Machine learning for chaotic time-series data generated from simple food webs

Abstract

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Mathematical models for simple food webs have been shown to exhibit chaotic dynamics which are difficult for ecologists to interpret or predict. The primary objective of this study was to test the ability of a convolutional neural network for classifying chaotic population data. This proved to be successful which led to the secondary goal which was to attempt to infer characteristics of the chaos by visualizing how the trained neural network processed the data. Filters were extracted representing the most common patterns in the chaotic data that were identified by machine learning. Utilizing machine learning and food web theory in this way could be a valuable tool in the future for directing conservation strategies toward a more holistic, network-based approach.

Keywords—chaos, machine learning, population dynamics, ecology, food webs

BACKGROUND

The complexity of nature is as beautiful as it is spirit-crushing for mathematical ecologists. That is because the central mathematical modeling involves nonlinear dynamics, often resulting in chaotic unpredictable systems. Ecologists first began applying nonlinear dynamics to population ecology 50 years ago (Zimmer, 1999), and the progress has been slow. The study of small food webs is especially difficult because community dynamics exhibited by simple food web topologies are chaotic and difficult to interpret. This is where machine learning could be useful, as it has been in many other fields of biology including other network systems such as protein interactions and nerve impulses (Holbrook, 2003).

In this project a convolutional neural network (CNN) was trained on time-series data generated from simple food webs. Inferring food web structure from population data has been attempted in the past using statistical methods such as Bayesian networks (Milns, Beale & Smith, 2010, Faisal et al., 2010, Shandilya & Timme, 2011, Aderhold et al., 2012, Derocles et al., 2018, Manna, Volpert & Banerjee,

2020). However, those methods require data from multiple species in order to test for correlation. The simple CNN used in this project only requires data for one species. This is much more efficient considering data availability in real life, and also beneficial because it reduces processing time and data storage. The other reason the CNN is interesting to apply to this problem is because the filters can be analyzed giving us insight into how the machine algorithm "learns" to recognize the data. This could reveal patterns about the attractors that were not noticeable by the naked human eye.

It has been shown that network structure and dynamics have substantial impacts on ecosystem performance (Bohan et al., 2013). The more that humans benefit from the ecosystem services that nature has to offer, the more we become integrated into the complex network of interactions between all organisms. Thus, nature needs to be preserved for the innate beauty of itself as well as for the ecosystem services it provides that improve the lifestyle of humans.

METHODS

Data was generated for various food webs which were previously described by Fussman and Heber in "Food web complexity and chaotic population dynamics" (Fussman & Heber, 2002). Parameters were set so that communities would coexist, such that the models would be feasible in nature. Python's built-in Runge-Kutta integration method was used to generate the time series, this numerical method ensures that the step size is small enough so that the values do not get chaotically out of control over time. Table 1 shows the three food web topologies that were analyzed in this project and their equations.

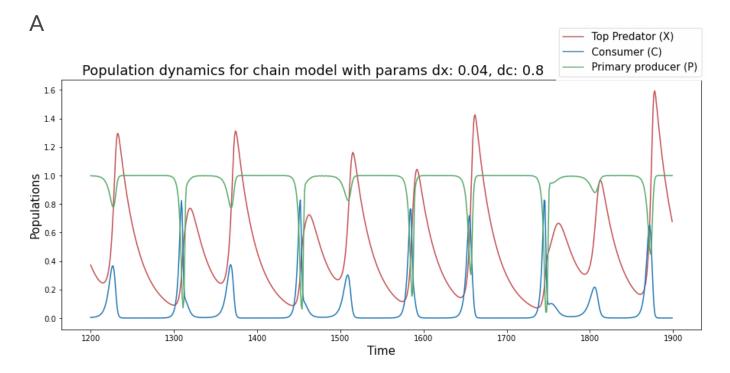
Data was only kept for co-existing communities, that is the ones in which all species survived (all stayed higher than a threshold value of $\epsilon=10^{-9}$). It took about 20 minutes to generate all the data, which traversed a grid of mortality rates. The differential equations were evaluated for 4000 time steps, omitting the first 1000 steps to remove initial transient behaviour of the system. Figure 1 shows an example of a time-series produced for the chain model. In preparation for machine learning, the data was shuffled and 20% was set aside for testing. The labels were hot encoded to remove bias.

Table 1: Simple food web models and their equations as described by Fussman and Heber.

Nickname	Model	Equations
Chain	X Predator C Consumer P Plants	$\frac{dx}{dt} = \frac{(a_3 \cdot c)}{1 + (b_3 \cdot c)} - dx$ $\frac{dc}{dt} = \frac{(a_4 \cdot p)}{1 + (b_4 \cdot p)} - \frac{(a_3 \cdot x)}{1 + (b_3 \cdot c)} - dc$ $\frac{dp}{dt} = r \cdot (1 - p) - \frac{(a_4 \cdot c)}{1 + (b_4 \cdot p)}$
Triangle	G P	$ \frac{dx}{dt} = \frac{(a_3 \cdot c) + (a_5 \cdot p)}{1 + (b_3 \cdot c) + (b_5 \cdot p)} - dx $ $ \frac{dc}{dt} = \frac{(a_4 \cdot p)}{1 + (b_4 \cdot p)} - \frac{(a_3 \cdot x)}{1 + (b_3 \cdot c) + (b_5 \cdot p)} - dc $ $ \frac{dp}{dt} = r \cdot (1 - p) - \frac{(a_4 \cdot c)}{1 + (b_4 \cdot p)} - \frac{(a_5 \cdot x)}{1 + (b_3 \cdot c) + (b_5 \cdot p)} $
Diamond	GI P	$ \frac{dx}{dt} = \frac{(a_3 \cdot c_1) + (a_3 \cdot c_2) + (a_5 \cdot p)}{1 + (b_3 \cdot c_1) + (b_3 \cdot c_2) + (b_5 \cdot p)} - dx $ $ \frac{dc_1}{dt} = \frac{(a_4 \cdot p)}{1 + (b_4 \cdot p)} - \frac{(a_3 \cdot x)}{1 + (b_3 \cdot c_1) + (b_3 \cdot p)} - dc $ $ \frac{dc_2}{dt} = \frac{(a_4 \cdot p)}{1 + (b_4 \cdot p)} - \frac{(a_3 \cdot x)}{1 + (b_3 \cdot c_2) + (b_3 \cdot p)} - dc $ $ \frac{dp}{dt} = r \cdot (1 - p) - \frac{(a_4 \cdot c_1)}{1 + (b_4 \cdot p)} - \frac{(a_4 \cdot c_2)}{1 + (b_4 \cdot p)} - \frac{(a_5 \cdot x)}{1 + (b_3 \cdot c) + (b_5 \cdot p)} $

Global parameters: $a_3 = 1.0$, $b_3 = 2.0$, $a_4 = 7.5$, $b_4 = 5.0$, $a_5 = 0.25$, $b_5 = 0.5$

Varying parameters: d_{y} , d_{z}



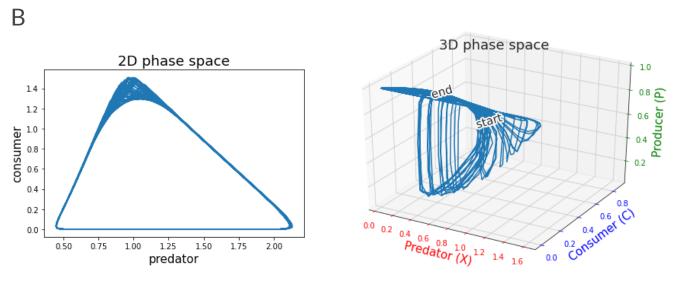




Figure 1: The Chain Model: Different ways to visualize a time series

This is a time series for the 3 species chain model with a low predator death rate (0.04) and high consumer death rate (0.8). A: Population trajectories for a short time range. B: Phase space with the start and end points labelled. It is clear from these graphs that the dynamics are not periodic, but instead follow a strange attractor.

Figure 1 only shows a single time series for a single food web model. For each model, hundreds of time series were generated by iterating over a grid of parameters corresponding to the death rates of the predator and consumer. Each time series had its own strange attractor, and its own unique phase space.

A convolutional neural network (CNN) was trained on this data to attempt to infer food web structure from the time-series for only a single species. The first layer of the 1 dimensional CNN took a single time-series as input and output 32 convolutions with a filter of size 500, although filter size surprisingly did not seem to be important for accuracy. The output was then passed through a max-pooling layer which protects against small shifts in the time series, and finally a fully connected layer with a dropout rate of 0.5, which helps reduce the effect of noise on the learning process.

Once it was established that the CNN could distinguish between food webs from minimal data (time-series for just one species), even when each food web varied in parameters and phase space, the most logical next step was to try to visualize the

filters of the CNN and see if we can make sense of the chaos. In order to do, specific parameters were chosen for a single food web for which the data appeared to oscillate chaotically around a strange attractor. This data was then combined with "random data" and labelled with a single value: 1 for the food web, and 0 for random. By hot-encoding the data (basically distributing the population values into binary bins), and then creating random data of the same shape except the bin chosen is for a random value between the min and max of the actual values, one can compare the likelihood of the data against the null expectation. When a CNN is trained on this data it will be able to optimize its filter accordingly. A slightly different CNN was used to process this data in that it only had 1 convolution in the first layer to allow for easy visualization of the weights

RESULTS

The CNN proved to be easily successful in classifying between the food webs from data for only a single species, which is not possible with simple statistical methods. Figure 2 shows a confusion matrix which can be used to assess the accuracy of the machine learning.

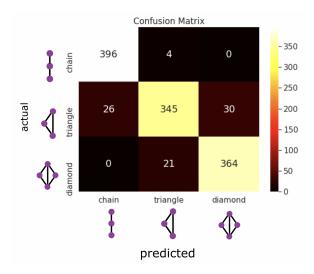


Figure 2: Confusion matrix showing the accuracy of the CNN in classifying between food webs. This is for test data that was not used in training. The diagonal shows all the food webs that were correctly guessed and the rest of the squares show the errors.

The interesting thing about these results is that the chain model is rarely mixed up with the other two models, whereas the triangle is equally mixed up with both, and the diamond is only mixed up with the triangle. This reflects the difference in complexity between the food webs that could be creating some invisible patterns in the time-series.

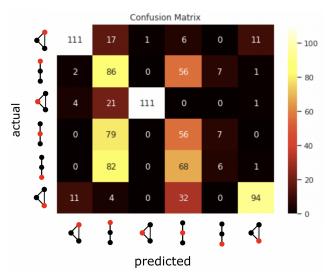
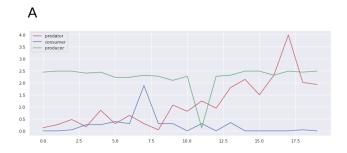
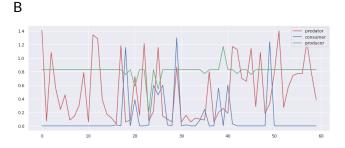


Figure 3: Confusion matrix showing the accuracy of the CNN in classifying between food webs, but also where the species is located within the network. One can observe that predators get confused as consumers, but consumers rarely get confused as predators.

In order to visualize the inner workings of the neural network, a separate dataset was created for a single set of parameters for just one food web model. The initial conditions were randomized and hundreds of time-series were produced, resulting in a variety of dynamics of which none were identical but all looked similar because they oscillated around the same strange attractor. The way that a CNN works is by applying a filter to the data which is then optimized gradually to be as close a match to the data as possible. By identifying the shapes or patterns that result in maximum activation of the filter, it is possible to visualize the inner workings of the deep learning neural network.





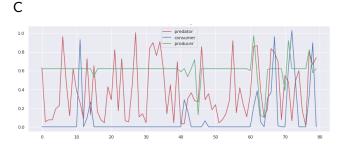


Figure 4: Visualization of the values that result in the maximum activation of the CNN's filter after being trained on chaotic time-series data. Filter size for A, B and C are 20, 60 and 80 respectively.

Visualizing the weights of the CNN produced various results depending on the size of the filter. The results are messy, although this is expected because it is impossible for a single filter to match the chaotic data

perfectly. The idea is to show how that time-series is most likely to look within a time range of the filter size. This is a novel method of visualizing patterns produced by chaotic oscillations around strange attractors.

DISCUSSION

As natural, unbothered habitats become smaller due to the expansion of human civilization, chaotic dynamics will become more prevalent in nature. With the growing population our need to understand and mitigate the impacts of climate change on natural resources is increasingly important. Chaotic dynamics are generally not favourable in nature due to their instability, yet in some cases they actually increase the resilience of ecosystems due to the de-syncing of populations between source and sink habitats. It is interesting to question what other types of functionality chaotic regimes may have.

An interesting aspect of chaotic dynamics is their tendency toward self-organization, autocatalysis, and autopoiesis as described eloquently by Holbrook in his essay "Adventures in Complexity" (Holbrook, 2003). The way that DNA randomly arranged itself into a self-reproducing structure, or that random genetic mutations gradually accumulate over millions of years into brilliant macroevolutionary adaptations, indicate that perhaps there is a sort of unknown deeper organization to chaos that is yet to be discovered. This theory can be applied to all sorts of chaotic network dynamics including those produced in ecological systems, business organizations, or even rhythms and melodies in jazz.

The ecological implication of this research is to be able to understand chaotic dynamics in nature as well as in the lab. From there we may be able to infer the types of chaos that are more likely to be seen in nature, or that lead to robust ecosystems. In some ecosystems where there is a source and sink population it can be advantageous to have chaotic dynamics because it prevents the populations from going extinct at the same time, thus the thriving population can always replenish the suffering one. It would be interesting to see future research in this field involving spatio-temporal data and machine learning.

CONCLUSION

This paper introduces a novel method of inferring ecological networks from minimal data, and is also useful in the broader sense of analyzing chaos. Utilizing machine learning and food web theory in this way could be a valuable tool in the future for directing conservation strategies toward a more holistic, network-based approach. Future research could include spatio-temporal simulations that incorporate factors such as nutrient diffusion, migration between habitats, weather, or seasonal effects. It would be interesting to see what kind of spatial dynamics allow for certain communities to co-exist when they normally would be too chaotic in a more simple model, as well as how the chaotic dynamics interact with other factors.

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REFERENCES

- Aderhold, A., Husmeier, D., Lennon, J. J., Beale, C. M., & Smith, V. A. (2012). Hierarchical bayesian models in ecology: Reconstructing species interaction networks from non-homogeneous species abundance data. *Ecological Informatics*, 11, 55-64. doi:10.1016/j.ecoinf.2012.05.002
- Bohan, D., Raybould, A., Mulder, C., Woodward, G., Tamaddoni-Nezhad, A., Bluthgen, N., ... Macfadyen, S. (2013). Networking Agroecology: Integrating the Diversity of Agroecosystem Interactions. doi:10.1016/B978-0-12-420002-9.00001-9
- 3. Derocles, S. A., Bohan, D. A., Dumbrell, A. J., Kitson, J. J., Massol, F., Pauvert, C., ... Evans, D.

- M. (2018). Biomonitoring for the 21st Century: Integrating next-generation sequencing into ecological network analysis. *Next Generation Biomonitoring: Part 1*, 1-62. doi:10.1016/bs.aecr.2017.12.001
- Faisal, A., Dondelinger, F., Husmeier, D., & Beale, C. (2010). Inferring species interaction networks from species abundance data: A comparative evaluation of various statistical and machine learning methods. doi:10.1016/j.ecoinf.2010.06.005
- Holbrook, B. M.,. (2003). Adventures in Complexity: An Essay on Dynamic Open Complex Adaptive Systems. Retrieved April 16, 2021, from https://issuu.com/gfbertini/docs/adventures_i n_complexity_-_an_essay_on_dynamic_ope
- 6. Fussmann, G. F., & Heber, G. (2002). Food web complexity and chaotic population dynamics. Ecology Letters, 5(3), 394-401. doi:10.1046/j.1461-0248.2002.00329.x
- 7. Tamaddoni-Nezhad, A. Bohan, D., A., Raybould, A., Muggleton, S. Machine Learning a Probabilistic Network of Ecological Interactions. (2012). *Lecture Notes in Computer Science* 7207:332-346 doi:10.1007/978-3-642-31951-8_28
- Manna, K., Volpert, V., & Banerjee, M. (2020). Dynamics of a diffusive two-prey-one-predator model with nonlocal intra-specific competition for both the prey species. Mathematics, 8(1), 101. doi:10.3390/math8010101
- 9. Milns, I., Beale, C. M., & Smith, V. A. (2010). Revealing ecological networks using Bayesian network inference algorithms. *Ecology*, *91*(7), 1892-1899. doi:10.1890/09-0731.1
- Shandilya, S. G., & Timme, M. (2011). Inferring network topology from complex dynamics. New Journal of Physics, 13(1), 013004. doi:10.1088/1367-2630/13/1/013004
- 11. Zimmer, C. (1999). Life after chaos. *Science*, 284(5411): 83-86. doi:10.1126/science.284.5411.8