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

PokMan HO

Department of Life Sciences, Faculty of Natural Sciences,

Imperial College London

Imperial College London

Approximate Word Count: 717

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

PokMan HO (CID: 01786076)

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 ^{o}C)", "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: $g1 \leq t.lag < g2 < t.K \leq g3$. 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.

Statistical analysis

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)[8] was used with following packages: "ggplot2"[9] was used for visualisation; "reshape2"[10] was used for converting dataset from wide to long format; "scales"[11] was used for improve "ggplot" graphs data presentation; and "minpack.lm"[12] was used for computing non-linear least square statistics for model comparisons.

Results

Discussion

Model fitness to real data and simplistic mathematics were favoured by both AIC[5–7] and BIC[5,13]. Apart from that, BIC also takes account of sample size effect[5,13].
comparisons in different fields[14–19]

Conclusion

Code and Data Availability

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

References

1. McKendrick, A. & Pai, M. K. XLV.—the rate of multiplication of micro-organisms: a mathematical study. *Proceedings of the Royal Society of Edinburgh* **31,** 649–653 (1912).
2. Gil, M. M., Brandão, T. R. & Silva, C. L. A modified Gompertz model to predict microbial inactivation under time-varying temperature conditions. *Journal of Food Engineering* **76.** Bugdeath, 89 –94. ISSN: 0260-8774. `http://www.sciencedirect.com/science/article/pii/S0260877405003389` (2006).
3. Baranyi, J, McClure, P., Sutherland, J. & Roberts, T. Modeling bacterial growth responses. *Journal of industrial microbiology* **12,** 190–194 (1993).
4. Buchanan, R., Golden, M. & Whiting, R. Differentiation of the effects of pH and lactic or acetic acid concentration on the kinetics of Listeria monocytogenes inactivation. *Journal of Food Protection* **56,** 474–478 (1993).
5. Johnson, J. B. & Omland, K. S. Model selection in ecology and evolution. *Trends in ecology & evolution* **19,** 101–108 (2004).
6. Akaike, H. in *Selected papers of hirotugu akaike* 199–213 (Springer, 1998).
7. Burnham, K. & Anderson, D. Model selection and multimodel inference: a practical information-theoretic approach. *Ecological Modelling.*
8. R Core Team. *R: A Language and Environment for Statistical Computing* R Foundation for Statistical Computing (Vienna, Austria, 2019). `https://www.R-project.org/`.
9. Wickham, H. *ggplot2: Elegant Graphics for Data Analysis* ISBN: 978-3-319-24277-4. `https://ggplot2.tidyverse.org` (Springer-Verlag New York, 2016).
10. Wickham, H. Reshaping Data with the reshape Package. *Journal of Statistical Software* **21,** 1–20. `http://www.jstatsoft.org/v21/i12/` (2007).

11. Wickham, H. *scales: Scale Functions for Visualization* R package version 1.0.0 (2018). `https://CRAN.R-project.org/package=scales`.

12. Elzhov, T. V., Mullen, K. M., Spiess, A.-N. & Bolker, B. *minpack.lm: R Interface to the Levenberg-Marquardt Nonlinear Least-Squares Algorithm Found in MINPACK, Plus Support for Bounds* R package version 1.2-1 (2016). `https://CRAN.R-project.org/package=minpack.lm`.

13. Turchin, P. *Complex population dynamics: a theoretical/empirical synthesis* (Princeton university press, 2003).

14. Kuha, J. AIC and BIC: Comparisons of assumptions and performance. *Sociological methods & research* **33,** 188–229 (2004).

15. Aho, K., Derryberry, D. & Peterson, T. Model selection for ecologists: the worldviews of AIC and BIC. *Ecology* **95,** 631–636 (2014).

16. Yang, Y. Can the strengths of AIC and BIC be shared? A conflict between model indentification and regression estimation. *Biometrika* **92,** 937–950 (2005).

17. Vrieze, S. I. Model selection and psychological theory: a discussion of the differences between the Akaike information criterion (AIC) and the Bayesian information criterion (BIC). *Psychological methods* **17,** 228 (2012).

18. Wang, Y. & Liu, Q. Comparison of Akaike information criterion (AIC) and Bayesian information criterion (BIC) in selection of stock–recruitment relationships. *Fisheries Research* **77,** 220–225 (2006).

19. Acquah, H. D.-G. Comparison of Akaike information criterion (AIC) and Bayesian information criterion (BIC) in selection of an asymmetric price relationship. *Journal of Development and Agricultural Economics* **2,** 001–006 (2010).

20. Zwietering, M., De Wit, J., Cuppers, H. & Van't Riet, K. Modeling of bacterial growth with shifts in temperature. *Appl. Environ. Microbiol.* **60,** 204–213 (1994).

21. Schwarz, G. Estimating the dimension of a model. *Ann. Stat.* **6,** 461–464 (1978).

22. Kelley, C. T. *Iterative methods for optimization* (SIAM, 1999).