

Machine learning evaluating evolutionary fitness in complex biological systems

1st Oleg Kuzenkov
Institute of Information Technology
Lobachevsky State University
Nizhni Novgorod, Russia
kuzenkov_o@mail.ru

2nd Andrew Morozov
Department of Mathematics
University of Leicester
Leicester, UK
Institute of Ecology and Evolution
Moscow, Russia
am379@leicester.ac.uk

3rd Galina Kuzenkova
Institute of Information Technology
Lobachevsky State University
Nizhni Novgorod, Russia
galina.kuzenkova@itmm.unn.ru

Abstract—Here we suggest a novel computational approach based on artificial neural network technologies to be able to evaluate evolutionary fitness in both theoretical models of population dynamics and empirical biological systems from data. Our approach uses long-time population time series (obtained either from a model or from data) and establishes the ranking order of inherited strategies reflecting their selective advantages. We approximate the fitness surface in the space of a few key parameters based on Taylor expansion. To do this, we create learning and testing samples and then apply artificial neural networks to build a fitness surface separating the domains of interior and superior ranking in the space of parameters. Using the obtained approximation of the fitness function we can find the evolutionarily stable (optimal) strategy by maximising evolutionary fitness. We demonstrate the efficiency of our approach by applying it to some classical population models where the exact fitness function can be derived analytically as well as to empirical systems. In the considered study cases, both the fitness function and the optimal strategy obtained via our computational method are close to the ones provided by analytical solutions or observed in natural systems. We apply our method to predict the evolutionarily stable diel vertical migrations (DVM) of zooplankton in the ocean and lakes, the phenomenon, which is considered as the most significant synchronous biomass movement on Earth.

Index Terms—zooplankton, diel vertical migration, evolutionarily stable strategy, fitness, recognition, neural network, machine-learned ranking, validation.

I. INTRODUCTION

Currently, artificial intelligence systems are widely implemented in various research areas (see [1] for a short review) in particular, in life sciences. For example, methods of patterns recognition and neural networks are applied in computational biology for ranking candidate 3-D structures of protein complexes [2]. Another important application is predicting outcomes of biological evolution and selection [3].

In evolutionary biology, the key issue is understanding and predicting which inherited behavioural strategy or a life history trait would be eventually selected as a result of interspecies and intraspecific competition under given environmental conditions. The naturally selected strategy is called the evolutionarily stable strategy [4]. Modern approaches to mathematical modelling of biological evolution are often based on the maximization of some prescribed criterion – evolutionary fitness

[4]–[6], that reflects selective advantages of inherited elements (genotype, life trait, behavior, etc.). This approach was firstly developed in the works of Haldane, Fisher and Wright [7] and was the implementation of Darwin’s fundamental idea – “survival of the fittest”.

However, to practically implement Darwin’s seminal idea, we need to choose some key characteristics of hereditary strategies that determine their impact on evolutionary success. Each hereditary strategy will determine a set of life traits under given environmental conditions. Then it becomes necessary to be able to compare selective advantages of different hereditary strategies with each other, i.e. to introduce a certain ranking order based on available information on long-term population success. Finally, we should determine a fitness function that quantitatively expresses the ranking order and relates it to the key characteristics of organisms. Predicting the evolutionarily stable strategy consists of finding the optimal argument of fitness function (e.g. via calculus of variations or other methods). Thus, by maximizing evolutionary fitness one can predict the evolutionary outcomes in biological systems [8], [9]. The central point of evolutionary modelling based on the above paradigm is the ability to rank inherited strategies. Therefore, it would be logical to apply the existing machine-learned ranking techniques to tackle this problem [10], [11]. Currently, there exist various algorithms of learning to rank such as pointwise, pairwise, and listwise algorithms [12].

In this study, we apply the pairwise method of machine-learned ranking to construct a fitness function based on empirical observations and theoretical models. We create an artificial neural network to rank inherited strategies and derive the fitness function of diel vertical migrations (DVM) of zooplankton in the water column.

The problem of reconstructing fitness using machine learning has several important features (caveats) that makes it complicated. Firstly, we require a sample of the time series to be sufficiently long [9]. Secondly, we assume that the set of evolving strategies is not finite but is a certain continuum (e.g. function space) [6]. Thirdly, the main task is not to establish ranking order by itself, but by using it to derive fitness function following this order with the final goal being to predicting the

evolutionary stable strategy [9]. Finally, it is often practically hard to validate the appropriate software.

In this study, we are particularly focused on problems of software validation when we reveal evolutionary fitness by machine learning techniques. We use two different conceptual approaches. For some models, we can analytically derive the corresponding fitness function that reflects the selective advantages of strategies. In this case, we can directly compare the obtained fitness via our numerical methods and the exact analytical solution. The second approach includes the comparison of the numerically found evolutionary stable strategy and the one obtained using the exact analytical solution for the relevant model. Here we apply the methods to reveal optimal patterns of diel vertical migration of zooplankton in the ocean and lakes.

II. METHODOLOGY

Evolutionary fitness has been always a controversial issue in the literature since different authors have proposed distinct definitions of fitness [13]–[19], etc. The approach of adaptive dynamics to this problem uses local stability of an equilibrium state in the space of inherited elements [4], [17], [20]. However, the problem of how to define evolutionary fitness is still far from its final solution. Currently, the choice of fitness is generally subjective and depends on the personal preference of the modeller. As a result, different approaches to fitness may produce conflicting predictions of evolutionary outcomes [17], [21].

Recently, a new mathematically rigorous framework has been proposed to deal with the problem of fitness [22], [23]. The main idea is to consider the long-term dynamics of inherited elements in function spaces which is mathematically described as dynamics of measure of sets. The corresponding dynamical models of self-replicating systems are given by differential equations or differential equations with delay [6], [22]. In this case, the fitness function is expressed as a long-term per capita rate of a subpopulation corresponding to a particular inherited element. On the other hand, we often do not know the underlying differential equations but only have empirical time series of population dynamics of competing species and subpopulations. Thus, we only know a posteriori result of long-term selection in the system.

It was recently demonstrated that evolutionary fitness can be estimated directly from empirical data by following long-term population dynamics [9], [23]–[25]. The main idea is to assume that an inherited strategy A is better (fitter) than a strategy B if the ratio between the number of individuals applying B and that of individuals using A tends to zero over time [25]. In the case of limited environmental capacity, this signifies that the group of individuals using A will eventually be displaced by those using B . As such, from population time series, we can easily rank all strategies on the base of the partial ordering of their per capita growth rates. This allows us to introduce ranking using the data-defined partial order. Finally, we need to build a function preserving ranking order

of strategies, such a function becomes the evolutionary fitness [9], [24].

According to the computational method presented in this study, the evolutionary fitness function J can be directly constructed by studying the selection among competing strategies taking place in the system. The population dynamics time series required to establish the ranking order can be either taken from empirical data or by simulating theoretical models. Here we apply the pairwise method of machine-learning to restore the ranking order for all inherited strategies. We have developed an algorithm to reconstruct the evolutionary fitness as a function of the key parameters which are determined by a strategy. The fitness function in this approach is approximated using Taylor expansion. Below we provide a brief description of the computational framework of the method (for more details see [9], [25]).

Consider v to be a hereditary strategy from some space V of hereditary strategies of the population; $\rho(v, t)$ is the number of individuals realizing strategy v ; this can be also understood as the density distribution of the population over V . We formally define the strategy v to be better (or fitter) than w if the ratio $\rho(w, t)/\rho(v, t)$ tends to zero, i.e.

$$\lim_{t \rightarrow \infty} \rho(w, t)/\rho(v, t) = 0.$$

If the above ranking order does not depend on the initial condition and there exists a functional $J(v)$ such that it preserves the ranking order of the elements, i.e. $J(v) > J(w) \Leftrightarrow v \succ w$, then this functional is referred to as the evolutionary fitness. Functional J will play the role of the ranking function. Note that in many models, ranking order can depend on the initial conditions. Such complicated situations are partially discussed in [9], [24] and we do not consider them in this note.

Temporal dynamics of $\rho(v, t)$ are usually determined by few key characteristics ('macroparameters') $M = (M_1(v), \dots, M_n(v))$ such as foraging rates, mortalities, maturation times, etc, which are function(al)s of the strategy v . Thus, fitness J will be a multivariable function of M , i.e. $J(v) = J(M(v))$. We assume that we can approximate J using Taylor expansion around a certain point M_0 :

$$J(M) = J(M_0) + dJ|_{M_0} + \dots + d^k J|_{M_0} + o(\|M - M_0\|^k).$$

Thus, to find evolutionary fitness we need to estimate the coefficients in the above Taylor expansion. We can also always remove the constant $J(M_0)$ since we are not interested in finding the absolute value of J .

Assume that we have long-term data on the joint dynamics of $\rho(v_1, t), \dots, \rho(v_m, t)$ for certain finite subset of hereditary elements with known v_1, \dots, v_m . This should allow us to approximate the limit of the ratio $\rho(v_j, t)/\rho(v_i, t)$ for all pairs (v_i, v_j) from this set. Comparing the magnitude of this ratio, we can obtain ranking order for the subset of elements (and their corresponding parameters M). In the case $v_i \succ v_j$, the inequality $J(M(v_i)) > J(M(v_j))$ should hold. The based on the Taylor approximation, we obtain the inequality for Taylor coefficients for J .

We can solve the corresponding system of linear inequalities using methods of linear programming [9]. However, here we suppose a new approach for finding the coefficients via modern methods of pattern recognition.

The crux of the method is the following. Let us assign the pair (v, w) to the point $(M(v), M(w))$, the pair (w, v) to the point $(M(w), M(v))$ in the $2n$ -dimensional space of parameters. In the considered $2n$ -dimensional space, we explore samples of pairs of hereditary elements, with known comparison results in terms of ranking order. We can separate the two sets using a surface which will be related to fitness. Consider a separating surface given by the following parameterization

$$\begin{aligned}
Y(v, w) \equiv & \sum_{i=1}^n \lambda_i (M_i(v) - M_i(w)) + \\
& + \sum_{j=1}^n \sum_{i=1}^n \lambda_{ij} (M_i(v)M_j(v) - M_i(w)M_j(w)) + \\
& + \sum_{i_1=1}^n \sum_{i_2=1}^n \dots \sum_{i_k=1}^n \lambda_{i_1 i_2 \dots i_k} \left(\prod_{j=1}^k (M_{i_j}(v) - \prod_{j=1}^k M_{i_j}(w)) \right) = 0.
\end{aligned}$$

The above problem of separation of sets is a typical pattern recognition problem (known as classification) that can be solved with the help of learning neural networks [26]–[28]. Such a comparison boils down to determining whether the ordered pairs of elements "first, second" belong to one of two classes: "the first is better than the second" or "the first is worse than the second". The coefficients of the separating surface will be those of Taylor approximation of fitness function.

Note that separation of two finite sets of points from the learning sample with the surface $Y(u, v)$ is generally non-unique. The concrete realisation of the separation procedure (and the corresponding approximation of fitness) depends on the method of constructing the separating surface. For example, in the simplest case where $k = 1$, the function Y is linear and the separating surface is a hyperplane. The location of this hyperplane can be slightly different depending on the methods used in neural networks. In the case where one implements a simple single-layer neural network, constructing a separating hyperplane will be equivalent to the gradient descent for a certain function depending on the coefficients of the hyperplane. There also exists the concept of an optimal hyperplane which can be constructed using, for example via the Gauss-Seidel method. The problem of fitness reconstruction can be also solved using pointwise methods of machine-learning ranking, for example, OPRF (polynomial regression) [29].

Note that evolutionary fitness can be analytically derived for several relevant population models (Verhulst, von Foerster, Lotka-Volterra, etc., see for details [6], [23], [24], [30]). Thus we can use the analytical results to validate the efficiency of the developed software as it is done in the next sections.

Finally, after revealing the evolutionary fitness function it is possible to derive the evolutionary stable behaviour (strategy) by methods of calculus of variations or the optimal control theory. In this case, the fitness function will be the objective functional of the corresponding optimizing problem [9], [24]. We have developed the program complex to solve this problem numerically for any known objective functional [3]. We can compare the numerical results with those empirically observed in nature (suggesting that the current strategy, life trait or behavior pattern is the result of long term selection) to validate the created software. Moreover, we can solve the optimizing problem analytically for some population dynamics models. Then we can easily perform a comparison between analytical and numerical solutions for the validation of our software (see some examples below).

III. DIEL VERTICAL MIGRATIONS OF ZOOPLANKTON

The phenomenon of diel vertical migration (DVM) of aquatic organisms was discovered two hundred years ago [14]. It was found that a large number of zooplankton species move up and down between deep and surface layers on a regular daily basis. It is recognised that the DVM of zooplankton plays an important role in the dynamics of the organic matter of the ocean. This phenomenon is considered to be the greatest synchronous migration of biomass on Earth [31] and can potentially influence the climate on the planetary scale [32]. Zooplankton is regarded as a key element in aquatic food chains, in particular, they present the main food source for fish. Identifying the causes and mechanisms of DVM of zooplankton is an important problem in modern ecology and is crucial for an efficient fishery.

The mechanisms and ecological significance of DVM have been largely both empirically and theoretically [14]–[16], [18], [21], however many aspects of this phenomenon are still poorly understood. In particular, this is due to the wide variety of patterns of DVM observed in nature [14]. Various mathematical models of DVM were considered in the literature [9], [23], [24], [33]–[36]. In this study, we reconsider recent data from the long-term observations of zooplankton DVM and evaluate evolutionary fitness and optimal DVM using our computation method. The data considered here is publically accessible, taken from the literature [14], [21], [36] as well as from the following websites: <http://www.oceannetworks.ca/zap-data-saanich-inlet> <http://www.oceannetworks.ca/zap-data-saanich-inlet> and <http://hdl.handle.net/1828/4630> <http://hdl.handle.net/1828/4630>.

Mathematical models and empirical data suggest that the timing and the amplitude of DVM of herbivorous zooplankton are mainly determined by various environmental factors: spatial distributions of food $E(x)$ at the depth x of the column, spatial distribution of predators $S_x(x)$, extra mortality $G(x)$ due to unfavourable temperature or/and radiation level, the daily predator activity $S_t(t)$, in this case, $S(x, t) = S_x(x)S_t(t)$ is the predator pressure depending on the depth and time of day [14], [21]. All of these factors can be considered as mathematical functions of the vertical coordinate x (e.g.

measured in meters) or time of day t (e.g. measured as a fraction of the day). We suggest that the environment is stable.

Let x be the vertical coordinate of the position of zooplankton in the column; t is the time of day varying from 0 to 1. Let zooplankton have N developmental stages characterized by different life traits and distinct patterns of DVM. Then mathematically the inherited strategy v of a subpopulation is the set of N periodic functions $X(t) = (x_1(t), \dots, x_N(t))$ corresponding to different developmental stages. We assume that every $x_i(t)$ is a continuously differentiable function on the segment $[0, 1]$, satisfying conditions $x_i(0) = x_i(1)$. We can study dynamics of m different competing subpopulations (or species) using strategies v_1, \dots, v_m . Then mathematically we have the set of vector functions $X_j, j = 1, m$, corresponding to these different strategies and the set of the derivatives X'_j .

We can analyze the long-term dynamics of $\rho(v_i, t)$, where ρ is the sum of individuals of all age stages realizing strategy v_i with the time of observation T being sufficiently long, i.e. $T \gg 1$. We use data on long-term persisting species to derive fitness function.

We can derive the fitness function using the separating surface $Y(v, w)$ in the space of parameters introduced in Section II. The primary analysis of the data shows that the impact of some terms in Y is relatively small and they can be neglected without affecting the quality of the approximation. Therefore, for the given problem, we can use a reduced form of $Y(v, w)$.

To separate two sets (domains) of pairs with different ranking order, we can use either the classifier based on the nearest neighbour method or a two-layer neural network. We found that using artificial networks technology solves the problem more efficiently. Moreover, using the classifier makes the further building of fitness function more complicated. Whereas the implementation of neural networks would allow us to make it easier: using the weight coefficients of individual neurons of the first layer of the network one can easily determine the coefficients of the separating surface Y corresponding to the coefficients in the Taylor approximation of fitness.

IV. RESULTS. SINGLE-STAGE MODEL

The above methodology was applied to find fitness of zooplankton DVM based on one- and two-stages models. We firstly assume a single developmental stage ($N = 1$). The fitness function is given by the following integral

$$F = \int_0^1 (\alpha(t)E(x(t)) - \gamma(t)S(x(t), t) - \beta(t)(x'(t))^2 - \delta(t)(G(x(t))))dt.$$

The weighting functions $\alpha, \gamma, \beta, \delta$ quantify the relative contribution of the corresponding environmental factors at the moment t .

Note that in practice we can only observe discrete values of E, S and G through the day, i.e. we should formally use the

discrete version (approximation) of the above integral given by

$$Y(v, w) \equiv \sum_{l=1}^L (\alpha_l(E(x(v, t_l)) - E(x(w, t_l))) + \gamma_l(S(x(v, t_l), t_l) - S(x(w, t_l), t_l)) + \beta_l(x'(v, t_l)) - x'(w, t_l)) + \delta_l(G(x(v, t_l)) - G(x(w, t_l)))$$

We considered eight data time points for the zooplankton positions during a day ($L = 8$) following the observation data [36]. Note that time increment $\Delta t = t_{l+1} - t_l$ is constant.

We found that the separation of sets of pairs with different ranking can be satisfactorily done by reducing the system complexity and assuming α, β, γ and δ to be constant; this assumption largely simplifies functioning of the method. In this case, evolutionary fitness is given by

$$F(v) = \alpha M_1(v) + \gamma M_2(v) + \beta M_3(v) + \delta M_4(v),$$

where

$$M_1 = \int_0^1 E(x(t))dt, M_2 = \int_0^1 S_t(t)S_x(x(t))dt, \\ M_3 = - \int_0^1 (x'(t))^2 dt, M_4 = - \int_0^1 G(x(t))dt.$$

Our training set contains 132 samples, whereas the testing set is formed of 110 samples using [14]. As a result of training, the neural network can learn to compare the test sample pairs without any mistakes.

To give a clear geometric interpretation of the obtained result let us fix two parameters M_3 and M_4 . Then we may plot points $(M_1(v) - M_1(w), M_2(v) - M_2(w))$ in the plane of two remaining parameters M_1 and M_2 corresponding to the considered pairs of strategies (v, w) (see fig. 1). These pairs belong to two different classes corresponding to the different ranking $w \succ v$ or $w \prec v$. It can be seen from the figure that a straight line with fitted coefficients (α, γ) unmistakably separates these classes.

After we find the coefficients α, β, γ and δ (we can always normalize $\alpha = 1$) we can find the evolutionary optimal trajectory of DVM by analytically maximizing the fitness functional F . This can be done, for example using calculus of variations. The obtained optimal trajectory can be compared with the observed DVM.

Good agreement between the predicted and observed trajectories supports validation of the developed software. We found that per the recent data provided at <http://www.oceannetworks.ca/zap-data-saanich-inlet>, zooplankton was located at a depth of 10 meters for one-half day and a depth of 100 meters for the second half of the day. If we expand the DMV trajectory in a Fourier series and take into account the first three terms, we get the following approximation $x = -55 - 70 \cos 2\pi t + 0.4 \cos 6\pi t$. In accordance with [21], the amount of food $E(x)$ typically

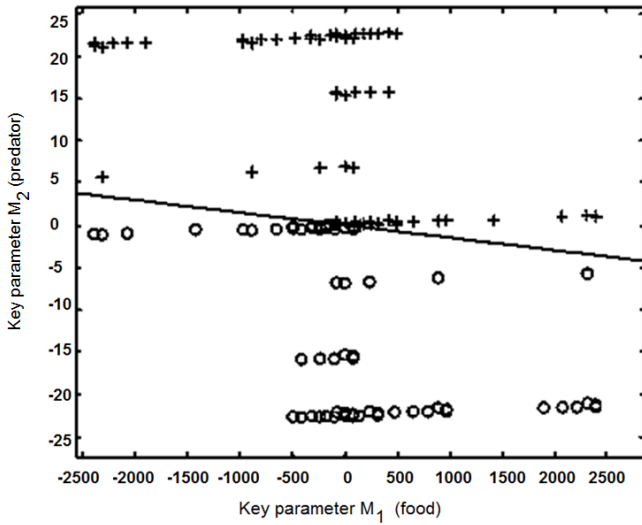


Fig. 1. The set of points $(M_1(v) - M_1(w), M_2(v) - M_2(w))$ corresponding piers of strategies (v, w) in the plain of key parameters M_1 (food) and M_2 (predator). \circ denotes the pair where $v < w$; $+$ denotes the pair where $v > w$.

varies from 20 in the upper water layers ($x = -10m$) to 0 in the lower ($x = -100m$), the predator pressure $S_x(x)$ varies from 70 to 0, respectively. We use a linear approximation of these quantities and a quadratic approximation of negative factors $G(x) = -(x - 50)^2$ when approaching the boundaries of comfort zones and $S_t(t) = \cos 2\pi t + 1$. Our fitness estimations give $\alpha \approx 1, \delta \approx 0.001, \beta \approx 0.00001, \gamma \approx 0.29$. We then analytically find the following optimal solution $x \approx -51.5 - 72.7 \cos 2\pi t$ by the methods of variation calculus. This shows a good agreement between predictions and the data.

Let us now consider a more accurate approximation of the variation of the predator pressure through time $S_t(t) = \cos 2\pi t - \varepsilon \cos 6\pi t + 1$ with $\varepsilon = 0.013$ [14]. In this case solution of the variation problem (assuming the fitness coefficients $\alpha, \delta, \beta, \gamma$ to be the same) is given by $x \approx -51.5 - 72.7 \cos 2\pi t - 0.41 \cos 6\pi t$, which is even in a better agreement with empirical observation [14], [36].

V. RESULTS. TWO-STAGE MODEL

Now consider a two-stage model. We construct the fitness function using the following quadratic form

$$F = \sum_{i=1}^8 \lambda_i M_i + \sum_{i=1}^8 \sum_{j=1}^8 \lambda_{ij} M_i M_j,$$

where the parameters M_i are time discrete approximations of integrals

$$\begin{aligned} M_1 &= \int_0^1 E(x_1(t)) dt, M_2 = \int_0^1 S_t(t) S_x(x_1(t)) dt, \\ M_3 &= - \int_0^1 (x_1'(t))^2 dt, M_4 = - \int_0^1 G(x_1(t)) dt, \\ M_5 &= \int_0^1 E(x_2(t)) dt, M_6 = \int_0^1 S_t(t) S_x(x_2(t)) dt, \end{aligned}$$

$$M_7 = - \int_0^1 (x_2'(t))^2 dt, M_8 = - \int_0^1 G(x_2(t)) dt.$$

Following previous studies [6], [28], we consider the following two-stage model. We denote $\xi(v_i)$ to be the population density of the juvenile (non-reproducible) stages of zooplankton; $\eta(v_i)$ is the population density of adults which can reproduce. In both cases, v_i denotes the corresponding strategy of DVM. The model is described by the following system of ODEs:

$$\xi'(v_i) = r(v_i)\eta(v_i) - \xi(v_j)(p(v_i) + q(v_i) + \sum_{j=1}^m (\xi(v_j) + \eta(v_j)))$$

$$\eta'(v_i) = p(v_i)\xi(v_i) - \eta(v_i)(s(v_i) + \sum_{j=1}^m (\xi(v_j) + \eta(v_j))),$$

$i = 1, m$. In the model, the coefficients r, s, p and q describe, respectively, the reproduction, mortality of juveniles, maturation of juveniles and mortality of adults. They are all functions of the strategy v . In [6], [28] it was shown that the analytical expression for fitness function for the given model is the following

$$J = -s - p - q + \sqrt{4rp + (p + q - s)^2}$$

Following previous studies we can take

$$p = \theta_1 M_1 + \phi_1 M_3 + \psi_1 M_4, q = \zeta_1 M_2,$$

$$r = \theta_2 M_5 + \phi_2 M_7 + \psi_2 M_8, s = \zeta_2 M_6.$$

We fix coefficients $\theta_1, \phi_1, \psi_1, \zeta_1, \theta_2, \phi_2, \psi_2, \zeta_2$.

For each inherited strategy v_i we can calculate the values of the parameters p, q, r, s . Let us consider such strategies that (p, q, r, s) is located near some point (p_0, q_0, r_0, s_0) . Then we can approximate J according to the Taylor formula up to the second-order to obtain

$$\begin{aligned} J \approx & J_0 + h_{11}p + h_{22}q + h_{33}r + h_{44}s + h_{11}p^2 + h_{22}q^2 + h_{33}r^2 + h_{44}s^2 + \\ & + h_{12}pq + h_{13}pr + h_{14}ps + h_{23}qr + h_{24}qs + h_{34}rs. \end{aligned}$$

We can perform computer simulations to integrate model equations for an arbitrary set of inherited strategies. Using the obtained long-term dynamics time series we can reconstruct the fitness function of the following form

$$\begin{aligned} F = & h_1(\theta_1 M_1 + \phi_1 M_3 + \psi_1 M_4) + h_2(\zeta_1 M_2) + \\ & + h_3(\theta_2 M_5 + \phi_2 M_7 + \psi_2 M_8) + h_4(\zeta_2 M_6) + \\ & + h_{11}(\theta_1 M_1 + \phi_1 M_3 + \psi_1 M_4)^2 + h_{22}(\zeta_1 M_2)^2 + \\ & + h_{33}(\theta_2 M_5 + \phi_2 M_7 + \psi_2 M_8)^2 + h_{44}(\zeta_2 M_6)^2 + \\ & + h_{12}(\theta_1 M_1 + \phi_1 M_3 + \psi_1 M_4)(\zeta_1 M_2) + \\ & + h_{34}(\theta_2 M_5 + \phi_2 M_7 + \psi_2 M_8)(\zeta_2 M_6) + \\ & + h_{13}(\theta_2 M_5 + \phi_2 M_7 + \psi_2 M_8)(\theta_2 M_5 + \phi_2 M_7 + \psi_2 M_8) + \\ & + h_{14}(\theta_1 M_1 + \phi_1 M_3 + \psi_1 M_4)(\zeta_2 M_6) + \end{aligned}$$

$$+h_{23}(\zeta_1 M_2)(\theta_2 M_5 + \phi_2 M_7 + \psi_2 M_8) + \\ +h_{23}(\zeta_1 M_2)(\zeta_2 M_6).$$

We can next compare the numerically estimated values of coefficients h_i and h_{ij} with the known coefficients coming from the above Taylor expansion for J .

An example of the comparison between the analytical and our computational method is provided in Table 1. The coefficients in the Taylor expansion of J were computed in the vicinity of the point $r = 35.11, s = 0.73, q = 0.36, p = 0.03$. The coefficients present in fitness function F were found based on the mentioned neural networks for fixed coefficient $h_3 = 0.023$ (that is equal to the corresponding Taylor coefficient). Technically, we implemented classification using a sample consisting of 15 pairs of points.

TABLE I
COMPARISON OF FITNESS FUNCTION COEFFICIENTS

	Taylor's expansion	Recognition of pairs
h_4	-0.8343	-0.3923
h_2	-1.1657	-1.0015
h_1	33.848	29.0951
h_{33}	-0.0002	-0.000001
h_{34}	-0.0023	-0.0020
h_{23}	0.0023	0.0086
h_{13}	0.5199	0.0204
h_{44}	0.2449	0.1511
h_{14}	-3.4120	-2.6510
h_{22}	0.2449	0.1318
h_{12}	3.4120	2.2154
h_{11}	-305.6119	-282.7759

From the table, one can see that the applied here method provides a good approximation of fitness function in the two-stage model.

We also considered another way of verification of the computational method and the software. To do it we can use analytical evaluation of the optimal trajectories of DVM. We considered the same parameterisations for $E(x)$ and $S_x(x, t), G(x)$ of the functions as in the single-stage model. We considered the following weights in the fitness function $\theta_1 = 14, \phi_1 = 0.0008, \zeta_1 = 1$ (here we can normalise ζ_1), $\psi_1 = 0.13, \theta_2 = 11, \phi_2 = 0.0008, \zeta_2 = 18.2, \psi_2 = 0.13$. The optimal DVM obtained via maximisation of fitness is given by $x_1 \approx -10 - 10 \cos 2\pi t, x_2 \approx -50 - 50 \cos 2\pi t$, which is in a good agreement with observed patterns in the ocean [14], [36].

SHORT SUMMARY

In this study, we develop a novel computational method and the appropriate software to be able to reconstruct the evolutionary fitness function from both data and theoretical biological models. The method combines a previous powerful theoretical approach, to define evolutionary fitness in self-replicating systems, and some recent computational methods of artificial neural networks as well as machine-learned ranking. As an important study case, we apply our method to explore evolutionary stable strategies of regular diel vertical

migration (DVM) of zooplankton in the ocean and lakes. Our straightforward tests of the proposed methodology demonstrated its great potential in revealing DVM of zooplankton. As a future extension, we are planning to analyse a large number of reported empirical cases of DVM and include more complicated theoretical models of zooplankton population growth to better train neural networks.

ACKNOWLEDGMENTS

The work was supported by the Ministry of education and science of the Russian Federation (Project No. 14.Y26.31.0022).

REFERENCES

- [1] O. I. Abiodun, A. Jantan, A. E. Omolara, K.V. Dada, N.A. Mohamed, H. Arshad, "State-of-the-art in artificial neural network applications: A survey", 2018, Heliyon 4:e00938.
- [2] K. Duh, "Learning to Rank with Partially-Labeled Data", University of Washington. Washington, 2009.
- [3] O. Kuzenkov, A. Morozov, G. Kuzenkova, "Recognition of patterns of optimal diel vertical migration of zoo-plankton using neural networks", IJCNN 2019 – International Joint Conference on Neural Networks, Budapest Hungary, 2019, DOI: 10.1109/IJCNN.2019.8852060
- [4] M. Gyllenberg, J. H. Metz, R. Service, "When do optimisation arguments make evolutionary sense?", in "The Math-ematics of Darwin's" Legacy, Birkhauser, Basel, 2011, pp. 233–268.
- [5] J. Birch, "Natural selection and the maximization of fitness," Biol Rev Camb Philos Soc, 2016, vol. 91(3), pp. 712–727.
- [6] O. Kuzenkov, A. Morozov, "Towards the construction of a mathematically rigorous framework for the modelling of evolutionary fitness", Bulletin of Mathematical Biology, 2019, vol. 81, pp. 1–22 doi.org/10.1007/s11538-019-00602-3
- [7] S. Wright, "Surfaces of selective value revisited", Am Nat, 1988, vol. 131, pp. 115–123.
- [8] S. Gavrilits, "Fitness landscapes and the origin of species (MPB-41)", Princeton University Press, 2004, vol. 41, p. 476.
- [9] S. K. Sandhu, A. Morozov, O. Kuzenkov, "Revealing Evolutionarily Optimal Strategies in Self-Reproducing Systems via a New Computational Approach", Bulletin of Mathematical Biology, 2019, vol. 81, issue 11, pp. 4701–4725. DOI: 10.1007/s11538-019-00663-4.
- [10] M. Mohri, A. Rostamizadeh, A. Talwalkar, "Foundations of Machine Learning", The MIT Press, 2012.
- [11] N. Tax, S. Bockting, Dj. Hiemstra, "A cross-benchmark comparison of learning to rank methods", Information Processing & Management, 2015, vol. 51 (6), pp. 757–772.
- [12] T.-Y. Liu, "Learning to Rank for Information Retrieval", Foundations and Trends in Information Retrieval, 2009, vol. 3, pp. 225–331.
- [13] J. Sainmont, K. H. Andersen, U. H. Thygesen, O. Fiksen, A. W. Visser, "An effective algorithm for approximating adaptive behavior in seasonal environments", Ecological Modelling, 2015, vol. 311, pp. 20–30.
- [14] C.W. Clark, M. Mangel, "Dynamic State Variable Models in Ecology: Methods and Applications", Oxford Series in Ecology and Evolution, 2000, Oxford University Press, Oxford.
- [15] S. H. Liu, S. Sun, B. P.Han, "Viewing DVM via general behaviors of zooplankton: a way bridging the success of individual and population", J. Theor Biol., 2006, vol. 238, pp. 435–48.
- [16] B. P. Han, M. Strakraba, "Control mechanisms of diel vertical migration: theoretical assumptions", J. Theor. Biol., 2001, vol. 210(3), pp. 305–318.
- [17] K. Parvinen, U. Dieckmann, M. Heino, "Function-valued adaptive dynamics and the calculus of variations", J. Math. Biol., 2006, vol.52, pp.1–26.
- [18] A. De Robertis, "Size-dependent visual predation risk and the timing of vertical migration: An optimization model", Limnol. Oceanogr., 2002, vol. 47, pp. 925–933.
- [19] A. Y. Klimenko, "Entropy and equilibria in competitive systems", Entropy, 2014, vol. 16, pp. 1–22.
- [20] U. Dieckmann, M. Heino, K. Parvinen, "The adaptive dynamics of function-valued traits", J. Theor. Biol., 2006, vol. 241, pp. 370–389.

- [21] O. Fiksen, J. Giske, "Vertical distribution and population dynamics of copepods by dynamic optimization", *ICES J. mar. Sci.*, 1995, vol. 52, pp. 483–503.
- [22] A. N. Gorban, "Selection Theorem for Systems with Inheritance", *Math. Model. Nat. Phenom.*, 2007, vol. 2(4), pp. 1–45. DOI: <https://doi.org/10.1051/mmnp:2008024>
- [23] O. Kuzenkov, E. Ryabova, "Variational Principle for Self-replicating Systems", *Math. Model. Nat. Phenom.*, 2015, vol. 10, N 2, pp. 115–128.
- [24] A. Y. Morozov, O. A. Kuzenkov, "Towards developing a general framework for modelling vertical migration in zooplankton", *Journal of Theoretical Biology*, 2016, vol. 405, pp. 17–28. DOI: 10.1007/s11538-019-00602-3
- [25] O. A. Kuzenkov, E. A. Ryabova, "Limit possibilities of solution a hereditary control system", *Differential Equations*, 2015, vol. 51, N 4, pp. 523–532.
- [26] A. K. Jain, R. P. W. Duin, J. Mao, "Statistical pattern recognition: a review", *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2000, vol. 22(1), pp. 4–37.
- [27] M. Kudo; J. Sklansky, "Comparison of algorithms that select features for pattern classifiers", *Pattern Recognition*, 2000, vol. 33(1), pp. 25–41.
- [28] Ch. M. Bishop, "Pattern Recognition and Machine Learning", Heidelberg, Germany: Springer, 2006.
- [29] N. Fuhr, "Optimum polynomial retrieval functions based on the probability ranking principle", *ACM Transactions on Information Systems*, 1989, vol. 7(3), pp. 183–204.
- [30] O. A. Kuzenkov, G. V. Kuzenkova, "Optimal control of self-reproduction systems", *Journal of Computer and Systems Sciences International*, 2012, V. 51, N 4, pp. 500–511.
- [31] G. Hays, "A review of the adaptive significance and ecosystem consequences of zooplankton diel vertical migrations", *Hydrobiologia*, 2003, vol. 503(1), pp. 163–170.
- [32] K. Buesseler, C. Lamborg, P. Boyd, et al., "Revisiting carbon flux through the oceans twilight zone", *Science*, 2007, vol. 316, pp. 567–570.
- [33] A. Morozov, E. G. Arashkevich, "Towards a correct description of zooplankton feeding in models: Taking into account food-mediated unsynchronized vertical migration", *Journal of Theoretical Biology*, 2009, vol. 262(2), pp. 346–360.
- [34] A. Morozov, E. Arashkevich, A. Nikishina, K. Solovyev, "Nutrient-rich plankton communities stabilized via predator-prey interactions: revisiting the role of vertical heterogeneity", *Mathematical medicine and biology: a journal of the IMA*, 2011, vol. 28, N 2, pp. 185–215.
- [35] W. Gabriel, B. Thomas, "Vertical migration of zooplankton as an evolutionarily stable strategy", *Am. Nat.*, 1988, vol. 132(2), pp. 199–216.
- [36] A. Morozov, O. Kuzenkov, E. Arashkevich, "Modelling optimal behavioural strategies in structured populations using a novel theoretical framework", *Scientific Reports*, 2019, Vol. 9, N 1, 15 p. DOI: 10.1038/s41598-019-51310-w