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A METHOD FOR IDENTIFICATION OF HOMOCLINIC TRAJECTORIES

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For the incorrect problem of calculation of homoclinic trajectories of systems of ordinary differential equations a new approach is proposed based on solving a boundary value problem for the system of Euler-Lagrange equations for minimization of the functional which is an integral over the infinite interval of the sum of squares of the equation from the original set. Difference scheme, iterative procedure and numerical algorithm for minimization of golden-section type are devised. The performance of the method is displayed on the case of Lorenz system. The main advantage of the new method is that the computations are easily automatized and do not require a-priori information about solution.

Introduction. In recent years the identification of homoclinic solutions of ordinary differential equations has attracted considerable attention in connection with application to soliton phenomena. A number of research papers has been devoted to solitons occurring in different physical situations. It goes well beyond the frame of the present paper to give a detailed survey on solitons. Instead here are only mentioned a few works which are close to the author's interests. The most popular example of soliton solutions is the flow of thin liquid film down an inclined or vertical plate (see for details [1]). Another customer of homoclinic solutions is the theory of stochastic regimes of dynamic systems. When the stochastic process is considered as a random train of soliton-like structures one can derive equations for the structures and calculate the homoclinic trajectories of these systems. For the case of so-called Burgers turbulence this approach is outlined in the author's work [7] . It turns out that in the general scheme of functional expansions (see [2]) for stochastic problems once again soliton-like solutions of many independent variables are needed in order to evaluate the higher-order terms of expansion. Similar solutions with summable over infinite region square are obtained in [8] concerning the stochastic regime of plane Poiseuille flow and identified as so-called large eddies of turbulent flow. All the examples cited involve partial differential equations. Among those described by ordinary differential equations the most studied is, perhaps, the system proposed by Lorenz [3] who showed the stochastic behaviour of its trajectories. In [9] is proved that Lorenz system (or as it is called currently "Lorenz attractor") possesses also homoclinic solution. The latter is related to the stochastic regime in [10] . Shtern [11] reported the shape of homoclinic trajectory which he supposedly obtained as an initial value problem but there is no clear indication in his work exactly what type of method is used.

Obtaining homoclinic solutions on the base of initial value numerical procedures is an extremely difficult task and as a rule requires sizable amount of a-priori information about the solution itself. For this reason the quest for alternative numerical approaches is still under way. Here should be mentioned the works [12] , [13] concerned with solutions in falling thin liquid films where Fourier integral and Fourier series are employed, respectively. Completely different way is persued in [4] where a complete orthonormal system of functions in $L^2(-\infty,\infty)$ space is introduced and applied to stochastic solution of Burgers equation. The necessary technique for practical application of this system is developed in [5] for the case of plane Poiseuille flow.

All the methods cited in the above have their advantages and shortcomings as always but the meanest enemy lurks in the very problem and more specificly in the fact that the homoclinic trajectory exists only for special values of parameters and as a rule cannot be obtained by means of iterating the original systems of equations starting from the solution for specific set of parameters. In the present paper one more approach to the problem of identification of homoclinic trajectories which is free of the shortcomings listed is proposed. The new method is displayed on the problem arising when the homoclinic solution of Lorenz system is to be calculated.

1. Lorenz attractor. Consider the following dimensionless system of ordinary differential equations

$$(1) \qquad \frac{dx}{dt} = \sigma(y-x) , \quad \frac{dy}{dt} = -xz+rx-y , \quad \frac{dz}{dt} = xy-bz ,$$

which is derived in [3] for the amplitudes of the first three Fourier modes of the solution for the natural convection in an unbounded region. In the above equations r is a version of Rayleigh number. The most interesting feature of (1) is that for certain values of Rayleigh number r its trajectories exhibit stochastic behaviour. Usually this is observed for $\sigma = 10$ and $b = 8/3$ so our results shall be concerned only with these values of σ and b .

As it is mentioned in the above, in [9] is proved that at $r = r_{hc} = 13.926$ a homoclinic trajectory occurs which with an increase of r becomes instable giving birth to various stochastic and periodic regimes.The main significance of homoclinic solution is that it raises from zero at $t = -\infty$ and again decays to zero at $t \to \infty$, i.e. it satisfies the following conditions:

$$(2) \qquad x = y = z = 0 \quad at \quad t = -\infty , \ t \to \infty .$$

So we have arrived at the boundary-value problem (1), (2) which is apparently incorrect since the number of boundary conditions (2) is greater than the order of the system (1). On the other hand the homoclinic solution hardly could be obtained as an initial value problem by means of a kind of shooting procedure because exactly in the vicinity of $r = r_{hc}$ the initial value problem for (1) becomes instable.

2. Correct boundary value problem. The main idea of the present work is to replace solving the incorrect boundary value problem (1), (2) by the minimization of the following integral

$$I(r) = \min \int_{-\infty}^{\infty} [(\frac{dx}{dt} + \sigma x - \sigma y)^2 + (\frac{dy}{dt} + xz - rx + y)^2 + (\frac{dz}{dt} - xy + bz)^2] dt \qquad (3)$$

which we shall call further "residuals functional". The integral in (3) is divergent if $x, y, z \in L^2(-\infty, \infty)$ and if there exist no singularities, i.e. $\dot{x}, \dot{y}, \dot{z} \in L^2(-\infty, \infty)$.

As $I(r)$ is a sum of squires its infinum is equal to zero. This value is attained either on the trivial solution or on homoclinic solution if the latter exists. Residuals functional can have a local minimum for each value of r but this minimum need not be equal to zero except for $r = r_{hc}$. This means that for the beginning one has to devise an efficient procedure for minimizing the integral in (3) for an arbitrary and given r and afterwards to couple this procedure with a method for minimization of the real function $I(r)$. A necessary condition for existing of a local minimum of the integral are the Euler-Lagrange equations:

$$(4) \quad \begin{aligned}
&\frac{d^2x}{dt^2} - [\sigma^2 + (r-z)^2 + y^2]x = (\sigma - r + z)\frac{dy}{dt} - y\frac{dz}{dt} \\
&\qquad - y[\sigma^2 + r + (b-1)z] , \\
&\frac{d^2y}{dt^2} - [1 + \sigma^2 + x^2]y = -2x\frac{dz}{dt} - (\sigma + z)\frac{dx}{dt} \\
&\qquad - x[\sigma^2 + r + (b-1)z] , \\
&\frac{d^2z}{dt^2} - (b^2 + x^2)z = 2x\frac{dy}{dt} + y\frac{dx}{dt} + xy - bxy - rx^2 .
\end{aligned}$$

Unlike (1) the order of this system is in accordance with the number of boundary conditions (2) and can be easily solved numerically. So far we have succeeded to pose a correct boundary value problem (4), (2) among whose solution is present the required homoclinic solution of (1). The most important feature of (4) is that that it is a bifurcation problem since the trivial solution is always present under the provision of boundary conditions (2). This fact additionally complicates the solution.

3. Difference scheme. System (4) is very tractable for numerical treatment since for each of the operators in left-hand sides the principle of maximum holds when considering in the respective equation two of the functions as known and only the third one which enters through its second derivatives as unknown. This enables one to construct the following simplified linearization for the discretized equations:

$$(5) \quad \begin{aligned}
&\frac{1}{h^2}x_{i+1}^{n+1} - [\frac{2}{h^2} + \sigma^2 + (r - z_i^n)^2 + (y_i^n)^2] x_i^{n+1} + \frac{1}{h^2}x_{i-1}^{n+1} \\
&= (\sigma - r + z_i^n)\frac{1}{2h}(y_{i+1}^n - y_{i-1}^n) - \frac{1}{2h}y_i^n(z_{i+1}^n - z_{i-1}^n) - y_i[\sigma^2 + r + (b-1)z_i^n] , \\
&\frac{1}{h^2}y_{i+1}^{n+1} - [\frac{2}{h^2} + 1 + \sigma^2 + (x_i^{n+1})^2] y_i^{n+1} + \frac{1}{h^2}y_{i-1}^{n+1} = x_i^{n+1}\frac{1}{h}(z_{i+1}^n - z_{i-1}^n) \\
&- (\sigma + z_i^n)\frac{1}{2h}(x_{i+1}^{n+1} - x_{i-1}^{n+1}) - x_i^{n+1}[\sigma^2 + r + (b-1)z_i^n] , \\
&\frac{1}{h^2}z_{i+1}^{n+1} - [\frac{2}{h^2} + b^2 + (x_i^{n+1})^2] z_i^{n+1} + \frac{1}{h^2}z_{i-1}^{n+1} = \frac{1}{h}x_i^{n+1}(y_{i+1}^{n+1} - y_{i-1}^{n+1})
\end{aligned}$$

$$+y_i^{n+1}\frac{1}{2h}(x_{i+1}^{n+1}-x_{i-1}^{n+1})+x_i^{n+1}y_i^{n+1}(1-\delta)-r(x_i^{n+1})^2,$$

where h is the time increment. The superscript n refers to the number of iteration, subscript i - to the location of the point from the interval $t\in(-\infty,\infty)$ for which the approximation (5) is valid.

For the purposes of numerical implementation the infinite time interval is reduced to a finite one $t\in[-\frac{T}{2},\frac{T}{2}]$, where T is certain sufficiently large number. The total number of grid points is denoted by N and then

$$(6)\qquad t_i=(i-1)h-\frac{T}{2},\quad h=T/(N-1)$$

is the mesh and by definition of set function $x_i=x(t_i)$. Boundary conditions (2) give the following difference boundary conditions

$$(7)\qquad x_1=x_N=0.$$

The total order of approximation of (5) is $O(h^2)$.

Concerning the computational algorithm it is to be mentioned that the principle of maximum results (5) in the fact that the matrix of the system is tridiagonal and the elements of the main diagonal dominate the sum of elements of the other two diagonals. The latter enables one to use the simplest variant of Gaussian elimination method called "progonka" (see [14]).

4. Results and discussions. The first problem which has to be tackled in numerical solution is to estimate the magnitude of T. If the latter is chosen too large more mesh points are needed and the computational time amounts to intolerable value. If T is chosen too small the solution obtained is distorted and often happens the worst - only the trivial solution persists in computations. In our computations $T\simeq 6$ is the lower limit for which reasonable results are obtained. In order to have some margin of safety for arbitrary r we settle $8\leqq T\leqq 10$.

The second crucial point in algorithm is the selection of the initial condition since starting the iterations from an inappropriate initial condition one is bound to obtain only the trivial solution. Fortunately, the nontrivial solution of (4), (2) proves numerically to be a strong attractor so that quite different in shape and amplitude initial conditions resulted in the same soliton-like solution. The most attractive feature of the method proposed is that the non-trivial solution exists for a wide range of the governing parameter r. At least we had successful calculations for $5\leqq r\leqq 300$. In order to avoid lengthy calculations the solution obtained for $r=28$ (see fig.1) is employed as an initial condition for computations with different r. It is noteworthy that always less than 80 iterations were needed to obtain the solution within the relative accuracy of 0.01%.

The accuracy of difference scheme proposed is checked through the mandator tests involving different grid spacings h. In this instance the solution presented on fig.1 is obtained with $h=0{,}02$. The trajectory calculated with $h=0{,}01$ is hardly distinguished if plotted along with the previous one. The difference is about 2.8%. If the spacing is further reduced to $h=0{,}008$ the

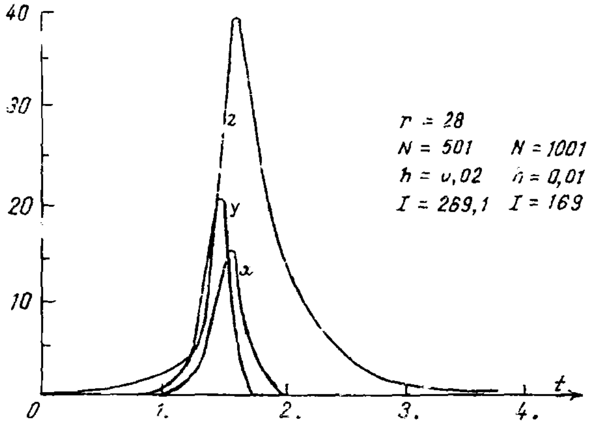

Fig. 1

difference between the respective solutions is about 0.2%. It is instructive to note the considerable jump in the value of the functional $I(r)$ (see the caption to fig. 1) with decreasing the grid of spacing. The conclusion is that the optimal mesh size for $r=28$ is $h=0{,}01$. Calculations confirmed that it is so and for the rest of the values of r which are of interest.

So far a practical procedure capable of solving the boundary value problem (4), (2) is constructed and we can effectively compute the real function $I(r)$. As stated in the above, our purpose is to find the minimum of I with respect to the independent variable r. Obviously, the dependence of I on r is too complicated conveyed by the solution of (4), (2). Hence a method of minimization which does not employ derivative is chosen. Initially, starting from $r=28$ and decreasing it by step 1 the minimum is roughly located and then a procedure implementing the method of golden section (see [6]) is activated and the value of r at which minimum occurs is estimated within the accuracy of 0.1%. On fig.2

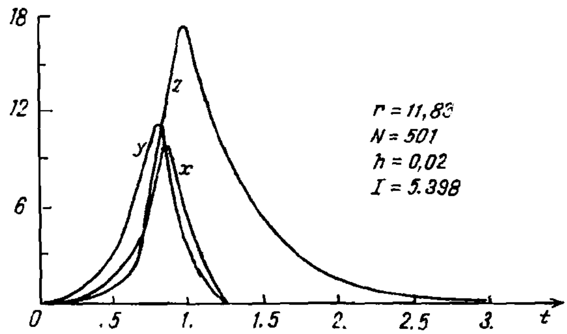

Fig. 2

is shown the homoclinic trajectory obtained with $h=0{,}02$ as well as the value of r^* at which the minimum occurs. It is important to note that similarly to the value of the minimum the argument at which the minimum takes place is highly susceptible to the mesh size too. This is clearly displayed by the comparison between fig. 2 and fig. 3. The difference between those two results is considerable.

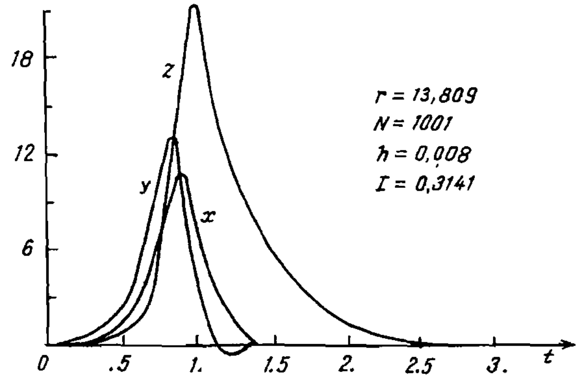

Fig. 3

It is interesting to stress however, that the difference of the I_{min} and r_{min} for solutions with $h = 0,01$ and $h = 0,008$ is less than 1% while the very solutions for x, y, z compare even better - within 0.3%. So one can state that $h = 0,01$ is the optimal mesh size even for the whole problem, including the minimization process.

The way in which I_{min} depends on the size of grid spacing when the latter is decreased to zero hints that the value of minimum of I is equal to zero within the order of magnitude of truncation error. Moreover, $I(r)$ has a sufficiently steep shape in the vicinity of minimum. All this allows us to conclude that the sought homoclinic trajectory is found. The value of Rayleigh number for which the homoclinic exists is calculated to be approximately $r_{hc} = 13,809$ which compare quantitatively well with $r_{hc} = 13,926$ reported in [9] , [11] . The agreement is within 1% which is fully compatible with the magnitude of truncation error and the error of estimation of minimum.

In conclusion it can be said that a simple and robust method for identification of homoclinic trajectories is developed. It is a promising one and can be used in other areas where incorrect problems are to be treated numerically.

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ЕДИН МЕТОД ЗА ОПРЕДЕЛЯНЕ НА ТРАЕКТОРИИ ОТ ТИПА НА ХОМОКЛИНИКА

Христо И. Христов

За пресмятане на решения на системи от обикновени диференциални уравнения от типа на хомоклиника е предложен нов подход, основан на решаване на гранична задача за уравненията на Ойлер-Лагранж за минимизиране на функционала, получен след интегриране върху безкраен интервал на сумата от квадратите на изходните уравнения. Предложена е диференчна схема и итеративна процедура за решаване на тази задача и числен алгоритъм от типа на златното сечение за минимизиране на функционала като функция на изходните параметри. Методът е демонстриран върху системата на Лоренц. Основно негово преимущество е, че пресмятанията се автоматизират лесно и че за успешното числено решаване не е необходима предварителна информация за самото решение.