x_1 + p_{11}x_1^2 + q_{13}x_1x_3 + q_{14}x_1x_4 + \beta x_2 + \gamma x_1$, $B_{22} = a_2x_2 + p_{22}x_2^2 + \beta x_2 + \gamma x_1$, $B_{33} = c_3x_3 + p_{33}x_3^2 + q_{34}x_3x_4 + d_{13}x_1x_3$, $B_{44} = c_4x_4 + p_{44}x_4^2 + d_{34}x_3x_4 + d_{14}x_1x_4$.

Thus, using the software package the construction of the "prey–migration area–predator–superpredator" model is constructed for both stochastic and deterministic cases. After constructing the models other modules of the software package can be applied for the numerical investigation of the system based on Runge–Kutta methods [12].

The results of the numerical experiments are presented in Fig. 5. The same parameter values are used as those for the numerical solution of the SDE with additive and multiplicative noise. The plots show the dynamics of the phase variables (population densities) x_1, x_2, x_3, x_4, respectively.

Based on the results of the numerical experiments it can be concluded that the self-consistent stochastic model exhibits a different qualitative behavior. The solutions of the SDE also reach a stationary regime. However, for this model the introduction of stochasticity in the described manner leads to the extinction of both predators populations while the prey continues to exist in both the main habitat and the refuge.

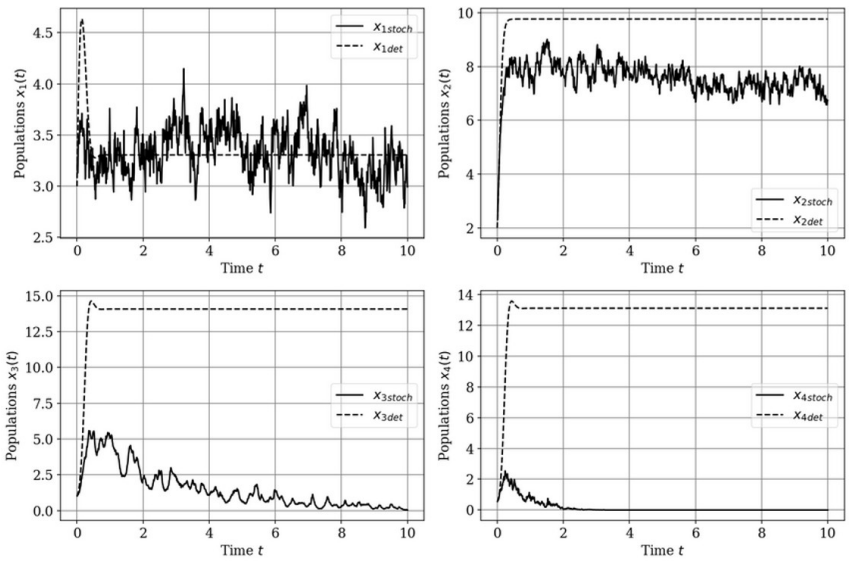

Figure 5. Visualization of the numerical solution

4. Discussion

In this paper a four-dimensional dynamic population model of the "prey–migration area–predator–superpredator" type which accounts for complex trophic interactions, intraspecific and interspecific competition as well as prey migration to a refuge are investigated. For the model with complex trophic interactions and migration flows, stochastization are performed using various approaches: the approach with additive and multiplicative noises, the approach involving stochastic parametric perturbations and the approach based on constructing self-consistent one-step models.

Using the scheme of stages of applying the differential evolution algorithm presented in Fig. 2 for the study of model (1), a parameter set ensuring the coexistence of populations in the main habitat and the survival of the prey population in the refuge is obtained. It is worth noting the universal nature of the developed algorithm which can be applied to various types of dynamic models.

According to Fig. 3 the introduction of additive noise has a minor effect on the behavior of the model. Adding a random process to the migration parameters significantly affects not only the population density of prey that can migrate to the refuge but also the population densities of predator and superpredator in the main habitat. The introduction of multiplicative noise influences the trajectory dynamics; however, this influence is less significant compared to the stochastization of migration parameters. The solution trajectories of the system of stochastic differential equations reach a stationary regime. According to Fig. 5 the introduction of stochasticity using the method of constructing self-consistent one-step models leads to the extinction of both predator populations while the prey continues to exist in both the main habitat and the refuge.

Figure 6 shows a diagram illustrating the types of stochastization of a deterministic dynamic population model with migration flows.

The results of this paper are obtained using two software packages. One of the two software packages is developed for finding the optimal parameters of the deterministic "prey–migration area–predator–superpredator" model, constructing and analyzing the trajectory dynamics of stochastic models based on additive and multiplicative noise, as well as for building a stochastic model with

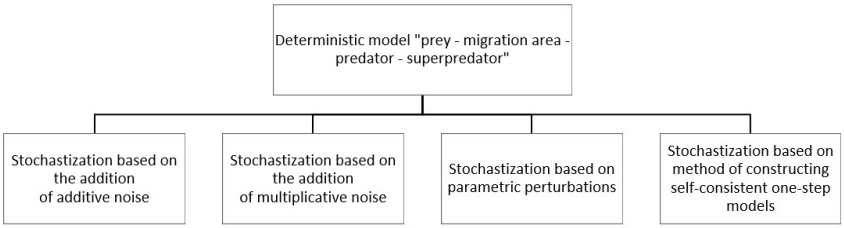

Figure 6. Stochastization directions of a deterministic dynamic population model with migration flows

random migration parameters. The other software package [12, 16] is designed for stochastization based on the method of constructing self-consistent one-step models. The study results of the "prey–migration area–predator–superpredator" model obtained using these software tools enabled a comparative analysis of the trajectory dynamics for the deterministic population system with migration flows and its corresponding stochastic variants.

5. Conclusion

The paper uses an approach to the study of population models with trophic interactions and migration flows which is based on the use of evolutionary algorithms for finding parameters, additive and multiplicative noises, the method of constructing self-consistent stochastic models and modified numerical methods for solving systems of stochastic differential equations. Solving the optimization problem using differential evolution allowed to find the optimal parameters of the "prey–migration area–predator–superpredator" model with species competition in the main habitat and prey migration to a refuge. For this model an approximate positive equilibrium state corresponding to the obtained set of parameters is found.

In this paper the use of the applied methods made it possible to construct new stochastic models of population dynamics that take into account trophic interactions, competition and bidirectional prey migration. The implementation of algorithms for the stochastization of model (1) through the introduction of additive and multiplicative noises as well as stochastization based on given interaction schemes enabled an analysis of the trajectory dynamics for the stochastic variants of the model in comparison with the deterministic model.

As directions for further research one can consider the construction of new modifications of multidimensional population models based on model (1) and the identification of parameter sets that lead to significant differences in the dynamics of deterministic and stochastic models. Additionally future research prospects include modeling complex trophic interactions involving several types of prey or predator species as well as accounting for the nonlinear nature of migration flows.

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Анализ стохастической модели “жертва–ареал миграции–хищник–суперхищник”

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Аннотация. К актуальным направлениям исследования динамических миграционно-популяционных моделей относятся анализ траекторной динамики и решение задач параметрической оптимизации с применением компьютерных методов. В настоящей работе рассматривается популяционная модель «жертва–ареал миграции–хищник–суперхищник», которая задаётся системой четырёх дифференциальных уравнений. В модели учитываются трофические взаимодействия, внутривидовая и межвидовая конкуренция, а также миграция жертвы в убежище. С помощью дифференциальной эволюции найдены параметры, обеспечивающие сосуществование популяций жертвы, хищника и суперхищника соответственно в основном ареале обитания и существование популяции жертвы в убежище. Выполнен переход к стохастическим вариантам модели на основе аддитивных шумов, мультипликативных шумов и метода построения самосогласованных моделей. Для описания структуры стохастической модели использованы уравнения Фоккера–Планка и выполнен переход к системе уравнений в форме Ланжевена. Численное решение стохастических систем дифференциальных уравнений реализовано методом Эйлера–Маруямы. С помощью программного комплекса на языке Python проведены компьютерные эксперименты, построены траектории для детерминированного и стохастических случаев. Проведён сравнительный анализ детерминированной и соответствующих ей стохастических моделей. Результаты могут найти применение при решении задач математического моделирования биологических, экологических, физических, химических и демографических процессов.

Ключевые слова: система дифференциальных уравнений; миграционные потоки; стохастизация; метод построения самосогласованных моделей; дифференциальная эволюция

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Using NeuralPDE.jl to solve differential equations

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Abstract. This paper describes the application of physics-informed neural network (PINN) for solving partial derivative equations. Physics Informed Neural Network is a type of deep learning that takes into account physical laws to solve physical equations more efficiently compared to classical methods. The solution of partial derivative equations (PDEs) is of most interest, since numerical methods and classical deep learning methods are inefficient and too difficult to tune in cases when the complex physics of the process needs to be taken into account. The advantage of PINN is that it minimizes a loss function during training, which takes into account the constraints of the system and th e laws of the domain. In this paper, we consider the solution of ordinary differential equations (ODEs) and PDEs using PINN, and then compare the efficiency and accuracy of this solution method compared to classical methods. The solution is implemented in the Julia programming language. We use NeuralPDE.jl, a package containing methods for solving equations in partial derivatives using physics-based neural networks. The classical method for solving PDEs is implemented through the DifferentialEquations.jl library. As a result, a comparative analysis of the considered solution methods for ODEs and PDEs has been performed, and an evaluation of their performance and accuracy has been obtained. In this paper we have demonstrated the basic capabilities of the NeuralPDE.jl package and its efficiency in comparison with numerical methods.

Key words and phrases: physics-informed neural networks, numerical methods, differential equations, Julia programming language, NeuralPDE

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1. Introduction

Physics-informed neural networks (PINNs) are deep learning methods designed to solve various types of differential equations (DEs) that arise in computational science and engineering [1]. By integrating data and physical laws, PINNs construct a neural network that approximates the solution of a DE system. Such a network is obtained through the minimization of a loss function that encodes any prior knowledge about the DEs and the available data.

To demonstrate the functionality of PINNs, we employ the NeuralPDE.jl library [1], implemented in Julia programming language [2, 3]. We consider a simple mathematical model based on a system of ordinary differential equations (ODEs). The system is solved numerically and using PINNs, then the resulting solutions are compared with the first integral of a system.

2. Physics-informed neural networks

Physics-informed neural networks (PINNs) have become an increasingly effective approach for solving differential equations and constructing neural equivalents of physical models. Classical neural networks derive solutions solely based on data represented as pairs of "state–value." A key feature of PINNs is that they take into account the physical laws behind the problem, which are expressed as ordinary or partial differential equations. In other words, the loss function explicitly includes the ODE/PDE terms as well as the initial and boundary conditions. The term PINN was introduced in [4], where it was defined as a new class of universal function approximators capable of encoding fundamental physical laws that can be described by partial differential equations.

2.1. Overview

Consider a differential equation of the following form:

$$F(u(x);\lambda) = 0,$$

where F is a differential operator, u is the solution of the differential equation, λ denotes the parameters of the equation, and $x = x_1, \dots, x_n \in \Omega$ is an n-dimensional coordinate vector defined on the domain Ω.

Let B denote the boundary operator, and let the function u satisfy the following boundary conditions:

$$B(u(x);\lambda) = 0$$

And I denotes the initial condition operator, while the function u satisfies the following initial conditions:

$$I(u(x);\lambda) = 0.$$

PINNs solve partial differential equations (PDEs) by utilizing the Universal Approximation Theorem [5], which states that for any measurable function u, there exists a sufficiently large neural network N with weights w such that $||N(x;w) - u(x)|| < \varepsilon$ for all $x \in \Omega$. This implies that an arbitrary differential equation can be solved by replacing the unknown solution $u(x)$ with a neural network $N(x;w)$ and finding the weights w such that $F(N;\lambda) \approx 0$ for all $x \in \Omega$. Formally, this condition can be expressed as a single equation by summing the the residuals over all points x.

$$L(w) = \int_{\Omega} ||F(N(x;w);\lambda)||dx, \tag{1}$$

where the objective is to determine the neural network weights w that minimize the loss function $L(w)$. In contrast to the exact analytical solution, if $L(w) = 0$, the neural network can be regarded, by definition, as the solution of the corresponding differential equation.

Since the boundary conditions must be satisfied only on a certain subset $\partial\Omega$, it is useful to separate the boundary and initial conditions into their own equation. Thus, we obtain:

$$L(w) = \int_{\Omega\setminus\partial\Omega} ||F(N(x,w);\lambda)||dx + \int_{\partial\Omega} ||B(N(x,w);\lambda)||dx + ||I(N(x,w);\lambda)||. \tag{2}$$

Equation (1) is equivalent to (2), but it provides a clearer view of the implementation. Let us rewrite it using the following notation:

$$L(w) = L_r + L_{ic} + L_{bc},$$

where L_r is the differential equation residual, L_{ic} is the initial condition error, and L_{bc} is the boundary condition error.

2.2. General workflow

The workflow of PINNs consists of the following main steps:

1. Definition of the problem based on physical laws and formulation of the governing equations describing the system.
2. Collection of data representing the system's behavior from experiments, simulations or other sources.
3. Selection of the neural network architecture and initialization of its parameters.
4. Formulation of the loss function, which incorporates both the agreement with experimental data and the satisfaction of the physical equations.
5. Training of the neural network by minimizing the loss function.
6. Verification of the training stopping criteria (e.g., reaching a predefined number of epochs or achieving minimal loss).
7. Analysis and interpretation of the obtained results.

A more detailed workflow of PINNs can be outlined as follows:

1. Definition of the physics-based problem:
   - formulate the governing equations that describe the behavior of the system (these equations may be derived from fundamental principles such as conservation laws or constitutive equations);
   - specify the boundary and initial conditions for the problem.
2. Data collection:
   - obtain data representing the behavior of the system from experiments, simulations, or other sources;
   - prepare the training data by selecting the points (spatial or temporal coordinates) at which predictions and losses will be evaluated.
3. Design and configuration of the neural network architecture:
   - define the type of neural network (e.g., fully connected network);
   - select the number of layers and neurons per layer;
   - choose activation functions;
   - initialize network parameters (weights and biases).
4. Formulation of the loss function:
   - include two main components in the loss function:
     - data fidelity term — measures the discrepancy between network predictions and observed data;
     - physics-informed term — enforces the satisfaction of the governing physical equations as constraints;
   - adjust the weighting of the loss components to balance data accuracy and physical consistency.
5. Training of the neural network:
   - feed input data into the network and compute predictions;
   - evaluate the loss using the formulated loss function;
   - update the network parameters using an optimization algorithm;

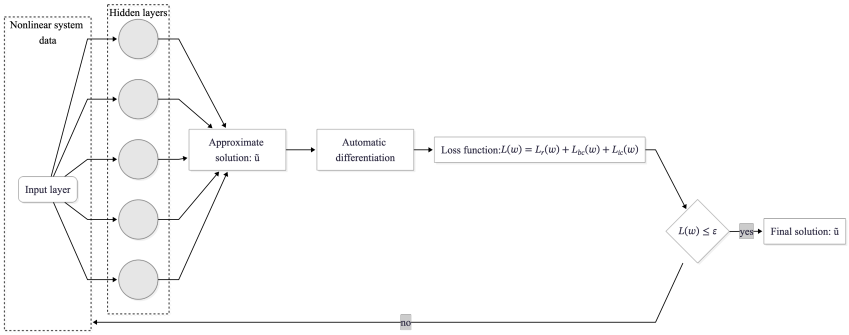

Figure 1. Flow diagram of the PINN training process

- apply automatic differentiation to compute the derivatives required for training.

6. Verification of stopping criteria:
   - monitor whether a predefined number of training epochs (iterations) has been reached;
   - track the minimization of the loss function or other convergence criteria;
   - assess the stability and quality of the predictions.
7. Iterative refinement of training and validation until the stopping conditions are met. This process can be represented by a block diagram (Fig. 1).
8. Evaluation of results:
   - analyze network predictions for consistency with both experimental data and physical laws;
   - assess the accuracy and interpretability of the obtained solution.
9. Interpretation and application of results:
   - use the trained model to predict system behavior under new conditions;
   - apply the model to solve forward and inverse problems, data assimilation tasks, and related applications.
10. Model optimization and refinement (if required):
    - adjust the network architecture, loss function, or training process to improve performance;
    - retrain the model with updated parameters if the results are unsatisfactory.

2.3. Overview of the NeuralPDE package

The `NeuralPDE` package [6] is part of the SciML [7] ecosystem for the Julia programming language. This collection includes packages that enable the computation of mathematical models based on various types of differential equations, combining traditional numerical methods with machine learning techniques.

The `NeuralPDE` package employs neural networks whose loss function incorporates the differential equations defining the mathematical model. This enables the training process to account for the underlying physical laws governing the problem, thereby implementing the concept of PINNs [8].

NeuralPDE is used to address three broad classes of problems:

- approximation of solutions to systems of ordinary differential equations (ODEs);
- approximation of solutions to partial differential equations (PDEs);

– solution of inverse problems, which involve determining the coefficients of ODEs and PDEs from known solutions.

The `NeuralPDE` package has been in active development since 2019 [9]. It can be installed through Julia's standard package manager by executing the command `add NeuralPDE`. Installation involves downloading a substantial number of dependencies, including both additional Julia packages and artifacts. In the Julia ecosystem, artifacts refer to external binary files of libraries or auxiliary utilities required by dependent packages. By default, `NeuralPDE` performs computations on the central processing unit (CPU). To enable graphics processing unit (GPU) acceleration, one must additionally install either `Flux.jl` [10] or `Lux.jl` [11]. The formulation of ordinary and partial differential equations relies on the syntax provided by the `ModelingToolkit.jl` package [12], which is also part of the SciML ecosystem. According to its official documentation, `ModelingToolkit.jl` is a framework for high-performance symbolic–numerical computation designed for mathematical modeling and scientific machine learning. It enables high-level symbolic specification of problems for subsequent numerical computation and analysis. The symbolic representation is built upon the `Symbolics.jl` package [13], which serves as a computer algebra system (CAS) within the Julia environment.

2.4. Solving ODEs in Julia

In mathematical terms, `ODEProblem` represents the following formulation:

$$u' = f(u, p, t)$$

for the interval $t \in (t_0, t_f)$ with the initial condition $u(t_0) = u_0$.

Let us solve a simple ordinary differential equation (ODE):

$$u' = cos(2\pi t)$$

for $t \in (0, 1)$ with $u_0 = 0$, we use `NNODE` and a numerical method, and then compare the results.

The problem is defined using the `ODEProblem` method by specifying the equation, initial condition, and time interval.

```
linear(u, p, t) = cos(t * 2 * pi)
tspan = (0.0, 1.0)
u0 = 0.0
prob = ODEProblem(linear, u0, tspan)
```

We set `NeuralPDE.NNODE()`, an algorithm for solving ordinary differential equations with a neural network. It represents a specialized form of the physics-informed neural network approach that serves as a solver for standard ODE problems. We then specify the neural network architecture using `Lux.jl` by defining a multilayer perceptron (MLP) with one hidden layer of 5 units and a sigmoid activation function, as follows:

```
rng = Random.default_rng()
Random.seed!(rng, 0)
chain = Chain(Dense(1, 5, σ), Dense(5, 1))
ps, st = Lux.setup(rng, chain) |> Lux.f64
```

We use the `solve` method to compute the solution of the defined problem, applying the `Tsit5()` solver with a step size of 0.01 (see Fig. 2):

```
sol_num = solve(prob, Tsit5(), saveat = 0.01)
```

A similar procedure is applied to produce the plot for the time interval $[0, 15]$ (Fig. 3).

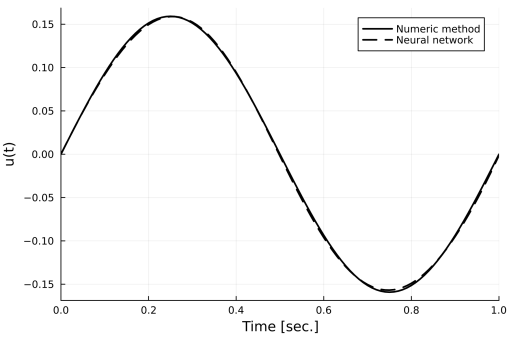

Figure 2. Comparison of solutions over the interval [0, 1]

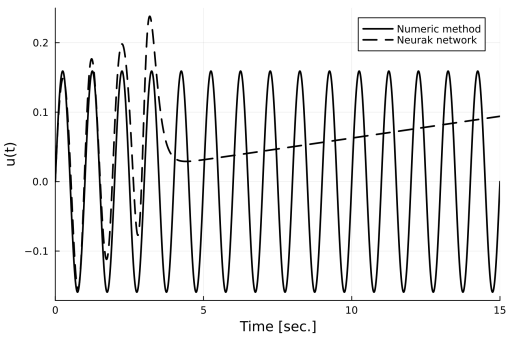

Figure 3. Comparison of solutions over the interval [0, 15]

3. Lotka–Volterra model

3.1. Description of the Lotka–Volterra model

Let us consider the Lotka–Volterra mathematical model (predator–prey model), which describes the interaction between two species of animals. One species preys on the other, while the prey population has access to unlimited food resources [14, 15]. The model is represented by the following system of equations:

$$\begin{cases} \dfrac{dx}{dt} = \alpha x(t) - \beta x(t) y(t), \\ \dfrac{dy}{dt} = -\gamma y(t) + \delta x(t) y(t). \end{cases}$$

In this model x denotes the number of prey and y the number of predators. The coefficient a represents the natural growth rate of the prey population in the absence of predators, while c describes the natural mortality rate of predators deprived of food (prey). The probability of interaction between prey and predators is assumed to be proportional to both their population sizes. Each interaction decreases the prey population but contributes to the growth of the predator population (the terms $-bxy$ and dxy in the right–hand side of the equations).

The first integral of the system can be written as follows:

$$\alpha \log y - \beta y + \gamma \log x - \delta x = C, \ C = \text{const}.$$

To solve the system, we set the parameters $\alpha = 1.5$, $\beta = 1.0$, $\gamma = 3.0$, $\delta = 1.0$. We consider the initial value problem (Cauchy problem) with the following initial conditions:

$$\begin{cases} x(0) = 1, \\ y(0) = 1. \end{cases}$$

3.2. Numerical investigation

We solve the system numerically using `Tsit5()` with a step size of 0.01 from the `DifferentialEquations.jl` library [16]. We consider the time interval $[0, 4]$. The results obtained by the numerical method are shown in Figs. 4, 5.

As shown in Fig. 4, the trajectory of the numerical solution forms a closed curve, indicating that the phase volume is conserved, similar to the analytical case.

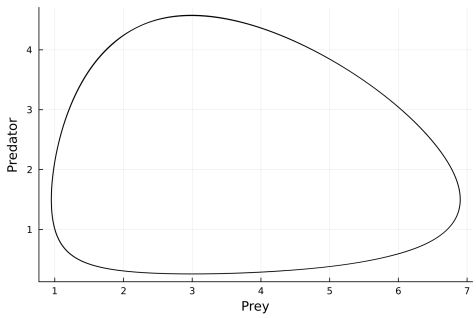

Figure 4. Phase portrait of the Lotka–Volterra model. Numerical method

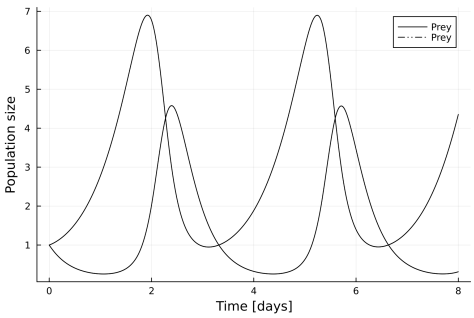

Figure 5. Numerical solution of the Lotka–Volterra model

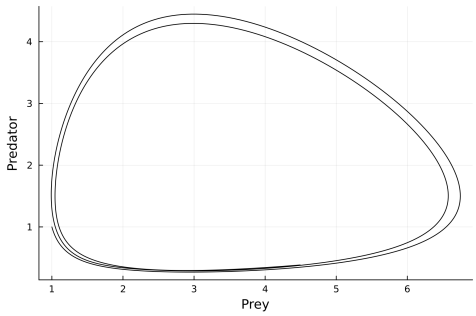

Figure 6. Phase portrait of the Lotka–Volterra model obtained using PINN

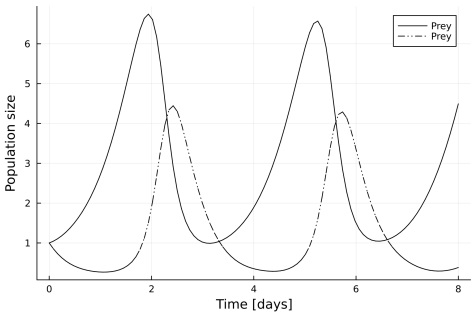

Figure 7. PINN-based solution of the Lotka–Volterra model

3.3. PINN-based solution of the model

We now solve the system using the `NeuralPDE.jl` library. The neural network architecture is defined with the `Lux.jl` library. A three-layer neural network is employed, consisting of one input neuron, two output neurons, and sixteen neurons in the hidden layer. The activation function for the first two layers is the hyperbolic tangent. Parameter optimization is carried out using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm from the `OptimizationOptimJL.jl` package. The `NeuralPDE.NNODE()` algorithm is used to solve the system of ordinary differential equations. This algorithm is a specialization of the physics-informed neural network (PINN) approach applied to standard ODE problems.

```
chain = Lux.Chain(Lux.Dense(1, 16, tanh),  Lux.Dense(16, 16,tanh),
 ↪  Lux.Dense(16, 2))
opt = OptimizationOptimJL.BFGS()
alg = NeuralPDE.NNODE(chain, opt)
```

We proceed by calling `solve` as in a typical `ODEProblem`. The `verbose` option is enabled to monitor the loss evolution during training. The maximum number of training epochs (iterations) is set to 1000:

```
sol = solve(prob, alg, verbose = true, abstol=1e-8, maxiters = 1000)
```

As a result we obtain the following plots (Fig. 6, 7).

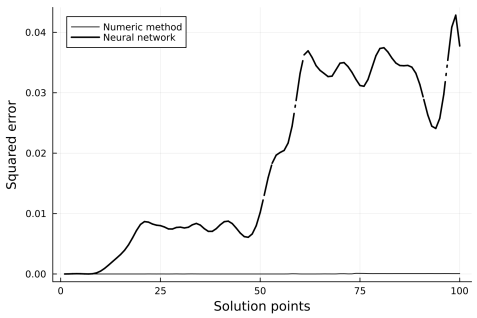

Figure 8. Comparison of solution errors

3.4. Comparative analysis of methods

We compare the phase trajectories obtained from the numerical solution and from the neural network with the first integral of the system. The corresponding squared error plots are shown in Fig. 8.

The plot indicates that the numerical solution provides higher accuracy than the PINN-based one. A performance comparison of the two approaches is then conducted using the `BenchmarkTools.jl` package. The efficiency of the numerical method is assessed in terms of computation time and memory consumption:

```
233.154 μs (7052 allocations: 567.62 KiB)
```

A similar evaluation is performed for the `NeuralPDE.jl` library:

```
2463.046 s (3569138613 allocations: 2682.28 GiB)
```

Neural networks require significantly more computational resources and time compared to numerical methods.

4. SIR model

Consider a system of differential equations whose solutions are aperiodic.

Compartmental models represent a general framework for modeling dynamic systems. They are widely used in the mathematical modeling of infectious diseases, where the population is divided into compartments labeled, for example, S, I, or R (susceptible, infectious, or recovered). Individuals can move between compartments according to the transition rules defined by the model.

The SIR model is one of the simplest compartmental models, and many other models are derived from this basic form. The model consists of three compartments:

- S: the number of susceptible individuals. When a susceptible and an infectious individual come into "infectious contact", the susceptible individual becomes infected and moves to the infectious compartment.
- I: the number of infectious individuals. These are individuals who have been infected and are capable of transmitting the disease to susceptible individuals.
- R: the number of recovered (and immune) individuals. These are individuals who have been infected and recovered from the disease and moved to the recovered compartment. This compartment may also be referred to as "resistant."

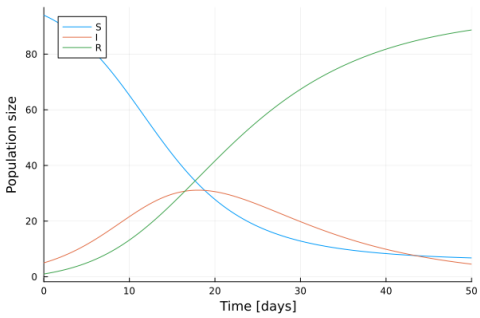

Figure 9. Numerical solution of the SIR model

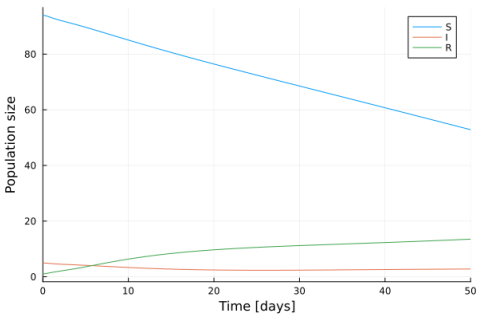

Figure 10. PINN-based solution of the SIR model

As long as the number of infected individuals does not exceed a critical threshold I^*, all infected persons are assumed to be isolated and unable to transmit the disease. Once $I(t) > I^*$, the infected individuals begin to spread the infection among the susceptible population.

The SIR model without vital dynamics (birth and death processes, sometimes referred to as demographic effects) can be formulated as the following system of ordinary differential equations:

$$\begin{cases} \dfrac{dS}{dt} = -\dfrac{\beta IS}{N}, \\ \dfrac{dI}{dt} = \dfrac{\beta IS}{N} - \gamma I, \\ \dfrac{dR}{dt} = \gamma I, \end{cases}$$

where S is the number of susceptible individuals, I is the number of infected individuals, R is the number of recovered individuals, and N is the total population given by the sum of these three compartments. The parameters β and γ represent the infection and recovery rates, respectively.

The system is solved numerically using the `Tsit5()` method with a step size of 0.1 from the `DifferentialEquations.jl` library [16]. We consider the time interval $[0, 50]$ with the initial conditions $S = 990.0$, $I = 10.0$, and $R = 0.0$. The resulting solution is shown in Fig. 9.

Next, we solve the same system using the `NeuralPDE.jl` library. We employ a three-layer neural network with one neuron in the input layer, three neurons in the output layer, and thirty-two neurons in the hidden layer. The activation function in the first two layers is the sigmoid function. The optimization is performed using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm from the `OptimizationOptimJL.jl` package.

```
chain = Lux.Chain(Lux.Dense(1, 32, σ), Lux.Dense(32, 32, σ), Lux.Dense(32,
 ↪  3))
opt = OptimizationOptimJL.BFGS()
alg = NeuralPDE.NNODE(chain, opt)
```

With the maximum number of training epochs set to 1000, the resulting solution is shown in Fig. 10.

In the case of a simple epidemic model the solution obtained using a physics-informed neural network demonstrated low accuracy. Therefore, this approach cannot be recommended for solving the given problem.

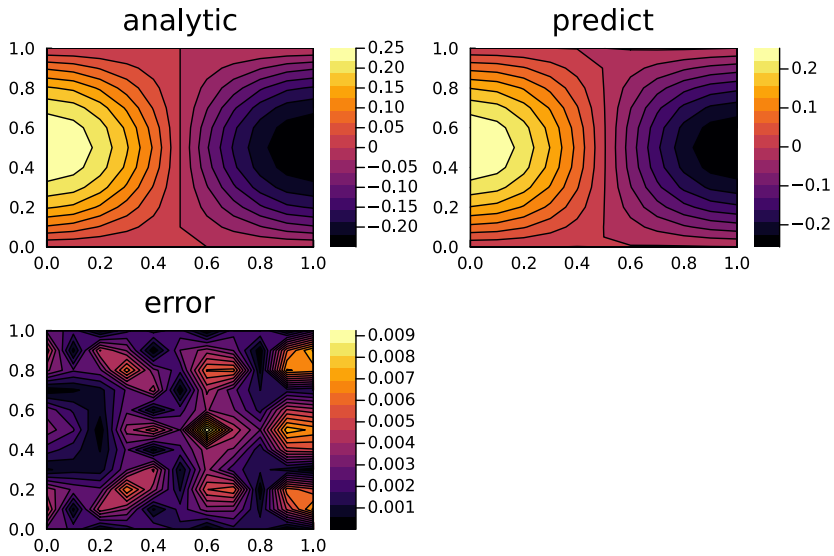

Figure 11. Visualization of the Poisson's equation solution based on the official NeuralPDE documentation

5. Eikonal equation

5.1. Poisson's equation

The official `NeuralPDE` documentation provides an example illustrating the solution of the two-dimensional Poisson's equation.

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = -\sin(\pi x)\sin(\pi y),$$

in a rectangular domain defined by the intervals $x \in [0,1]$ and $y \in [0,1]$, with the following boundary conditions:

$$u(0,y) = 0, u(1,y) = 0,$$
$$u(x,0) = 0, u(x,1) = 0.$$

The computation took approximately 30–40 minutes, resulting in plots consistent with those presented in the official documentation (Fig. 11).

5.2. Solving the Eikonal equation with NeuralPDE

Let us write the Eikonal equation [17–20] in Cartesian coordinates on the plane.

$$\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 = n^2(x,y).$$

The function $n(x,y)$ is piecewise continuous.

This example employs the function describing the two-dimensional Maxwell lens [21].

$$n(r) = \begin{cases} \dfrac{n_0}{1 + \left(\dfrac{r}{R}\right)^2}, & r \leqslant R, \\ n_0, & r > R, \end{cases}$$

where $r = \sqrt{(x - x_0)^2 + (y - y_0)^2}$ is the distance from the center of coordinates to points on the lens, which has a circular shape. The center of the lens is located at $(x_0, y_0) = (0, 0)$. The lens radius is $R = 1$, and the refractive index of the medium is $n_0 = 1$.

The example from the official documentation was modified by replacing the Poisson's equation and its boundary conditions with the Eikonal equation. The first modification involved substituting the second derivatives with the squares of the first derivatives:

```
Dx = Differential(x)
Dy = Differential(y)
```

Additionally, for the Maxwell lens:

```
eq = Dx(u(x, y))*Dx(u(x, y)) + Dy(u(x, y))*Dy(u(x, y)) ~ n(x, y)
```

In the `Differential` function, the symbol `^` specifies the order of differentiation rather than exponentiation. For this reason, it was replaced by an explicit multiplication of the derivative by itself. Also the boundary conditions and the domains of x, y were adjusted:

```
# Boundary condition (indicating that the point source is located at the
 ↪ origin)
bcs = [
    u(-1, 0) ~ 0.0
]
# Domain (x, y)
domains = [x in (-1.0, 2.0), y in (-1.0, 2.0)]
```

After several simplifications and the elimination of most internal variables, the `n(x, y)` function was represented as follows:

```
function n(x, y)
  r = hypot(x, y)
  if r <= 1
    return 1 / (1 + r^2)
  else
    return 1
  end
end
```

However, the program failed to execute in this configuration. After neural network initialization (which took about 10 minutes), the program crashed with the error about a non-Boolean value used in a Boolean context: `ERROR: TypeError: non-boolean (Num) used in boolean context`.

According to the official documentation, this error is documented and can arise from two primary causes:

- the `hypot` function is not available in symbolic form, meaning it is not implemented within the `Symbolics.jl` package;
- the **`if`**–**`else`**–**`end`** construct is not supported for symbolic expressions and must be replaced with the `Base.ifelse` function from the standard library.

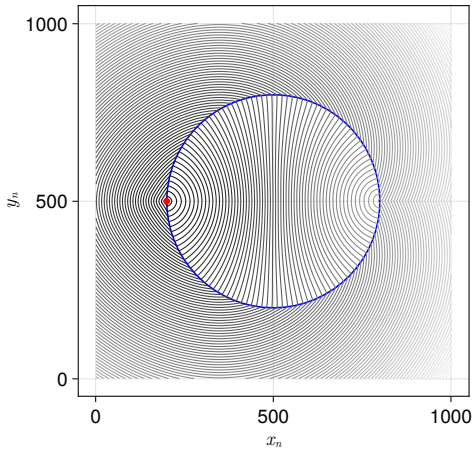

Figure 12. Wavefronts for the Maxwell lens

After applying these modifications, the refraction function was expressed as follows:

```
n(x, y) = ifelse(sqrt(x^2+y^2) <= 1, 1 / (1 + (x^2 + y^2))^2, 1)
```

After these modifications, the program executed successfully.
The processed results are presented in Fig. 12.

6. Discussion

The analysis of the `NeuralPDE` package revealed several drawbacks:

- The package has a large number of dependencies (over one hundred), including both other Julia packages and external binary files (utilities and libraries). As a result, it requires significant disk space and installation time. However, the main issue with the large dependency set is the reduced reliability and stability of the package.
- The differential equation and boundary conditions are defined in symbolic form, which provides only limited support for standard language constructs. Even for a simple function $n(x, y)$, the **`if-else-end`** statement and the standard `hypot` function did not work as expected. It is particularly unintuitive that **`if-else-end`** must be replaced with `Base.ifelse`.
- Computation time is significantly greater compared to classical numerical methods. While traditional numerical schemes complete calculations within tens of seconds, execution time using `NeuralPDE` reaches several tens of minutes.

7. Conclusion

A comparative analysis was carried out for solving the Lotka-Volterra system of differential equations, the epidemiological (SIR) model, and the eikonal equation using both a numerical method and a physics-informed neural network. The implementation was performed in the Julia programming language using the `DifferentialEquations.jl` and `NeuralPDE.jl` libraries. It was concluded

that currently neural network-based numerical methods cannot be regarded as a “silver bullet”. Further research is required to determine the scope and limitations of their applicability.

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Применение NeuralPDE.jl для решения дифференциальных уравнений

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Аннотация. Работа описывает применение Physics Informed Neural Network (PINN) для решения уравнений в частных производных. Physics Informed Neural Network — это вид глубокого обучения, который учитывает физические законы для более эффективного решения физических уравнений по сравнению с классическими методам. Наибольший интерес представляет решение уравнений в частных производных (УЧП), так как численные методы и классические методы глубокого обучения не эффективны и слишком сложно настраиваемы в случаях, когда необходимо учесть сложную физику процесса. Преимуществом PINN является то, что при обучении она минимизирует функцию потерь, которая учитывает ограничения системы и законы предметной области. В работе мы рассматриваем решение обыкновенных дифференциальных уравнений (ОДУ) и УЧП с помощью PINN, а затем сравниваем эффективность и точность этого метода решения по сравнению с классическими. Решение реализовано на языке программирования Julia. Мы используем NeuralPDE.jl - пакет, содержащий методы решения уравнений в частных производный с помощью нейронных сетей, основанных на физике. Классический метод решения УЧП реализован посредством библиотеки DifferentialEquations.jl. В результате был проведен сравнительный анализ рассматриваемых методов решения для ОДУ и УЧП, а также получена оценка их производительности и точности. В этой статье мы продемонстрировали базовые возможности пакета NeuralPDE.jl и его эффективность по сравнению с численными методами.

Ключевые слова: нейронные сети на основе физики, численные методы, дифференциальные уравнения, язык программирования Julia, пакет NeuralPDE.jl

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Dark matter hypothesis and new possibilities of the Skyrme–Faddeev chiral model

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Abstract. New possibilities of the 16-spinor realization of the Skyrme–Faddeev chiral model are discussed. Using gauge invariance principle, it is shown that there exist two independent ways for breaking the isotopic invariance symmetry. The first one concerns the interaction with the electromagnetic field (ordinary photons generated by the electric charge) and the second one includes the interaction with the new vector field (shadow/dark photons generated by the special neutrino charge). The neutrino oscillation phenomenon is explained.

Key words and phrases: chiral model, 16-spinor field, shadow/dark photons, neutrino charge

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1. Introduction. Structure of the $\mathrm{SO}(3)$ generators

The main idea behind this research concerns the problem of unifying the approaches suggested by Skyrme [1] and Faddeev [2] for interpreting baryons and leptons as topological solitons. To this aim, the 16-spinor Ψ realization of the Skyrme–Faddeev chiral models was considered some years ago [3]. Within the scope of this spinor realization there exist two kinds of the internal SO(3) generators:

$$\Lambda_i/2 = I_8 \otimes \sigma_i/2$$

and also

$$\lambda_i/2 = I_4 \otimes \sigma_i \otimes I_2/2,$$

where σ_i, $i = 1, 2, 3$, stands for the Pauli matrices and I_n denotes the unity matrix of the n-th order. The generators $\Lambda_i/2$ are used for constructing the S^2 manifold $(\bar{\Psi}\Lambda_i\Psi)^2 = \text{const}$ determining the Hopf invariant Q_{H}, which is interpreted as the lepton charge $\mathbb{L}$ according to Faddeev. As for the generators $\lambda_i/2$, they determine the isotopic space symmetry, with its localization implying the Yang–Mills axial vector field, which gives the main contribution to strong interactions.

2. Breaking the isotopic symmetry

However, the isotopic symmetry is broken by the electromagnetic interactions due to the extension of derivatives:

$$\partial_\mu \Psi \to \partial_\mu \Psi - \imath e_0 \Gamma_e A_\mu \Psi; \quad \mu = 0, 1, 2, 3,$$

where the electromagnetic coupling constant e_0 and the corresponding charge generator $\Gamma_e = P_3 \Lambda$ are introduced. Here the denotations are used: $P_3 = (1 - \lambda_3)/2$; $\Lambda = (1 - \Lambda_3)/2$. We are now in a position to mention the other possibility of the isotopic symmetry breaking due to extending the derivatives:

$$\partial_\mu \Psi \to \partial_\mu \Psi - \imath \tilde{e}_0 \Gamma_c C_\mu \Psi,$$

where the new massless vector field C_μ, the new coupling constant $\tilde{e}_0$ and the corresponding generator $\Gamma_c = N_3 \Lambda$, are introduced. Here the new isotopic projector $N_3 = (1 + \lambda_3)/2$ is used. It is worth while to underline that this new vector field should be generated by the special charge, which is similar to the electromagnetic one. However, only neutral leptons (neutrinos) should be endowed with this charge, so it can be called "the neutrino charge" [4, 5], and the corresponding vector field C_μ describes the unusual photons called "shadow" or "dark" ones. It should be also stressed that the universal vacuum state Ψ_0 there exists in this model, with the natural projector property being $\Lambda \Psi_0 = 0$, where the boundary condition at space infinity reads:

$$\Psi_0 = \lim_{|\vec{x}| \to \infty} \Psi. \tag{1}$$

3. Correspondence with quantum mechanics. Lepton part of the Lagrangian

The other problem to be solved in this model concerns the correspondence with quantum mechanics. According to Einstein [6, 7], particles should be represented as soliton-like configurations described by some regular solutions to field equations. Let us consider small excitations of the particle-soliton near the vacuum: $\Psi = \Psi_0 + \xi$, where $\xi \to 0$ as $|\vec{x}| \to \infty$. Correspondence with quantum mechanics means that the field ξ should satisfy the Klein–Gordon equation of the form

$$\left(\partial_\mu \partial^\mu + M^2\right) \xi = 0, \tag{2}$$

where M stands for the mass of the particle-soliton in natural units $\hbar = c = 1$. The latter condition implies the special structure of the Lagrangian density of the model in question [3]:

$$\mathcal{L} = \mathcal{L}_{\text{spin}} + \mathcal{L}_{\text{em}} + \mathcal{L}_c + \mathcal{L}_g,$$

where the following denotations are used:

$$\mathcal{L}_{\text{spin}} = \frac{1}{2\lambda^2} D + \frac{\varepsilon^2}{4} f_{\mu\nu} f^{\mu\nu} - V,$$

$$D = \overline{D_\mu \Psi} \gamma^\nu J_\nu D^\mu \Psi,$$

$$f_{\mu\nu} = (\bar{\Psi} \gamma^\alpha D_{[\mu} \Psi)(\overline{D_{\nu]} \Psi} \gamma_\alpha \Psi),$$

$$V = -\frac{2D^3}{\lambda^2 K^2 \ell_{\text{Pl}}^4 \varkappa_0^8} (J_\mu J^\mu - \varkappa_0^2)^2,$$

$$D_\mu \Psi = \partial_\mu \Psi - \left(\imath e_0 \Gamma_e A_\mu + \imath \tilde{e}_0 \Gamma_c C_\mu + \Gamma_\mu\right) \Psi.$$

Here the extended derivative contains the spinor affine connection Γ_μ. The Lagrangian includes the sigma-model part D with the projector $\gamma_0 J_\nu \gamma^\nu$ on the positive energy states. The first two terms in the Lagrangian $\mathcal{L}_{\text{spin}}$ imply the lower estimate of the energy through the corresponding topological charge (lepton or baryon one). Here the Dirac current reads $J_\mu = \bar{\Psi}\gamma_\mu \Psi$. At last, the Higgs potential V has the special structure based on the boundary condition:

$$\lim_{|\vec{x}|\to\infty} J_\mu J^\mu = \varkappa_0^2. \tag{3}$$

For providing the compatibility of the conditions (1), (3) and (4) the Higgs potential V includes the special gravitational invariant known as that of Kretschmann:

$$K = R_{\mu\nu\sigma\lambda} R^{\mu\nu\sigma\lambda},$$

that is the square of the Riemann curvature tensor. Finally, the Einstein gravitational term is included:

$$\mathcal{L}_g = -\frac{1}{2\varkappa} R,$$

where $\varkappa = 8\pi G/(c^4)$ and R, G stand for the scalar curvature and the Newton gravitational constant, respectively.

4. Quantization of the electric and the neutrino charges

It is worth while to underline that the discrete nature of the charges mentioned above can be provided through the special structure of the electromagnetic Lagrangian density and that of the dark/shadow photons part. Introducing intensity tensors for the electromagnetic and shadow fields respectively: $F_{\mu\nu} = \partial_{[\mu} A_{\nu]}$; $G_{\mu\nu} = \partial_{[\mu} C_{\nu]}$, let us write down the corresponding Lagrangian densities:

$$\mathcal{L}_{\text{em}} = -\frac{1}{16\pi} F_{\mu\nu} F^{\mu\nu} \left[1 + \mu_0 \sin^2 \frac{\pi U}{2e}\right], \quad \mu_0 = \text{const};$$

$$\mathcal{L}_c = -\frac{1}{16\pi} G_{\mu\nu} G^{\mu\nu} \left[1 + \nu_0 \sin^2 \frac{\pi \tilde{U}}{2\tilde{e}}\right], \quad \nu_0 = \text{const};$$

where the special denotations are used:

$$U = (n_\mu A^\mu)^2 (-E_\nu E^\nu)^{-1/2}; \quad \tilde{U} = (n_\mu C^\mu)^2 (-G_\nu G^\nu)^{-1/2}.$$

Here the following quantities are introduced: $E_\nu = n^\mu F_{\mu\nu}$; $G_\nu = n^\mu G_{\mu\nu}$, where $n^\mu = J^\mu/J$ is the unit vector. It can be shown that at the space infinity the asymptotic behavior of the vector fields coincides with that of the Coulomb potential: $A_0 = q/r$; $C_0 = \tilde{q}/r$, where $r = |\vec{x}|$, with the corresponding charges taking integer values of the fundamental charges e and $\tilde{e}$.

5. Mirror symmetry and the intersection problem of lepton and baryon states

Let us now recall the Skyrme's idea [1] to determine the S^3 manifold by the O(4) invariant condition

$$(\bar{\Psi}\Psi)^2 + (\imath \bar{\Psi}\gamma_5 \vec{\lambda} \Psi)^2 = \text{const} \tag{4}$$

and identify the baryon charge $\mathbb{B}$ with the winding number $\deg(S^3 \to S^3)$. However, the main question arises: how to exclude the intersection of baryon and lepton sectors? The answer is given by the special mirror symmetry that should be attributed to the states in the lepton sector:

$$\Psi_{\mathrm{L}} = \gamma_{(0)}\Psi_{\mathrm{L}}. \tag{5}$$

The similar mirror symmetry but in the isotopic space should be attributed to the states in the baryon sector:

$$\Psi_{\mathrm{B}} = \gamma_{(0)}\gamma_5\gamma_{(2)}\lambda_2\Psi^*_{\mathrm{B}}. \tag{6}$$

Here the following structure of the plane Dirac γ-matrices are used:

$$\gamma_{(0)} = I_2 \otimes \sigma_1 \otimes I_4; \quad \gamma_{(k)} = -\imath\sigma_k \otimes \sigma_2 \otimes I_4,$$

where $k = 1, 2, 3$, and $\gamma_5 = I_2 \otimes \sigma_3 \otimes I_4$. The physical origin of the symmetry (6) reduces to the fact of charge independence of strong interactions. To prove the impossibility of intersecting lepton and baryon states let us introduce the following representation of the 16-spinor [8]:

$$\Psi = \oplus_{j=1}^{2}\left(\varphi_j \oplus \chi_j \oplus \xi_j \oplus \zeta_j\right), \tag{7}$$

where φ_j, χ_j, ξ_j, ζ_j stand for some 2-spinors. Applying the symmetry (6) to (7), one finds $\varphi_j = \chi_j$, $\xi_j = \zeta_j$ for the Weyl representation of γ-matrices. For this effective 8-spinor one obtains $(\bar{\Psi}\vec{\Lambda}\Psi) \neq 0$, but $(\bar{\Psi}\gamma_5\vec{\lambda}\Psi) = 0$. Therefore, in view of (5) one gets $\mathbb{B} = 0$, $\mathbb{L} \neq 0$.

On the contrary, applying the symmetry (6) to (7), one finds for the baryon sector $\xi_j = \imath\sigma_2\varphi_j^*$, $\zeta_j = \imath\sigma_2\chi_j^*$. For this effective 8-spinor one gets $(\bar{\Psi}\Lambda_2\Psi) = 0$, but $(\bar{\Psi}\Psi) \neq 0$, $(\bar{\Psi}\gamma_5\vec{\lambda}\Psi) \neq 0$. Thus, as a consequence, $\mathbb{B} \neq 0$, $\mathbb{L} = 0$. Taking these facts into account, one concludes about impossibility of intersecting lepton and baryon states.

Finally, one can deduce the structure of the vacuum state Ψ_0. To this end, due to the universal character of the vacuum state, let us apply to Ψ_0 both (6) and (6) symmetries, with the result being:

$$\Psi_0 = \mathrm{col}\left\{\begin{bmatrix} a_0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} a_0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ -a_0^* \end{bmatrix}, \quad \begin{bmatrix} 0 \\ -a_0^* \end{bmatrix}\right\}.$$

Here $4|a_0|^2 = \varkappa_0$ is the new fundamental constant, characterizing the vacuum state.

6. Axially symmetric states

First one remarks that due to space reflection symmetry of the lepton sector one gets $\varphi_j = \chi_j$ and also $\xi_j = \zeta_j$. To study the angular structure of the spinor field let us use the principle of symmetric criticality [9] and consider a class of axially symmetric states invariant under the special group of combined space and isotopic rotations:

$$G = \mathrm{diag}\left[\mathrm{SO}(2)_S \otimes \mathrm{SO}(2)_I\right], \tag{8}$$

with the corresponding generators reading: $\bar{J}_3 = -\imath\partial_\phi + \sigma_3/2$; $T_3 = \lambda_3\Lambda_3/2$, respectively. Solving the invariance equations:

$$\bar{J}_3\Psi_1 = \frac{\lambda_3}{2}\Psi_1, \quad \bar{J}_3\Psi_2 = -\frac{\lambda_3}{2}\Psi_2,$$

one can find the dependence of the fields on the azimuth angle ϕ:

$$\varphi_1 = \begin{bmatrix} f_1 \\ g_1 \exp[\imath\phi] \end{bmatrix}; \quad \zeta_1 = \begin{bmatrix} u_1 \exp[-\imath\phi] \\ v_1 \end{bmatrix};$$
$$\varphi_2 = \begin{bmatrix} g_2 \exp[-\imath\phi] \\ f_2 \end{bmatrix}; \quad \zeta_2 = \begin{bmatrix} u_2 \\ v_2 \exp[\imath\phi] \end{bmatrix}.$$

It should be also underlined that the fields satisfy the vacuum boundary condition at the space infinity $\Psi \underset{r\to\infty}{\to} \Psi_0$, if the following nontrivial boundary conditions read:

$$f_1 \underset{r\to\infty}{\to} a_0, \tag{9}$$
$$v_1 \underset{r\to\infty}{\to} -a_0^*. \tag{10}$$

7. Structure of the lepton charge

First of all one should remark that all calculations in the lepton sector appear to be drastically simplified through using the toroidal coordinates $x \geq 0$, $\xi \in [-\pi, \pi]$. Their connection to the cylindrical ones reads:

$$\rho = a\frac{\sinh x}{\cosh x - \cos\xi}, \quad z = a\frac{\sin\xi}{\cosh x - \cos\xi},$$

where a stands for the length parameter. The explanation for this effect can be seen if one identifies, following Faddeev, the lepton charge $\mathbb{L}$ with the Hopf invariant $Q_{\mathrm{H}} = \mathbb{L}$. To define the structure of Q_{H}, let us introduce the unit 3-vector $\vec{n} = \vec{V}/|\vec{V}|$, where $\vec{V} = (\Psi^+\vec{\Lambda}\Psi)$, the manifold S^2 being determined by the condition $\vec{n}^2 = 1$. In view of the boundary conditions (9) and (10) one can put: $u_1 = g_1 = f_2 = v_2 = 0$ and also:

$$f_1 = sa_0, \quad v_1 = -sa_0^*, \quad s^* = s;$$
$$g_2 = a_0 v \exp[\imath\mu],\ u_2 = u,\ v^* = v,\ u^* = u,\ \mu^* = \mu.$$

As a result, one finds that the quantity $V_1 + \imath V_2 = 2\Psi_1^+\Psi_2$ reduces to the following one:

$$V_1 + \imath V_2 = \varkappa_0 sv \exp[\imath(\mu - \phi)]. \tag{11}$$

On the other hand, there exists the following correspondence between the 3-vector n^a, $a = 1, 2, 3$, and the special 4-vector a^μ:

$$\partial_\mu a_\nu - \partial_\nu a_\mu = 2\epsilon_{abc}\partial_\mu n^a \partial_\nu n^b n^c. \tag{12}$$

On the basis of the relation (12) one can construct the identically conserved topological current:

$$j^\mu_{\mathrm{H}} = -(128\pi^2)^{-1}\epsilon^{\mu\nu\sigma\tau}\left(\partial_\nu a_\sigma - \partial_\sigma a_\nu\right)a_\tau, \tag{13}$$

the conservation equation $\partial_\mu j^\mu_{\mathrm{H}} = 0$ being implied by the S^2-condition $\vec{n}^2 = 1$. Identifying the conserved charge $\int dV j^0_{\mathrm{H}}$, where dV is the element of the 3-volume, with the Hopf topological invariant, one finds the well-known Whitehead formula for the degree of knottedness or link invariant [10, 11]:

$$Q_{\mathrm{H}} = -(8\pi)^{-2}\int dV\big([\nabla\vec{a}]\vec{a}\big). \tag{14}$$

In our case of axially symmetric configurations the expression (14) can be reduced to the standard winding number $\deg(S^3 \to S^3)$ through applying the Hopf mapping $S^3 \to S^2$ and the definitions (12), (13), (14). To this end, let us introduce the auxiliary 2-spinor:

$$\chi = \mathrm{col}\Big[\cos\tilde{A} + \imath \sin\tilde{A}\cos\tilde{B}, \sin\tilde{A}\sin\tilde{B}\exp(\imath\tilde{C})\Big] \tag{15}$$

and calculate the following 3-vectors:

$$\vec{n} = \chi^{+}\vec{\sigma}\chi, \quad \vec{a} = -\imath\chi^{+}\nabla\chi, \quad [\nabla\vec{a}] = -2\imath[\nabla\chi^{+}\nabla\chi].$$

As a result, one gets from (15) the desired form of Q_{H}:

$$Q_{\mathrm{H}} = \frac{1}{2\pi^2}\int dV \sin^2\tilde{A}\sin\tilde{B}\big(\nabla\tilde{C}[\nabla\tilde{A}\nabla\tilde{B}]\big). \tag{16}$$

However, the integral (16) can be calculated exactly for the axially symmetric states via the substitution:

$$\sin\tilde{A}\sin\tilde{B} = \sin(\tilde{\sigma}/2), \quad \tan\tilde{A}\cos\tilde{B} = \tan\varphi.$$

Thus, the integral (16) takes the form:

$$Q_{\mathrm{H}} = \frac{1}{8\pi^2}\int dV\big([\nabla(\varphi\nabla n_3)]\nabla\tilde{C}\big), \tag{17}$$

where $n_3 = \cos\tilde{\sigma}$. Comparing the phases in (11) and in $n_1 + \imath n_2 = 2\chi_1^{+}\chi_2 \sim \exp[\imath(\tilde{C} - \varphi)]$, one finds $\tilde{C} = -\phi$ and $\varphi = -\mu$. First, one deduces from (17) that

$$Q_{\mathrm{H}} = \frac{1}{8\pi^2}\int dV\big([\nabla(\mu\nabla n_3)]\nabla\phi\big).$$

Using the Stokes theorem and performing the ϕ-integration, one gets the contour integral:

$$Q_{\mathrm{H}} = -\frac{1}{4\pi}\oint\limits_{L}\mu dn_3. \tag{18}$$

It is worth while to stress that the contour L in (18) contains the z-axis, the large asymptotic circumference, where $\sin\tilde{\sigma} = 0$, and also surrounds the interval $0 \le \rho \le a$, $z = 0$. Therefore, one concludes that the integral (18) reduces to the jump $[\mu]$ of the function μ on that interval, the latter one connecting the north and the south poles of the sphere S^2, i. e. the points $n_3 = \pm 1$, respectively. Finally, one obtains the value of the lepton number $\mathbb{L} = n$ characterizing our particle-soliton, since

$$\frac{1}{4\pi}\int_{-1}^{+1}[\mu]dn_3 = n.$$

Here the evident property of the angular variable ξ was taken into account:

$$\lim_{z\to+0}\xi = \pi, \quad \lim_{z\to-0}\xi = -\pi.$$

Therefore, the following relations hold: $\mu = n\xi$, $[\mu] = n[\xi] = 2\pi n$, with n being some integer number.

Let us now recall the final angular structure of the spinor field Ψ:

$$\begin{aligned} \varphi_1 &= \begin{bmatrix} sa_0 \\ 0 \end{bmatrix}, \qquad \varphi_2 = \begin{bmatrix} \upsilon a_0\exp[\imath(n\xi - \phi)] \\ 0 \end{bmatrix}, \\ \zeta_1 &= \begin{bmatrix} 0 \\ -sa_0^{*} \end{bmatrix}, \qquad \zeta_2 = \begin{bmatrix} u \\ 0 \end{bmatrix}; \end{aligned} \tag{19}$$

with s, v, u being some real functions of the radial toroidal coordinate x. Inserting (19) into the current $J_\mu = \bar{\Psi}\gamma_\mu\Psi$, one gets $J_\mu J^\mu = J^2$, where $J = 2\left[|a_0|^2(2s^2 + v^2) + u^2\right]$. This structure of the current J_μ suggests the following simplifying substitution:

$$s|a_0| = \frac{\sqrt{J}}{2}\sin A\cos B, \quad u = \left(\frac{J}{2}\right)^{1/2}\cos A, \quad v|a_0| = \left(\frac{J}{2}\right)^{1/2}\sin A\sin B.$$

8. Neutrino dark charge and spin. Neutrino oscillations

Let us first recall the invariant definition of the neutrino charge (or shadow/dark charge):

$$\tilde{U} = \frac{C_0^2}{|\dot{C}_0|} = \tilde{e} \equiv \tilde{e}_0(\hbar c).$$

Solving this equation, one finds $C_0 = \tilde{e}(1+t)^{-1}$; $t = -\log\tanh(x/2)$, that corresponds to the closed string approximation $x \to \infty$, or $t \to 0$. On the other hand, one can use the charge conservation law due to the Nœther's theorem:

$$\tilde{U} = \int \frac{\partial\mathcal{L}}{\partial\dot{C}^0}dV = \tilde{e}. \tag{20}$$

However, there exists the definition of the spin z-projection:

$$S_3 = \int 2\Re\left[\frac{\partial\mathcal{L}}{\partial(D^0\Psi)}\bar{J}_3\Psi\right]dV,$$

which is equivalent, in view of the symmetry group (8), to the relation:

$$S_3 = \frac{1}{2c}\int \frac{\partial\mathcal{L}}{\partial(\tilde{e}_0\dot{C}^0)}dV. \tag{21}$$

Therefore, unifying (20) and (21), one gets

$$S_3 = \tilde{U}(2c\tilde{e}_0)^{-1} = \hbar/2.$$

Fixing the neutrino charge $Q_\nu = 1$ in the units of $\tilde{e}$, it is possible to attack the very old neutrino oscillations problem. According to observations [12–20], in the flux of ν_τ some time later there can be found a mixture of ν_μ, ν_e, $\bar{\nu}_\mu$, $\bar{\nu}_e$. The same concerns the flux of ν_μ. First of all, one should take into account the conservation law of the lepton number $\mathbb{L}$ due to its topological origin. Let us recall the properties of the lepton family:

$$\mathbb{L} = 1 : (e^-, \nu_e); \quad \mathbb{L} = 2 : (\mu^-, \nu_\mu); \quad \mathbb{L} = 3 : (\tau^-, \nu_\tau).$$

Taking into account the neutron decay: $n \to p + e^- + \bar{\nu}_e$, one should attribute to the neutron the neutrino charge $Q_\nu = -1$. The conservation laws of $\mathbb{L}$ and Q_ν imply the following reaction and its inversion process (in a medium):

$$\nu_\tau \to 2\nu_\mu + \bar{\nu}_e, \quad 2\nu_\mu + p \to \nu_e + \nu_\tau + p,$$

that explains the oscillations of ν_τ.

Now let us consider the flux of high energy ν_μ in a medium: Then the following reactions hold:

$$\nu_\mu + n \to p + \mu^-, \quad \mu^- \to e^- + \bar{\nu}_e + \nu'_\mu,$$

that explains the oscillations of ν_μ.

9. Results and Discussions

Some aspects of the dark matter problem are discussed in this paper. First, one remarks two possibilities of breaking the isotopic invariance, which imply the existence of two kinds of electric charges and corresponding electromagnetic fields and photons: ordinary and dark/shadow ones. The realization of this program specifies the adequate structure of the basic field model, the Skyrme–Faddeev chiral model. The topological solitons in this model correspond to the two classes of particles: leptons and baryons, endowed with the lepton $\mathbb{L}$ and baryon $\mathbb{B}$ charges, respectively. The intersection problem of these classes can be solved via introducing the Brioschi 16-spinors Ψ as fundamental unitary fields advocated by Einstein. The hypothesis of the alternative (dark) electric charge, called the neutrino charge Q_ν, permits one to attack and to solve the neutrino oscillation problem.

10. Conclusion

Basing on the dark matter hypothesis, the neutrino oscillation problem is attacked. The solution of this problem is given due to the conservation laws of the lepton and of the neutrino charges.

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Гипотеза о тёмной материи и новые возможности киральной модели Скирма–Фаддеева

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Аннотация. Обсуждаются новые возможности 16-спинорной реализации киральной модели Скирма–Фаддеева. Используя принцип калибровочной инвариантности, показывается, что есть два независимых способа нарушения изотопической симметрии. Первый способ состоит в том, чтобы включить взаимодействие с электромагнитным полем (обыкновенными фотонами, порождаемыми электрическим зарядом), а второй опирается на взаимодействие с новым векторным полем (теневыми/тёмными фотонами, порождаемыми специальным нейтринным зарядом). Объясняется явление нейтринных осцилляций.

Ключевые слова: киральная модель, 16-спинорное поле, теневые/тёмные фотоны, нейтринный заряд

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Research of hieroglyphic signs using audiovisual digital analysis methods

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Abstract. A study of ancient written texts and signs showed that the hieroglyphs and structure of the archaic sentence have much in common with the modern Chinese language. In the context of the history and evolution of the Chinese language, its characteristic tonality and melody are emphasized. The main focus of the work is on the study of the sound properties of hieroglyphs (keys / Chinese radicals) found simultaneously in ancient inscriptions as well as in modern text messages. The article uses modern digital methods of sound analysis with their simultaneous visualization. To characterize the sound of hieroglyphs (in accordance with the Pinyin phonetic transcription adopted in China), two (FI, FII), three (FI, FII, FIII) or four (FS, FI, FII, FIII) formants are used, which create a characteristic F-pattern. Our proposed model of four formants for typical hieroglyphs is called the basic one "F-model", it's new and original. To visualize the formants, digital audio signal processing programs were used. The data obtained were compared with the corresponding spectrograms for Mandarin (standard) Chinese. Their correspondence to each other has been established. When analyzing F-patterns, an original model was used, which made it possible to characterize spectrograms in the frequency and time domains. The formalized description of basic components of basic "F-model" of a pronunciation of hieroglyphs is given. In conclusion, several areas are noted in which the use of various methods of audiovisual research is promising: advanced innovative technologies (artificial intelligence and virtual reality); television, theatrical video production; evaluation of the quality of audiovisual content; educational process. The present study has shown that described promising research methods can be useful in analyzing similar ancient hieroglyphs.

Key words and phrases: speech analyzing, Chinese hieroglyphs, spectrogram, formants, subharmonics, basic "F-model", linguistics, data processing, computer modeling

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1. Introduction

Sound waves are an example of an oscillatory process. The simplest sound wave is a periodic (i.e., the amplitude values are repeated at regular intervals) oscillation described by a sinusoid. The sound is characterized by a number of parameters (see e.g. [1, 2]). The human vocal cords produce complex sounds. The presence of complex vibration movements, which form both the main tone and overtones, is one of the reasons for the appearance of complex sounds [2].

The history of the Chinese language has more than three thousand years [3–7]. The Chinese language, the Chinese (Sinitic) family, is a language branch that includes language and dialect groups united by a common script. In its standard form, Chinese is the official language of the PRC and Taiwan, and one of the six official and working languages of the United Nations. Modern Chinese language Putonghua was created artificially in the middle of the 20th century. It is based on the vocabulary and grammar of "Mandarin" (Mandarin Chinese or Northern Chinese) and Beijing dialect is the source for pronunciation, i.e. Putonghua phonetics and vocabulary is based on the pronunciation norm of the Beijing dialect, which belongs to the northern group of dialects of Chinese language [4–9].

The modern Chinese language Putonghua (普通话) is tonal, that is, each syllable that has an accent is pronounced in one tone or another [7–9]. Since the meaning of the word depends on the tone of the sound, new words must be learned along with the tones. There are four tones in Mandarin (the fifth tone is conditional and has no special voice coloring): the first tone is high, even, its melody gives the impression of an unfinished statement; the second tone is an average ascending one, it gives the impression of a second question; the third tone is descending-ascending, gives the impression of a bewildered question; the fourth tone is a high descending one, giving the impression of a categorical command.

2. Materials and Methods

Recall that sound is a mechanical vibration that propagates in the form of elastic waves in various media (gaseous, solid or liquid) [1, 2, 10, 11]. In a narrower sense, sound refers to mechanical vibrations perceived by the senses, in particular the ear (see the Appendix for more details). Among the audible sounds, phonetic sounds, speech sounds, phonemes (which make up speech) and musical sounds (which make up music) are distinguished [10–13].

Sounds can be divided into *tones (simple, complex), noises* and *sonic booms*. A *simple (pure) tone* is a sound that has only one frequency f; it is described by a harmonic oscillation. *The acoustic spectrum* $A(f)$ *of a tone* is the totality of all its frequencies f with an indication of their amplitudes A or intensities $I = |A|^2$. *The main tone* corresponds to the largest amplitude of the spectrum $A(f)$. It is this tone that is perceived by the ear as the *pitch of the sound*. Overtones create the "color" of the sound. Sounds of the same pitch, created by different instruments, are perceived differently by the ear precisely because of the different ratio between the amplitudes of the overtones. *A complex tone* is a sound that contains several frequencies; it is described by a non-harmonic oscillation.

Musical sounds are an example of a complex tone; they contain not one, but several tones, and sometimes noise components in a wide range of frequencies. The acoustic spectrum $A(f)$ of a complex tone is lined; it contains a set of multiple frequencies f [1, 10]. *Noise* is a set of randomly (randomly) changing complex tones of any frequency. The noise spectrum is continuous. *A sonic boom* is a brief sonic impact, such as a bang.

The line spectrum $A(f)$ in the form of a set of individual harmonic components with multiple frequencies f is inherent in musical sounds. In this case, the fundamental frequency determines the pitch of the sound perceived by the ear, and the set of harmonic components determines the timbre of the sound. We also note that there are so-called *formants* in the sound spectrum $A(f)$; the *formants* are stable groups of frequency f components corresponding to certain phonetic elements [10–12]. Formant denotes a certain frequency region in which, due to resonance [1, 14], a certain number of harmonics of the tone produced by the vocal cords are amplified [11–14].

In the sound spectrum $A(f)$, the formant is a fairly distinct region of enhanced frequencies. Formants are denoted by the letter "F". Four formants are usually distinguished to characterize speech sounds (FI, FII, FIII, FIV), which are numbered in ascending order of their frequency: the formant with the lowest frequency is FI, then FII, etc. [2, 10–14]. Formant frequencies are denoted as follows: f_0, f_1, f_2, f_3, f_4 (sometimes use capital letters and start numbering with "1"). For different speech sounds, certain frequency ranges of formants are characteristic. The set of formant values is called the F-picture. Usually, the first two formants are sufficient to distinguish between vowels, but the number of formants in the sound spectrum is always more than two. This indicates more complex relationships between articulation and the acoustic characteristics of sound than if only formants were taken into account: FI, FII. Formants are visualized using spectrograms obtained using digital audio signal processing programs [2, 10, 11, 15].

The formant structure of a particular sound is determined by the characteristics of the formants, i.e. those areas of energy concentration in the acoustic spectrum that are associated with the characteristics of articulation and are necessary for the correct identification of a given sound. The number of formants essential for characterizing speech sounds is defined in different ways. The most common point of view is that four formants are sufficient to characterize the sound, while the first and second formants (FI, FII) are more important than the third and fourth (FIII, FIV).

Two classical theories explain the formation of formants as follows [10]. According to the first theory (Krantzenstein, Helmholtz), the characteristic timbre of a vowel is formed due to the amplification in the supraglottic cavities of one or several harmonic overtones, which arise together with the fundamental tone of the voice in the larynx as a result of complex vibrations of the vocal cords. Due to the vibrations of the vocal cords in the larynx, the fundamental tone of the voice arises together with harmonic overtones. In this case, the supraglottic cavities act as resonators in which amplification of certain overtones occurs, which determines the timbre of the vowel.

The second theory (Hermann) explains the formation of vowel formants as a result of the superposition of the proper tone of the supraglottic cavities, which arises from blowing a stream of air through them, onto the fundamental tone coming from the larynx. Here the formants arise in the oral cavity and are not in a harmonic relationship to the fundamental tone of the voice.

It is important to emphasize the recognition by both theories of the fact that vowel formants are determined by the position of the organs of pronunciation in the supraglottic cavities, and not in the larynx. In this sense, the two theories do not contradict each other.

Earlier in our works, we proposed a number of original approaches for the study of ancient hieroglyphs [8, 9, 16]. In particular, a comparison was made of typical hieroglyphs (keys or Chinese radicals) from modern text messages with hieroglyphs on typical Jiaguwen (Jiǎgǔwén / 甲骨文 are inscriptions on tortoise shells and fortune-telling bones that date back to the 14th–11th centuries BC) and Jinwen (Jīnwén / 金文 are ancient inscriptions on bronze vessels, around the 2nd-1st millennium BC) [3–9, 16, 17]. As a result, matching hieroglyphs and keys were found. An analysis of the most ancient written signs and texts showed that both the hieroglyphs themselves and the structure of the archaic sentence have much in common with the sentence structure of the modern Chinese language. In sum, through the prism of the modification of writing, the historical link between the past and the present day of Chinese civilization was presented.

The articles [9, 16] explored a number of typical hieroglyphs (keys / graphemes / Chinese radicals), such as, 土 (tu) earth, soil; 天 (tian) sky; 卜 (bu) fortuneteller, guess, divination; 册 (ce) letter, message, writing boards; 京 (jing) capital; 宫 (gong) castle; 家 (jia) home, family; 立 (li) stand; 交 (jiao) exchange, transfer, give; and so on. We emphasize that the research methods described in these works are also applicable to other hieroglyphs.

The article [9] examined the history and evolution of the Chinese language. We considered it right to talk about the written language of the Chinese language as the main link between the ancient

Chinese, Middle Chinese and modern Chinese languages. To study the hieroglyphic inscriptions on the ancient Jiaguwen and Jinwen artifacts, some typical hieroglyphs from text messages were compared with hieroglyphs depicted on a bone and a copper vessel. In that order 14 and 16 ancient symbols (hieroglyphs / Chinese radicals) were identified, which are also found in modern texts. At the same time, the possibility of developing methodological foundations for the selection of quantitative criteria is shown, which can be a good addition to traditional methods of studying prehistoric artifacts.

For a comprehensive perspective study, it is also of great interest to study the sound properties of hieroglyphs [18–20], for example, those present on typical samples of Jiaguwen and Jinwen described in our previous works (see [9, 16]). Various models can be used to study the sound spectrum, in particular, models of the following oscillations: a string, a thin plate, a pendulum, a plate in a resonator (see, for example, [1, 2, 10, 11, 13, 14]).

The object of research is the most ancient hieroglyphs (Chinese radicals) included in the hieroglyphic inscriptions on ancient artifacts. At the same time, the main goal (subject of research) is the study of the sound characteristics and parameters of hieroglyphs, i.e. features of their pronunciation, taking into account the syllabic structure (initials and finals) [3, 11–14]. In the future, for simplicity, we will talk about the pronunciation of hieroglyphs (in accordance with the phonetic transcription of Pinyin adopted in China). Note that the pronunciation of hieroglyphs in antiquity (more than 3000 years ago) is not known (see Appendix), so their modern sounding was studied in the work. The main criterion for the selection of hieroglyphs is the simultaneous presence, both in ancient inscriptions and in modern messages.

In our work, to study the characteristics and parameters of the pronunciation of hieroglyphs, we used methods and programs that are used in phonetics for the spectral analysis of sounds with their simultaneous visualization [15]. This eventually made it possible to identify formants in the sound spectrum. Formants are visualized using spectrograms obtained using specialized instruments or computer programs (e.g. “Spectrum Lab”, “TrueRTA (Real Time Audio Spectrum Analyzer)” for Windows) for digital processing of audio signals. These programs are essentially digital appliances capable of replacing specialized instruments as an audio spectrum analyzer. For this purpose, it is possible to use: computer, laptop, tablet or smartphone. The spectrum analyzer shows in real time the frequency spectrum of the analyzed sounds, which can be both audible and inaudible. As a result, the screen shows a spectrogram of the sound of the studied character in a fairly wide frequency range (usually from about 1 to 8000 Hz; there are also applications that have twice the frequency range).

Recall that *visualization* (from Latin *visualis*) is the creation of conditions for visual observation. In a general sense, this is a method of presenting information in the form of an optical image. *Sound visualization* includes methods for obtaining a visible picture of the distribution of certain quantities that characterize the sound (sound field).

The *notation (sheet music)* should also be noted, that is a traditional centuries-old way of visualizing music (musical sounds). This is a very harmonious and concise system, clear and symbolic. Musical notation uses a system of musical clefs and different ways of showing tones and their pitches. From this point of view, there is an analogy of music with the Chinese language.

We have analyzed several models that allow us to explain to a greater or lesser extent the results observed in the experiments. In particular, we revealed the possibility of using some equivalent simplified mathematical models (systems) that allow us to describe the corresponding processes. Within the framework of these different types of resonance phenomena and factors influencing them were also considered within the framework of these models. The conducted analysis has shown that there is a possibility to choose different fundamental frequencies (tones) of oscillations of the investigated equivalent systems. At this stage of research we have chosen as a basic model in which the observed speech spectrum is determined both by the complex oscillations of the vocal cords in the larynx and by the position of the pronunciation organs in the supraglottic cavities.

3. Results and discussion

To demonstrate the capabilities of the research method described in this article from previously studied hieroglyphic signs [8, 9, 16] as an example, the following three hieroglyphs (Chinese radicals) were chosen: 家 "home, family"; 立 "stand" and 交 "exchange, transfer, give". It can be noted that many hieroglyphs carry a certain historical context and symbolism that is still understood. For example, the upper part of the character house 家 means a roof, and the lower part means a pig. In ancient China, a pig under a roof (that is, in a house) was a sign of the wealth and success of a given family or clan.

To describe the spectrograms $A(f)$ of the pronunciation of hieroglyphs (keys / Chinese radicals), the pendulum model was used in the work (for more details, see the Appendix). This model is considered to be simplified, but it allows one to describe and study the spectra of sound vibrations, i.e. the resulting spectrograms $A(f)$ of the pronunciation of hieroglyphs [18–20]. We will consider the oscillation frequencies f found using the pendulum model as some parameters that allow us to characterize the pronunciation of hieroglyphs (see Appendix).

To receive digital audio files, pronunciation of hieroglyphs 家, 立 and 交 several sources were used, in particular: 1) audio files from open sources (see, for example, [18–20]); 2) digital software application "Trainchinese"; 3) professional Chinese translator. This article presents only the latest spectrograms; however, other sources were also used in the analysis of the obtained data. Fig. 1 shows successively some of the obtained sound spectra $A(f)$ (dependence of the amplitude A of sound vibrations on frequency f, i.e. spectrograms) of three studied hieroglyphs. Let's compare the found frequencies of model vibrations (see Appendix) with the spectrograms of the pronunciation of hieroglyphs corresponding to the selected hieroglyphs: 家 "home, family", 立 "stand" and 交 "exchange, transfer, give".

Recall that a spectrogram $A(f)$ is a visual representation of the frequency spectrum of a signal that changes with time t or frequency f [1, 2, 10, 11, 13]. When applied to an audio signal, spectrograms are sometimes referred to as sonographs, voice prints, or voice charts. Spectrograms are widely used, for example, in such areas as music, linguistics, speech processing, sonar, seismology, and others.

Any process (oscillation) $A(t)$ that is non-periodic in time can be represented as an infinite sum (the integral is taken over infinite limits) of oscillatory processes (oscillations) periodic in time:

$$A(t) = \frac{1}{2\pi} \int A(\omega) \exp(i\omega t) d\omega, \tag{1}$$

where $\pi \approx 3.14$; $A(\omega)$ (or $A(f)$) is the spectrum (spectrogram) or spectral amplitude density, $A(f)$ is the acoustic characteristic; in the quasi linear approximation $A(f) = E(f)K(f)$, where $E(f)$ is an input acoustic signal (its spectral amplitude density), and $K(f)$ is the transmission coefficient of the vocal tract (acoustic characteristic of a filtering process); $\omega = 2\pi f$ is the angular frequency of process (oscillation), f is the frequency measured in hertz (Hz). The expression (1) is usually called the Fourier integral of the oscillatory process. In practical applications, expansion $A(t)$ into a finite series (the sum of a finite number $M \ll \infty$ of harmonics) is used:

$$A(t) = A_0 + \sum_{m=1}^{M} A_M \cos(\omega m t) + B_m \sin(\omega m t), \tag{2}$$

where A_0, A_m and B_m are well known Fourier coefficients.

A spectrogram (see Eq. (1)) can be obtained using: a spectrometer, a band pass filter, a Fourier transform, or a wavelet transform (see e.g., [1, 2, 10–12]). The most common way to represent a spectrogram is a graph with two dimensions: one axis (horizontal) represents frequency f (or time t) and the other axis (vertical) represents the amplitude A of the sound for a particular time or frequency value (see Fig. 1). As a result, a spectrogram $A(f)$ of sounds is visible on the display screen. The spectrograms $A(f)$ of the sounds of the three hieroglyphs under study in the frequency f range from around 1 to 2000 Hz are shown in Fig. 1 (the vertical axis is the normalized level (loudness) of the sound A, and the horizontal axis is the frequency f in Hz).

A comparative analysis of the obtained data showed that in the initial interval (approximately from 1 up 800 Hz) all spectrograms $A(f)$ contain sufficiently intense low frequencies f, which contain a range from the fundamental frequency to a certain boundary value of about 1–5 Hz and which naturally have a low-pitched sound. The *fundamental tone* in our simple (basic) model has a *fundamental frequency* f_0 about 100 Hz, and the overtone frequencies are multiples of the fundamental tone (see the Appendix for more details). Moreover, in all spectra $A(f)$ there is a section in the frequency f range from around 1 Hz up about 25–30 Hz with characteristic maxima in the vicinity of about 10–20 Hz. Any oscillatory processes are accompanied by the generation of infrasonic waves. The most important source of infrasound for us is the process of speech production. This is precisely what spectrograms demonstrate.

As can be seen from the spectrograms $A(f)$, individual characteristic discrete components stand out against the background of continuous sound spectra (the line part of the spectrum). Vibrations that have a line spectrum give the impression of a sound with a more or less defined pitch. Such a sound is called *tonal*. On the spectrograms of the pronunciation of hieroglyphs, line spectral components stand out; this indicates the tonality of sounds.

The *pitch* of the tonal sound is determined by the fundamental (lowest) frequency. Oscillations with frequencies f that are multiples of fundamental frequency f_0 are *overtones*. The ratio of the intensities of the main tone and overtones determine the *timbre of the sound*; give sound a certain "color". The phases of harmonics do not affect the timbre of the sound. In the absence of overtones, a tonal sound is called a *pure tone*. A pure tone is given by tuning forks, which are used when tuning musical instruments.

In the study, one should also take into account that in the process of the formation of one Chinese language, there were many different dialects, where the same hieroglyph could be pronounced differently. This fact allows speaking about the possibility of using some extensive discrete set of sounds (quasi-continuum, i.e. a sufficiently large but finite set of close but not identical pronunciations) for each specific character (see comparison with Standard Chinese in Appendix).

The spectrogram $A(f)$ of the hieroglyph 家 is shown in Fig. 1(a). A study of the spectrogram $A(f)$ of this hieroglyphic sign showed that it contains at least 6 overtones corresponding to the fundamental frequency f_0. We emphasize that in the spectrogram $A(f)$ of the pronunciation of the hieroglyph "home, family" there are three characteristic local maxima in the vicinity of frequencies f about 300, 600 and 1000 Hz. The main audible frequency f (about 15–20 Hz) determines the audible pitch of the hieroglyph 家, and the set of harmonic components is the timbre of this sound.

The spectrograms $A(f)$ of other hieroglyphs 立 and 交 (see Fig. 1) reveal similar features. Note that the maximum in the vicinity of 300 Hz is the main one in the spectrum; the amplitude $A(f)$ of the sound wave in the vicinity of this frequency f is greater than all other amplitudes of sound waves in the spectrogram of the hieroglyph "stand" 立.

At this stage of research, it is possible to propose as the simplest sound model for these hieroglyphic characters the basic model of hieroglyphic pronunciation, in which the spectrum $A(f)$ is limited from above by a frequency f, for example, close to 1200 Hz. Then their spectrograms $A(f)$ in the range from about 1 up 1200 Hz will have 3 spectral components f (formants F), which are overtones for the

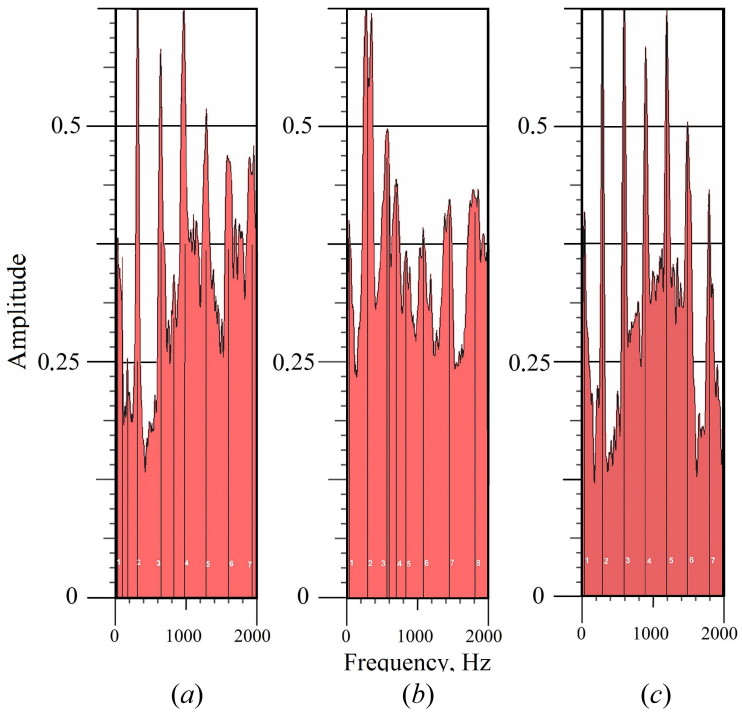

Figure 1. Spectrograms $A(f)$ of the pronunciation of hieroglyphs in the range from 0 to 2000 Hz: (a) 家; (b) 立; (c) 交

fundamental frequency $f \approx 100$ Hz and one ($f \approx 10$ or $f \approx 30$ Hz) that corresponds to the inverse bifurcation. These low frequency components correspond to sub harmonics of the following type: $f_0/10$ or $f_0/3$. It should be noted that the last two cases correspond to an increase in the oscillation period by 10 and 3 times, respectively. Since the oscillation period depends directly proportionally on the resonator size [1, 14], we can conclude that the (effective) resonator size increases dynamically during pronunciation. In simple terms, we can assume that the fundamental tone of the voice (along with harmonic overtones) arises in the larynx due to the oscillations of the vocal cords, and then in the supraglottic cavities, which increase the size of the effective resonator, some overtones are amplified. As can be seen from Fig. 1, discrete harmonic components are observed in the spectra against the background of continuous spectral bands. This indicates the presence of quasi-harmonic and non-periodic (noise) components in the original spectrum. It can be seen that subharmonics near the fundamental frequency have the highest intensity. It can be assumed that the appearance of non-periodic oscillations of different components of the speech tract up to a certain point contributes to the generation of subharmonic components. A more detailed analysis of the phenomenon of the appearance of subharmonics will be considered in one of the subsequent works.

We will name this simple model including overtones and subharmonics a fundamental (basic) "F-model" of the pronunciation of hieroglyphs in accordance with the phonetic transcription of Pinyin adopted in China. Taking a subharmonic component into account highlights the difference between our model and others, and also demonstrates the novelty of our scientific approach and its relevance.

Within the framework of this model, the hieroglyphic signs under consideration will have the following four bands containing four main approximate frequency maxima in spectrograms $A(f)$

(Hz): 1) 家 “home, family”: 10, 300, 600, 1000; 2) 立 “stand”: 30, 300, 600, 1000; 3) 交 “exchange, transfer, give”: 30, 300, 600, 900 (or more exactly: a frequency band near 850–1050 Hz). At this stage, the possibility of distinguishing sounds will remain if they are synthesized from these frequencies within the framework of this model. Indeed, a sequential comparison of two of the three spectrograms $A(f)$ shows that there is at least one non-coinciding spectral component, which will make it possible to distinguish these sounds.

This analysis suggests that the model vibration frequencies found by us can correspond to at least some (low-frequency) part in the spectrograms $A(f)$ of the original (dialect) sounds of the 3 studied hieroglyphs: 家, 立 and 交. At the same time, a correspondence was found between the overtones of the found frequencies of the model oscillations and some parts of the spectrograms of these hieroglyphs.

Using the methods of harmonic analysis, the spectra $A(f)$ were numerically synthesized, which made it possible to approximately describe the found values of the formants of the studied hieroglyphs. To do this, we used the values of the fundamental frequency of about 100 Hz and its overtones and subharmonics in the frequency range from about 10 to 1200 Hz. The study took into account that the spectrograms of the corresponding hieroglyphic signs 家, 立 and 交 in a given range have accordingly 4 spectral frequency components f (Hz): 10 (or more precisely: a band around 5–20 Hz), 300, 600, 1000; 30, 300, 600, 1000; 30, 300, 600, 900. To control the accuracy, audiograms in the time domain were also used dynamic spectrograms $A(t)$ (see Appendix). In particular, the time taken for the decrease in the volume of experimental and calculated sounds to zero was taken into account. In this parameter, the experimental and calculated data are in good agreement with each other.

In the future, this procedure can be extended, for example, to a frequency of 2000 Hz or more. However, it is clear that the expansion of the spectral range will complicate the solution of this problem. For a more accurate synthesis of model spectra $A(f)$, in addition to the main harmonics (tones), one can add a certain set of auxiliary spectral components such as overtones and subharmonics or noise-like sound components (we will speak next only about spectral components without distinguishing between them). It should be noted that such signals are approximate models of the studied sounds.

So, at this stage, some basic principles for constructing formant models for the hieroglyphic signs “home, family”, “stand” and “exchange, transfer, give” in the selected frequency range are formulated. Such a construction can be based, for example, on the principle of specifying a certain frequency range in the studied spectrograms, taking into account the presence of certain spectral components in them. At this point, one should rely on the form of the original acoustic spectrograms.

We have shown that these three groups of frequencies f (spectral components 10, 300, 600, 1000; 30, 300, 600, 1000; 30, 300, 600, 900 Hz) can be considered as some formants F of the first (basic) model of the pronunciation of the hieroglyphs “house, family”, “stand” and “exchange, transfer, give” in the frequency range from about 10 to 1200 Hz. These stable groups of frequency components correspond to a simple model of phonetic sounds for given hieroglyphs: 家, 立 и 交. As a result we can construct a simplified basic pronunciation “F-model”, containing two FI, FII or four formants FS, FI, FII, FIII (FS denotes a subharmonic formant). We will call this model a basic “F-model” of the pronunciation of hieroglyphs in accordance with the phonetic transcription of Pinyin adopted in China. A further simplification of this model is to use the concept of resonant bands (spectral bands concentrated near resonant frequencies) and their weight contribution to the spectrum, taking into account their amplitude. As can be seen from Fig. 1, from this point of view the components below 10 Hz can be neglected at the initial analysis. Therefore in this case our simplified pronunciation “F-model” can include: 1) two formants (FI, FII), contained in frequency bands around approximately 300, and 600 Hz respectively; 2) or four formants (FS, FI, FII, FIII): 20 (average for two subharmonics; there formant is denoted as “FS”), 300, 600, and 1000 Hz.

The data obtained by us were compared with the spectrograms of the pronunciation of hieroglyphs in Mandarin (standard) dialect of the Chinese language [18–20]. It is established that they correspond to each other. In addition, our results were compared with some data from the paper [11].

The results obtained by us testify to the correctness of the assumptions made and chosen research methods, which made it possible to propose formant models for hieroglyphs that are found simultaneously in ancient inscriptions and in modern texts. So an idea was obtained not only about the place and role of formants in the spectrograms of the Chinese language, but also about their certain universality.

Within the framework of the described model, it is possible to create a library of basic pronunciations of hieroglyphs for a typical 100-character key table of Chinese characters (an example of some conditional analogy with a 100-word Swadesh list). Such a music library will be useful, for example, for automatic preliminary recognition of digitized spectrograms of the pronunciation of hieroglyphs depicted on artifacts. Experts can work at the next stage, carrying out a qualified systematization of the studied ancient hieroglyphic inscriptions.

In conclusion, it is worth noting several areas in which various methods of audiovisual research are used, demonstrating their purpose, features, capabilities and differences (see, for example, [15, 21, 22]). The growing interest in this area is partly due to the recently actively developing trend of visualization of various Internet resources, as well as the increasingly widespread use of advanced innovative technologies (Artificial Intelligence (AI) and Virtual Reality (VR)). Due to the large number of publications on these topics, we will consider only three works as examples [15, 21, 22] (see the list of references for this article, as well as the literature cited in these publications [15, 21, 22]).

One of these areas is related to television [15]. Here, audiovisual analysis aims primarily at understanding the ways in which a sequence (or an entire film) uses a combination of sound and image. At the same time, it is proposed to give answers to the questions: “What do I see?”, “What do I hear?” Audiovisual analysis must be word-based at its core and attempt to develop ways of classifying sound using new descriptive criteria. Thus, audiovisual analysis is considered in the work [15] as a descriptive analysis which should avoid any interpretation of a psychoanalytic, psychological, social or political nature. However, the interpretation can follow based on the results of the analysis done. An example of an approach to audiovisual analysis of images of water and waves is given. It is noted that the analysis is not interested in the symbolism of water and waves, but in the wave as a dynamic model [15]. From our point of view, this approach is a systems approach, when a complex phenomenon is studied as an integral system. A similar approach is quite applicable to theatrical video productions, as well as to traditional theater, Pantomime Theater, theater of facial expressions and gestures, and shadow play when sounds may be present in a minimal amount or absent altogether. In the latter case, the absence of sounds is replenished or supplemented by each viewer individually in accordance with his life experience, individual skills, education, knowledge of languages and cultural traditions.

The article [21] analyzes subjective experiments examining the relationship between audio and video quality measured separately and the overall quality of the audiovisual experience. At the same time, the paper provides a statistical analysis of this experiment within the framework of model approaches. From the analysis of the data obtained, we come to the conclusion that there is no obvious natural relationship between the accuracy of the multiplicative model and the authors’ conclusions as the dominant factor (sound quality or video quality) on the overall audiovisual quality. In the multiplicative model, people combine audio and video errors together using the multiplicative rule. And the true formula that describes the statistical data depends on the context and the test material in question. All of this indicates that audio quality and video quality are equally important to the overall audiovisual quality. In particular, one important factor that can affect audiovisual quality is noted: audiovisual synchronization errors (for example, lip synchronization).

The use of audiovisual analysis methods for the purpose of selecting and forming the necessary audiovisual content can be also promising in a variety of educational processes. The effective use of such an approach, for example, in the creation of audiovisual media presented as new perspective educational platforms, can contribute to the formation of the necessary professional competencies, for example, in the training of specialists in the field of journalism, public relations and advertising [22].

We presented in this paper a fundamental (basic) "F-model" of the pronunciation of hieroglyphs in accordance with the phonetic transcription of Pinyin adopted in China. This model includes overtones and subharmonics. Taking a subharmonic component into account highlights the difference between our model and others, and also demonstrates the novelty of our approach, its relevance and the prospect of its development in further studies.

Appendix

Let us give brief information about the sound (sound waves). Sound waves are an example of an oscillatory process [1, 2, 10]. The simplest sound wave is a periodic (i.e., the amplitude values are repeated at regular intervals) oscillation described by a sinusoid. The sound is characterized by a number of parameters. Here are some of these parameters: amplitude, intensity, wavelength, oscillation period, oscillation frequency. Only the last two parameters are important to us for research: the period of oscillations is the smallest time interval for the repetition of oscillations (time t is measured in seconds (s)); the oscillation frequency f is inversely proportional to the period T (the unit of frequency is Hertz (Hz)). The human ear perceives sound frequencies f in the range of approximately 15 up 20000 Hz. A more detailed description of sound waves is beyond the scope of the article (see details in [1, 2, 10, 11, 13, 21]).

Let us recall the model of an ideal pendulum. In this model, the load is suspended on a thread and performs harmonic oscillations about the equilibrium position (see below Eq. (4) and accompanying explanations). In this case, the deviation angle is small, the mass of the load is greater than the mass of the thread, and the length of the thread is greater than the dimensions of the load. The period of oscillation in this mathematical model can be found as:

$$T = 2\pi\sqrt{l/g}, \tag{3}$$

where l is the length of the pendulum; g is the gravity acceleration ($g \approx 10$ м/с^2); $T = 2\pi/\omega_0$, so $\omega_0 = \sqrt{g/l}$, $\omega_0 = 2\pi f_0$, f_0 is the own frequency of the system. The pendulum can be considered as a kind of mechanical resonator.

This model describes the vibrations of a tuning fork characterized by a pure tone. That model will be closer to the real system it describes, in which the oscillations are complex, if the action of some external driving force is introduced into it. This will result in more frequency components than just one fundamental tone. In our case, this may be due to some influence on the pendulum (located, for example, in a cavity resonator): pushing the swinging weight, changing the length of the thread. If the impact, for example, a light push on the load on the thread, is in time with the oscillations, then both the fundamental frequency of oscillations and the occurrence of some resonances in this system are possible [1, 2, 10, 14]. In the resulting overtones (or harmonics), the frequency is an integer number of times higher than the frequency of the fundamental tone, and the intensity is weaker, the higher the frequency. The human vocal cords make complex sounds. The presence of complex vibration movements, which form both the main tone and overtones, is one of the reasons for the emergence of complex sounds.

We will consider the pendulum as some simplified (basic F-model) that allows us to describe the main properties of the spectrograms of the pronunciation of hieroglyphs. Indeed, the oscillations are nearly harmonic only at very small angles. At large angles oscillations turn into anharmonic vibrations. As a result, oscillations with frequencies 2ω, 3ω , etc., appear where the fundamental frequency of the oscillator is ω. Moreover, the frequency ω deviates from the frequency ω_0 of the harmonic oscillations. As the first approximation, the frequency shift $\Delta\omega = \omega - \omega_0$ is proportional to the square of the oscillation amplitude: $\Delta\omega \propto A^2$. In a system of oscillators with different natural frequencies anharmonicity results in additional oscillations with combined frequencies and one can observe, for example, intermodulation and combination tones.

Consequently, we replace the complex movements of the human tongue in the process of pronunciation with simpler pendulum oscillations. We will call appropriate model like basic "F-model" of the pronunciation of hieroglyphs (in accordance with the phonetic transcription of Pinyin adopted in China). Obviously, this is a fairly simplified mathematical model of the pronunciation of hieroglyphs. However this model allows us to find the frequency of fundamental vibrations and frequencies of overtones, i.e. desired sound spectrum $A(\omega)$. And this allows finally explaining the identified features of F-pictures of hieroglyphs.

The tongue is one of the main articulators in the production of speech. For example, different vowels are pronounced by changing the pitch of the tongue and retracting it to change the resonant properties of the vocal tract. These resonant properties enhance certain harmonic frequencies (formants), which are different for each vowel, and attenuate other harmonics. Consonants are articulated by constricting the flow of air passing through the vocal tract. Then, many consonants have a narrowing between the tongue and some other part of the vocal tract.

The solution of such problems, even in the first approximation, encounters serious theoretical and computational difficulties. At the same time, studies of such systems are undoubtedly relevant and promising, since they make it possible to describe the behavior of a number of biological and social processes. We only note that the main problem is connected with the fact that there is no general theory of oscillations of strongly nonlinear systems. To study the model of a pendulum under the action of a quasi-periodic driving force, one can use, for example, a theory describing the interaction of two coupled (quasi-)linear oscillators. It is important to note that even in the absence of resonances; there is instability in the behavior of this system. If we introduce into the model some slight "jitter" of the axis of rotation of the pendulum (relative to the suspension point), then we can make the behavior of the system more stable. In non-resonant (rather far from resonance regions of the studied structure) and resonant (near resonance regions) cases, asymptotic stability is possible in such a system.

To illustrate, we can cite the case when the external driving force changes according to an (almost) harmonic law. Then the oscillations are described by the following second order differential equation:

$$\frac{d^2A}{dt^2} + 2\beta\frac{dA}{dt} + \omega_0^2 A = B_0\cos(\omega t), \tag{4}$$

where β is the damping coefficient, ω_0 is the own frequency of the system, B_0 is the amplitude of the driving force, ω is the frequency of the driving force.

The dependence of the amplitude A of forced oscillations on the frequency ω of the forcing force leads to the fact that at some frequency determined for a given system (4), the amplitude of oscillations reaches its maximum value.

The vibrating system is particularly responsive to the action of the forcing force at this frequency. This phenomenon is called *resonance*, and the corresponding frequency is called the *resonant frequency*. The value of the resonance frequency ω_r is equal to the value:

$$\omega_r = \left(\omega_0^2 - 2\beta^2\right)^{1/2}. \tag{5}$$

It follows from the obtained expression (5) that, in the absence of medium resistance, the amplitude of oscillations at resonance theoretically tends to infinity. According to (5), the resonance frequency at condition $\beta = 0$ coincides with the own frequency ω_0 of oscillations of the system. The dependence of the amplitude $A(\omega)$ of forced oscillations on the frequency of the forcing force (or on the frequency of oscillations) has a well-known form of resonance curves similar in shape to a Gaussian curve.

We emphasize that the smaller β is, the higher and to the right lies the maximum of the resonance curve. At large damping (when $2\beta^2 > \omega_0^2$) the expression for the resonance frequency becomes imaginary. This means that in this case resonance is not observed in the system. With increasing frequency, the amplitude of forced oscillations monotonically decreases, i.e., asymptotic stability is observed in the system.

Another type of influence on the system consists in the (almost) periodic change of some parameter of the system, for example, the length of the pendulum, in time with the oscillations. In this case, resonance is also possible, which is called *parametric resonance*. For this purpose, it is necessary, for example, to periodically change the length of the pendulum, increasing it at the moments when the pendulum is in extreme positions, and decreasing it at the moments when the pendulum is in the middle position. As a consequence, the pendulum will swing wildly. By controlling the moments of influence on the pendulum length, one can also provide asymptotic stability.

To reveal the effect of asymptotic stability in spectrograms, experimental frequency (amplitude-frequency) and dynamic (time) spectrograms were studied. As an example, one can see Fig. 2 (the vertical axis is the frequency f in Hz, and the horizontal axis is the time t in seconds). The growth of the sound amplitude in Fig. 2 is shown by the darkening of the spectrogram $A(f)$. For comparison, using harmonic analysis methods, the spectra $A(f)$ of sound signals (having three main spectral components f in the range from about 1 up 700 Hz), similar to the experimental ones, were numerically synthesized.

Then, using the inverse Fourier transform of the data of the amplitude-frequency spectra $A(f)$, the corresponding audiograms in the time domain were obtained: dynamic spectrograms $A(t)$. Their analysis showed that the asymptotic stability of the studied sounds is indeed observed, which manifests itself in the gradual decay of the amplitude $A(t)$ of the sound signals with time (see Fig. 3, where the vertical axis is the normalized amplitude of the sound, and the horizontal axis is the time in seconds). It can be seen that the decrease in the calculated amplitude occurs rather quickly, approximately in 0.2 s. This decay process in time can be described by the normalized exponential decreasing dependence with an attenuation coefficient about 50:

$$A(t) \propto A_0 \exp(-50t), \tag{6}$$

where A_0 is the initial value of the amplitude $A(t)$, e.g. for $t = 0$.

It is important to emphasize that the effect of the asymptotic stability of dynamic spectrograms $A(t)$ manifests itself not only in the temporal, but also in the energy localization of the corresponding sounds. This effect causes the volume of sounds to fade gradually over a period of approximately 0.02–0.05 s.

The effect mentioned above is based on both the actual short-term nature of the pronunciation of hieroglyphs (localization of the process in time) and the properties of the human vocal tract (localization of the process in space). Thus, in the characteristics (spectrograms) and parameters (formants, time intervals) of the pronunciation of hieroglyphs, their syllabic structure (initials and finals) was naturally reflected. From a theoretical point of view, this two-component "initial-final" structure can be described as the interaction of two connected oscillators, each of which is responsible for its own zone in the human cerebral cortex. In this case, one oscillator can be assigned a zone that causes excitation, and the second — a zone that causes inhibition. As a consequence, there

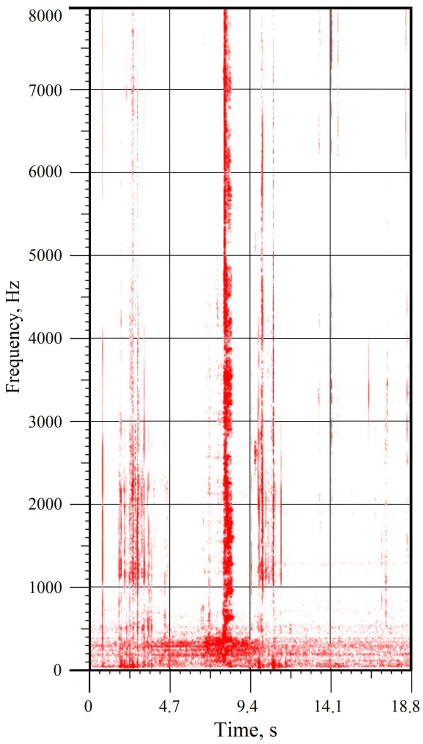

Figure 2. Dynamic spectrogram $A(t)$ of the hieroglyph "home, family" 家

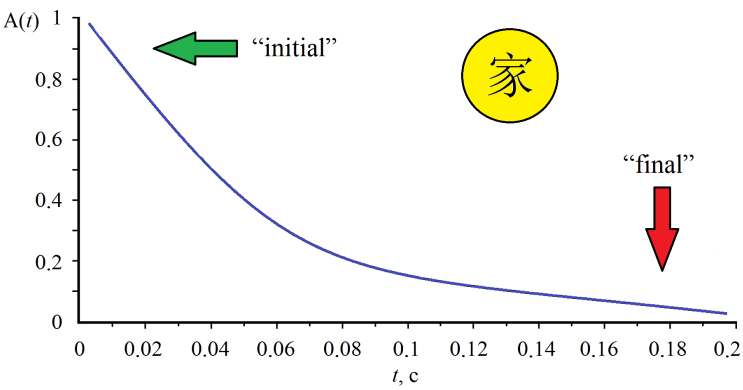

Figure 3. Estimated dynamic spectrogram $A(t)$ of the hieroglyph 家

is a certain balance of these processes and the final asymptotic stability, which is shown in Fig. 3. A more detailed analysis of this phenomenon is beyond the scope of this article (see e.g. [1, 2, 11, 13, 14]).

Note that the decrease in the calculated amplitudes for dynamic spectrograms $A(t)$ almost to zero occurs approximately in 0.2–0.7 s (see Eq. (6) and Fig. 3). Let us compare these data with the

experimental data shown in Fig. 2. Dynamic spectrogram $A(t)$ of the actual pronunciation of the hieroglyph 家 observed over a period of time from 7.7 to 8.2 seconds, i.e. about half a second and corresponds to the time predicted by calculations (similar data were also obtained for a number of other hieroglyphs). We emphasize that the darker region on the dynamic spectrogram $A(t)$ (see Fig. 3, center of the time interval approximately from 7.5 to 8.5 seconds in the frequency band from 1 to 8000 Hz) correspond to a greater sound volume (on Fig. 4 is an interval from approximately 0 to 0.1 s).

As a consequence, for the study of such complex systems, preference is given to approximate qualitative and numerical analysis. In this case, the possibility of reducing such quasi linear systems to simpler equivalent systems can be used. So we can replace the complex movements of different components of the human speech tract with simpler oscillations (see Eq. (3) and Eq. (4)). A more detailed description is beyond the scope of this article (see, for example, [1, 2, 10–14, 21]).

From Fig. 1 and Fig. 2 we can see the effects of the sound source (generator) (larynx and vocal cords) on the filtering system of the speech tract (pharynx, oral and nasal cavities). To separate the contributions of the sound source and the speech path, we can take for simplicity in expression (1) (or its corresponding Fourier image in the time domain) E as a delta function type, i.e., a unit pulse with spectral density equal for all frequencies of the speech path. Then the spectral density $A(f)$ of the acoustic signal at the output is equal to $K(f)$, i.e. the transmission coefficient of the speech path (reflecting the filtering property of the delta function).

In this case, the contribution of elements to the characterization of the speech path can be most simply described: $K(f) = k(f)K_1(f)K_2(f)K_3(f)K_4(f)$, where $k(f)$ is the correction factor, $K_{1-4}(f)$ are the resonant frequency responses (in general, complex-valued) of the corresponding formants FI–FIV. As a result we can propose a corresponding basic "F-model" for the pronunciation of hieroglyphs.

Under this assumption, we see in Fig. 1 the actual characteristic $K(f)$ of the speech path fully describing the F-pattern. In our simple base "F-model" the component corresponding to the fundamental frequency near 100 Hz characterizes the sound source (larynx and vocal cords). As a consequence, our base "F-model" describes in this approximation exactly F-patterns of the pronunciation of hieroglyphs. From Fig. 2 for the moment of pronunciation of the hieroglyph 家, observed during a period of time from 7.7 to 8.2 seconds, we can see the vertical profile of $A(f) \approx K(f)$ for any fixed moment in the specified time interval about 0.5 s. Further complication of the base "F-model" can be done in particular by taking into account the formant corresponding to the fundamental frequency.

Now we can give a brief description of our proposed model "F-model" of the studied phenomenon of the pronunciation of hieroglyphs. In addition, we will give some explanations to this model, allowing us to understand the essence of the key idea and its relationship to the phonetic transcription of Pinyin adopted in China. This is a rather simple mathematical model of the pronunciation of hieroglyphs. However this model allows us to find the frequency of fundamental vibrations and frequencies of overtones, i.e. desired sound spectrum $A(f)$ (and $K(f)$). This ultimately allows us to explain the recognized features of F-patterns of hieroglyphs. Using the inverse Fourier transform of the data of the amplitude-frequency spectra $A(f)$, the corresponding audiograms in the time domain can be obtained, i.e. dynamic spectrograms $A(t)$. In useful applications, expansion $A(t)$ into a finite series (the sum of a finite number of harmonics, see Eq. (2)) is used.

This model also includes an investigation of the temporal asymptotic stability of these sound characteristics of hieroglyphs, as it is one of the most important indicators of the phenomenon of the pronunciation of hieroglyphs under study. For this purpose, the study of dynamic dependence $A(t)$ is carried out; in particular, the type of a suitable function approximating the experimental one $A(t)$ under study is found. It is convenient to take an exponential damped function as the latter. The degree of its closeness to the dynamical dependence $A(t)$ under study can be estimated, for example,

in the mean-square metric (i.e. RMS error). In our case, the RMS error of approximation using functions of the form in Eq. (6) for a number of conducted experiments did not exceed 10–20%.

4. Conclusion

In summary, the construction of the base "F-model" boils down to obtaining the following 8 main components. 1) Images of studied hieroglyphs (Chinese radicals) and their digital files; all with detail descriptions. 2) Digital audio files of pronunciation of studied hieroglyphs. 3) Experimental sound spectrum $A(f)$ of the studied hieroglyphs and $K(f)$. Highlighting four basic formants in $A(f)$ (and $K(f)$). 4) Construction based on the experimental amplitude-frequency spectrum $A(f)$ a simplified basic "F-model" pronunciation of hieroglyphs under study, containing two, three or four formants (FI, FII; FI, FII, FIII; or FS, FI, FII, FIII, where FS denotes a subharmonic formant). We will call this models a basic "F-model" of the pronunciation of hieroglyphs in accordance with the phonetic transcription of Pinyin adopted in China. If the components below 300 Hz are neglected, a simplified pronunciation "F-model" will include only three formants FI, FII, FIII, contained in frequency bands around approximately 300, 600 and 1000 Hz respectively. 5) Computation of the inverse Fourier transform of the data of the amplitude-frequency spectra, i.e. dynamic spectrograms $A(t)$. 6) Study of temporal asymptotic stability of dynamic spectrograms $A(t)$ of the studied hieroglyphs. 7) Study of peculiarities of the pronunciation of hieroglyphs (localization of the process of pronunciation in time and localization of the process of the pronunciation in space), enabling the identification of the syllabic structure of hieroglyphs, i.e. initials and finals. Calculation of frequency and time localization parameters characterizing this two-component "initial-final" structure of the pronunciation of hieroglyphs. 8) Creation of a digital databank of the hieroglyphs under study within the framework of this basic "F-model". This databank should include the following elements in digital formats: images of studied hieroglyphs; audio and audio-visual files of pronunciation of studied hieroglyphs; $A(f)$ (and $K(f)$); formants FI, FII, FIII, FIV (or FS); formant frequencies f_{1-4}; $A(t)$; set of suitable functions like $\exp(-at)$ (a is a certain constant), approximating with the required accuracy the experimental data under study; set of localization parameters in frequency and time domain, characterizing two-component "initial-final" structure of the pronunciation of hieroglyphs. It is important to underline that there are no analogous models of the pronunciation of hieroglyphs presented and described in similar formalized and structured way in the scientific literature.

For an introduction to more complex models, including physical models, as well as studying speech production in different specific languages, which attempt to describe the features of a human speech, we recommend, for example, the following publications [23–28]. At the same time, we consider that our "F-model" can also be used in innovative technologies like AI and VR.

Recall that a periodic oscillation can be represented as a sum of harmonic oscillations. A real pendulum has complex oscillations, therefore, in addition to the fundamental tone; oscillations with a higher frequency are also formed. The frequency of these oscillations corresponds to the frequency of sound waves, the spectrum of which also contains frequencies that are multiples of the fundamental tone, i.e., exceeding it by a multiple number of times: 2, 3, 4, etc. (these numbers are the spectrum harmonic number M, see Eq. (2)).

A more detailed examination of the type of the calculated approximate dynamic spectrogram near zero showed that there is a section of increasing amplitude to the maximum shown in Fig. 3. Next, using the Fourier transform of the data of the dynamic spectrogram of hieroglyph 家, the corresponding amplitude-frequency spectra in the frequency domain were obtained (it looks like a Gaussian curve modulated by a damped cosine). Analysis of the obtained data demonstrated that the experimental subharmonic formants about 12 and 30 Hz are slightly less than calculated

model subharmonic formant values: 18 and 36 Hz. This indicates the need for further theoretical, computational and experimental study of the behavior of the audio spectrum in the frequency range below 300 Hz to understand the nature of this frequency shift, especially in the subharmonic region.

Preliminary we put forward a hypothesis that this frequency shift in a spectrum can be partly caused by a little change of a modern pronunciation of hieroglyphs in comparison with their most ancient sounding. This idea made it possible to explain partly and approximately the identified features of F-patterns of hieroglyphs. The essence of the hypothesis is that these features are associated with the process of historical formation of the Chinese people, the most important stage of which is the transition from a sedentary lifestyle to a more mobile, active lifestyle. Probably similar phenomena can be found in F-patterns of other people. To analyze the peculiarities of linguistic information $I(x)$ dissemination in a similar community, one can use, for example, such a mathematical nonlinear model: $I(x) = \lambda_1 x(1-x) + \lambda_2 x(1-x)^2$ (see e.g. [8, 9]). Parameters of this model: x is the independent variable (varies from 0 to 1); $\lambda_{1,2}$ are coefficients (or control parameters) of the analyzed model (see for more details [8]).

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Исследование иероглифов с помощью методов аудиовизуального цифрового анализа

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Аннотация. Проведённое исследование античных письменных текстов и знаков показало, что иероглифы и строение архаического предложения имеют много общего с современным китайским языком. В контексте истории и эволюции китайского языка подчёркнуты его характерные тональность и мелодичность. Основное внимание в работе уделено исследованию звуковых свойств иероглифов (ключей), встречающихся одновременно в древнейших надписях, а также в современных текстовых сообщениях. В статье использованы современные цифровые методы анализа звуков с одновременной их визуализацией. Для характеристики звучания иероглифов (в соответствии с принятой в Китае фонетической транскрипцией Пиньинь) использованы две (FI, FII), три (FI, FII, FIII) или четыре форманты (FS, FI, FII, FIII), которые создают характерную F-картину. Предложенная нами модель четырёх формант для типовых иероглифов (ключей) названа базовой «F-моделью», она является новой и оригинальной. Для визуализации формант применены программы цифровой обработки звуковых сигналов. Полученные данные сравнивались с соответствующими спектрограммами для мандаринского (стандартного) диалекта китайского языка. Установлено их соответствие друг другу. При анализе F-картин использовалась оригинальная модель, которая позволила охарактеризовать спектрограммы в частотной и временной областях. Дано формализованное описание основных компонентов базовой «F-модели» произношения иероглифов. В заключение отмечено несколько областей, в которых перспективно использование различных методов аудиовизуального исследования: передовые инновационные технологии (искусственный интеллект и виртуальная реальность); телевидение, театральное видеопроизводство; определение качества аудиовизуального контента; образовательный процесс. Проведённое исследование показало, что описанные перспективные методы исследования могут быть полезны при анализе подобных античных иероглифов.

Ключевые слова: анализ речи, китайские иероглифы, спектрограмма, форманты, субгармоники, базовая «F-модель», лингвистика, обработка данных, компьютерное моделирование

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Methods for developing and implementing large language models in healthcare: challenges and prospects in Russia

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Abstract. Large language models (LLMs) are transforming healthcare by enabling the analysis of clinical texts, supporting diagnostics, and facilitating decision-making. This systematic review examines the evolution of LLMs from recurrent neural networks (RNNs) to transformer-based and multimodal architectures (e.g., BioBERT, Med-PaLM), with a focus on their application in medical practice and challenges in Russia. Based on 40 peer-reviewed articles from Scopus, PubMed, and other reliable sources (2019–2025), LLMs demonstrate high performance (e.g., Med-PaLM: F1-score 0.88 for binary pneumonia classification on MIMIC-CXR; Flamingo-CXR: 77.7% preference for in/outpatient X-ray re-ports). However, limitations include data scarcity, interpretability challenges, and privacy concerns. An adaptation of the Mixture of Experts (MoE) architecture for rare disease diagnostics and automated radiology report generation achieved promising results on synthetic datasets. Challenges in Russia include limited annotated data and compliance with Federal Law No. 152-FZ. LLMs enhance clinical workflows by automating routine tasks, such as report generation and patient triage, with advanced models like KARGEN improving radiology report quality. Russia's focus on AI-driven healthcare aligns with global trends, yet linguistic and infrastructural barriers necessitate tailored solutions. Developing robust validation frameworks for LLMs will ensure their reliability in diverse clinical scenarios. Collaborative efforts with international AI research communities could accelerate Russia's adoption of advanced medical AI technologies, particularly in radiology automation. Prospects involve integrating LLMs with healthcare systems and developing specialized models for Russian medical contexts. This study provides a foundation for advancing AI-driven healthcare in Russia.

Key words and phrases: large language models, healthcare, deep learning, clinical text analysis, radiology report generation, interpretability, Russian healthcare

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1. Introduction

Artificial intelligence (AI) is reshaping healthcare by enhancing diagnostics, treatment planning, and medical data management. Large language models (LLMs), leveraging transformer architectures, have emerged as pivotal tools for processing clinical texts and multimodal data, achieving performance comparable to human experts (e.g., Med-PaLM: F1-score 0.88 on MIMIC-CXR for pneumonia classification) [1]. LLMs also support literature analysis, personalized medicine, and automated radiology report generation, with applications in oncology and chronic disease management [2, 3]. In Russia, AI adoption is supported by the National Strategy for AI Development until 2030, but challenges such as data scarcity and regulatory constraints hinder progress. LLMs are increasingly integrated with electronic health record (EHR) systems to provide real-time clinical insights, reducing diagnostic delays. Russia's National Strategy emphasizes data interoperability to support LLM deployment across regions, including for automated radiology reporting. Emerging applications, such as AI-driven epidemiology and radiology report generation, enable proactive disease surveillance and workflow efficiency, critical for public health and radiologist workload reduction. Partnerships with global tech leaders could enhance Russia's capacity to develop scalable AI healthcare solutions. This review analyzes the evolution, applications, limitations, and prospects of LLMs in healthcare, with a focus on adapting these technologies to Russian medical systems, particularly in radiology automation.

The paper is structured as follows: Section 2 outlines the methodology; Section 3 traces LLM evolution; Section 4 details healthcare applications; Section 5 addresses challenges; Section 6 discusses prospects; and Section 7 concludes with recommendations.

2. Methods

This systematic review, conducted between January and May 2025, analyzed 40 peer-reviewed articles from Scopus, PubMed, and other reliable sources (2019–2025) focusing on LLMs in healthcare, including automated radiology report generation. Inclusion criteria comprised articles with empirical data on LLM performance (e.g., F1-score, AUC, MCC) in medical tasks, with full-text access. Exclusion criteria included non-empirical reviews and duplicates. Keywords included "large language models," "healthcare," "deep learning," and "radiology report generation." Models were classified by architecture (e.g., transformers, MoE), application (e.g., diagnostics, radiology reporting), and performance metrics. Interpretability was assessed using SHAP (SHapley Additive exPlanations) adapted for medical data, with additional evaluation of RadGraph scores for radiology reports. A Mixture of Experts (MoE) model, implemented in TensorFlow 2.12, was tested on a synthetic dataset ($n = 500$, 10 rare pathology classes), achieving promising results for diagnostics and report generation. The review employed a mixed-methods approach, combining quantitative performance metrics with qualitative insights from clinician feedback. Synthetic datasets were generated to simulate Russian medical records, addressing data scarcity in model training. Cross-lingual validation ensured applicability to Russia's multilingual population. Standardized evaluation protocols, aligned with international benchmarks like MIMIC-CXR, were used to assess model generalizability. Results are presented in tables and discussed below.

3. Evolution of large language models

The development of LLMs has progressed through several stages, each addressing limitations of prior approaches and expanding applications in healthcare.

3.1. Early neural networks and RNNs

Natural language processing (NLP) began with multilayer perceptrons (MLPs) in the 1980s, limited by fixed input windows. Recurrent neural networks (RNNs) enabled sequential data processing but suffered from vanishing gradients, limiting their ability to capture long-range dependencies in medical texts (e.g., case histories). Early RNNs faced challenges in processing complex medical terminologies, limiting their utility in multilingual settings like Russia. Long short-term memory (LSTM) networks partially addressed vanishing gradient issues, but scalability remained a constraint. Pre-transformer models required extensive manual feature engineering, unsuitable for dynamic clinical environments. These limitations underscored the need for transformer-based architectures in modern healthcare AI, particularly for automated radiology reporting.

3.2. Transformer breakthrough

The transformer architecture revolutionized NLP by enabling parallel processing of text. BERT-based models, pre-trained on large corpora, improved performance in healthcare tasks. BioBERT, pre-trained on 18 billion PubMed words, attained an F1-score of 0.84 for named entity recognition (NER) of diseases and drugs [4]. ClinicalBERT, trained on MIMIC-III (2M records), achieved an AUC of 0.89 for readmission prediction [5]. Transformers' self-attention mechanisms enable efficient handling of large-scale clinical datasets, critical for Russia's diverse healthcare records. Pre-trained models like BioBERT reduce training time for domain-specific tasks, such as drug interaction prediction and radiology report generation. Fine-tuning on Russian medical guidelines could improve model relevance for local practices. Scalable transformer architectures support real-time clinical decision-making and report generation in high-pressure environments.

3.3. Specialized and multimodal models

Specialized models like Med-PaLM integrate text and images, achieving an F1-score of 0.88 for pneumonia classification on MIMIC-CXR [1]. Multimodal models, such as BLIP-2 and Flamingo-CXR, combine text and visual data, achieving an AUC of 0.92 for diabetic retinopathy detection and 77.7% preference for in/outpatient X-ray reports [6]. The Mixture of Experts (MoE) architecture dynamically selects submodels, improving performance on rare diseases and radiology report generation [7]. Emerging models process genomic sequences, predicting molecular properties with high accuracy [8]. Multimodal LLMs process heterogeneous data, such as clinical notes and imaging, enabling holistic patient assessments and automated radiology reporting. In Russia, integrating LLMs with regional EHR systems could standardize diagnostics and reporting across urban and rural facilities. Model compression techniques, like quantization, ensure deployment on low-resource devices, critical for remote clinics. Recent advances in temporal learning and knowledge-enhanced models like KARGEN enhance longitudinal imaging analysis and report quality, improving recurrence prediction in pediatric gliomas and chest X-ray reporting [9, 10].

4. Applications in healthcare

LLMs are applied across multiple healthcare domains, as summarized in the Table.

Application	Model	Dataset	F1-score	AUC	Source
Diagnostics	Med-PaLM	MIMIC-CXR	0.88	0.91	[1]
Diagnostics	Med-PaLM	CheXpert	0.85	0.88	[1]
Patient Care	ClinicalBERT	MIMIC-III	0.78	0.89	[5]
Literature Analysis	BioBART	PubMed	0.90	0.92	[11]
Drug Discovery	ChemBERTa	ChEMBL	0.85	0.87	[12]
Radiology Report Generation	Flamingo-CXR	MIMIC-CXR	0.80	0.85	[13]
Radiology Report Generation	KARGEN	IU-Xray	0.82	0.87	[10]
Radiology Report Generation	RaDialog	MIMIC-CXR	0.79	0.84	[14]
Diagnostics	CathEF	Angiograms	0.82	0.85	[9]
Literature Analysis	LLM (unspecified)	Medical Literature	0.87	0.90	[15]

4.1. Medical diagnostics

Large language models (LLMs) have advanced medical diagnostics by analyzing multimodal data, including clinical texts, medical imaging, and laboratory results. Med-PaLM achieved an F1-score of 0.88 for binary pneumonia classification on MIMIC-CXR (2M chest X-rays) and 0.85 on CheXpert (224,316 radiographs) [1]. Globally, LLMs like BioMedLM achieved an AUC of 0.90 for sepsis detection from EHRs [16]. AI-powered thermography analysis has shown promise in diagnosing heart failure with an AUC of 0.87 [17]. In Russia, LLMs are being adapted for diagnostics, but limited annotated data (5% of medical records) poses challenges [18]. Techniques like federated learning have improved performance for rare diseases, such as rheumatic autoimmune conditions [19, 20]. LLMs integrate patient histories with diagnostic imaging to enhance differential diagnosis accuracy, particularly for complex diseases like cancer. In Russia, aligning LLMs with EGIISZ (Unified State Healthcare Information System) could streamline data access for diagnostics. Techniques like zero-shot learning allow LLMs to generalize to rare conditions with limited training data. Continuous model retraining ensures adaptability to evolving clinical guidelines.

4.2. Patient care

LLMs enhance patient care by generating personalized treatment plans and supporting chronic disease management. ClinicalBERT, fine-tuned on MIMIC-III, achieved an AUC of 0.89 for predicting hospital readmissions [5]. Llama 2 supports patient-provider dialogues, achieving an F1-score of 0.83 for patient interactions [21]. In Russia, telemedicine platforms use LLMs to monitor chronic conditions, but linguistic diversity and inconsistent EHR formats limit performance [18]. Guidelines for medical professionals emphasize the need for training to integrate LLMs effectively [22]. LLMs support chronic disease management by predicting patient deterioration through longitudinal data analysis. In Russia, telemedicine platforms leveraging LLMs could improve care access in remote regions with limited specialists. Patient-facing AI systems must incorporate cultural and linguistic

nuances to ensure effective communication. Training clinicians to use LLM outputs enhances trust and adoption in clinical workflows.

4.3. Literature analysis

LLMs transform biomedical literature analysis by summarizing articles and identifying trends. BioBART processes 10,000 PubMed articles per minute, achieving an F1-score of 0.90 for oncology research trends [11]. SciBERT, fine-tuned on 1.14M scientific papers, achieved an F1-score of 0.87 for NER on CORD-19 [23]. Recent studies demonstrate LLMs assisting in literature searches for surgical approaches, achieving an F1-score of 0.87 [15]. In Russia, analyzing local literature (e.g., eLibrary) is limited by metadata inconsistencies [18]. Multimodal LLMs predict research trends with an AUC of 0.89 [24]. LLMs enable rapid synthesis of global and Russian medical literature, supporting evidence-based practice. Integration with eLibrary and Russian medical journals could address metadata inconsistencies, improving research accessibility. Automated summarization reduces literature review time, aiding clinicians in staying updated with advancements. Advanced LLMs can identify research gaps, guiding future studies in Russia's healthcare landscape.

4.4. Drug discovery

LLMs predict molecular properties and drug-target interactions. ChemBERTa, pre-trained on ChEMBL, achieved an F1-score of 0.85 for compound activity prediction [12]. AlphaFold enhances drug discovery by predicting protein-ligand interactions (AUC=0.90) [8]. GPT-3 identified drug candidates for COVID-19 with an F1-score of 0.88 [25]. AI-driven precision oncology leverages LLMs to select personalized treatments, improving outcomes in pediatric cancer care [3]. In Russia, data scarcity (10% digitized pharmacological data) limits LLM applications [18]. LLMs accelerate drug repurposing by predicting novel indications from existing compounds. In Russia, digitizing pharmacological databases could enhance LLM-driven drug discovery. Collaborative AI platforms enable integration of Russian research with global datasets, fostering innovation. Real-world evidence from clinical trials can refine LLM predictions for drug efficacy.

4.5. Radiology report generation

Automated radiology report generation using LLMs reduces radiologist workload and enhances report consistency, addressing the growing demand for imaging in healthcare [26, 27]. Models like Flamingo-CXR achieve an F1-score of 0.80 on MIMIC-CXR, with 77.7% of in/outpatient chest X-ray reports rated as preferable or equivalent to human reports by radiologists [28]. KARGEN, a knowledge-enhanced LLM, integrates disease-specific knowledge graphs to improve report quality, achieving an F1-score of 0.82 on IU-Xray [29]. RaDialog, a vision-language model, supports interactive report generation and clinician dialogue, with an F1-score of 0.79 on MIMIC-CXR, surpassing larger models like Med-PaLM in natural language generation metrics [30]. In Russia, integration with EGIISZ and DICOM-compatible systems could standardize reporting across facilities, but only 10% of radiology data is digitized, limiting model training [31]. Challenges include model hallucinations (10% of outputs) and the need for robust validation to ensure clinical accuracy [10, 13, 14, 32]. Techniques like retrieval-augmented generation (RAG) and fine-tuning on Russian medical datasets could mitigate errors and enhance report reliability [33]. On-premise models like Llama-2-70B ensure compliance with Federal Law No. 152-FZ, achieving an MCC of 0.75 for structured reporting in English and 0.66 in German [34]. Multimodal LLMs, combining imaging and clinical notes, prioritize critical findings, reducing diagnostic turnaround time and supporting rural clinics with limited resources.

5. Challenges and limitations

LLMs face challenges in data scarcity, interpretability, security, accuracy, and ethics, particularly in radiology report generation.

5.1. Data scarcity

Only 5% of Russian medical records are annotated, limiting supervised learning for diagnostics and radiology reporting [18]. Synthetic data generation (e.g., SynthMed) improves accuracy by 8% [26]. Crowdsourcing annotation is promising but faces terminology inconsistencies [18]. Russia's low digitization rate (10% of medical and radiology records) limits LLM training, necessitating innovative solutions like transfer learning. Generative adversarial networks (GANs) create synthetic datasets compliant with Russian data protection laws. Crowdsourcing platforms could engage medical students to annotate records, expanding datasets. Public-private partnerships are critical to fund large-scale digitization efforts for radiology data.

5.2. Interpretability in large language models

The adoption of large language models (LLMs) in radiology report generation has been met with both enthusiasm and caution. While LLMs have demonstrated remarkable capabilities in processing and generating natural language, their "black-box" nature—the opacity of their decision-making processes—poses a significant barrier to clinician trust [27]. This challenge is particularly acute in radiology, where accurate and timely diagnoses are critical, and misinterpretations can have severe consequences for patient outcomes. Clinicians, accustomed to understanding the rationale behind diagnostic decisions, find it difficult to rely on AI systems whose inner workings remain obscure. This lack of interpretability undermines confidence in automated reports, especially in high-stakes medical applications.

5.3. SHAP analysis and over-reliance on common symptoms

To address the interpretability challenge, researchers have employed methods like SHAP (SHapley Additive exPlanations), which attributes the output of a machine learning model to its input features [18]. In the context of LLMs for radiology report generation, SHAP analysis can reveal which parts of the input text or image the model prioritizes when generating its predictions. However, recent studies have highlighted a critical issue: LLMs may over-rely on common symptoms or frequently occurring phrases, potentially leading to inaccurate or biased reports [18]. For example, if an LLM is trained on a dataset where certain symptoms like "shortness of breath" are overrepresented, it might incorrectly associate those symptoms with a diagnosis like pneumonia, even when other, less common indicators — such as subtle imaging findings — are present. This over-reliance can result in reports that overlook critical nuances, such as rare conditions or atypical presentations, thereby compromising their accuracy and reliability.

5.3.1. Lightweight interpretability frameworks for real-time use

Given the time-sensitive nature of clinical workflows, interpretability methods must be computationally efficient to be viable in real-time applications [17, 28]. Traditional interpretability techniques, while insightful, often demand significant computational resources, making them impractical for use during patient consultations. Consequently, there is a pressing need for lightweight

interpretability frameworks that can provide meaningful explanations without introducing latency. These frameworks might involve approximations or simplifications of more complex methods, such as focusing on the most influential features or employing faster approximation algorithms instead of computing SHAP values for every input feature. The goal is to strike a balance between interpretability and computational efficiency, ensuring that clinicians can access explanations in real-time without disrupting their workflow.

5.3.2. Model calibration for trustworthy confidence scores

Beyond understanding how a model makes decisions, clinicians also need to gauge the model's confidence in its predictions. Model calibration ensures that the confidence scores output by the LLM accurately reflect the likelihood of correctness [28]. A well-calibrated model assigns high confidence to predictions that are likely accurate and lower confidence to uncertain ones. This is crucial for building trust, as clinicians can use these scores to decide when to rely on the AI's report and when to seek additional verification. Techniques for model calibration include temperature scaling or ensemble methods, which adjust the model's output probabilities to align more closely with actual outcomes. Without proper calibration, even interpretable models may mislead clinicians by presenting overconfident predictions, thereby eroding trust in AI-generated reports.

5.3.3. Explainable AI frameworks: attention heatmaps and beyond

Explainable AI (XAI) frameworks, such as attention heatmaps, offer visual representations of the model's focus areas, providing intuitive insights into its decision-making process. In radiology, attention heatmaps can highlight regions of an image or sections of text that the LLM deems most relevant for generating the report. For instance, in analyzing a chest X-ray, a heatmap might illuminate areas indicative of pneumonia, helping clinicians understand why the model suggested a particular diagnosis. By making the model's reasoning more transparent, these frameworks can significantly increase clinician confidence in automated reports. Other XAI methods, such as LIME (Local Interpretable Model-agnostic Explanations), can also be employed to generate local explanations for specific predictions, further enhancing interpretability.

5.3.4. Regulatory mandates in Russia: transparency and accountability

In regions like Russia, the adoption of AI in clinical settings may be subject to specific regulatory mandates aimed at ensuring transparency and accountability. While the exact nature of these mandates is not detailed, it is plausible that they would require AI systems to provide clear explanations for their outputs, particularly in high-stakes applications like radiology. Such regulations might stipulate that AI-generated reports include interpretability features—such as attention heatmaps or confidence scores—to facilitate clinician validation. Compliance with these mandates would be essential for the clinical approval and widespread adoption of LLMs in Russian healthcare systems, ensuring that AI tools meet stringent standards for safety and reliability.

5.3.5. Real-time interpretability tools for clinical validation

For interpretability to be truly useful in clinical practice, it must be accessible in real-time, allowing clinicians to validate LLM-generated reports during patient consultations. Real-time interpretability tools could take the form of interactive dashboards or integrated software modules within existing radiology information systems. These tools might display attention heatmaps, highlight key phrases

in the report, or provide natural language explanations of the model's reasoning. For example, a clinician reviewing an AI-generated report could click on a highlighted section to understand why the model emphasized certain findings. By enabling immediate validation, these tools can bridge the trust gap and facilitate the seamless integration of LLMs into routine clinical workflows.

5.3.6. Standardized metrics for interpretability: the role of RadGraph

To systematically evaluate and compare the interpretability of different LLMs in radiology, standardized metrics are essential. RadGraph, presumably a metric designed for assessing radiology reports, could provide a quantitative measure of how well the model's explanations align with expert interpretations or ground truth data. Standardization is crucial for benchmarking, as it allows researchers and developers to objectively assess improvements in interpretability over time and across different models. Furthermore, standardized metrics can inform regulatory bodies and healthcare providers about the reliability and transparency of AI systems, aiding in their evaluation and selection. Without such metrics, the assessment of interpretability remains subjective, hindering the development of best practices and the establishment of trust in AI-driven diagnostics.

The interpretability of LLMs in radiology report generation is a multifaceted challenge that requires a combination of technical innovations and regulatory considerations. By leveraging methods like SHAP analysis, lightweight interpretability frameworks, model calibration, and explainable AI techniques such as attention heatmaps, researchers can make significant strides toward demystifying the decision-making processes of LLMs. Additionally, real-time interpretability tools and standardized metrics like RadGraph are vital for ensuring that these advances translate into practical benefits for clinicians and patients. As regulatory mandates evolve, particularly in regions like Russia, the emphasis on transparent and accountable AI will only grow, underscoring the importance of continued research and development in this critical area.

5.4. Data security

Compliance with Federal Law No. 152-FZ is mandatory for Russian healthcare data, including radiology reports. Federated learning preserves 99.8% data privacy [19]. Differential privacy reduces risks but lowers accuracy by 5–10% [18]. Secure multi-party computation ensures LLM training on encrypted Russian medical and radiology data, aligning with Federal Law No. 152-FZ. Blockchain-based data sharing enhances transparency while protecting patient privacy. Russia's cybersecurity advancements support secure LLM deployment in national healthcare systems. Regular audits mitigate risks of data breaches in AI-driven radiology workflows.

5.5. Improving the accuracy and reliability of radiology reports using LLMs

Hallucinations, which are plausible but incorrect or meaningless outputs generated by large language models (LLMs), have a significant impact on their reliability, affecting approximately 10% of all outputs, including critical areas such as radiology reports. In radiology, such errors can lead to serious consequences, including incorrect diagnoses or inadequate treatment plans, emphasising the need to develop and apply effective strategies to address them. One approach is ensemble methods, which combine multiple models or variations of a single model to generate output, selecting the most consistent or highest confidence result. Research shows that such methods can improve accuracy by 5%, which is a marked improvement, especially when you consider that this could mean a reduction in errors in tens of thousands of reports each year when used on a mass scale.

To further validate LLM output data, regular auditing is applied using auxiliary classifiers. These classifiers are specifically designed to identify certain types of errors or inconsistencies, such as made-up anatomical details or inconsistencies in image descriptions. This approach allows hallucinations to be detected and corrected before reports enter clinical practice, which is particularly important in a high workload environment for radiologists. Another important technique is knowledge distillation, in which a smaller and more efficient model is trained to mimic the behaviour of a larger and more complex model. This not only reduces computational resource requirements, which is relevant for radiology departments with limited equipment, but also maintains or even improves accuracy, speeding up the report generation process without loss of quality.

In Russia, clinician-led validation is of particular importance to ensure that LLM-generated reports comply with local medical standards and practices. Clinicians involved in the validation process bring expertise and context, which helps to tailor models to the specifics of Russian medicine, such as unique protocols or terminology used in radiology. This process builds confidence in automated systems and minimises the risk of errors due to cultural or system differences. In addition, augmented generation (RAG), which combines the capabilities of generative models with mechanisms for extracting data from validated medical knowledge bases, is used. This allows outputs to be 'grounded' in factual information, such as data from radiology atlases or clinical guidelines, which significantly reduces the likelihood of hallucinations.

Finally, continuous monitoring systems are being implemented into real-time radiology workflows. These systems use automated checks to instantly identify potential hallucinations or inconsistencies, such as abnormal organ sizes or fictitious pathologies, and provide the opportunity for immediate correction. For example, if the model indicates the presence of a tumour where it cannot be, the system signals this to the radiologist for verification. The combination of these strategies — ensemble methods, auditing with classifiers, knowledge distillation, clinician validation, RAG and continuous monitoring — creates a comprehensive system that not only reduces the risks associated with hallucinations in the LLM, but also improves the accuracy and reliability of radiological reports, ultimately improving the quality of care and patient safety.

5.6. Ethical and legal issues in AI-driven radiology

The integration of artificial intelligence (AI) into healthcare, particularly in radiology, has introduced transformative potential alongside significant ethical and legal challenges. These challenges span bias in training data, fairness in AI predictions, transparency, liability frameworks, and patient consent, all of which have profound implications for patient care and societal equity. Below, we explore these issues in depth, drawing comparisons between regions like Russia and the European Union (EU) and proposing pathways for improvement.

5.6.1. Bias in training data and its impact on fairness

A foundational ethical concern in AI-driven radiology is bias in training data. When datasets used to train AI models are skewed—such as being predominantly composed of male subjects—the resulting models often exhibit reduced accuracy for underrepresented groups, including females and minority ethnic populations. This bias directly undermines the fairness and reliability of radiology reports. For example, an AI system trained primarily on male chest X-rays may misinterpret female anatomy due to differences in tissue composition or presentation, potentially leading to misdiagnoses [30]. Studies have substantiated these concerns, demonstrating that AI models can perpetuate gender and racial biases, resulting in unequal healthcare outcomes across demographic groups [30]. This

disparity raises critical ethical questions about equitable access to accurate diagnostics and highlights the need for diverse, representative datasets in AI development.

5.6.2. Ethical frameworks for AI in healthcare

To address such issues, ethical frameworks have emerged as essential guides for the responsible use of AI in healthcare. These frameworks emphasize core principles: fairness, accountability, transparency, and privacy. In contexts beyond radiology, such as vaccine supply chains, ethical AI frameworks have proven effective in ensuring equitable resource distribution and transparent decision-making that accounts for diverse population needs [31]. In radiology, these principles translate into designing AI systems that minimize health disparities and prioritize patient welfare. For instance, an ethical framework might mandate regular audits of AI performance across demographic groups to identify and correct biases, ensuring that technological advancements do not widen existing inequities.

5.6.3. Comparing AI liability frameworks: Russia vs. the EU

A stark contrast exists between AI liability frameworks in different regions, notably between Russia and the EU. The EU AI Act represents a pioneering effort to regulate AI technologies, including those in healthcare, by establishing clear liability provisions [18]. This legislation ensures that developers and users of AI systems can be held accountable for harms caused by their technologies, fostering trust and safety in their deployment. In radiology, this might mean liability for an AI system that fails to detect a condition due to biased training data. Conversely, Russia currently lacks a specific AI liability framework for radiology applications, leaving a legal void. This absence creates uncertainty for patients and healthcare providers, as there are no standardized mechanisms to address AI-related errors or harms. Aligning Russia's regulations with global standards like the EU AI Act could enhance patient protections and encourage responsible AI innovation.

5.6.4. Fairness in LLM predictions for diverse populations

Fairness in AI predictions, particularly those driven by large language models (LLMs), is a pressing concern in multi-ethnic societies like Russia. With its diverse population, Russia requires AI systems in radiology to be trained on datasets that reflect this diversity to avoid biased outcomes. An LLM that inaccurately interprets radiological data for certain ethnic groups—due to underrepresentation in training data—could lead to suboptimal care, eroding trust in healthcare systems. Ethical AI frameworks prioritize fairness as a non-negotiable principle, advocating for inclusive data collection and model validation across all population segments. This is not just a technical challenge but a moral imperative to ensure equitable healthcare delivery.

5.6.5. Transparent reporting of model biases

Transparent reporting of model biases is a cornerstone of ethical AI deployment. By documenting and disclosing biases inherent in AI models, developers enable stakeholders—clinicians, regulators, and patients—to understand limitations and take corrective actions. In clinical radiology, transparency might involve publishing performance metrics disaggregated by gender, ethnicity, and age, revealing any disparities in accuracy. This openness fosters accountability, allowing for independent scrutiny and continuous improvement of AI systems. Without such transparency, the risks of undetected biases persist, potentially compromising patient safety and trust in AI-driven diagnostics.

5.6.6. Russia's opportunity to develop AI liability regulations

Given the global proliferation of AI in healthcare, Russia has a critical opportunity to develop its own AI liability regulations. Modeling these after frameworks like the EU AI Act could provide a robust legal structure for the development, deployment, and use of AI systems in radiology. Such regulations would clarify responsibilities, protect patients from AI-related errors, and incentivize developers to prioritize safety and fairness. For example, a Russian liability framework might mandate compensation for patients harmed by AI misdiagnoses, aligning with international norms and enhancing the credibility of its healthcare technology sector.

5.6.7. Integrating patient consent protocols in LLM-driven systems

Finally, the integration of patient consent protocols into LLM-driven radiology systems is essential for ethical practice. Patients must be fully informed about how their data is used—whether for diagnostics or to train AI models—and retain the right to opt out. Consent processes should also clarify the role of AI in their care, including potential risks like bias or errors. This transparency is vital for maintaining patient autonomy and trust, core tenets of medical ethics. In practice, this might involve digital consent forms embedded in healthcare systems, ensuring that patients actively participate in decisions about AI's role in their treatment.

The ethical and legal landscape of AI in radiology is complex, requiring a multifaceted approach to ensure fairness, accountability, and patient-centered care. Mitigating bias in training data, adhering to ethical frameworks, establishing liability regulations, promoting fairness and transparency, and prioritizing patient consent are all critical steps. For Russia, developing a comprehensive AI liability framework could bridge existing gaps, aligning its practices with global standards and enhancing the equity and reliability of AI-driven healthcare. By addressing these issues holistically, stakeholders can harness AI's potential to improve patient outcomes while safeguarding societal values.

6. Current challenges in LLM interpretability

6.1. The "Black-Box" problem

The inherent complexity of LLMs, driven by billions of parameters and intricate neural architectures, renders their decision-making processes difficult to interpret. In radiology report generation, this lack of transparency is particularly problematic, as clinicians require clear rationales to trust automated outputs [27]. For instance, an LLM might generate a report identifying a pulmonary nodule, but without insight into why it prioritized certain imaging features, radiologists may hesitate to rely on the output, fearing potential errors or biases. This distrust is compounded by the high-stakes nature of radiology, where misinterpretations can lead to incorrect diagnoses or delayed treatments, adversely affecting patient outcomes.

6.2. Over-reliance on common symptoms

SHAP (SHapley Additive exPlanations) analysis, a widely used interpretability method, has revealed that LLMs often exhibit over-reliance on common symptoms or frequently occurring phrases in their training data, which can compromise report accuracy [18]. For example, an LLM trained on a dataset with a high prevalence of "chest pain" may disproportionately associate this symptom with conditions like myocardial infarction, potentially overlooking less common but critical findings, such as subtle vascular anomalies visible on coronary angiography. This bias can lead to incomplete or misleading

reports, particularly for atypical presentations or rare pathologies, highlighting the need for more nuanced interpretability methods that capture the full spectrum of clinical indicators.

6.3. Strategies for enhancing interpretability

Lightweight interpretability frameworks

Given the time-sensitive nature of clinical workflows, interpretability methods must be computationally efficient to support real-time applications [17, 28]. Traditional methods like SHAP, while insightful, often require significant computational resources, making them impractical for use during patient consultations. Lightweight interpretability frameworks offer a solution by providing rapid, actionable explanations without introducing latency. These frameworks might employ simplified algorithms, such as feature importance approximations or attention-based visualizations, to highlight key inputs driving the model's predictions. For instance, a lightweight framework could prioritize the top 10% of features contributing to a radiology report, enabling clinicians to quickly validate the model's focus on relevant imaging findings, such as calcified plaques in coronary arteries.

6.4. Model calibration for reliable confidence scores

Model calibration is critical for ensuring that LLM confidence scores accurately reflect the likelihood of correct predictions [28]. A well-calibrated model assigns high confidence to accurate reports and lower confidence to uncertain ones, providing clinicians with a reliable metric to guide decision-making. Techniques such as temperature scaling or Platt scaling can adjust output probabilities to align with actual outcomes, reducing the risk of overconfident predictions. For example, a calibrated LLM generating a report for a chest CT scan might assign a 95% confidence score to a confirmed pneumonia diagnosis but a lower score to an ambiguous finding, prompting further clinician review. Calibration enhances trust by ensuring that the model's confidence aligns with its performance, a critical factor in clinical settings.

6.5. Explainable AI frameworks: attention heatmaps and beyond

Explainable AI (XAI) frameworks, such as attention heatmaps, provide visual insights into LLM decision-making by highlighting regions of an image or text that influence the model's output. In radiology, attention heatmaps can illuminate areas of a medical image—such as a region of stenosis in a coronary angiogram—that the LLM deems significant, thereby clarifying its reasoning [35]. For instance, a heatmap might highlight a narrowed vessel segment, enabling radiologists to confirm whether the model's focus aligns with clinical findings. Other XAI methods, such as LIME (Local Interpretable Model-agnostic Explanations) and Integrated Gradients, can complement heatmaps by providing local explanations for specific predictions, further enhancing interpretability. These methods are particularly valuable for complex cases, such as multi-vessel stenosis, where understanding the model's focus is essential for validation.

6.6. Real-time interpretability tools

To integrate seamlessly into clinical workflows, real-time interpretability tools are essential. These tools, potentially embedded in radiology information systems or Picture Archiving and Communication Systems (PACS), could provide interactive interfaces displaying heatmaps, feature importance scores, or natural language explanations during consultations. For example, a radiologist reviewing an LLM-generated report could interact with a dashboard that highlights key phrases (e.g.,

"moderate stenosis") and their corresponding image regions, enabling rapid validation. Such tools bridge the trust gap by allowing clinicians to verify AI outputs in real time, ensuring that automated reports align with clinical observations and reducing the risk of errors.

6.7. Standardized metrics for interpretability

To systematically evaluate LLM interpretability, standardized metrics like RadGraph are critical [36]. RadGraph, a metric designed for radiology report analysis, quantifies the alignment between model-generated explanations and expert annotations, providing a benchmark for interpretability. For instance, RadGraph could measure how accurately an LLM's attention heatmap corresponds to a radiologist's identification of a pulmonary lesion. Standardized metrics enable objective comparisons across models, facilitating the identification of best practices and informing regulatory standards. Without such metrics, interpretability assessments remain subjective, hindering the development of reliable AI systems.

6.8. Future directions by 2030

6.8.1. Multimodal LLMs and federated learning

By 2030, multimodal LLMs, which integrate text, imaging, and other data modalities, are projected to reduce healthcare costs by approximately 30% by streamlining radiology workflows and improving diagnostic accuracy [37]. These models can process both radiological images and clinical notes, generating comprehensive reports that account for patient history and imaging findings. Federated learning, which enables model training across distributed datasets without sharing sensitive patient data, will further enhance efficiency by leveraging diverse, multi-center data while preserving privacy. This approach is particularly promising for Russia, where integrating LLMs with healthcare systems could improve diagnostics and patient care, especially in rural clinics with limited access to advanced imaging technologies.

6.8.2. Cloud platforms and model optimization

Cloud platforms and model optimization techniques, such as quantization and pruning, will enhance the accessibility of LLMs for rural clinics by reducing computational requirements [37]. Quantization, for instance, compresses model weights to lower precision (e.g., 8-bit integers), enabling deployment on standard hardware without significant performance loss. This is critical for Russia's vast rural regions, where high-end GPUs may be unavailable. By 2030, cloud-based LLM solutions could enable real-time radiology report generation in remote settings, democratizing access to advanced diagnostics.

6.8.3. Policy advancements and GOST-compliant standards

In Russia, the development of GOST-compliant standards for AI in healthcare is essential for ethical deployment [18]. These standards could mandate transparent model outputs, such as requiring attention heatmaps or confidence scores in radiology reports, to ensure clinical accountability. Aligning with global frameworks like the EU AI Act (EU AI Act) could further strengthen Russia's regulatory landscape, ensuring that AI systems meet international safety and fairness standards. Such policies would foster trust among clinicians and patients, facilitating widespread adoption.

6.8.4. Training programs for clinicians

Training programs for medical professionals are crucial for LLM adoption in radiology [36]. These programs should educate clinicians on interpreting AI outputs, understanding interpretability tools like heatmaps, and integrating AI into clinical workflows. In Russia, tailored training could address local medical practices and terminology, ensuring that LLMs align with regional standards. By 2030, comprehensive training initiatives could empower radiologists to leverage AI effectively, enhancing diagnostic accuracy and patient care.

6.8.5. Predictive analytics and epidemic preparedness

Russia's investment in AI-driven healthcare platforms could enable predictive analytics for epidemic preparedness, such as forecasting disease outbreaks based on radiological data [37]. For example, LLMs could analyze chest X-rays to detect early signs of infectious diseases, informing public health strategies. Standardized radiology reporting, supported by localized LLMs trained on Russian medical texts and imaging, would enhance diagnostic accuracy across diverse populations, addressing the needs of Russia's multi-ethnic society.

6.8.6. Global collaborations

Global collaborations with AI research hubs, such as those in the EU or North America, could accelerate LLM development for radiology. Collaborative efforts could involve sharing anonymized datasets, developing open-source interpretability tools, or co-creating standardized metrics like RadGraph. By 2030, such partnerships could position Russia as a leader in ethical healthcare AI, particularly in radiology automation, by leveraging global expertise while addressing local needs.

6.8.7. Challenges and limitations

Despite these advancements, several challenges remain:

- Computational Demands: Multimodal LLMs and federated learning require significant computational resources, which may limit adoption in resource-constrained settings without optimization [37].
- Regulatory Gaps: Russia's lack of a comprehensive AI liability framework, unlike the EU AI Act, could delay ethical deployment and erode trust [18].
- Bias in Localized Models: Training localized LLMs on Russian medical texts and imaging must account for ethnic and regional diversity to avoid biases that could compromise diagnostic fairness.
- Clinician Resistance: Without adequate training, clinicians may resist adopting LLMs due to concerns about interpretability and reliability [27].

6.8.8. Recommendations for improvement

To align with global standards by 2030, the following strategies are recommended:

1. Develop Lightweight Multimodal LLMs: Invest in model optimization techniques, such as quantization and knowledge distillation, to reduce computational demands, enabling deployment in rural clinics.
2. Establish GOST-Compliant Standards: Create regulatory frameworks that mandate interpretability features and align with global standards like the EU AI Act (EU AI Act).

3. Enhance Training Programs: Implement nationwide training initiatives for radiologists, focusing on AI interpretability and integration, to facilitate adoption.
4. Leverage Federated Learning: Use federated learning to train LLMs on diverse Russian datasets, ensuring privacy and inclusivity across multi-ethnic populations.
5. Foster Global Collaborations: Partner with international AI research hubs to develop standardized interpretability metrics and share best practices, positioning Russia as a leader in ethical AI.

7. Conclusion

LLMs, from RNNs to multimodal transformers, offer transformative potential for healthcare (e.g., Med-PaLM: F1=0.88; Flamingo-CXR: 77.7% preference) [1, 13]. In Russia, challenges like data scarcity, regulatory compliance, and radiology data digitization persist. Recommendations include expanding annotated radiology datasets, developing specialized LLMs for report generation, and standardizing data formats to position Russia as a leader in AI-driven healthcare by 2030. Russia's focus on AI-driven healthcare aligns with global trends, emphasizing data standardization and ethical deployment. Investments in clinician training and public awareness will drive LLM adoption in radiology workflows. Collaborative research with international AI communities could enhance Russia's healthcare AI ecosystem. GOST-compliant AI frameworks could set a precedent for responsible AI use globally, particularly in automated radiology reporting.

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Методы разработки и внедрения больших языковых моделей в здравоохранении: проблемы и перспективы в России

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Аннотация. Большие языковые модели (LLM) трансформируют здравоохранение, позволяя анализировать клинические тексты, поддерживать диагностику и упрощать принятие решений. В этом систематическом обзоре рассматривается эволюция LLM от рекуррентных нейронных сетей (RNN) до основанных на трансформаторах и многомодальных архитектур (например, BioBERT, Med-PaLM), с акцентом на их применение в медицинской практике и проблемы, с которыми они сталкиваются в России. Согласно 40 рецензируемым статьям из Scopus, PubMed и других надёжных источников (2019–2025 гг.), LLM демонстрируют высокую производительность (например, Med-PaLM: F1-критерий 0,88 для бинарной классификации пневмонии на MIMIC-CXR; Flamingo-CXR: предпочтение 77,7% для стационарных/амбулаторных рентгенологических заключений). Однако к ограничениям относятся дефицит данных, трудности с интерпретацией и вопросы конфиденциальности. Адаптация архитектуры «Смесь экспертов» (MoE) для диагностики редких заболеваний и автоматизированного создания отчётов по радиологии дала многообещающие результаты на синтетических наборах данных. В России существуют такие проблемы, как ограниченный объём аннотированных данных и соблюдение Федерального закона № 152-ФЗ. LLM улучшают клинические рабочие процессы, автоматизируя рутинные задачи, такие как создание отчётов и сортировка пациентов, благодаря передовым моделям, таким как KARGEN, повышающим качество отчётов по радиологии. Ориентация России на здравоохранение на основе ИИ соответствует мировым тенденциям, однако лингвистические и инфраструктурные барьеры требуют разработки индивидуальных решений. Разработка надёжных фреймворков валидации для LLM обеспечит их надёжность в различных клинических сценариях. Совместные усилия с международными исследовательскими сообществами в области ИИ могут ускорить внедрение в России передовых медицинских технологий ИИ, особенно в области автоматизации радиологии. Перспективы включают интеграцию LLM с системами здравоохранения и разработку специализированных моделей для российского медицинского контекста. Данное исследование закладывает основу для развития здравоохранения на основе ИИ в России.

Ключевые слова: большие языковые модели, здравоохранение, глубокое обучение, анализ клинических текстов, создание отчётов по рентгенологии, интерпретируемость, российское здравоохранение