Department of Scientific Computing

Spring 2019

New model for population genetics

CONTENTS

Traditionally, fractional calculus has been used to model highly complex phenomena in biological physics (e.g. arterial viscoelasticity), mechanical engineering (e.g. controller tuning, legged robots, redundant robots, heat diffusion, and digital circuit synthesis) and acoustics (speech signal models); it has never been applied in population genetic processes. Recently, two Scientific Computing research scholars, Somayeh Mashayekhi, a postdoctoral researcher, and her advisor, Professor Peter Beerli, proposed and implemented the fractional coalescent in studying genetic datasets, including mitochondrial sequence data of humpback whales, mitochondrial data of a malaria parasite [Plasmodium falciparum], and complete genome data of the H1N1 influenza virus strain collected in Mexico City in 2014.

Postdoctoral Associate Somayeh Mashayekhi

Population genetics is a field of biology that studies the genetic composition of biological populations and the changes in genetic composition that result from the operation of various factors, including natural selection. Population geneticists pursue their goals by developing abstract mathematical models of gene frequency dynamics; they attempt to draw conclusions from those models about the likely patterns of genetic variation in actual populations, then test the conclusions using empirical data.

“The theory of population genetics is based on the coalescent theory. In this research, we have used the fractional Poisson process to introduce the fractional coalescent. The fractional coalescent is the extension of Kingman’s coalescent which uses the Poisson process,” Mashayekhi explained.

Population genetic analyses commonly assume that all individuals within a population are affected in the same way by the environment. Populations, however, show heterogeneity; neglecting this heterogeneity can lead to biased parameter estimates. Previous approaches have focused on strong selection or large offspring variance but have not allowed estimates to reflect these differences. Mashayekhi and Beerli base their fractional coalescent model by building on and extending Cannings’ model.

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SC Fulbright Scholar featured in new video

Professor Anke Meyer-Baese, Fulbright Scholar

The Office of Faculty Development and Advancement developed a new video that features FSU faculty who have participated in the Fulbright Program. The video features Scientific Computing professor and Fulbright Scholar, Anke Meyer-Baese along with a core collection of FSU faculty. The video was created at the GEOSET studio in Dirac Science Library, an academic recording studio which serves as a conduit for the university community to showcase their

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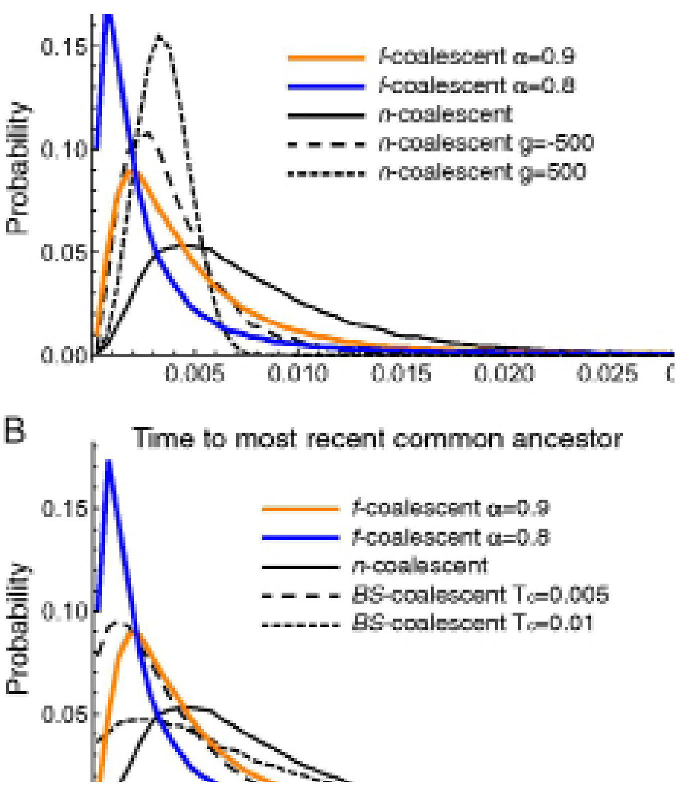

Empirical distribution of the time of the most recent common ancestor for various coalescents: strictly bifurcating (A) and f-coalescent vs. n-coalescent and multifurcating BS-coalescent (B). The x axis is truncated at 0.03. Each curve represent a histogram of 100,000 draws of the TMRCA.

Cannings' model allows for a fixed variance of the offspring number; this concept was expanded by Mashayekhi and Beerli by assuming that this variance is not fixed but has a probability distribution; the nestsite model, where individuals can pick among a set of favorable or not so favorable nestsites is a discrete version of this concept. Extending the nestsite model to a continuous framework allows to fit the model into an existing probability framework in fractional calculus, that is based on the Mittag-Leffler function. Using this Mittag-Leffler function allowed Mashayekhi and Beerli develop a computer program that can take into account heterogeneity that has an influence on the offspring variance. The new model introduces an additional parameter which could reflect hidden population heterogeneity. The f-coalescent is able to accommodate extreme waiting time intervals better than the previous model. Mixtures of very short genetic branches with very large genetic branches are possible; the f-coalescent shows a better fit when the immigration rate is 1 per 10 generations. The f-coalescent may improve our understanding of evolution of long-lived, versus short-lived organisms, or fast evolving organisms that are under selection.

Beerli gave an example of how this affects the populations: "Assume an influenza virus infects different people in a population, some who received the flu vaccine, others who received no vaccine. The virus that ends up in work and bring creative ideas to life through digital film.

Meyer-Baese was awarded the Fulbright to Strasbourg, France in 2016 to study dementia with Lewy bodies (DLB), a common form of dementia. Distinguishing between DLB and Alzheimer's, both neurodegenerative diseases, can be difficult, as the diseases tend to have overlapping clinical symptoms. By using neuroimaging methods, Meyer-Baese has uncovered important information which helps researchers and medical practitioners differentiate between specific, important structures; this helps contribute to fast, accurate diagnostics for Alzheimer's disease and DLB patients at a critical, early stage. With accurate evidence, clinical neuroscientists can evaluate properly the next steps in treating the actual disease.

In addition to Professor Meyer-Baese, the video features Bruce Locke, Engineering; Carol Weissert, Political Science; Bruce Lamont, Business; Barbara Parker-Bell, Art Education; and Jean Munn, Social Work.

To see the video that features Professor Meyer-Baese, go to https://www.youtube.com/watch?v=BmEOqAUelRQ.

For more on her research, go to https://people.sc.fsu.edu/~ameyerbaese/.

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a person who was vaccinated against influenza will have by chance fewer offspring than the virus that infects a non-vaccinated person. Our model allows for such differences in the environment, whereas the original model assumes all virus particles have the same chance," Beerli said.

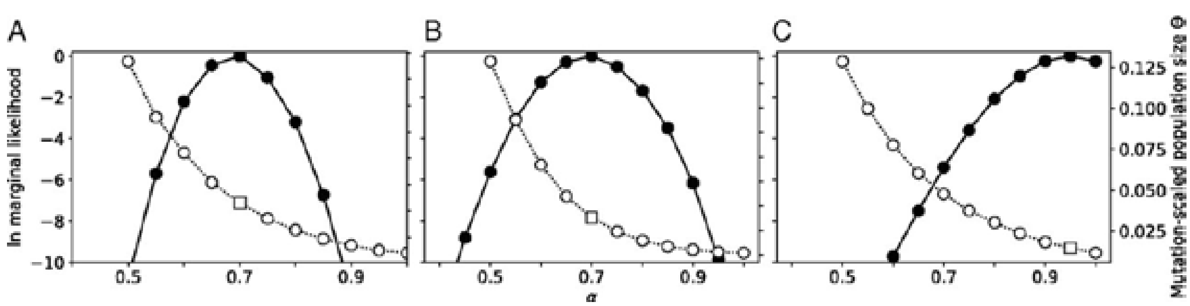
Mashayekhi and Beerli plan to continue and extend this research, refining the model over time. "We have only started to explore the effects of the fractional coalescent. Our theory works for a single population, and we hope to extend the model soon to several populations, because that will allow analyses of many important data sets ranging from pathogens to humans."

To read Mashayekhi and Beerli's article, *The Fractional Coalescent*, go to: https://www.pnas.org/content/pnas/116/13/6244.full.pdf.

For information about Mashayekhi, her background and research, go to: http://myweb.fsu.edu/smashayekhi/.

For more on Peter Beerli, go to: http://peterbeerli.com/beerli-lab-html5/index.html

Professor Peter Beerli



Model selection using relative mLs of an H1N1 influenza eight-locus (A), a P. falciparum mtDNA (B), and a humpback whale mtDNA (C) dataset. The solid line connects the ln mLs of models with different α values; the dashed line marks the mutation-scaled effective population size Θ; and the square marks Θ of the best model for each dataset.

Faculty receive grant awards for summer research

Florida State University's Council on Research & Creativity selected two Department of Scientific Computing faculty projects for grant support. In the coming months, Professor Peter Beerli and Assistant Professor Bryan Quaife will receive $14,000 each for their respective research.

Quaife's research, titled "Augmented Reality Simulations of Fire Dynamics with Topography," proposes to study fire dynamics as they involve relationships with topography. Fire dynamics is the study of how fires start, spread and develop. Fire dynamics is a blend of chemistry, fire science, materials science, fluid dynamics and heat transfer that influence fire behavior. With the use of algorithms and a sand box in augmented reality, Quaife will study fluid flow, a particularly complex topic, with the goal of developing models that simulate real-time fire behavior. This research is particularly relevant given annual wildfire events in the western states.

For his research, Beerli plans to use the summer semester to improve and extend a new Bayesian algorithm for assigning individuals to populations, starting with a two-population scenario with asymmetric migration. Beerli's proposal seeks to improve existing models for inferring individuals' genetic ancestry. In addition, the proposed approach will take the genetic relationships among known populations into account. The outcome of this work can be applied to studying the origins of invasive species.

These developments will form the preliminary data for an NSF proposal in Fall 2019 that will extend the algorithm for multiple populations and will ultimately be implemented in MIGRATE, Beerli's widely-used software program.

The Council on Research & Creativity supports research and creative activity, project related travel, and stipends for grant-funded students. Through the Committee on Faculty Research Support (COFRS), CRC provides faculty with summer salary or allowable research related expenses to assist with research and creative endeavors that encourage external funding.

For more on CRC, COFRS or related awards, go to https://www.research.fsu.edu/research-offices/opd/crc/. For more on Beerli's and Quaife's research, go to http://peterbeerli.com/beerli-lab-html5/index.html and https://people.sc.fsu.edu/~bquaife/.

Bryan Quaife talking to students at the department's annual research exposition.

Alum advances and excels

After graduating from Reed College with an undergraduate degree, SC alum Verónica Vergara Larrea received the Masters of Science in Computational Science in 2011. For her thesis, Vergara Larrea explored improvements in the construction of Delaunay Triangulations on the sphere by designing and implementing a parallel alternative to then current software. The research gave an introduction to Delaunay Triangulations on the plane and presented current methods available for their construction. These concepts were then mapped to the spherical case [Spherical Delaunay Triangulation (SDT)].

SC Alum Veronica Vergara Larrea at Oak Ridge National Laboratory.

Immediately after graduation in 2011, she accepted a position at Purdue University's Research Computing group; by 2014 she was working as HPC User Support Specialist at Oak Ridge National Laboratory, working to provide assistance to users and programming the sophisticated, powerful computers used for research at the lab.

Recently, ORNL acquired one of the world's most powerful supercomputers, the IBM AC922, and Vergara Larrea was an essential part of the implementation team. The AC922 boasts unprecedented speeds and performance capabilities, with peak performance of 200,000 trillion calculations per second (200 petaflops), and Oak Ridge research staff have successfully run the world's first exascale scientific calculations.

As part of the System Test Working Group, Vergara Larrea led the design and selection of test codes and problem cases to ensure the stability of the system. For months, she coordinated and organized test development and benchmarking of the supercomputer's complex, massive architecture. Diagnostics, functionality testing, performance measurement were all part of acceptance testing, a process that lasted over a period of two years. Scientists studying astrophysics, materials science, cancer surveillance, and systems biology will use the supercomputer for their research.

Verónica Vergara Larrea is user support specialist and programmer at the OLCF, a US Department of Energy (DOE) Office of Science User Facility at DOE's Oak Ridge National Laboratory (ORNL). Her excellent work on the IBM AC922 machine, Oak Ridge's new supercomputer, was highlighted in ORNL's Faces of Summit Series. To see the article lauding Vergara Larrea's work, go to https://www.olcf.ornl.gov/2018/01/17/faces-of-summit-putting-the-system-to-the-test/. .

Summit, ORNL's new supercomputer, is eight times more powerful than ORNL's previous top-ranked system. Summit is providing scientists with incredible computing power to solve challenges in energy, artificial intelligence, human health, and other research areas, that were simply out of reach until now.

New student organization formed

Fellowship of Computational Scientists founder Jack Keen

Undergraduate student Jack Keen recently began the Fellowship of Computational Scientists, a university Recognized Student Organization designed to provide academic support to undergraduate students. The organization helps students by providing resources, services, and assistance to students with courses, events, tutoring, and developmental opportunities. Below, Keen talks about the organization, its catalyst, purpose, and scope.

When and why did you decide to do this?

I decided to do this last semester, during Fall 2018. Originally, Nathan Crock, one of the doctoral candidates in the Department of Scientific Computing, asked me to start an "undergraduate engagement group." We were thinking along the lines of coding competitions. From this stemmed the math review groups, an extension of a project I started in the summer with Dr. Lemmon's lab. I felt like the competitions would be more fun if there was a "prepping" process. The review groups give less-experienced students a stronger foundation to work with.

A big reason why I decided to do this is because I remember feeling really overwhelmed my first semester. I had just transferred from Tallahassee Community College, and I was filled with a lot of self-doubt. I eventually found my place, thanks to many kind professors and students, but I know a lot of new students going through the same process. I wanted to create a sense of community between the whole department—professors, graduates students, and undergraduate students.

There are so many friendly people in this department, but in the beginning it's hard to figure out how to ask for help. For example, a lot of new students want to get engaged in research, but they don't know who to ask. One of our goals is to facilitate this process, working with the graduate students and faculty. I'm hoping this organization helps new students get involved in the department quickly.

Who's invited?

Everyone is invited! We're really trying to focus on collaboration and interdepartmental reach. There are so many ways to cross computational science with other disciplines—biology, physics, chemistry, even music and literature. One of the fascinating areas I've read about is computational linguistics. I want people to be able to meet other people and create novel ideas with this organization.

What do you hope to accomplish?

We hope to create a collaborative, interdepartmental network of undergraduate and graduate students using computational science. We really want to pull people from all departments—statistics, mathematics, etc. Our main goals include:

- Review groups to strengthen core subjects
- Coding competitions to encourage teamwork
- Project presentation events to develop public speaking skills
- Interdepartmental events to foster collaboration

Where will you meet?

We will primarily meet in the Department of Scientific Computing, but ideally we want to be able to attend conferences and large events too! I want to do events within other areas of the College of Arts and Sciences so that other people can see what scientific computing is all about.

What type of activities will the organization do?

We're starting off with the review groups from the past couple of semesters. We're working towards creating review groups for calculus, linear algebra, differential equations, and numerical analysis. We want these to be "fixed" review groups, available every semester, for all students. Our coursework is very math-intensive, and sometimes extenuating circumstances mean undergrads have to take courses out of sequence in order to graduate on time. And sometimes you just forget something from linear algebra or calculus, and you need a refresher!

What are the benefits of becoming an 'official' university organization?

Becoming an official Registered Student Organization means we have certain privileges within the university: we're automatically included in the list of current organizations in Nole Central, making it easier for all students to find us; we have access to more material resources (e.g. 5,000 free black and white copies each year on the copy machine in the Student Activities Center); we are eligible to win awards such as "Student Organization of the Year"; we can set up a table during Market Wednesday; and more. Our networking ability has increased a lot!

Since becoming a university Registered Student Organization in February, the Fellowship of Computational Scientists has held general body meetings, sponsored a meet-and-greet for all current members, provided tutoring and study sessions in numerical analysis, review groups on Sine Orthogonality, Partial Differential Equations, and Calculus II. For more information on the Fellowship, go to https://nolecentral.dsa.fsu.edu/organization/focs or email Jack Keen at kmk17e@my.fsu.edu.

Keen and fellow FCS officers discussing organizational issues.

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The department's mission is to be the focal point of science and computation at Florida State University. Gordon Erlebacher is Chair of the Department of Scientific Computing. He can be reached at 850.644.7024. Newsletters are issued three times each year. Subscriptions and single copies are available by calling 850.644.0196. This publication is available in an alternative format on request.

Soda moves to Connecticut university

Morphometrician and computational scientist K. James Soda.

After completing his Masters in 2013 and Ph.D. in 2017, SC alum K. James Soda accepted a postdoctoral associate position at the Department of Biological Sciences and Eck Institute for Global Health, University of Notre Dame where he continued to use geometric morphometric analytic tools for shape analysis research. While at Notre Dame, Soda, along with his colleagues, published papers on disease progression -- *Local and regional dynamics of chikungunya virus transmission in Colombia: the role of mismatched spatial heterogeneity* and *DTK-Dengue: A new agent-based model of dengue virus transmission dynamics*.

Recently, Soda completed his postdoc appointment, and accepted a faculty position at Quinnipiac University. Soda is an assistant professor of mathematics, and will, in addition to his teaching and research duties, be a primary contributor in the development of a new major at Quinnipiac, data science and applied statistics. He will teach probability and data analysis in the fall.

Soda was mentored by Dennis Slice.

For more on Soda, go to www.qu.edu. For more on the department, go to www.sc.fsu.edu.

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