NUMERICAL TREATMENT OF THE MODEL VALIDATION INDEX: COMPARISON OF NUMERICAL METHODS AND SELECTION OF BEST-FIT DATA

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Abstract
In the scenario of the competition between two biological species, we have applied the method of a simulation analysis to study the impact of the initial condition variation on the concept of the model validation index which has not been previously studied. In this study, one has found the numerical method of the ODE 23 to have the value of 2.3547 when the initial condition boundary values are 0.45 and 0.55. In each group of the initial condition variation and its corresponding numerical method implementation, we have observed that the numerical method of the ODE 15s irrespective of the choice of the initial condition is a poor predictor of the model validation index. However, when the initial condition is (0.45, 0.55), the ODE 15s can be considered to be a relatively better predictor of the model validation index when compared with the scenarios of the initial condition data of (0.5, 0.6) and (0.55, 0.65). We would expect these contributions to provide a further insight in the prediction of some elements of biodiversity (loss or gain in the yields of yeast species). The full novel results that we have obtained which we have not seen elsewhere are presented and discussed.

Keywords: *Numerical, Treatment, Model Validation Index, Comparison, Numerical Methods.*

Introduction

Since a mathematical model is only an approximate description of a real life phenomenon, it is ideal to measure the fitness of the derived data by using the method of a model validation index which is based on the implementation of the infinity-norms error analysis. From the theory of mathematical analysis, the smaller value of the inifinity-norms value which forms part of the p-vector norms is an indication of the best-fit characteristic of the data sets. To tackle this challenging numerical analysis research problem, we have utililised four (4) distinct numerical methods of different numerical computational efficiency namely the ODE 45, the ODE 15s, ODE 23, and ODE 23tb. From these numerical methods, we will be in a firm position to select the numerical method that is associated with the smallest model validation index in the context of the initial condition variation of (0.5, 0.6), (0.45, 0.55), and (0.55, 0.65). Other related numerical treatments of scientific phenomena have cited in the contributions of [1-10] without a detailed numerical simulation analysis of the model validation index.

Mathematical Formulations

Following Pielou (1977), we have considered the following continuous dynamical system of a non-linear first order ordinary differential equations with the mathematical structure

$$\frac{dx}{dt} = \alpha_1 x - \beta_1 x^2 - r_1 xy \qquad (1)$$

$$\frac{dy}{dt} = \alpha_2 y - \beta_2 y^2 - r_2 xy \qquad (2)$$

Such that $x(0) = x_0 > 0$ and $y(0) = y_0 > 0$. For the purpose of this study, the precise values of the growth rate model parameter values are 0.1 and 0.08, the intra-species coefficients of 0.0014 and 0.001 followed by the inter-species coefficients of 0.0012 and 0.0009 such that x(0) = 4 grams per area of grass cover and y(0) = 10 grams of grass cover. Here, the independent variable is denoted by t in the unit of time whereas the two dependent variables x(t) and y(t) define the biomasses of two competing yeast species.

Method of Analysis

On the simplifying assumption of three (3) variations of the initial condition boundary specified values of (0.5, 0.6), (0.45, 0.55), and (0.55, 0.65), we have implemented a Matlab numerical algorithms in terms of the ODE 45, ODE 15s, ODE 23 and ODE 23tb to compute the infinity-norms error which represents the model validation index. For the purpose of interpreting the results, the first column data stand for the variation of the time independent variable, the second column data stand for the variation of the solution trajectories growth pattern of the first yeast species, the third column data stand for the variation of the solution trajectories growth pattern of the second yeast while the fourth column data stand for the difference between each time-dependent pair of data from which the metric is mathematically defined and calculated as the absolute value of the difference between the boundaries for each pair of data values.

Results

The full results of this study are presented in Table 1- Table 12.

Table 1: Numerical quantification of the model validation index using ODE 45 numerical method using the initial condition (0.5, 0.6)

0	0.5000	0.6000	-0.1000
1.0000	0.5518	0.6115	-0.0597
2.0000	0.6089	0.6231	-0.0143
3.0000	0.6718	0.6350	0.0368
4.0000	0.7411	0.6470	0.0941
5.0000	0.8175	0.6592	0.1583
6.0000	0.9017	0.6716	0.2301
7.0000	0.9944	0.6842	0.3103
8.0000	1.0965	0.6969	0.3996
9.0000	1.2088	0.7098	0.4991
10.0000	1.3325	0.7228	0.6096
11.0000	1.4684	0.7360	0.7324
12.0000	1.6179	0.7494	0.8685
13.0000	1.7822	0.7629	1.0194
14.0000	1.9627	0.7764	1.1863
15.0000	2.1608	0.7901	1.3707
16.0000	2.3782	0.8039	1.5743

17.0000	2.6166	0.8178	1.7989
18.0000	2.8779	0.8317	2.0462
19.0000	3.1640	0.8456	2.3183
20.0000	3.4770	0.8596	2.6174
	8.0442	5.3592	**2.6174**

Table 2: Numerical quantification of the model validation index using ODE 15s numerical method using the initial condition (0.5, 0.6)

0	0.5000	0.6000	-0.1000
1.0000	0.5525	0.6115	-0.0590
2.0000	0.6100	0.6232	-0.0131
3.0000	0.6734	0.6350	0.0383
4.0000	0.7430	0.6471	0.0960
5.0000	0.8198	0.6593	0.1605
6.0000	0.9043	0.6716	0.2327
7.0000	0.9975	0.6842	0.3133
8.0000	1.0999	0.6969	0.4030
9.0000	1.2128	0.7098	0.5029
10.0000	1.3368	0.7229	0.6140
11.0000	1.4734	0.7361	0.7373
12.0000	1.6234	0.7494	0.8740
13.0000	1.7884	0.7629	1.0255
14.0000	1.9695	0.7764	1.1930
15.0000	2.1684	0.7901	1.3783
16.0000	2.3866	0.8039	1.5827
17.0000	2.6259	0.8178	1.8081
18.0000	2.8881	0.8317	2.0564
19.0000	3.1751	0.8456	2.3295
20.0000	3.4892	0.8595	2.6296

18.1473 5.3871 **2.6296**

Table 3: Numerical quantification of the model validation index using ODE 23 numerical method using the initial condition (0.5, 0.6)

0	0.5000	0.6000	-0.1000
1.0000	0.5518	0.6115	-0.0597
2.0000	0.6088	0.6231	-0.0143
3.0000	0.6718	0.6350	0.0368
4.0000	0.7411	0.6470	0.0940
5.0000	0.8175	0.6592	0.1582
6.0000	0.9016	0.6716	0.2300
7.0000	0.9943	0.6842	0.3101
8.0000	1.0963	0.6969	0.3994
9.0000	1.2086	0.7098	0.4988
10.0000	1.3321	0.7228	0.6093
11.0000	1.4681	0.7360	0.7320
12.0000	1.6175	0.7494	0.8681
13.0000	1.7817	0.7629	1.0188
14.0000	1.9620	0.7764	1.1856
15.0000	2.1601	0.7901	1.3699
16.0000	2.3774	0.8039	1.5734
17.0000	2.6156	0.8178	1.7979
18.0000	2.8767	0.8317	2.0450
19.0000	3.1626	0.8456	2.3170
20.0000	3.4755	0.8596	2.6159

18.0343 5.3562 **2.6159**

Table 4: Numerical quantification of the model validation index using ODE 23tb numerical method using the initial condition (0.5, 0.6)

0	0.5000	0.6000	-0.1000
1.0000	0.5518	0.6115	-0.0597
2.0000	0.6089	0.6231	-0.0142
3.0000	0.6720	0.6350	0.0370
4.0000	0.7414	0.6470	0.0944
5.0000	0.8181	0.6592	0.1588
6.0000	0.9023	0.6716	0.2307
7.0000	0.9953	0.6842	0.3112

8.0000	1.0976	0.6969	0.4007
9.0000	1.2103	0.7098	0.5005
10.0000	1.3341	0.7228	0.6113
11.0000	1.4706	0.7360	0.7346
12.0000	1.6204	0.7494	0.8710
13.0000	1.7853	0.7628	1.0225
14.0000	1.9662	0.7764	1.1898
15.0000	2.1652	0.7901	1.3750
16.0000	2.3832	0.8039	1.5793
17.0000	2.6225	0.8177	1.8048
18.0000	2.8846	0.8317	2.0529
19.0000	3.1719	0.8456	2.3263
20.0000	3.4857	0.8595	2.6262
	18.1009	5.3767	**2.6262**

Table 5: Numerical quantification of the model validation index using ODE 45 numerical method using the initial condition (0.45, 0.55)

0	0.4500	0.5500	-0.1000
1.0000	0.4967	0.5606	-0.0639
2.0000	0.5481	0.5713	-0.0232
3.0000	0.6049	0.5823	0.0226
4.0000	0.6674	0.5933	0.0741
5.0000	0.7364	0.6046	0.1317
6.0000	0.8123	0.6161	0.1963
7.0000	0.8960	0.6277	0.2684
8.0000	0.9882	0.6394	0.3488
9.0000	1.0897	0.6514	0.4383
10.0000	1.2014	0.6634	0.5380
11.0000	1.3244	0.6757	0.6487
12.0000	1.4596	0.6880	0.7716
13.0000	1.6083	0.7006	0.9078
14.0000	1.7718	0.7132	1.0586
15.0000	1.9513	0.7259	1.2254
16.0000	2.1485	0.7388	1.4097
17.0000	2.3648	0.7517	1.6131

18.0000	2.6021	0.7647	1.8374
19.0000	2.8622	0.7778	2.0844
20.0000	3.1470	0.7909	2.3561
	16.1179	4.8037	**2.3561**

Table 6: Numerical quantification of the model validation index using ODE 15s numerical method using the initial condition (0.45, 0.55)

0	0.4500	0.5500	-0.1000
1.0000	0.4973	0.5606	-0.0633
2.0000	0.5492	0.5714	-0.0222
3.0000	0.6063	0.5823	0.0240
4.0000	0.6691	0.5934	0.0757
5.0000	0.7384	0.6046	0.1337
6.0000	0.8147	0.6161	0.1986
7.0000	0.8988	0.6277	0.2711
8.0000	0.9913	0.6395	0.3518
9.0000	1.0932	0.6514	0.4419
10.0000	1.2054	0.6635	0.5419
11.0000	1.3288	0.6757	0.6531
12.0000	1.4646	0.6881	0.7765
13.0000	1.6139	0.7006	0.9133
14.0000	1.7779	0.7132	1.0647
15.0000	1.9582	0.7259	1.2323
16.0000	2.1561	0.7388	1.4173
17.0000	2.3733	0.7517	1.6216
18.0000	2.6114	0.7647	1.8467
19.0000	2.8724	0.7778	2.0946
20.0000	3.1581	0.7909	2.3673
	16.2117	4.8291	**2.3673**

Table 7: Numerical quantification of the model validation index using ODE 23 numerical method using the initial condition (0.45, 0.55)

0	0.4500	0.5500	-0.1000
1.0000	0.4967	0.5606	-0.0639
2.0000	0.5481	0.5713	-0.0232
3.0000	0.6048	0.5823	0.0226
4.0000	0.6674	0.5933	0.0740
5.0000	0.7363	0.6046	0.1317
6.0000	0.8122	0.6161	0.1962
7.0000	0.8959	0.6277	0.2682
8.0000	0.9880	0.6394	0.3486
9.0000	1.0895	0.6514	0.4381
10.0000	1.2011	0.6634	0.5377
11.0000	1.3240	0.6757	0.6484
12.0000	1.4592	0.6880	0.7711
13.0000	1.6078	0.7006	0.9073
14.0000	1.7712	0.7132	1.0580
15.0000	1.9507	0.7259	1.2247
16.0000	2.1477	0.7388	1.4089
17.0000	2.3639	0.7517	1.6122
18.0000	2.6010	0.7647	1.8363
19.0000	2.8609	0.7778	2.0831
20.0000	3.1456	0.7909	2.3547
	16.1088	4.8009	**2.3547**

Table 8: Numerical quantification of the model validation index using ODE 23tb numerical method using the initial condition (0.45, 0.55)

0	0.4500	0.5500	-0.1000
1.0000	0.4967	0.5606	-0.0639
2.0000	0.5482	0.5713	-0.0231
3.0000	0.6051	0.5823	0.0228
4.0000	0.6677	0.5933	0.0743
5.0000	0.7368	0.6046	0.1322
6.0000	0.8129	0.6161	0.1968
7.0000	0.8968	0.6277	0.2692
8.0000	0.9892	0.6394	0.3497

9.0000	1.0910	0.6513	0.4397
10.0000	1.2030	0.6634	0.5395
11.0000	1.3263	0.6757	0.6507
12.0000	1.4619	0.6880	0.7738
13.0000	1.6111	0.7005	0.9106
14.0000	1.7750	0.7132	1.0618
15.0000	1.9553	0.7259	1.2294
16.0000	2.1530	0.7388	1.4142
17.0000	2.3702	0.7517	1.6185
18.0000	2.6082	0.7647	1.8435
19.0000	2.8694	0.7778	2.0917
20.0000	3.1550	0.7908	2.3641
	16.1698	4.**8196**	**2.3641**

Table 9: Numerical quantification of the model validation index using ODE 45 numerical method using the initial condition (0.55, 0.65)

0	0.5500	0.6500	-0.1000
1.0000	0.6069	0.6624	-0.0555
2.0000	0.6696	0.6749	-0.0054
3.0000	0.7386	0.6877	0.0509
4.0000	0.8148	0.7006	0.1141
5.0000	0.8986	0.7138	0.1848
6.0000	0.9910	0.7271	0.2639
7.0000	1.0926	0.7406	0.3520
8.0000	1.2045	0.7543	0.4502
9.0000	1.3276	0.7681	0.5595
10.0000	1.4630	0.7821	0.6809
11.0000	1.6119	0.7962	0.8157
12.0000	1.7755	0.8105	0.9650
13.0000	1.9552	0.8249	1.1303
14.0000	2.1525	0.8394	1.3130
15.0000	2.3689	0.8541	1.5149
16.0000	2.6063	0.8687	1.7375
17.0000	2.8664	0.8835	1.9829

18.0000	3.1511	0.8983	2.2529
19.0000	3.4627	0.9130	2.5497
20.0000	3.8033	0.9278	2.8755
	19.9546	5.9097	**2.8755**

Table 10: Numerical quantification of the model validation index using ODE 15s numerical method using the initial condition (0.55, 0.65)

0	0.5500	0.6500	-0.1000
1.0000	0.6077	0.6624	-0.0547
2.0000	0.6709	0.6750	-0.0041
3.0000	0.7404	0.6877	0.0526
4.0000	0.8169	0.7007	0.1162
5.0000	0.9011	0.7138	0.1873
6.0000	0.9938	0.7271	0.2667
7.0000	1.0959	0.7406	0.3553
8.0000	1.2083	0.7543	0.4540
9.0000	1.3319	0.7681	0.5638
10.0000	1.4678	0.7821	0.6857
11.0000	1.6173	0.7963	0.8210
12.0000	1.7814	0.8105	0.9709
13.0000	1.9619	0.8249	1.1369
14.0000	2.1598	0.8394	1.3204
15.0000	2.3772	0.8540	1.5231
16.0000	2.6154	0.8687	1.7466
17.0000	2.8764	0.8835	1.9929
18.0000	3.1622	0.8982	2.2639
19.0000	3.4748	0.9130	2.5618
20.0000	3.8165	0.9277	2.8887
	20.0667	5.9400	**2.8887**

Table 11: Numerical quantification of the model validation index using ODE 23 numerical method using the initial condition (0.55, 0.65)

0	0.5500	0.6500	-0.1000
1.0000	0.6069	0.6624	-0.0555
2.0000	0.6695	0.6749	-0.0054
3.0000	0.7386	0.6877	0.0509
4.0000	0.8147	0.7007	0.1140
5.0000	0.8985	0.7138	0.1847
6.0000	0.9908	0.7271	0.2637
7.0000	1.0924	0.7406	0.3518
8.0000	1.2043	0.7543	0.4500
9.0000	1.3274	0.7681	0.5592
10.0000	1.4627	0.7821	0.6806
11.0000	1.6115	0.7962	0.8152
12.0000	1.7750	0.8105	0.9645
13.0000	1.9546	0.8249	1.1297
14.0000	2.1518	0.8394	1.3123
15.0000	2.3681	0.8541	1.5141
16.0000	2.6053	0.8687	1.7366
17.0000	2.8653	0.8835	1.9818
18.0000	3.1499	0.8983	2.2516
19.0000	3.4613	0.9130	2.5482
20.0000	3.8017	0.9278	2.8739
	19.9439	5.9064	**2.8739**

Table 12: Numerical quantification of the model validation index using ODE 23tb numerical method using the initial condition (0.55, 0.65)

0	0.5500	0.6500	-0.1000
1.0000	0.6069	0.6624	-0.0555
2.0000	0.6696	0.6749	-0.0053
3.0000	0.7389	0.6877	0.0512
4.0000	0.8151	0.7006	0.1144
5.0000	0.8992	0.7138	0.1854
6.0000	0.9916	0.7271	0.2645
7.0000	1.0936	0.7406	0.3530
8.0000	1.2057	0.7543	0.4514
9.0000	1.3292	0.7681	0.5611

10.0000	1.4649	0.7821	0.6828
11.0000	1.6142	0.7962	0.8180
12.0000	1.7782	0.8105	0.9677
13.0000	1.9585	0.8249	1.1336
14.0000	2.1563	0.8394	1.3169
15.0000	2.3736	0.8540	1.5196
16.0000	2.6116	0.8687	1.7429
17.0000	2.8727	0.8834	1.9893
18.0000	3.1584	0.8982	2.2602
19.0000	3.4712	0.9130	2.5582
20.0000	3.8127	0.9277	2.8850
	20.0160	5.9285	**2.8850**

Discussion of Results

From Table 1 to Table 4 when the initial condition boundaries are 0.5 and 0.6, the smallest model validation index value is 2.6159 which is associated with the numerical method of ODE 23 while the other model validation index values are 2.6174, 2.6262 and 2.6296 with respect to the numerical methods of ODE 45, ODE 23tb and ODE 15s. On the basis of this numerical simulation analysis, we have observed that the ODE 23 is considered to produce best-fit time dependent solution trajectories which is followed by the ODE 45, ODE 23tb and ODE 15s which is a relatively poor predictor of best-fit data.

In the scenario of the initial condition boundary values of 0.45 and 0.55, the best-fit data are associated with the ODE 23 numerical method which has the model validation index value of 2.3547 (Table 5 to Table 8). In contrast, when the initial condition boundary values of 0.55 and 0.65 were considered, the best-fit data are associated with the ODE 23 numerical method which has the model validation index value of 2.8739 (Table 9 to Table 12).

Conclusion and Further Research

In the specific Pielou (1977) model formulation of the competition between two yeast species which did not study the prediction of the model validation index so as to select the best-fit data, the present study has found that the best model validation index is 2.3547 which is associated with the numerical method of ODE 23 when the initial condition boundaries are 0.45 and 0.55. This numerical mathematics idea in solving and analyzing the model validation index can be extended to tackle similar interaction problems in the context of commensalistic, mutualistic and predation types of yeast species which we did not consider and study in this present analysis.

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