

SCINet Newsletter: January 2023

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RESEARCH SPOTLIGHT

Research Spotlight: Modeling the Spread of a Livestock Disease With Semi-Supervised Spatiotemporal Deep Neural Networks

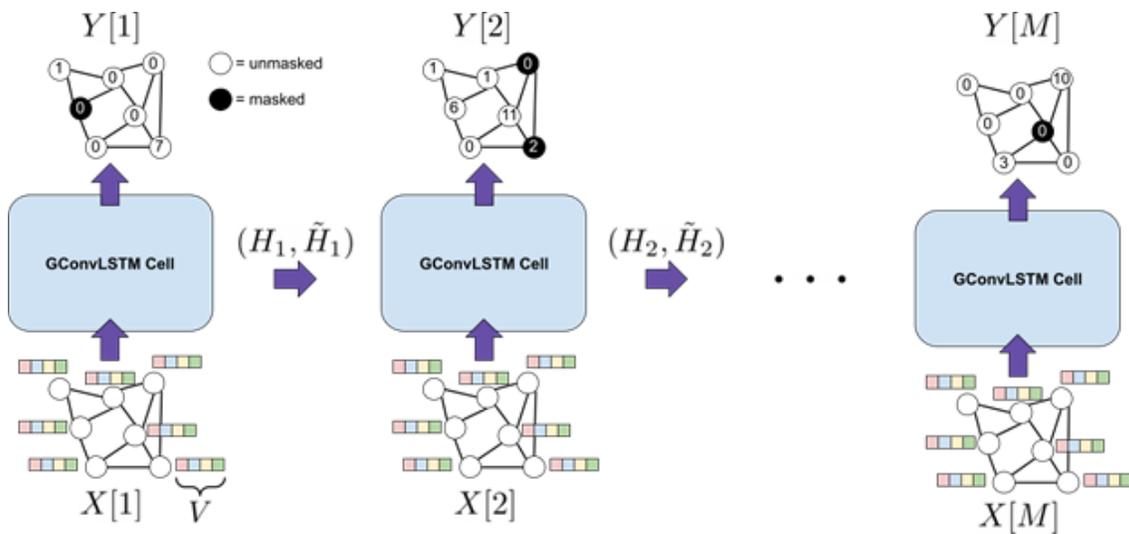


Figure 1. An overview of the graph spatiotemporal deep neural network that was trained to model the spread of vesicular stomatitis. The input to the model is a sequence of graphs where each node contains environmental and anthropogenic variables for a specific county in a specific month. The output of the model is also a sequence of graphs where each node indicates the reported number of vesicular stomatitis cases for a specific county in a specific month.

By Michael A. Alcorn; AI Center of Excellence Fellow

Over the past 20 years, the Western United States has experienced several widespread outbreaks of vesicular stomatitis (VS), a disease that affects livestock. Although infected animals generally clear VS without serious long-term effects, the initial symptoms (e.g., blisters on the lips) resemble foot-and-mouth disease (FMD), which is a much more severe illness that can wreak havoc on the agriculture sector of the economy. As a result,

developing methods for determining as early as possible whether VS/FMD-like symptoms are actually VS or FMD is of pressing importance. One potentially informative signal for assessing the likelihood of a VS infection is the likelihood that the disease is spreading in nearby regions.

AI Center of Excellence Fellow Dr. Michael Alcorn has been researching the potential for using spatiotemporal deep neural networks (STNNs) to model VS risk through both space and time. Specifically, he has investigated two alternative approaches for encoding spatial inputs—grids and graphs—and two corresponding STNNs—convolutional long short-term memory recurrent neural networks (ConvLSTMs) and graph ConvLSTMs (GConvLSTMs).

To train the STNNs, Dr. Alcorn worked with former SCINet Fellow Dr. Kerrie Geil and collaborators to construct the largest dataset so far of geotagged case reports for VS in the U.S. and Mexico from 2001 to 2020. These case reports were then linked to temporally varying environmental and anthropogenic variables recorded at a 30 km² resolution on a national scale, all of which was accomplished using SCINet's high-performance computing clusters.

When modeling reported VS cases in the U.S. spatially, the ConvLSTM struggled—likely because of the rarity of reported VS cases in the dataset; however, the ConvLSTM was more effective than a non-STNN and linear model when modeling the aggregated VS cases per month. In contrast, the GConvLSTM was more effective than a non-STNN and linear model when modeling reported VS cases in the U.S. county-wise, and it identified plausible regions of VS risk. Additionally, when jointly trained on U.S. and Mexico data, the GConvLSTM's performance on U.S. counties slightly improved, which suggests there are shared factors influencing VS spread between the two countries. Together, these results (a) highlight the importance of accounting for spatiotemporal dynamics when modeling the spread of livestock diseases and (b) lay a foundation for further exploration of STNNs as models for investigating these systems.

The code for implementing and training the STNNs was written in Python and uses the deep learning library PyTorch. The code for the project will be released as an open-source GitHub repository soon, which will allow other scientists to easily adapt these state-of-the-art machine learning techniques to their own projects. This work was presented at the 2022 AGU Fall Meeting, and slides for that presentation can be found [here](#).

SCINet and AI COE Fellows



Welcome **Dr. Sanghyun Lee**, SCINet/AI-COE Postdoctoral Fellow. Dr. Lee completed his PhD in Agricultural and Biological Engineering at the University of Illinois at Urbana-Champaign with a Computational Science and Engineering concentration in 2022. His dissertation revolves around surface and subsurface hydrology, sediment fate and transport, analyses of geospatial data, development, and integration of hydrologic models, algorithms, and analyses of ecosystem responses under environment changes. He received his M.S. in Civil and Environmental Engineering

from the University of Illinois at Urbana-Champaign, and his undergraduate degree in Civil and Environmental Engineering from Dankook University, South Korea. As a USDA-ARS SCINet Postdoctoral Fellow working with ARS Scientist Dr. Daniel Moriasi, Dr. Lee will develop a drought prediction tool using AI technology and HPC environment. This effort will provide critical information for timely decision-making to agricultural producers and water resource managers to address water stress and determine plausible systems.



Welcome **Dr. Jihyun Park**, SCINet/AI-COE Postdoctoral Fellow. Dr. Park was first introduced to molecular biology research at Rutgers University, where she received her B.S. in Chemical Engineering. Dr. Park completed her Ph.D. in Chemical Engineering at Georgia Institute of Technology in 2022, where her work focused on kinetically modelling a plant sugar membrane transporter and using

cheminformatics to explore its substrate specificity. Dr. Park is now a SCINet Postdoctoral fellow under the mentorship of Dr. Clifton Fagerquist at USDA Western Regional Research Center in Albany, CA. Dr. Park's current project focuses on predicting structural features of proteins from pathogenic bacteria and analyzing how these features affect their fragmentation in mass spectrometry.



Welcome **Dr. Laura Tibbs-Cortes**, SCINet/AI-COE Postdoctoral Fellow. Dr. Tibbs-Cortes earned a B.A. in Biology from Benedictine College in Atchison, KS in 2017. She then began her graduate studies at Iowa State University in Ames, Iowa as an NSF Graduate Research Fellow. Dr. Tibbs-Cortes completed her Ph.D. from ISU in Genetics and Genomics with a minor in Statistics in 2022. Her dissertation research focused on identifying genetic and environmental factors underlying nutritional and agronomic traits in maize. In addition, she has conducted research on the microbiome of tardigrades. In her research, she enjoys

integrating multiple types of big, “omic” data (genome, transcriptome, envirome, microbiome, etc.) to understand biological questions from a whole system approach. As a SCINet/AI-COE Postdoctoral Fellow, Dr. Tibbs-Cortes is working with Dr. Xianran Li studying phenotypic plasticity of crop performance and how it is affected by climate. She is excited to be working with new (to her) species including wheat and switchgrass.



Welcome **Dr. Collins Wakholi**, SCINet/AI-COE Postdoctoral Fellow. Dr. Wakholi is an agricultural engineer with a PhD from Chungnam National University in South Korea. He has extensive experience in agricultural engineering, particularly in the design and implementation of computer vision systems. Dr. Wakholi is currently working on the research and development of AI-driven image analysis algorithms aimed at facilitating the extraction of valuable insights from image data for scientists and researchers. Dr. Wakholi joins the lab of ARS Scientist Dr. Devin Rippner in Corvallis, OR.



Welcome **Dr. Rachel R. Harman**, SCINet/AI-COE Postdoctoral Fellow. Dr. Harman is a behavior and landscape ecologist who studies the responses of plants and insects to anthropogenically altered habitats. She received her B.S. in biology teaching and M.S. in biological science at Indiana University-Purdue University Fort Wayne. In 2020, she received her Ph.D. in biological sciences from Louisiana State University. Since then, Dr. Harman has worked at Kansas State University as a postdoc researching spillover movement and developing entomology-based coursework. Her research encompasses a wide spatio-temporal scale, from the immediate movement decisions of individuals in a single patch to multi-generational behavioral changes of communities in a landscape. As a SCINet Postdoctoral Fellow at the USDA-ARS Center for Animal Health and Grain Research, Dr. Harman brings an ecological perspective to an applied pest management program. Her research involves modeling the potential distribution, movement, species competition, and niche overlap of grain pest species. Dr. Harman is excited about the prospect of improving her quantitative skills and producing manuscripts that can be used to decrease biosecurity risks through timely surveillance programs and management implementation.



Welcome **Amira Burns**, SCINet/AI-COE Fellow. Amira Burns received her B.A. in English from the University of Pennsylvania and her M.B.A. from the University of Wisconsin – Milwaukee and worked in corporate sales before falling in love with statistics and deciding to change careers. She completed her Masters in Applied Statistics from Colorado State University in 2022, focusing on Bayesian and Frequentist applications to research in human and animal health. She first joined USDA – APHIS in 2021

as a Research Associate through CSU to provide statistical support in surveillance and disease monitoring, transitioning to model evaluation and post-processing analyses for Dr. Ryan Miller's CameraTrapDetector tool – a deep learning object detection model for classifying and counting animals in camera trap images.

As a SCINet Fellow under the mentorship of Dr. Miller and Dr. Hailey Wilmer with ARS, Amira will use her expertise in applied statistics and machine learning to further develop the model, its associated R package, and workflows within a scientific research framework; facilitate collaboration related to the tool's use and development; and provide statistical support to projects using the model. She is excited to continue developing expertise in deep learning to facilitate research into animal behavior and connect with subject experts. On weekends you will find her out on the trails around Jackson Hole, behind a pair of binoculars, looking for birds.



Welcome **Dr. Kevin Li**, SCINet/AI-COE Postdoctoral Fellow. Dr. Li is interested in understanding the effects of the landscape on ecosystem services. He received master's degrees in Landscape Architecture and Conservation Ecology from the University of Michigan. He went on to complete a PhD at the University of Goettingen (Germany) in 2020, studying the impacts of an oil palm transformation landscape on pollination ecology in Jambi, Indonesia. Since then he has studied critical transitions in coffee rust epidemics and worked with UAV remote sensing data to

understand coffee farm management as a postdoc at the University of Michigan. He is excited to return to pollination research and join Dr. Sarah Goslee's collaboration in State College, Pennsylvania. He will support ongoing work to model floral resources in the landscape over space and time and begin work on modeling tradeoffs between multiple ecosystem services resulting from land management decisions, using SciNet's computing resources to implement multi-criterion optimization to consider costs and benefits in an artificial intelligence framework.

NEWS

Atlas Improvements

Over the last several months, we've made a variety of changes to Atlas intended to improve the overall user experience. Most notably, all nodes on Atlas can now access resources on the Internet, which drastically simplifies many scientific computing workflows. For example, it is now possible to update software packages or access external data resources from any node on the system. Another key improvement is command-line histories now persist across Atlas sessions, which makes it much easier to repeat work from one session to the next. We want our clusters to be as user-friendly as possible, so please share any feedback or suggestions with us!

New SCINet Website Launched



The new SCINet [website](#) has launched!

The redesigned site includes a consolidated event calendar, improved user guide navigation, and a more informative landing page. Please send feedback to Moe Richert, Lead Developer (moe.richert@usda.gov).

AI Training Images Workshop

Are you interested in AI-based image analysis methods for scientific research? If so, please join us for an AI training images workshop at the end of February! What are “AI training images”? AI-based image analysis techniques typically require relatively large image datasets – “training images” – to help the AI system improve its performance on a given analysis task. Obtaining suitable training images is often one of the most expensive and time-consuming aspects of applying AI image analyses in scientific research. On February 28, 2023, from 12-4 pm EST, ARS’s AI Center of Excellence will host a virtual workshop to help lay the foundations for building shared AI training image resources for ARS research. We will a) help attendees gain a better understanding of AI image analysis methods, how they are used in ARS, and why we need agency-wide training image resources; b) identify training image requirements and use cases; and c) begin to develop an inventory of extant training image datasets. At the beginning of the workshop, we will host a lightning talk session for attendees to share their work using AI-based image analyses. If you would like to attend the workshop, please fill out [this brief form](#).

Fungal Bioinformatics Working Group

As technology advances in the field of molecular biology, so does the need for accurate and robust bioinformatics data analyses. The Fungal Bioinformatics Working Group was formed in December 2022 with the goal of developing centralized resources and a networking community for pathologists analyzing fungal and oomycete genomes. These resources are to include links to genome databases, optimized workflows and pipelines, and computing environments designed for fungal genome analyses. The group will meet once a month to discuss research, projects, and resource development.

Additionally, the working group hosts a bi-weekly journal club where participants take turns choosing research papers to read and discuss as a group. We also hope to host a Fungal Bioinformatics Workshop virtually in Spring 2023.

If you are interested in joining this group, please contact Kayla Pennerman (kayla.pennerman@usda.gov) or Olive Stanley (olive.stanley@usda.gov).

Protein Function and Phenotype Prediction Working Group

The Protein Function and Phenotype Prediction Working Group held their FY2023 second quarter meeting on January 11. Dr. Carson Andorf presented on emerging tools in protein structure and folding prediction on SCINet. The presentation recording and slides are available to USDA employees on the Working Group [web page](#).

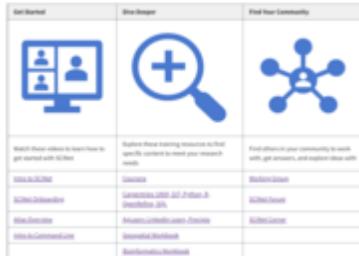
This working group will be hosting a third quarter workshop for interested scientists the first week of May 2023. Scientists can provide input into what content would be of most interest by filling out this [form](#).

Biological Invasion Working Group

We are seeking inquiries from those that would like to join a new working group on big data applied to ag-related biological invasions. Our goal is to bring together scientists from diverse disciplines such as genomics, ecology, economics, and conservation to help understand how big data can help predict, detect, prevent, and control biological invasions. We will meet quarterly to develop a review paper and then use that review paper as a jumping off point to develop new datasets and novel solutions. If interested, please email us (christopher.owen@usda.gov, rebeclem@gmail.com) with a few sentences about how you plan to contribute and what you hope to get out of this working group. We invite people from all career stages to respond.

TRAINING

Training Opportunities



Getting Started: With the expansive list of free training available online, finding the right training to meet your learning needs can be daunting. Take the first steps in getting started with the [SCINet Introductory Learning Pathway](#). Learn about SCINet, how to sign up for an account, and what is possible when supported by SCINet infrastructure. Then dive in with hands-on tutorials available across multiple searchable platforms to find the information you need for just in time learning.

AI Practicum Series: We are excited to announce a new collaboration with the University of Florida (UF) to provide hands-on, practical training for ARS scientists who want to apply artificial intelligence (AI) methods and techniques to their research. UF has developed a new, in-house AI training curriculum in support of a major initiative to deploy AI throughout UF's research enterprise. The SCINet Office is working with the UF training team to customize this curriculum for ARS, including developing new training modules to address specific ARS training needs. We plan to offer the first workshops in this series, designed for learners who are new to AI, in early 2023. If you are interested in participating, please sign up [here](#). Once we have a core group of participants signed up, we will decide on a workshop schedule.

In addition, the first new training module we will develop with the UF team will cover AI methods for biological sequence analysis. We are looking for ARS scientists who would like to participate in a steering committee to guide module content and development. If you are interested, please contact Dr. Brian Stucky (brian.stucky@usda.gov) or Dr. Ryan Lucas (ryan.lucas@usda.gov).

The Carpentries Workshops: With an influx of newly certified The Carpentries Instructors from ARS, we now can self-host Carpentries workshops. There are already four workshops scheduled for the second and third quarters of FY2023. These courses, listed below, will each be conducted over 4 days in 4-hour sessions.

Workshop	Dates
Software Carpentry with Python	Feb. 23-24, Mar. 2-3
Software Carpentry with R	Mar. 27-28, Apr. 3-4
Software Carpentry with Python	Apr. 11-12, 18-19
Software Carpentry with R	May 2023, exact dates TBD

Sign up for one or more of these courses by filling out this [form](#).

Courses by Mississippi State University: Mississippi State regularly offers [Introduction to Atlas](#) courses. Additionally, there are waiting lists available for several other courses, including an Intensive R course to help scientists with no R experience become familiar with the programming language and start performing statistical analyses in 4 days. [Sign up](#) to get notified when these courses are offered.

Coursera.org Courses: The SCINet Office and the AI-COE are excited to provide training opportunities through Coursera. Coursera licenses are available to ARS scientists and support staff for training focused on scientific computing, data science, artificial intelligence, and related topics. Successful completion of courses and specializations result in widely recognized certificates and credentials. Please visit the SCINet [Coursera Training Page](#) to request a license. Licenses will be assigned on a rolling basis and are active for three months. Users may be able to extend their licenses upon request.

Training opportunities are continuously being updated on the [SCINet Upcoming Training webpage](#). For more information on any of the above trainings, registration questions or suggestions, please email SCINet-training@usda.gov.

SUPPORT

Getting Started with SCINet is as Easy as 1,2,3

In October, we reached the milestone of having 2,000 registered SCINet users. If you do not already have a SCINet account, we hope you will consider joining the 2,000+ researchers who do. Follow the steps below to get your SCINet account.



1. [Request a SCINet account](#) to get started.
2. Read the [SCINet FAQs](#) covering general info, accounts/login, software, storage, data transfer, support/policy/O&M, parallel computing, and technical issues.
3. Register for a [SCINet Forum](#) account to connect to other users, ask questions, and learn how SCINet can enable your research.

P.S. Don't forget to complete your annual security training! This is required to maintain your account.

For technical assistance with your SCINet account, please email scinet_vrsc@usda.gov.

SCINet User Tip

If you are working with data on the HPC clusters that exceed your current storage quota in /project, you can request an increase to your /project storage quota. The only requirement for a quota increase is a clear explanation of why the increased space is necessary for the research project's success.

To request project quota increase for storage on Ceres, Atlas, and/or Juno, fill out this application [form](#).

Please Note: Only the project manager or the project PI can request a quota increase. Any requests sent by other individuals will be declined.

Do you have tips to share? Email them to SCINet-Newsletter@usda.gov to be included in future newsletters.

SCINet Corner: First Thursdays Each Month

SCINet Corner is a VRSC moderated virtual space for people to share knowledge, discuss best practices, learn about new opportunities, and explore resources to support progress on their projects.

The next SCINet Corner will be held Thursday, February 2, 2023 at 1 pm EST. The topic of discussion will be Exploratory Data Analysis in R. You can register for this and future SCINet Corners [here](#).

Have a question that just can't wait? Want to see what other users are doing? Reach out to the ever-expanding SCINet Forum community for ideas, support, or just someone to bounce ideas off of at <https://forum.scinet.usda.gov/>.

CONNECT

The SCINet Team

Every newsletter highlights SCINet community members as a way to connect the ARS scientific computing community. To see all the SCINet community and review past newsletters, visit the [Newsletter Archive](#).

Contribute

Do you use SCINet for your research? We would love to share your story! Email SCINet-Newsletter@usda.gov to contribute content, ask questions, or provide feedback on the SCINet newsletter or website.

SCINet Leadership Team

Brian Stucky, Acting Chief Science Information Officer
Rob Butler, Acting SCINet Project Manager
Adam Rivers, Science Advisory Committee (SAC) Chair
Steve Kappes, Associate Administrator

Note: This newsletter is edited to comply with ARS editorial standards.

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