Phenological models on microbial growth – which model is better and why?

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Abstract

Introduction

Phenological models are expected to fit data trends within its biological field. Yet due to different reasons, models developed and published from one sample may not fit the others. These reasons may be due to data variabilities, confounding factors, inaccurate assumptions or models being too-specific. This project is aimed at compare and contrast published phenological models on microbial population size data, highlighting which is a better model under what conditions. The hypotheses are:

- published phenological models are better than polynomials in describing microbial population size;
- appropriate phenological model(s) can be identified through distinguishable shapes of microbial population size; and
- parameters of data under each phenological model is clustered, similar with dataset best-described by the same model but different from those described by other models.

Methods

Experimental microbial population growth data library were divided into individual data subsets through six filters ("Temperature (in ^oC)", "Microbial clade", "growth substrate materials", "experimental replicate number", "population data recording unit" and "data source"). Records with data unit "OD_595" were scaled into optical density percentages (i.e. data*100) to facilitate general analyses workflow. Independent (or explanatory) variable was “Time (hr)” and dependent (or response) variable was “population size”.

Some raw data were recorded in minutes (instead of hour). This record artifact was not corrected because of two reasons: 1. shape of curves were the main concern instead of independent variable’s scale; and 2. the unit was consistent within each data subset.

Model assessment

Six candidate models were assessed, four phenological and two polynomial equations. They were “Verhulst (classical)”[1], “modified Gompertz”[2], “Baranyi”[3], “Buchanan”[4], “quadratic” and “cubic”. NLLS was used only on the four phenological models and linear model-fitting was done on the two polynomials. Starting values selection (for phenological models only) was described below:

Initial (N0) and final (K) population sizes were selected to be the minimum and maximum values of each data subset respectively. Maximum growth rate (r.max) was selected by linear model through a recursive manner. For every iteration, population size data from the top 5% independent variable values were excluded from the linear model calculation. The data and slope would only be recorded if it was positive, higher adjusted R^2 value and larger slope than the recorded “best slope” value. After scanning from the maximum side, the best slope and its respective data were taken out and screened from the minimum side. Final best slope and x-intercept were regarded as the r.max and relative time lag (t.lag) of the population (in the source experiment) respectively. Time which this linear model intersected with K was regarded as the time achieving carrying capacity (t.K). Population data was then classified into three groups (gx) according to the time: $\text{g1} \leq \text{t.lag} < \text{g2} < \text{t.K} \leq \text{g3}$. 5% was chosen as the scanning threshold because I assumed this resolution was fine enough for achieving good starting values for NLLS fitting. Inputs for phenological modelswere listed below (popn & time were the dependent and independent variables respectively):

$$\begin{aligned}
\text{Verhulst (classical):} \quad & \text{popn} = f(\text{N0, K, r.max, time}) \\
\text{modified Gompertz:} \quad & \text{popn} = f(\text{N0, K, r.max, time, t.lag}) \\
\text{Baranyi:} \quad & \text{popn} = f(\text{N0, K, r.max, time, t.lag}) \\
\text{Buchanan:} \quad & \text{popn} = f(\text{N0, K, r.max, time, t.lag, gx})
\end{aligned}$$

All test starting values were than sampled from normal distribution with mean as the estimated value and standard deviation (sd) of 1. The sd value was chosen because of different reasons for each parameters. N0 and K were directly extracted from the raw experimental data, which could be assumed being an accurate estimate for that data subset (hence a small sd was logical). r.max was a guesstimated value from fitting linear models. This process could potentially be affected by extreme values in the data and hence a large sd should be preferred. 100 trials were done as a optimal value under a trade-off between efficiency and accuracy.

Only AIC[5–7] was used to select for optimal parameter values within each phenological model and best model between the six candidates for a data subset. Reasons would be listed in Discussion section. For models with more than one parameter sets as sharing the lowest AIC value, the first set of values from the random sampling trials were used for downstream analyses. AIC tolerance threshold was expanded to min(AIC)+2[8] to incorporate more accepted models for analyses.

Statistical analysis

Kruskal test was used for identify the best-fit model among all included model because the count was categorical and not assumed being normally-distributed. Pairwise Nemenyi comparisons would be carried out to identify the best test if p-value of the above test was significant.

Main Assumptions

- there was no negative population growth (i.e. starting population was always lower than carrying capacity), so negative population growth data were set to zeros;
- estimated parameter estimates would always result in a global optimal status in parameter space through the non-linear least squares method (NLLS)

Computing tools

R (ver 3.6.0)[9] was used with "minpack.lm"[10] for computing non-linear least square statistics for model comparisons. "PMCMR"[11] was used for carrying out statistical analyses.

Results

From Fig.1, large fluctuations between each model to be described as "best-fit" were observed. However the occurrence difference was not statistical significant. Among the counts, there were

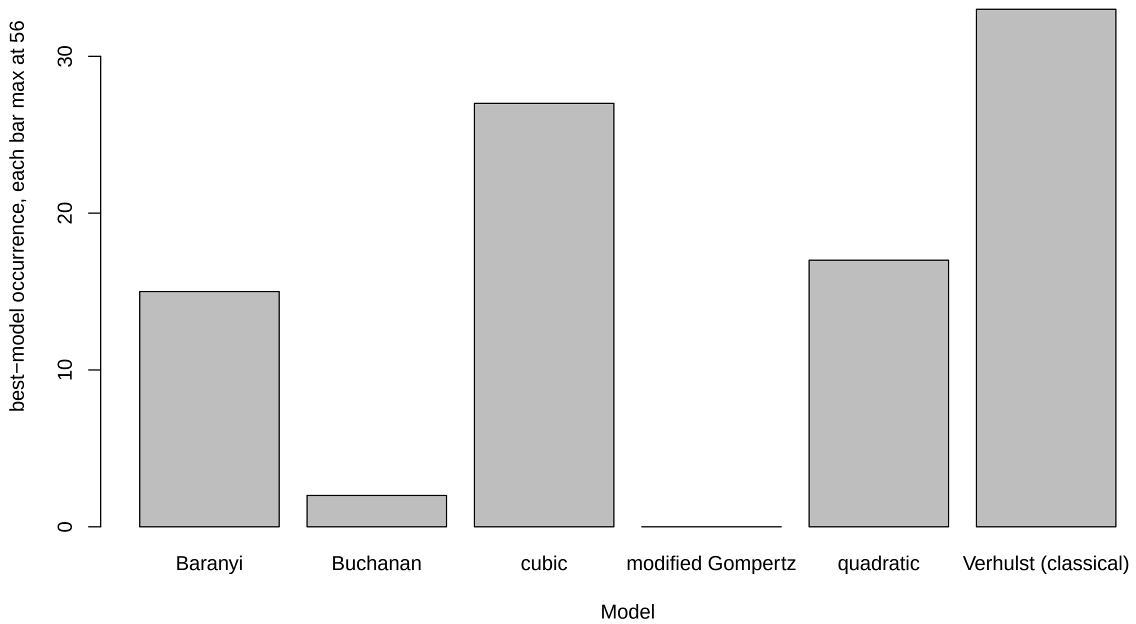

Figure 1: Barplot showing the number of "best model" identification under AIC model-selection methods with " Kruskal-Wallis rank sum test " statistic $X^2 = 5$, df = 5 , p = 0.42

56 datasets with more than one "best-fit" models. Verhulst (classical) and cubic were the top two models selected as "best-fit" for the 38 datasets (33 for Verhulst (classical) and 27 for cubic). There are 9 datasets calling both "best-fit" at the same trial. Between Baranyi and quadratic, the counts were 15 and 17 respectively with 6 datasets calling both models "best-fit".

Discussion

Model fitness to real data and simplistic mathematics were favoured by both AIC[5–7] and BIC[5,12]. Apart from that, BIC also takes account of sample size effect[5,12]. comparisons in different fields[13–18]

Conclusion

Code and Data Availability

All scripts and data used for this report were publicity available at GitHub.

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