Gauze' experiments vs. mathematical models

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Abstract

For the approximation of some of well-known time series of *Paramecia aurelia* population size changing in time, some well-known models with continuous time were used. For all considering models values of parameters were estimated with least square method in two different ways: with and without additional limits for parameter's values. In the case without additional limits for model's parameters deviations between theoretical (model) trajectories and experimental time series were tested for Normality (Kolmogorov–Smirnov test, and Shapiro–Wilk test) with zero average, and for existence/absence of serial correlation (Durbin–Watson criteria). The best results were observed for Gompertz' and Rosenzweig' models. This indicates that self-regulative mechanisms are not so strong as it is postulated in Verhulst model. Under the assumption that parameter K (maximum value of population size) is greater than all elements of initial sample the best results were observed for Rosenzweig' model only. Gompertz' model cannot be applied for fitting of experimental time series – hypothesis about Normality for the set of deviations between theoretical and experimental trajectories must be rejected. Verhulst' model cannot be applied for fitting too – there is strong serial correlation in the sequence of residuals.

Introduction

It is difficult to point out a textbook on ecological modeling without the presentation of the results of well-known experiments by G.F. Gause (1933, 1934). Results obtained by G.F. Gause on *Paramecia aurelia* population dynamics are normally used for demonstration of good correspondence between theory (Verhulst' model of isolated population dynamics; Verhulst, 1838)

and experiment. It is also used for demonstration of the legality of use of such mathematical models for the approximation of real datasets.

But it is important to note that in original publication by G.F. Gause (1934) statistical analysis of the correspondence of theoretical (model) results with experimental time series is absent. Comparison of model trajectories with real datasets of population fluctuations had pure visual nature, and estimations of values of model parameters were obtained with very low precision (Tutubalin et al., 1997, 1999). Additionally, there are no comparisons of the results of approximations which can be obtained with Verhulst' model and other models of population dynamics (for example, with Gompertz' model; Gompertz, 1825). It means, that **de facto** Verhulst' model was postulated as a unique applicable model for the approximation of real datasets. This point of view may be truthful and can be accepted, but if and only if comparisons of results of approximation of experimental time series by various models of one and the same class (Table 1) give a support for this hypothesis.

Table 1 Models which are used for approximation of time series

	Models	Sources	Name of the model (common and/or used in current publication)
1	$\dfrac{dx}{dt} = \alpha x\left(1 - \dfrac{x}{K}\right)$	Verhulst (1838)	Verhult model, logistic model
2	$\dfrac{dx}{dt} = \alpha x \ln \dfrac{K}{x}$	Gompertz (1825)	Gompertz model
3	$\dfrac{dx}{dt} = \alpha x^2\left(1 - \dfrac{x}{K}\right)$	Svirezhev (1987)	Svirezhev model
4	$\dfrac{dx}{dt} = \alpha x\left(1 - \left(\dfrac{x}{K}\right)^{\gamma}\right)$	Rosenzweig (1969), Rosenzweig, MacArthur (1963)	Rosenzweig model
5	$\dfrac{dx}{dt} = \alpha x(x - \gamma)\left(1 - \dfrac{x}{K}\right)$	Bazykin (1985)	Bazykin model

Note: The model's numbers are the same in all tables

In our previous publications (Nedorezov, 2011, 2012) there are the analyses of some experimental trajectories obtained by G.F. Gause (1933, 1934). It was obtained that for considered time series (presented on Fig. 24 in the book by G.F. Gause) there are no reasons to say that approximations with Verhulst' model give better results than approximations which were obtained with the use of Gompertz' model.

In current publication we continue analyses of time series by G.F. Gause (presented on Fig. 25 in the book by G.F. Gause). Results of approximation of time series by the models from the Table 1 are compared in two different ways. In first case we use least square method with global fitting (approximation of time series by the trajectories of differential equations from Table 1; Wood, 2001a, b) without additional conditions on the values of model parameters. In the second case we use also the global fitting under the condition that population size cannot be bigger than amount K (see table 1).

Datasets

At present time monograph by G.F. Gause (1934) can be free downloaded in Internet, www.ggause.com. Time series on the fluctuations of *Paramecia aurelia* which is used in current publication, can be found on the Fig. 25. Transformation of graphic information into sequences of numbers was realized with the help of graphic software, and all obtained numbers were round to nearest integer values.

Mathematical Models

In modern literature it is possible to find a big number of various models of population dynamics, which take into account the influence of intra-population self-regulative mechanisms on birth and death rates only (Bazykin, 1985; Svirezhev, 1987; Nedorezov, 1986, 1997, 2010; Brauer and Castillo-Chavez, 2001 and many others). In Table 1, there are simplest mathematical models of population dynamics, which can be presented in the following form:

$$\frac{dx}{dt} = F(x, \vec{\alpha}),$$
(1)

where F is the respective non-linear function in the right-hand side of equations, $\vec{\alpha}$ is a vector of non-negative and unknown parameters, $x(t)$ is population size at time moment t. In G.F. Gause' experiments initial value of population size x_0 was definitely determined, hence x_0 cannot belong to the set of unknown parameters, which have to be determined with analysis of experimental time series (Tonnang et al., 2009 a, b, 2010; Nedorezov and Sadykova, 2008, 2010). Part of considering models (Table 1) contains two unknown parameters, and Rosenzweig' model and Bazykin' model contain three parameters.

In Rosenzweig' model parameter γ plays the role of modifier of for self-regulative mechanisms influence on individual's death rate, and in Bazykin' model this parameter is equal to threshold value of population extinction.

Before applying of mathematical models for the approximation of experimental time series it is important to underline the biological sense of model parameters. First of all, parameter α is proportional to the speed of population growth: this speed increases with growth of value of this parameter for every fixed value of population size. But real role of this parameter is different for various models. In particular, in Verhulst' model and Rosenzweig' model parameter α is equal to the difference between intensity of birth rate and intensity of death rate of individuals. In this case it has a dimension time^{-1}. In Gompertz' model the product $\alpha \ln K$ has the same sense.

The second, in all considering models (table 1) parameter K is equal to limit population size, which can be achieved asymptotically if initial population size is less than K. But we may have two qualitatively different assumptions about the value of this parameter. For example, we may think a'priori that value K is stationary level of population size only. If so, in experiments we can observe values of population size which are bigger than level K.

It is possible to think that K is maximum limit of population size. It is possible to assume that every population tries to maximize the use all accessible resources (and, in particular, accessible space), and population tries to maximize its population size. If so, it means that in experiments we cannot observe the values of population size, which is bigger than K. Thus, under the estimation of values of models we have to take into account the following inequalities:

$$K \geq \max_{k} x_{k}, \tag{2}$$

where x_{k}, $k = 0,1,...,N$, are the elements of initial sample (values of population size obtained in experiments), $N+1$ is a sample size.

Consequently, we have to analyze two various situations which are determined by the biological interpretation of the sense of model parameter K. In first case, when K is a simple stationary level of population size, the following natural question arises: what are the reasons (mechanisms, conditions etc.) which don't allow the population to stabilize its size at maximum limit level? If parameter K is maximum limit population size then condition (2) arises, and we have to take it into account in a process of model's parameter estimations.

In current publication the question about correct or incorrect biological interpretation of the sense of parameter K isn't considered. Both possible variants are used, because the main

goal of publication is in comparison of models and its properties for approximation of real time series. Note, that in the first case there is the traditional problem of determination of non-linear regression, and all existing methods of analysis of deviations between theoretical and experimental datasets can be applied. In the second case there are some additional limits for the application of statistical methods for analysis of sets of deviations.

Statistical Criteria

Selection of statistical criterions and selection of mathematical models are most important steps in a process of finding a best model for the description of population dynamics. Results of selection process may have a strong influence on final results of analysis of population dynamics (Wood, 2001a, b; Nedorezov and Sadykova, 2005, 2008, 2010).

Let $\{x_k\}$, $k = 0,1,...,N$, be an initial time series on population size changing in time, x_k is a population size at time moment k, and $N+1$ is a sample size. Denote as $x = x(t, x_0, \vec{\alpha})$ a solution of equation (1) with initial population size x_0 and defined values of model parameters. Let's also note that initial population size x_0 and first element of considering sample is one and the same number (initial population size was fixed in G.F. Gause' experiments).

For every model from the Table 1 there was one and the same problem: for existing experimental sample $\{x_k\}$ it was necessary to estimate the values of parameters of model (1). For the solution of this problem the following statistical criteria was used:

$$Q(\vec{\alpha}) = \sum_{k=1}^{N} (x_k - x(k, x_0, \vec{\alpha}))^2 \to \min_{\vec{\alpha}} ,\qquad (3)$$

where $x(k, x_0, \vec{\alpha})$ are the values of the solution of equation (1) at the respective time moments. Choosing of this criterion means that a'priori it is assumed that time step in model $h = 1$ and it is equal to twenty-four hours (it is the time step between two nearest measurements of population size in G.F. Gause' experiments). It is important to note that in models of the type (1) there is no *real time*, and, respectively, it is possible to choose the amount of time step h from the standpoint of usability. Estimations of parameters will depend on the amount of selected time step.

Selection of criteria (3) means that in the set of model trajectories we have to find the best one, which gives a global minimum for expression (3) (*global fitting*). Finding the minimal values of the functional (3) allows ranking considering models with these numbers, but it doesn't

allow giving a final report on suitability or uselessness of one or other model for the approximation of datasets. If we follow the traditional views on mathematical models and have no additional limits for values of model parameters (in all situations we have obvious limits for parameters: K must be non-negative parameter, and α may have negative value if intensity of death rate is bigger than intensity of birth rate in population), we have to check several hypotheses for the set of deviations between theoretical and experimental datasets (Draper and Smith, 1986, 1987).

First of all, we have to check the hypothesis that average of the deviations is equal to zero (more precisely, we have to be sure that there are no reasons for rejecting this hypothesis; on the other words, we have to be sure that there are no *systematic components* in deviations). Density function of deviations must be symmetric and single-humped curve. At present time it is a generally accepted idea to check the set of deviations on "Normality": if we have no reasons to reject the hypothesis that deviations have Normal distribution, it gives us a certain background for conclusion that distribution of deviations is symmetric and single-humped curve. Thus, checking of the Normality of the distribution can be considered as sufficient condition for the respective properties of density function. For checking of the Normality of the distribution the Kolmogorov–Smirnov' test and Shapiro–Wilk' test were used (Draper and Smith, 1986, 1987; Shapiro et al., 1968). The sequence of deviations must also be checked for the absence/existence of serial correlation: we have to be sure that with a certain level of confidence we can consider the deviations as the values of independent stochastic variables. For these reasons the well-known Durbin–Watson criteria was used (Draper and Smith, 1986, 1987).

If we got a negative result with one or other statistical criteria, it allowed us concluding that assumption about suitability of the respective model for the approximation of real datasets isn't correct. Thus, we got the following final result: the respective model cannot be applied for fitting of time series. If all considering statistical criteria got positive results (i.e. there were no reasons for the rejecting of the hypothesis "average of deviations is equal to zero", there were no reasons for the rejecting of the hypothesis about "Normality" etc.), it allowed us concluding that respective model can be used for the approximation of initial datasets and for the explanation of population dynamics.

In the case, when criterion (3) was used together with condition (2), some problems in comparison of theoretical and experimental datasets can be observed (Nedorezov, 2011, 2012). It also leads to problems in comparison of various models. If condition (2) is true, starting from a

certain moment of time all experimental points will be at one side of theoretical curve. Consequently, if sample size is big enough, it is obvious that with small value of level of significance the hypothesis about equivalence of the average to zero will be rejected. It is also obvious that there will be a serial correlation in the sequence of residuals.

Results

Estimations of model parameters (with and without the additional condition (2)) are presented in Table 2. In both cases Rosenzweig' and Gompertz' models allowed obtaining better results in approximation than Verhulst' model (Fig. 1 and 2).

Table 2 Estimations of model's parameters and respective minimal value of functional (3) without the additional condition (2)

Models	Parameters			Functional
	α	K	γ	$Q_{\min}$
Results for time series without the additional condition (2)				
1	$5.03 \cdot 10^{-3}$	191.9	---	2043.77
2	0.407	202.83	---	1920.73
3	$7.18 \cdot 10^{-4}$	178.24	---	10231.85
4	1.513	196.75	0.395	1401.47
5	$7.18 \cdot 10^{-4}$	178.24	$3.52 \cdot 10^{-15}$	10231.85
Results for time series with the additional condition (2)				
1	$4.16 \cdot 10^{-3}$	214	---	5940.93
2	0.381	214	---	2551.03
3	$4.8 \cdot 10^{-4}$	214	---	20802.53
4	3.005	214	0.146	2690.66
5	$4.8 \cdot 10^{-4}$	214	$8.81 \cdot 10^{-17}$	20802.53

Results of analyses of deviations between theoretical and experimental trajectories are presented in Table 3. In all cases the Null hypotheses that mean values are equal to zero, cannot be rejected (with 5% significance level). In the first case (without additional condition (2)) three models showed the best results in fitting of considering dataset (Verhulst', Gompertz', and Rosenzweig' models; fig. 1), and two models (Svirezhev' and Bazykin' models) didn't allow obtaining good fitting (tabl. 2): there are the serial correlations in sequences of residuals for these models in both cases – with and without the condition (2) (tabl. 3; critical levels for Durbin – Watson two-side criteria with 5% significance level for sample size 17 and one predictable variable are the following: $d_L = 1.01$, $d_U = 1.25$; Draper, Smith, 1986, 1987). For both models

$d = 0.936 < d_L$, and thus with 5% significance level hypotheses about the absence of serial correlation in sequences of residuals must be rejected.
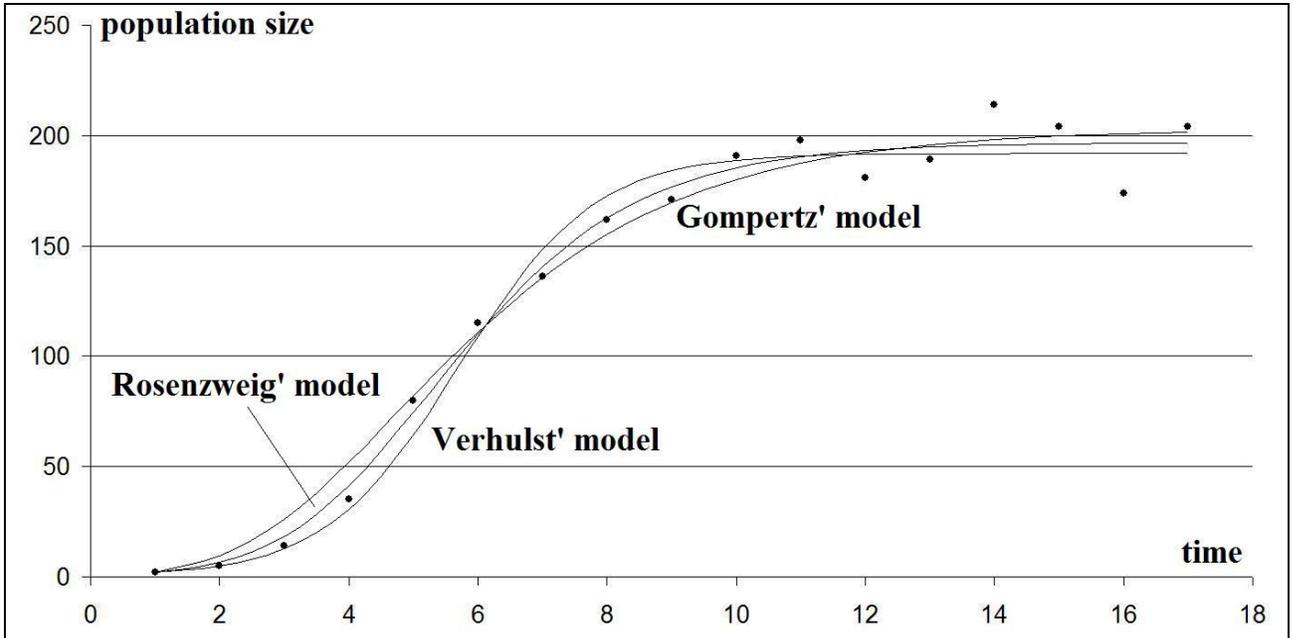

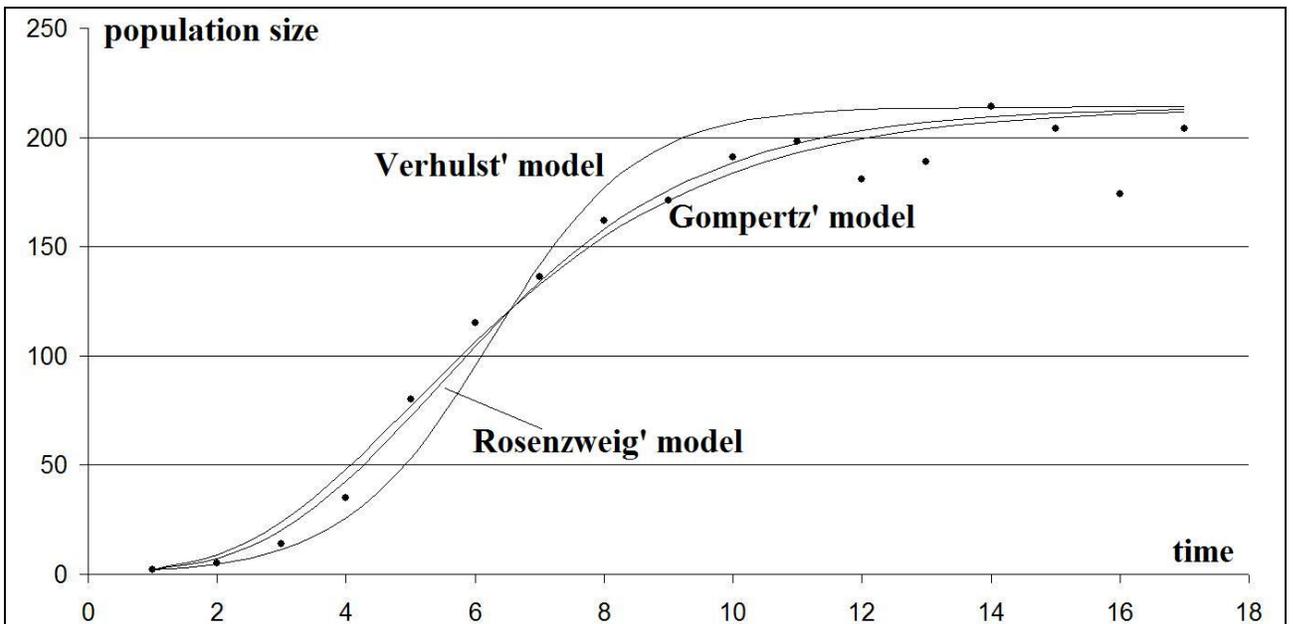Fig. 1. Approximation of real data by Verhulst, Gomprtz, and Rosenzweig models (without condition (2)).

Fig. 2. Approximation of real data by Verhulst, Gomprtz, and Rosenzweig models (with condition (2)).

In the second case approximation of time series obtained with Verhulst' model isn't so good with respect to Gompertz' and Rosenzweig' models. In sequence of residuals there is the

serial correlation (tabl. 3). It allows concluding that in this case Verhulst' model isn't suitable for fitting of considering dataset.

In the same case Gompertz' model allowed obtaining better results (in a comparison with Verhulst' model; table 2). But Shapiro – Wilk test shows (table 3) that hypothesis about Normality of the set of residuals for this model must be rejected. In this occasion Gompertz' model must also be rejected from the set of suitable for fitting models. Results of approximation of experimental time series by the models which allowed obtaining the best approximation, are presented on fig. 2.

Table 3 Analysis of deviations between real datasets and theoretical trajectories

Models	Av. ± S.E.	KS[1]	SW[2]	DW[3]
Analysis of dataset without the additional condition (2)				
1	-0.906±2.732	0.1374/p>0.2	0.9706/p=0.829	1.843
2	1.485±2.631	0.1427/p>0.2	0.9643/p=0.714	1.832
3	-2.295±6.106	0.176/p>0.2	0.8941/p=0.054	0.936
4	0.39±2.268	0.147/p>0.2	0.9576/p=0.586	2.398
5	-2.295±6.106	0.176/p>0.2	0.8941/p=0.054	0.936
Analysis of dataset with the additional condition (2)				
1	7.809±4.246	0.0982/p>0.2	0.9849/p=0.989	0.721
2	4.095±2.886	0.1526/p>0.2	0.8795/p=0.031	1.386
3	12.842±8.135	0.1473/p>0.2	0.9658/p=0.742	0.819
4	4.8±2.907	0.196/p>0.2	0.882/p=0.034	1.291
5	12.843±8.135	0.1473/p>0.2	0.9658/p=0.742	0.819

[1]KS: Kolmogorov–Smirnov test; [2]SW: Shapiro–Wilk test; [3]DW: Durbin–Watson criteria

Discussion

Analysis of time series for *P. aurelia* dynamics (from book by G.F. Gause, fig. 25) shows that self-regulative mechanisms are not so strong like it is assumed within the framework of Verhulst' model. In both considering cases (with and without additional condition for parameter which is equal to maximum of population size) Rosenzweig' and Gompertz' models (theta-logistic model) allowed obtaining better results (in fitting of experimental time series). Close results were obtained for the Rosenzweig' model in analysis of time series for *P. aurelia* and *P. caudatum* (Gause, 1934; fig. 24), which were analyzed in our previous publications (Nedorezov, 2011, 2012).

In the first case when population size can be bigger than amount of parameter K we have no reasons for rejecting hypothesis that Verhulst' model is suitable for fitting of experimental time series. At the same time we have no reasons for rejecting hypotheses that Gompertz' and

Rosenzweig' models are suitable for fitting of experimental time series. Taking into account that Gompertz' model has the same set of unknown parameters like Verhulst' model, and obtained better results in approximation of time series we can conclude that Gompertz' model is closer to real population dynamics law.

In second case (table 3) all used models didn't allow obtaining suitable approximation for time series. For Gompertz' and Rosenzweig' models we have to reject hypotheses about Normality of residuals (Shapiro – Wilk test showed negative results). For Verhulst' model there is the serial correlation in the sequence of residuals. In our previous publications (Nedorezov, 2011, 2012) it was pointed out that such situations can be observed but it doesn't mean that models are not suitable for fitting of considering time series. It means that used statistical criterions don't correspond to considering problem.

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