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An Applied Study on Converting Some Sigmoidal Models in Empirical Form to Meaningful Parameterized Mechanistic Models

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Abstract The growth models are used to estimate some unknown values of population for a given frame in time. The aim of this study is how and why some sigmoidal models which have empirical structure and are widely used in agriculture and biology are converted to mechanistic models which have biological meaning. For this purpose, four different commonly used models with sigmoidal structure were used. These models are the Logistic, Gompertz, Bertalanffy and Holling models, respectively. Firstly, we have given the models modified with three new parameters, namely lag time, maximum specific growth rate, reached maximum value for time approaching infinity. And we have also given the second models modified with three parameters. In this type of models we have used the value of initial time (t=0) instead of lag time. Only difference of two models modified is this: one of them has lag time, the other has the value of initial time (t=0). In this study, for the fork length of the flathead population from Zamanti Stream, Seyhan River; the models which have the smallest and the biggest lag time, reached maximum values, maximum specific growth rates and inflection points and maximum growth rates at these points were determined. Furthermore the smallest and the biggest values of initial time (t=0) were determined instead of lag time.

According to the least squares criterion, we found that the Bertalanffy model is the best growth model for the estimation of fork lengths of the flathead trout from Zamanti Stream and recommend its usage in scientific researches.

Keywords Empirical model, growth, Mechanistic model, Salmo platycephalus, Sigmoidal curve

Introduction

The main purposes of mathematical models used are to have a preliminary knowledge about the functioning of a system, reducing the product costs and improving the performance [1, 2].

Mathematical models can be divided into two classes; empirical models and mechanistic models [3]. Empirical models contain parameters such as a, b, c etc. Therefore, these models do not directly give an idea about the system. In these models, the parameters do not directly make sense. However, mechanistic models contain parameters with biological meaning $A, \mu_{max}, y(t_0)$, etc. Therefore, the researchers prefer mechanistic models in their studies [3, 4].

While empirical models simply describe the general shape of the data set, mechanistic models estimate real system properties (growth rate, maximum size, value of initial time,..., etc); therefore, mechanistic models are preferred to instead of empirical models. The aim of this study is related to how some of the sigmoidal models which have empirical structure and are widely used in agriculture and biology are converted to mechanistic models which have biological meaning. In this study, mean fork length measurements of the flathead trout (*Salmo platycephalus*), which is listed in the IUCN red list of threatened species, which were sampled from the Zamanti Stream of Seyhan River were used [5].



The growth curve of the flathead trout (*Salmo platycephalus*) found in the IUCN red list of threatened species in Zamanti Stream of Seyhan River has a sigmoidal shape. Kara *et al.* [5] were used the Von Bertalanffy model in their study. Since this model has not inflection point, we cannot get the maximum specific growth rate at the inflection point. Nevertheless, this model has the maximum growth rate at the initial year. In this study, the Logistic, Gompertz, Bertalanffy, and Holling models were used. By using various transformations on these models, these models have new parameters, value of initial time, maximum growth rate and reached maximum value for time approaching infinity. The differences and similarities among these models were evaluated.

Materials and Methods:

In this study, the mean fork length measurements of the flathead trout (*Salmo platycephalus*), which is listed in the IUCN red list of threatened species, which were sampled from the Zamanti Stream of Seyhan River were used [5]. For the presentation of the models, the measurements of the fork lengths (cm) in the age-structured female, male and combined sex groups of *S. platycephalus* from Zamanti Stream of the River Seyhan in Table 1 in their articles were used in this study in Table 1.

Table 1: The mean values of fork lengths (cm) of *S. platycephalus* from Zamanti Stream of the River Seyhan

Sex / Age (year)	1	2	3	4	5	6	7	8	9	10
Female	13.68	18.03	21.63	25.55	28.29	30.85	33.37	36.03	38.30	40.0
Male	15.15	18.72	20.91	25.11	27.97	30.88	33.13	35.94	37.04	39.20
Combined sex	13.26	18.17	21.21	25.33	28.16	30.86	33.28	35.79	37.88	39.73

There are many kinds of sigmoidal models used in empirical form. In this study, four of the widely used of these growth models are given in Table 2.

Table 2: The models used in the growth curves

Table 2: The models used in the growth curves								
Models	Equation							
Logistic	y=a/(1+exp(b-ct))							
Gompertz	y=a.exp(-exp(b-ct))							
Bertalanffy	$y=a(1-bexp(-ct))^3$							
Holling	$y = (a-b)t^2/(c^2+t^2)+b$							
where: y = the fork length (cm),								
exp(1)=e (the base of natural logarithm)								
a = the average asymptotic length,								
b and c= the coefficients about growth								

Most of the equations describing a sigmoidal growth curve contain mathematical parameters (a,b,c,...) rather than parameters with a biological meaning ($A,\mu_{max},\lambda,y(t_0),...$). The models which have mathematical parameters have been transformed into the models which have biologically meaningful parameters. The four growth models were firstly rewritten to substitute the mathematical parameters with A,μ_{max} and λ . And then the four growth models were rewritten to substitute the mathematical parameters with A,μ and $y(t_0)$. This was done by deriving an expression of the biological parameters as a function of the parameters of the basic function and then substituting them in the formula [4]. This was done by deriving an expression of the biological parameters as a function of the parameters of the basic function and then substituting them in the formula [4]. By using similar operations, the four growth models were rewritten to substitute the mathematical parameters with A,μ_{max} and λ and then with A,μ_{max} and $y(t_0)$. Many authors such as [6, 7] determined and used the time and values of the inflection point in different forms of the models of Gompertz and Richard in their studies. In addition, [8] used a similar study for the model of Richard to calculate the time and values of the inflection point in their studies.

We show here the modification of the Logistic model, which is written as:



$$y = \frac{a}{1 + \exp(b - ct)} \tag{1}$$

The three phases of the growth curve can be described by three parameters: the maximum growth rate, μ_{max} , is defined as the tangent in the inflection point; the lag time, λ , is defined as the x-axis intercept of this tangent; the value of initial time, $y(t_0)$ and the asymptote A=a is the maximal value reached (Figure 1).

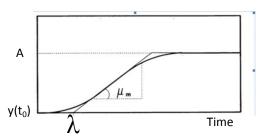


Figure 1: A growth curve

To obtain the inflection point of the curve, the first and the second derivatives of the function with respect to t are calculated respectively:

$$\frac{dy}{dt} = \frac{acexp(b-ct)}{(1+exp(b-ct))^2}$$
 (2)

$$\frac{d^2y}{dt^2} = \frac{2ac^2(exp(b-ct))^2}{(1+exp(b-ct))^3} - \frac{ac^2exp(b-ct)}{(1+exp(b-ct))^2}$$
(3)

At the inflection point, where $t = t_i$, the second derivative is equal to zero:

$$\frac{d^2y}{dt^2} = 0 \implies t_i = \frac{b}{c} \tag{4}$$

Now an expression for the maximum specific growth rate (μ_{max}) can be derived by calculating the first derivative at the inflection point.

$$\mu_{\text{max}} = \frac{\text{dy}}{\text{dt}} \Big|_{t_i} = \frac{\text{ac}}{4} \tag{5}$$

The parameter c in the Logistic equation can be substituted by $\,c = \frac{4\mu_{\text{max}}}{a}$

The description of the tangent line through the inflection point is:

$$y = \frac{a}{2} + \mu_{\text{max}}(t - t_{i})$$
 (6)

The lag time (λ) is defined as the t-axis intercept of the tangent through the inflection point:

$$0 = \frac{a}{2} + \mu_{\text{max}} (\lambda - t_i) \tag{7}$$

Using the equations 4, 5 and 7 yields:

$$\lambda = \frac{b-2}{c} \tag{8}$$

The parameter b in the Logistic equation can be substituted by:

$$b = \frac{4\mu_{\text{max}}}{a}\lambda + 2$$



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To obtain the value $y(t_0)$ of initial time $(t_0=0)$

$$y(t_0) = \frac{a}{1 + \exp(b - ct_0)} = \frac{a}{1 + \exp(b)}$$
(9)

The parameter b in the Logistic equation can be substituted by:

$$b = \ln(a / y(t_0) - 1) \tag{10}$$

The asymptotic value is attained by calculating the limit of the function "y" when t approaches infinity:

$$t \to \infty; y \to a \Longrightarrow A = a$$
 (11)

The parameter a in the Logistic equation can be substituted for by A, yielding the modified Logistic equation:

$$y = \frac{A}{1 + \exp(\frac{4\mu_{\max}(\lambda - t)}{\Delta} + 2)}$$
 (12)

and

$$y = \frac{A}{1 + (A / y(t_0) - 1) \exp(-(4\mu_{max} / A)t)}$$
 (13)

Absolute growth rate and relative growth rate can be calculated as the following formulas respectively;

$$\frac{dy}{dx}$$
 and $\frac{1}{y}\frac{dy}{dx}$

Table 3 shows modified forms of all models used in this study.

Table 3: Modified forms of the models used

Models	Modified Equation
Logistic	$y = A / (1 + \exp(2 + 4\mu_{max}(\lambda - t) / A))$
	$y = A/(1+(A/y(t_0)-1)\exp(-(4\mu_{max}/A)t))$
Gompertz	$y = A \exp(-\exp(1 + \exp(1)\mu_{max}(\lambda - t) / A))$
	$y=Aexp(-exp(ln(-ln(y(t_0)/A))-(2.718281828\mu_{max}/A)t))$
Bertalanffy	$y = -1/27A(-3 + \exp(2/3 + 9\mu_{max}(\lambda - t)/(4A)))^{3}$
	$y = A(1 - (1 - \sqrt[3]{y(t_0)/A}) \exp(-9\mu_{max}t/(4A)))^3$
Holling	$y = \frac{(27t^2\mu_{max}^2A - 6\mu_{max}\lambda A^2 - 15\mu_{max}^2\lambda^2A - 8\mu_{max}^3\lambda^3 + A^3)}{9(A^2 + 2A\mu_{max}\lambda + \mu_{max}^2\lambda^2 + 3t^2\mu_{max}^2)}$
	$y = \frac{(64At^2\mu_{max}^2 + 27A^2y(t_0) - 54A(y(t_0))^2 + 27(y(t_0))^3)}{(64t^2\mu_{max}^2 + 27A^2 - 54Ay(t_0) + 27(y(t_0))^2)}$

Results and Discussion

By using the modified models for the mean fork lengths of the growth features of the flathead trout (*Salmo platycephalus*) found in the IUCN red list of threatened species in Zamanti Stream of Seyhan River, number of parameters, the value of new parameters (λ ,A, μ_{max}), the inflection point and its relative growth rate of each model used for female, male and combined sex were given in Table 4. Kara *et al.* [5] found lag time, the hypothetical age for L(t)=0 and reached maximum value, the average asymptotic length as -1.72 year and 60.78 cm, respectively by using the von Bertalanffy model for combined sex.



Modified Models	Sex	Lag Time	The value of initial time	Asymptotic value (A)	Maximum Growth Rate	Relative Growth Rate	Inflection point		
		λ	$\mathbf{y}(\mathbf{t}_0)$		μ_{max}		t	y	
1. Logistic	F	-2.996	11.55	44.050	3.546	0.161	3.214	22.025	
	M	-3.613	12.46	44.192	3.256	0.147	3.172	22.096	
	C	-2.860	11.23	43.250	3.598	0.166	3.149	21.625	
2. Gompertz	F	-2.819	10.63	47.833	3.695	0.210	1.943	17.597	
	M	-3.487	11.82	48.748	3.351	0.187	1.865	17.933	
	C	-2.672	10.28	46.730	3.763	0.219	1.897	17.191	
3. Bertalanffy	F	-2.652	10.23	50.087	3.837	0.259	1.215	14.840	
	M	-3.335	11.55	51.520	3.456	0.226	1.082	15.265	
	C	-2.501	9.86	48.776	3.918	0.271	1.188	14.452	
4. Holling	F	-2.396	13.60	47.718	3.897	0.176	3.283	22.130	
	M	-3.041	14.80	47.793	3.510	0.152	3.525	23.047	
	C	-2.288	13.25	47.016	3.948	0.182	3.207	21.694	

Table 4: Number of parameters, the value of new parameters (λ , y(t₀), A, μ _{max}), relative growth rate, times of inflection point and their values of the models used for Female (F), Male (M) and Combined sex (C)

Lag time (λ) is the time when the fork length for each model is thought to be zero. In this study, for the fork length of female, male and combined sex; the lag time of the models were found between -2.40 and -3.00 year, -3.04 and -3.61 year, -2.29 and -2.86 year, respectively and while the Holling model has the biggest lag time, -2.40, -3.04, -2.29 year for female, male and combined sex, the Logistic model has the smallest lag time, -3.00, -3.61 and -2.86, respectively.

The value of initial time $y(t_0)$ is the value when the time is zero (t_0 =0). In this study, for the fork length of female, male and combined sex; the values of initial time were found between 10.23 and 13.60, 11.55 and 14.80, 9.86 and 13.25 year, respectively and and while the Holling model has the biggest value of initial time, 13.60, 14.80, 13.25 for female, male and combined sex, the Bertalanffy model has the smallest value of initial time, 10.23, 14.80 and 9.86, respectively.

The asymptotic value (A) of the fork length for each model is reached the maximum value for time approaching infinity. For the fork length of female, male and combined sex: The reached maximum values of the models were found between 44.05 and 50.09 cm, 44.19 and 51.52 cm, 43.25 and 48.78 cm, respectively and while the Logistic model has the smallest reached maximum values, 44.05, 44.19 and 43.25, the Bertalanffy model has the biggest reached maximum values, 50.09, 51.52, 48.78 cm, respectively.

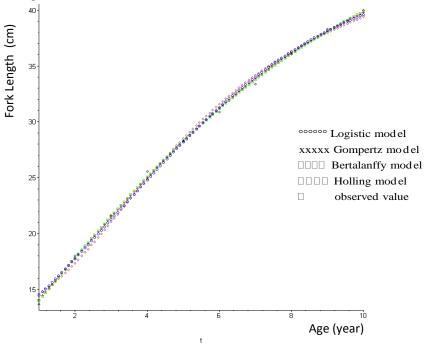
While the absolute growth rate increases until the inflection point, it has reached maximum value at the maximum specific growth rate point and after that point it decreases. Absolute growth rate of the fork length for each model has reached maximum value, maximum specific growth rate, (μ_{max}) at the inflection point of each model. For the fork length of female, male and combined sex: The maximum specific growth rates of the models were found between 3.55 and 3.90, 3.26 and 3.51, 3.60 and 3.95, respectively. While the Logistic model has the smallest maximum specific growth rates, 3.55, 3.26 and 3.60, the Holling model has the biggest maximum specific growth rates, 3.90, 3.51 and 3.95, respectively.

For the fork length of female, male and combined sex; the relative growth rates of the models were found between 0.16 and 0.26, 0.15 and 0.23, 0.17 and 0.27, respectively. While the Logistic model has the smallest relative growth rates, 0.16, 0.15 and 0.17, the Bertalanffy model has the biggest relative growth rates, 0.26, 0.23 and 0.27, respectively.

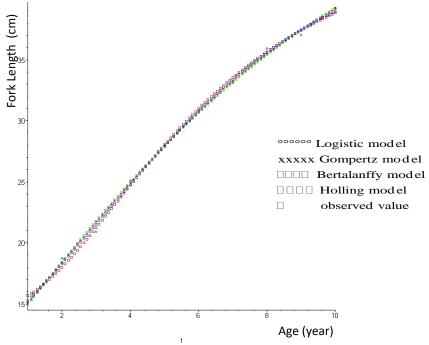
For the fork length of female, male and combined sex; the inflection points of the models were found as (time, length) between (1.22,14.84) and (3.28,22.13), (1.08,15.26) and (3.53,23.05), (1.19,14.45) and (3.21,21.69), respectively and while the Bertalanffy model has the smallest inflection points, (1.22,14.84), (1.08,15.26) and (1.19,14.45), the Holling model has the biggest inflection points, (3.28,22.13), (3.53,23.05) and (3.21,21.69), respectively.



The fork length curves of the Logistic, Gompertz, Bertalanffy and Holling models for female, male and combined sex were given in the same graph with the observed mean fork length for each year, respectively (Figures 2-4).

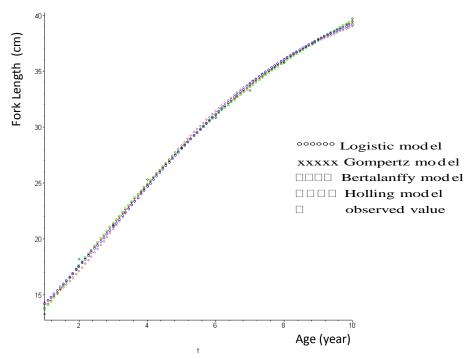


Colors of the Logistic, Gompertz, Bertalanffy and Holling models for female: blue, red, green and brown Figure 2: Fork length of Salmo platycephalus population for female according to the age.



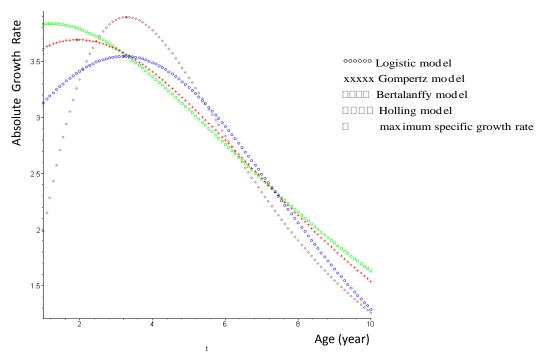
Colors of the Logistic, Gompertz, Bertalanffy and Holling models for male: blue, red, green and brown Figure 3: Fork length of Salmo platycephalus population for male according to the age.





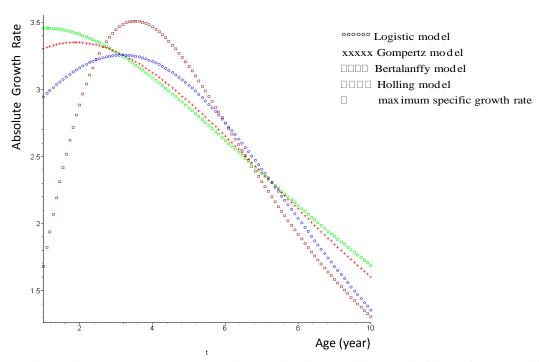
Colors of the Logistic, Gompertz, Bertalanffy and Holling models for combined sex: blue, red, green and yellow Figure 4: Fork length of Salmo platycephalus population for combined sex according to the age.

The Absolute growth rates of the fork lengths of the Logistic, Gompertz, Bertalanffy and Holling models for female, male and combined sex were given in the same graph with the maximum specific growth rate points of the models, respectively (Figures 5-7).

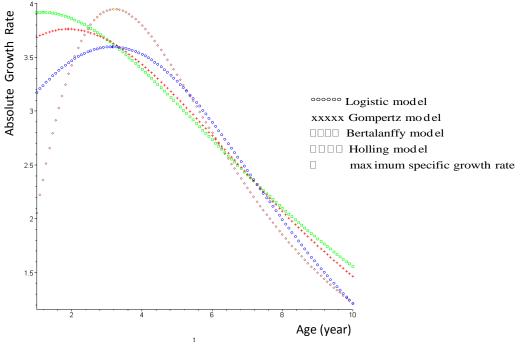


Colors of the Logistic, Gompertz, Bertalanffy and Holling models for female: blue, red, green and brown Figure 5: The Absolute growth rate of the fork length of Salmo platycephalus population for female according to the age.





Colors of the Logistic, Gompertz, Bertalanffy and Holling models for male: blue, red, green and brown Figure 6: The Absolute growth rate of the fork length of Salmo platycephalus population for male according to the age.

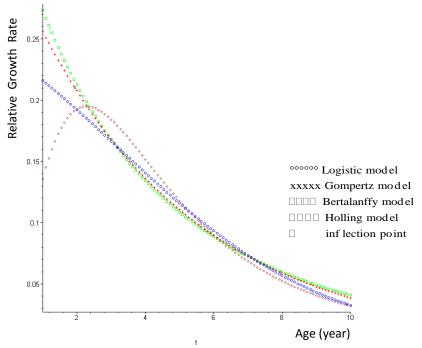


Colors of the Logistic, Gompertz, Bertalanffy and Holling models for combined sex: blue, red, green and brown Figure 7: The Absolute growth rate of the fork length of Salmo platycephalus population for combined sex according to the age.

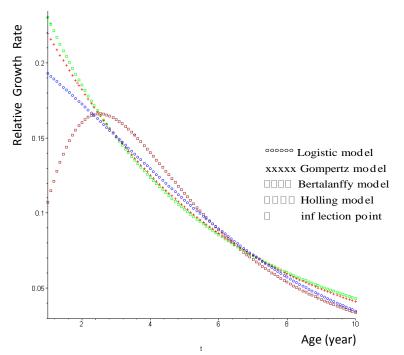
The Relative growth rates of the fork lengths of the Logistic, Gompertz, Bertalanffy and Holling models for female, male and combined sex were given in the same graph with the inflection points of the models,



respectively (Figures 8-10). For all the models used except the Holling model, while the relative growth rate declines rapidly until the inflection point, after that point the relative growth rate decreases slowly (Figures 8-10).

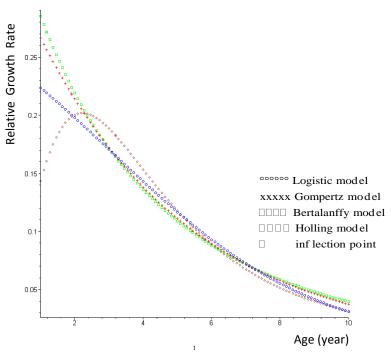


Colors of the Logistic, Gompertz, Bertalanffy and Holling models for female: blue, red, green and brown Figure 8: The Relative growth rate of the fork length of Salmo platycephalus population for female according to the age.



Colors of the Logistic, Gompertz, Bertalanffy and Holling models for male: blue, red, green and brown Figure 9: The Relative growth rate of the fork length of Salmo platycephalus population for male according to the age.





Colors of the Logistic, Gompertz, Bertalanffy and Holling models for combined sex: blue, red, green and brown Figure 10: The Relative growth rate of the fork length of Salmo platycephalus population for combined sex according to the age.

By using Table 1, the estimates with their Error Sum of Squares (SSE) of the Logistic, Gompertz, Bertalanffy and Holling models for the fork lengths were given in Table 5. According to the results of Table 5, while the Bertalanffy model has the minimum SSE, 0.76, 0.91, for female and combined sex, respectively, the Logistic model has the minimum SSE, 1.10, for only male.

Table 5. The observed and estimated fork length (cm) according to the Logistic, Gompertz, Bertalanffy and Holling models for female (F), male (M) and combined sex (C) with their Error Sum of Squares (SSE)

Sex					Age						SSE
	1	2	3	4	5	6	7	8	9	10	<u>-</u> '
F	13.68	18.03	21.63	25.55	28.29	30.85	33.37	36.03	38.30	40.0	
M	15.15	18.72	20.91	25.11	27.97	30.88	33.13	35.94	37.04	39.20	
C	13.26	18.17	21.21	25.33	28.16	30.86	33.28	35.79	37.88	39.73	
F	14.49	17.77	21.27	24.80	28.19	31.29	34.00	36.28	38.13	39.60	2.27
M	15.26	18.32	21.54	24.78	27.91	30.81	33.39	35.61	37.49	38.98	1.10
C	14.20	17.54	21.09	24.67	28.08	31.18	33.85	36.07	37.85	39.24	2.48
F	14.14	17.81	21.47	24.99	28.26	31.22	33.85	36.14	38.11	39.79	1.06
M	15.05	18.38	21.71	24.92	27.94	30.72	33.23	35.47	37.45	39.17	1.23
C	13.84	17.58	21.30	24.86	28.15	31.09	33.69	35.93	37.83	39.44	1.24
F	14.02	17.84	21.55	25.05	28.27	31.18	33.79	36.09	38.10	39.86	0.76
M	14.98	18.42	21.77	24.96	27.94	30.68	33.18	35.43	37.44	39.24	1.35
C	13.71	17.62	21.39	24.92	28.15	31.06	33.62	35.84	37.83	39.51	0.91
F	14.62	17.36	21.03	24.89	28.48	31.57	34.15	36.26	37.98	39.38	3.83
M	15.66	18.00	21.22	24.71	28.04	31.01	33.54	35.65	37.39	38.83	1.57
C	14.31	17.13	20.88	24.78	28.37	31.43	33.97	36.03	37.70	39.06	3.98
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Normally the curves of the functions or the models provide the best fit to the data in the sense that the error sum of squares is the smallest [9]. So, according to the error sum of squares, the Bertalanffy model has the best fit for female and combined sex and the Logistic model has the best fit for male. Although the Logistic, Gompertz, Bertalanffy models are slightly different, the Holling model is the worst model for female, male and combined sex. But the Holling model has the biggest maximum specific growth rate and fork length at the inflection point for female, male and combined sex. So we could say that the Bertalanffy model has the best fit as a growth model according to the error sum of squares in this study. In addition, we can recommend to use the Bertalanffy model for the fork length of female, male and combined sex. Since the Bertalanffy model has the best fit according to the error sum of squares in this study, we think that its estimate of the fork length at age zero is more realistic.

Conclusion

More information about the growth with the parameters of the new modified models could be obtained directly. So the models used in this way could be much more useful. Also, researchers could make more quick and accurate decisions about the issue concerned.

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