Generation of phase trajectories of experimental data

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Abstract. The phase plane method (PPM) is a graph-analytical approach for studying the stability and long-time behavior of systems described by differential equations. In order to apply the PPM to experimental data, it is necessary to identify these data with a first- or second-order differential equation. This work presents a numerical-analytical algorithm for obtaining phase trajectories from experimental data avoiding identification with a differential equation. For this purpose, the data are interpolated with a cubic spline. The first derivative was obtained analytically from the spline. The abscissa coordinates are the values of the spline at a given point, and the ordinate is the analytical representation of the first derivative. As an example, the phase trajectory of the dose-dependent curve of the drug tubazid is constructed by two methods - with identification of the differential equation describing the process and with the algorithm proposed in the article. The approach is implemented with Korelia software.

1. Introduction
The behavior of a system is described by differential equations. From them can be obtained data for equilibrium points, in which the system exhibits special qualities, e.g., loses stability and becomes unmanageable. Solving a differential equation (DE) is not always possible, especially if it is nonlinear. The problem of the solution can be avoided by using the phase plane method (PPM). The phase plane method is a graph-analytical approach for studying the stability and long-time behavior of systems described by DE. If DE is of the $n$-th order, with appropriate substitutions it is reduced to a system of $n$ first-order equations. The matrix presentation of this system is the state space of the system. Nonlinear equations can also be treated by this method, linearizing them in the vicinity of equilibrium points with a Jacobian matrix. Combining every two equations of the system, a phase plane is defined in which the phase trajectory is constructed. Algorithms for studying systems in the phase plane are well known. An inconvenience can be the high order of the DE. The number of phase planes will be combinations of $n$ elements chosen as 2. Therefore, the most suitable for studying using PPM are differential equations up to the second order. The two-dimensional phase space presents the data in a form that emphasizes the dynamic activity in the system. Another important limitation is that DE must be in an analytical form. When conducting experimental work, sets of discrete data are obtained with a clearly defined relation of independent-dependent sets. The construction of the data graph in the Cartesian plane is trivial. In order to apply the phase plane method, it is necessary to identify these data with a first- or second-order DE [1]. Once the analytical form of the DE is available, the application of the PPM follows. Identification in itself is a research process that requires specialized knowledge and skills to be realized. In addition, identification is an approximation method that introduces an error in the process study. There is another problem related to the processing of...
experimental data. There are processes, usually of a stochastic nature, that cannot be identified by an appropriate equation. Thus, the need arises to create an algorithm for generating phase trajectories, avoiding the requirement for identification.

In the widely used mathematical packages there are no specific functions for constructing phase trajectories. Algorithms for working with first and second-order differential equations in a Mathcad environment are given in [2,3], with Wolfram Mathematica in [4], with MatLab in [5], with Korelia in [6]. In these programs, appropriate commands must be written in a specialized language to implement the desired algorithm for constructing phase trajectories. This can be a significant difficulty for humanities researchers. This poses the task of constructing phase trajectories based on experimental data, avoiding the identification process, and without working with analytical expressions.

The aim of the present work is to create procedures and with the means of the interface to provide the user with the opportunity to perform analysis by the method of the phase plane without requiring specialized knowledge. A numerical-analytical algorithm for obtaining phase trajectories from experimental data avoiding identification with a differential equation in the Korelia program environment will be presented.

Korelia is a program for analyzing experimental data. In the present work, its possibilities for spline interpolation of data [7] and their identification with differential equations [8] will be used. The main users of Korelia are specialists in the biological and medical sciences.

2. Background and notations
The experiment is purposeful activity to obtain data about the nature and behavior of the studied systems [9]. Let $S$ is a system that is affected by the independent variable $x$. The finite number $N$ of input forces forms the input set $X$:

$$X = \{x_1, x_2, \ldots, x_N\} \quad (1)$$

The elements of this set satisfy the relation:

$$x_1 < x_2 < \ldots < x_{N-1} < x_N < \infty \quad (2)$$

No requirements are set for equality of the intervals between successive independent variables. Thus $X$ is defined as a closed set of ordered elements. The system response to input $x$ is output $y$:

$$y(x) = S(x) \quad (3)$$

As a result of the relation (3) $Y$ turns out to be a set with the same finite number of real values:

$$Y = \{y_1, y_2, \ldots, y_N\} \quad (4)$$

Thus, experiment $E$ upon the system $S$ can be defined by the relations:

$$E(S,X,Y): \quad S: x_i \rightarrow y_i \Rightarrow (x_i, y_i)$$

$$i=1,2,\ldots,N \quad (5)$$

The finite number of ordered data pairs $(x_i, y_i)$ will be called experimental base point or base element. The point graph $GP(S)$ represents the map of all pairs $(x_i, y_i)$ in Cartesian coordinate system:

$$GP(S): \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\} \quad (6)$$

The object of the approximation theory is to select one from a few candidate functions that approximate the base points according to a selected criterion. The identification evaluates and selects a single model $M(S)$ from multiple candidates. When constructing a phase trajectory, the candidates for identification are first or second order differential equations [6].

3. Phase plane generation
Let the system behavior is described by function $y(x)$. The change in the system is determined by the first derivative:

$$\frac{dy}{dx} = f(y) \quad (7)$$
\( f(y) \) is a function in which the independent variable \( x \) does not appear explicitly. The phase plane is defined by the pair of orthogonal axes \((y(x), dy/dx)\). Thus, the phase trajectory provides information about the process \( y(x) \) and its dynamics through its first derivative \( dy/dx \).

In an experiment, there are \( N \) in number ordered pairs with a graph \( GP(S) \). Due to the discrete nature of the base points, the "differentiation" operation is not applicable. The phase trajectory will look like:

\[
F(y, \Delta y): \{(y_1, \Delta y_1), (y_2, \Delta y_2), \ldots, (y_N, \Delta y_N)\}
\]

where \( \Delta y_i = \frac{y_{i+1} - y_i}{x_{i+1} - x_i} \)

The differences \( \Delta y \) are obtained by applying a suitable algorithm for numerical differentiation [10]. Several categories of algorithms are known. The finite-difference approximation uses the forward and backward Taylor series. The number of elected members determines the accuracy and duration of the calculation. Another approach is based on knowledge of the analytical type of a polynomial approximating the basis points. The first and subsequent derivatives of this polynomial make it possible to calculate the value of the derivative at any point in the definition domain of the independent variable.

The cubic spline interpolation of the experimental data was realized in the Korelia program. For intermediate point \( x \) between \( i \)-th and \((i+1)\) base points the ordinate \( g(x) \) is calculated by formula:

\[
g(x) = \frac{S}{6h_i} \left( x_{i+1} - x_i \right)^3 + \frac{S}{6h_i} \left( x - x_i \right)^3 + \frac{y_i}{h_i} \left( x_{i+1} - x_i \right) - \frac{y_{i+1}}{h_i} \left( x - x_i \right)
\]

where: \( x \in (x_i, x_{i+1}); h_i = x_{i+1} - x_i \);

\( S_i = f(x_i, y_i, g'(x_i), g''(x_i)) \) is the solution of the linear system satisfied continuous conditions for spline interpolation.

The number and coordinates of the internal points \( x \) for each interval can be chosen according to the specifics of the studied process. The interpolation formula (9) can be used to obtain the first derivative also in analytical form [7]. After differentiation, the first derivative for \( i \)-th interval is:

\[
g'(x) = \frac{S}{2h_i} \left( x - x_i \right)^2 - \frac{S}{h_i} \left( x_{i+1} - x_i \right)^2 + \frac{y_{i+1}}{h_i} - \frac{y_i}{h_i}
\]

This analytical expression can be used to generate and display the first derivative. Thus, the algorithm combines the analytical representation of the first derivative with the numerical calculation of points from the phase trajectory. The phase trajectory \( F(g, g') \) is the sequence of points \((g(x), g'(x))\).

Their number \( K \) may be greater than the number \( N \) of experimental points thanks to the interpolation algorithms (9) and (10).

\[
F(g, g') = \{(g(x_1), g'(x_1)), \ldots, (g(x_N), g'(x_N)), \ldots, (g(x_K), g'(x_K))\}
\]

The coordinates of the points forming the phase trajectory are determined parametrically by the independent variable \( x \). A sufficient close selection of abscissa points can contribute to the visualization of smooth graphics.

4. Example
An example with a dose-response curve for determining the effective dose of tubazid will be considered. Data published in [11] were used. In Figure 1, the experimental data are plotted with dots. Both approaches for obtaining the phase trajectory will be demonstrated - with the identification of a differential equation and with application of the algorithm described in the present work.

4.1. Identification of data with differential equation
The experimental data were identified by a logistic nonlinear differential equation [12]:

\[\text{(2021) 012078 doi:10.1088/1757-899X/1031/1/012078} \]
\[ \frac{dy(x)}{dx} = r \left[1 - y(x)\right] y(x) + b \cdot y(x) \]  
(12)

where:  
x - dose of a drug;  
y(x) - dose response curve;  
r - the rate constant of the process;  
b - parameter, presenting the influence of an ingredient.

The obtained values of the coefficients in the differential equation and the qualitative parameters of the identification are in Table 1.

| r     | b     | \( R^2 \) (coeff.determination) | Akaike’s Information Criterion AIC | Corrected AIC |
|-------|-------|---------------------------------|-----------------------------------|---------------|
| 0.182 | 0.15  | 0.998                           | -87.3583                          | -78.6440      |

The identified curve in Figure 1 is indicated by a triangular marker. Phase trajectory is determined by the equation:

\[ f(y) = r \left(1 - y\right) y + b \cdot y \]  
(13)

This is a parabola that defines equilibrium points with values 0 and 1. The identified phase trajectory of Figure 2 has a triangular marker.

4.2. Numerical-analytical algorithm

The solution is based on spline data interpolation. In Figure 1, spline interpolation connects the experimental points with a smooth curve. Visually, the differences between the two curves are not significant.

The data are differentiated by the algorithm (10). The numerical results are in Figure 3. The first column is the dose \( x \), which acts as a parameter for the phase trajectory. The second column is the phase independent variable \( y(x) \), and the third is the first derivative \( \frac{dy}{dx} \). The phase trajectory is formed by the coordinates represented by the second and third columns. In Figure 2 the calculated phase path is denoted by a dense dot. In this case, the equilibrium points are calculated by applying the numerical algorithm described in [6].
5. Results and discussions

The initial graph (Figure 1) shows a slight difference in dose-response curves obtained by the two methods. Passing into the phase plane, the differences become significant. In both methods of construction, the phase trajectory is a parabola and the fixed points coincide. The point with coordinates (0.0) is unstable - a small change in the dose leads to an effect of its application. Point (1.0) is stable, which means that a change in the dose does not lead to a significant change in the effect. A more accurate model is the one obtained with spline interpolation - it uses the exact coordinates of the base points.

6. Conclusions

In the present work, an algorithm for constructing phase trajectories of experimental data is considered. Cubic spline interpolation of data is applied. The first derivative is obtained analytically from the spline formula. The abscissa coordinates are the values of the spline at a given point, and the ordinate is the calculated value of the analytical representation of the first derivative at the same point. This algorithm avoids the need for more difficult and time-consuming data identification.
Some advantages of the numerical-analytical generation of phase trajectories.

- The exact coordinates of the basic points are taken into account and this leads to a phase trajectory, which is the carrier of only the error of the experiment, but not the error of approximation, typical of the identification.
- It is possible to construct phase trajectories of stochastic processes for which it would be difficult, if not impossible, to formulate an identification equation.
- Frees the researcher from the need to identify processes - the desired results are obtained easily, simplified by means of the graphical user interface. It is not necessary to write a program in a specialized programming language. This allows the analysis by PPM to be done by humanitarians.
- As an important drawback, it should be noted that the result obtained is valid only in the domain of definition of the experiment. Extrapolation beyond the original observation range of it would be problematic. In addition, the existence of an analytical model obtained with identification is a prerequisite for building more complex and generalizing models of the studied processes.
- As an example, the phase trajectory of the dose-dependent curve of the drug tubazid is constructed by two methods - with identification of the differential equation describing the process and with the algorithm proposed in the article. The approach is implemented with the software Korelia.

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