Dear ICME partners, faculty, and students,

I’m pleased to present the Stanford ICME Xpo research guide 2020, produced in support of the ICME Xpo research symposium, an annual event that provides an up-close and inside look at current research and future plans of ICME faculty and students. This symposium is a unique opportunity to see how computational mathematics, data science, machine learning, scientific computing, and related fields are applied across a wide range of domain areas. ICME Xpo 2020 is especially unique, as it is being held online in order to adhere to COVID-19 restrictions.

This research guide introduces the work of some of our MS and PhD students, as well as some students in related areas across campus. Please note that the content presented is only a subset of all the research activities currently ongoing in ICME and it is intended to provide a good glimpse of the interesting work being done by our faculty and students, and spark future collaborations.

The ICME and ICME-related students featured here work with or are advised by our 50+ ICME-affiliated faculty members from across campus, as well as external mentors. Some of the students presented at ICME Xpo and at NeurIPS 2019; some have participated in the ICME Xplore capstone program; and others are Schlumberger Innovation Fellows or TOTAL Innovation Fellows. All are doing interesting work in important application areas like healthcare (including COVID-19 research), genomics, environmental sciences, computational finance, education, public policy, and more. Note that you can search this guide using keywords in order to find areas that interest you most.

We invite you to read through the research abstracts, and connect with students who are working in your areas of interest.

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Confidence Intervals for Policy Evaluation in Adaptive Experiments
Monte Carlo (MC) sampling is the standard approach for uncertainty propagation in problems with high-dimensional stochastic inputs. The method is applied, for example, to wind farm flow models, which have stochastic wind direction, wind magnitude, and model parameters. Various acceleration techniques have been developed to overcome the slow convergence of MC estimates, such as Multilevel Monte Carlo (MLMC). MLMC uses approximations computed on a series of levels to reduce the estimator variance, where levels are models with different levels of accuracy and computational cost. MLMC analytically determines the number of samples required on each level to achieve a given accuracy at minimal cost. We extended the original MLMC theoretical framework for modern, heterogeneous computer architectures. In these architectures accelerators (GPUs) are available and, therefore, samples can be distributed on both different levels and different compute units (CPUs and GPUs). We derived the optimal sample allocation for the proposed MLMC extension by solving a convex optimization problem. We demonstrated that for a realistic range of CPU to GPU cost ratios the proposed approach leads to considerable total cost reduction (up to 90%) compared to MLMC using only GPUs. We applied the method to channel flow with stochastic heating. The work is under review for publication: Multilevel Monte Carlo Sampling on Heterogeneous Computer Architectures, C. Adcock, Y. Ye, L. Jofre, and G. Iaccarino, Int. J. for Uncertain. Quant.

Christiane is a second year ICME PhD candidate developing mathematical and computational methods to model, design, and control energy systems, such as wind turbines. She holds a BS in Mechanical Engineering from MIT. Previously she's worked at DNV GL forecasting wind farm power production and at the National Renewable Energy Laboratory incorporating atmospheric conditions into wind farm flow models.
Dimensionality reduction plays a crucial interpretative role in computational biology, and is increasingly important for human population genetics. However, most of the current methods for dimensionality reduction in genetics require single ancestry individuals. In cases of a mixture, substructure within the separate ancestry components cannot be resolved by these existing methods. In this project, we implement a series of novel ancestry-specific dimensionality reduction techniques in order to make them available for the wider medical genetics community as part of a publication. Our method reads in genomic data, available in several different formats. Using the output from local ancestry inference techniques, all segments from ancestries not under investigation are masked, generating a matrix completion problem. The masked matrix is completed using the Iterative SVD method. Finally, Principal Component Analysis is performed on the completed matrix for ancestry-specific dimensionality reduction.

Devang Agrawal graduated from ICME with MS in the Data Science track in April 2020. Prior to Stanford, he received his B.Tech in Mathematics and Computing from Indian Institute of Technology Delhi. He is interested in the applications of Machine Learning and Data Science in several industries.

Relevant Links:

DEVANG AGRAWAL
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The Human Genome project focuses on selecting SNPs (single nucleotide polymorphisms), which are genetic variants that consist of substitutions of a single nucleotide at a specific position in the genome) located in non-coding regions of the genome involved in craniofacial disorders for further biological validation. A pipeline has already been built and has allowed to select 193 unique SNPs that are likely to be involved in craniofacial disorders. In this project I leverage the Biomedical Data Common graph to conduct further analysis on this set of prioritized genetic variants. Especially after performing some statistical testing on the data, I worked on correlating the GTEx database with our SNP-gene pairs dataset to filter it according to the presence of those pairs in the GTEx database.

Leore Bensabath is a first year master's student in ICME in the data science track. She is especially interested in data science applied to biology and medicine.
In this work, we developed a novel general task-based runtime systems. TaskTorrent is simple (simple API, untouched user data), fast (minimal runtime overhead), task-based (operations are expressed as tasks triggering other tasks), distributed and easy to use (C++ library with only MPI as a dependency). We tests TaskTorrent on a wide range of linear algebra problems, and show that it is competitive with other state of the art runtime systems. We finally use TaskTorrent to parallelize the Sparsified Nested Dissection (spaND) algorithm. This allows us to run spaND on very large machine and to solve equations with hundreds of millions of unknowns. With Y. Qian, B. Klockiewicz, E. Darve, C. Chen, E. Boman, S. Rajamanickam, R. Tuminaro

Leopold Cambier is PhD student in ICME working with Professor Eric Darve. His current projects include runtime systems for scientific computing and fast parallel linear algebra. Leopold holds a BS in engineering and a M. in mathematical engineering from Université Catholique de Louvain in Belgium.
In this work we generalize recent results from E. Hallman and M. Gu who developed the LSMB algorithm, used to solve least square problems with an iterative Krylov method. They showed that the iterates generated by LSMB lie in a precise 1-dimensional subspaces. In this work, we relax the condition that the space be Krylov. We define the index of invariance of a subspace \( S \) w.r.t. \( A \) as \( \text{Ind}(A,S) = \dim(S + AS) - \dim(S) \), and show that the iterates lie in a \( \text{Ind}(A,S) \)-dimensional subspace. This result generalizes and explains the LSMB result. We study in detail that quantity and show multiple properties related to \( \text{Ind}(A,S) \).

Leopold Cambier is PhD student in ICME working with Professor Eric Darve. His current projects include runtime systems for scientific computing and fast parallel linear algebra. Leopold holds a BS in engineering and a M. in mathematical engineering from Université Catholique de Louvain in Belgium.

Rahul Sarkar is a PhD student in ICME, advised by Professors Biondo Biondi and András Vasy. Rahul holds a BS and MS degree from Indian Institute of Technology Kharagpur, India, as well as an MS degree from ICME. His current projects include computational inverse problems, quantum error correcting codes, and mathematical analysis.

LEOPOLD CAMBIER, RAHUL SARKAR

ICME MS & PHD STUDENTS

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Knowledge graph (KG) embeddings learn low-dimensional representations of entities and relations to predict missing facts. KGs often exhibit hierarchical and logical patterns which must be preserved in the embedding space. For hierarchical data, hyperbolic embedding methods have shown promise for high-fidelity and parsimonious representations. However, existing hyperbolic embedding methods do not account for the rich logical patterns in KGs. In this work, we introduce a class of hyperbolic KG embedding models that simultaneously capture hierarchical and logical patterns. Our approach combines hyperbolic reflections and rotations with attention to model complex relational patterns. Experimental results on standard KG benchmarks show that our method improves over previous Euclidean- and hyperbolic-based efforts by up to 6.1% in mean reciprocal rank (MRR) in low dimensions. Furthermore, we observe that different geometric transformations capture different types of relations while attention-based transformations generalize to multiple relations. In high dimensions, our approach yields new state-of-the-art MRRs of 49.6% on WN18RR and 57.7% on YAGO3-10.

Ines Chami is a PhD candidate in ICME where she is advised by Professor Chris Ré. Her research is focused on representation learning for graph-structured data and understanding how non-Euclidean geometries (e.g., hyperbolic geometry), can lead to more expressive representations for some types of relational structures. Her research also spans applications in the field of computer vision and natural language processing, such as understanding how objects interact in images or how entities are related in knowledge graphs.

Relevant Links:

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Understanding styles of furniture is important for an online furniture retailer to advertise their products and improve customer experience. Here we try to improve furniture (picture) classification by removing the background. We also extract features using color distribution, transfer learning, and embeddings from GANs to improve the classification. While we still could be conclusive in all these methods, some pretrained models and GANs seem promising.

Yuan Chen is a fifth year PhD student in applied physics working on numerical simulation of pump-probe spectroscopies. He just completed his MS degree at ICME in January 2020.

Relevant Links:
FAIR SUPERVISED LEARNING

As artificial intelligence and machine learning models have become more prevalent in human decision-making processes, there has been increased interest in understanding their fairness. Fairlearn is Microsoft’s opensource Python package that allows developers to both quantify the fairness of their models and mitigate any detected unfairness. The Fairlearn package contains algorithms that can be applied to mitigate unfairness based on different fairness definitions (equalized odds, demographic parity and bounded group loss) for regression and classification tasks.

We are working with the Microsoft team to further expand the capabilities of Fairlearn for regression. Specifically, we are implementing bounded group loss for exponentiated gradient. Bounded group loss is a fairness constraint for regression tasks where the overall loss is minimized while also bounding the worst loss on any protected group.

In addition, we are building a case study to demonstrate an application of Fairlearn for regression by mitigating disparities while predicting male and female student GPA based on entrance exam scores.

Davide Giovanardi is a first year master’s student in ICME. His research interests span deep learning and applied statistics areas. Previously, he received an MS in Finance from UCSD.

Andra Fehmiu is a first year master's student in ICME. Prior to that, she was an applied math in economics undergraduate at Harvard. Her research interests include deep learning and computer vision, particularly applied to healthcare.

Lauren Pendo is a first-year master's student in ICME, focusing on Data Science. Her research interests include machine learning and data analysis techniques.
Energy expenditure in buildings can be greatly reduced through advanced controls. However, building energy expenditure data often contains a large portion of missing values. The aim of this project is to explore the use of non-negative matrix factorization in filling the missing data based on the patterns of existing values. The filled-in data will be used to further analyze the behavior of sensors and cluster similar sensors into groups. The result of the project would be provided to energy experts for their research in reducing the energy usage in the buildings.

Yuan Gao is a second year master's student in ICME's general track. Her major research interest is in the application of machine learning and data analytics in environmental science.
Transformer models like BERT are used extensively in NLP tasks. We add to the growing literature on investigating how BERT works by analyzing the contribution of pre-trained knowledge on downstream tasks. We introduce a reinitialization method to better understand the performance gains related to having pre-trained parameters at the start of fine-tuning. In general, we see that when data is scarce, there is more reliance on pre-trained weights. Moreover, we study the synergies across layers and find that both the context in which the weights have been learned and the dependencies across the layers are critical factors of the model performance. Finally, we find that the parameters of the later layers get overwritten more during fine-tuning, while the earlier layers remain largely invariant.

Davide Giovanardi is a first year master's student in ICME. His main research interests are in the area of deep learning and applied statistics. Previously, he received an MS in Finance from UCSD.
My research is focused on developing fast approximate factorizations for large sparse matrices using orthogonal transformations. The factorization can be used as a fast direct solver or as a preconditioner to solve general linear systems and linear least squares problems. The method is based on limiting the fill-in generated in direct methods by using low-rank approximations. Using this, we can achieve close to linear complexity for the factorization. We also theoretically show the quality of the preconditioned system. Numerical experiments done on PDE discretizations and linear least-squares problems arising out of PDE constrained optimization validate our technique.

Abeynaya Gnanasekaran is a fourth year PhD student in ICME. Her research interests lie in numerical linear algebra and high performance computing. She works with Professor Eric Darve in developing fast algorithms for general sparse linear systems and sparse linear least-squares problems.
Recent machine learning models such as neural networks underpin many of the best-performing AI systems. Their success is largely due to their strong approximation properties, superior predictive performance, and scalability. However, a major caveat is explainability: these models are often perceived as black boxes that permit little insight into how predictions are being made. We tackle this issue by developing various tests to assess the statistical significance and importance of the input features of machine learning models with a special emphasis on neural networks. The tests enable one to discern the impact of individual variables as well as interactions of variables on the prediction of a model. The test statistics can be used to rank variables according to their influence but also to perform model and variables selection. Simulations and applications on various real datasets illustrate the computational efficiency and performance of the tests.

Enguerrand Horel is a final year PhD candidate in Applied Mathematics and Statistics from the Institute for Computational and Mathematical Engineering and part of the Advanced Financial Technology Lab at Stanford University. He has a M.Sc. in Applied Mathematics from École des Ponts ParisTech in France and a M.Sc. in Computational and Mathematical Finance from Stanford. His research interests include hypotheses testing, neural networks, nonparametric statistics, model explainability and their applications to finance.
**MARKETS FOR EFFICIENT PUBLIC GOOD ALLOCATION**

The over consumption of public goods results in a reduction in its value to customers, a phenomenon that has become more prominent with the Covid-19 pandemic, where strict social distance constraints are enforced to either prevent or limit the number of people who can share public spaces. In this work, we look to plug this gap through market based mechanisms designed to efficiently allocate capacity constrained public goods. To design these mechanisms, we leverage the theory of Fisher markets, wherein each agent in the economy is endowed with an artificial currency budget that they can spend to avail the public goods. However, the presence of additional physical constraints, such as the time of availability of agents when being allocated to time slots to use a public space, that are characteristic of public goods allocation problems are left unaccounted for in the Fisher market setup. We overcome this fundamental limitation by formulating two modifications to the Fisher market framework that account for a more general set of constraints that go beyond the capacity and budget constraints considered in Fisher markets. As a first step, we formulate a regularized version of the Fisher market individual optimization problem by replacing the physical constraints with a penalty in the objective for constraint violations and show the existence of market clearing conditions in this setup. Then, we develop a more robust approach in which we retain the additional physical constraints but instead perturb the budgets of agents in the Fisher market social optimization problem. The budget perturbations are set based on the dual variables of the additional physical constraints such that the KKT conditions of the social and individual optimization problems are equivalent. We then present a fixed point iterative procedure to determine the budget perturbation constants and establish the convergence of this fixed point iteration. Finally, we present numerical experiments that show strong convergence guarantees and highlight that convergence is invariant to perturbations in the data (i.e. the budgets and the utilities of consumers). This research is in collaboration with Professors Yinyu Ye and Marco Pavone.

Devansh is a PhD student in Computational and Mathematical Engineering at Stanford University. Prior to joining Stanford, he received his BS in Civil and Environmental Engineering and BA in Applied Mathematics with highest distinction from University of California Berkeley. His research interests span algorithmic game theory, market design and optimization and his current work is focused on the development of incentive schemes and market mechanisms for society to enable a smooth uptake of socially aware traffic routing strategies.
Identifying furniture styles is critical for e-commerce websites as they offer products to customers with different tastes and preferences. However, furniture style understanding is challenging as boundaries between styles can be fuzzy. In this project, we aim to improve furniture style understanding for product images by using self-supervised learning methods combined with Deep Learning techniques.

In this work, we employ Contrastive Predictive Coding, a universal (generalized over many modalities) unsupervised learning approach to extract useful representations from high-dimensional data. The key in-sight of CPC model is to learn such representations by predicting the future in latent space with the help of powerful autoregressive models combined with probabilistic contrastive loss. We then use these CPC representations to fine-tune deep learning models while leveraging transfer learning techniques.

Aasavari Kakne is a first year master's student in ICME and a recente graduate of IIT Delhi with B.Tech in mathematics and computing. Her research interests include weak- and semi- supervision techniques in NLP and computer vision. Yuan Fang is currently a first year master's student in ICME. Her research interests are data science, machine learning, and deep learning.
In severe viral pneumonias, including Coronavirus disease 2019 (COVID-19), the viral replication phase is often followed by a hyperinflammatory reaction (‘cytokine storm syndrome’) that leads to acute respiratory distress syndrome and death, despite maximal supportive care. Preventing hyperinflammation is key to avoiding these outcomes. We previously demonstrated that alpha-1 adrenergic receptor antagonists (α-blockers) can prevent cytokine storm syndrome and death in mice. Here, we conduct a retrospective analysis of patients with acute respiratory distress or pneumonia (n = 13,125 and n = 108,956, respectively) from all causes; patients who were incidentally taking α-blockers had a reduced risk of requiring ventilation (by 35% and 16%, respectively), and a reduced risk of being ventilated and dying (by 56% and 20%, respectively), compared to non-users. Beta-adrenergic receptor antagonists had no significant effects. These results highlight the urgent need for prospective trials testing whether prophylactic α-blockers improve outcomes in diseases with a prominent hyperinflammatory component such as COVID-19.

Allison Koenecke is a PhD candidate at Stanford's Institute for Computational & Mathematical Engineering. Her research interests lie broadly at the intersection of economics and computer science, and her projects focus on fairness in machine learning and causal inference in the public health space. She has held several data science roles in the Bay Area, and previously specialized in antitrust at NERA Economic Consulting after graduating from MIT with a Bachelor's in mathematics with computer science.

Relevant Links:
Automated speech recognition (ASR) systems are now used in a variety of applications to convert spoken language to text, from virtual assistants, to closed captioning, to hands-free computing. By analyzing a large corpus of sociolinguistic interviews with white and African American speakers, we demonstrate large racial disparities in the performance of popular commercial ASR systems developed by Amazon, Apple, Google, IBM, and Microsoft. Our results point to hurdles faced by African Americans in using increasingly widespread tools driven by speech recognition technology. More generally, our work illustrates the need to audit emerging machine-learning systems to ensure they are broadly inclusive.

Allison Koenecke is a PhD candidate at Stanford's Institute for Computational & Mathematical Engineering. Her research interests lie broadly at the intersection of economics and computer science, and her projects focus on fairness in machine learning and causal inference in the public health space. She has held several data science roles in the Bay Area, and previously specialized in antitrust at NERA Economic Consulting after graduating from MIT with a Bachelor's in mathematics with computer science.

Relevant Links:
http://fairspeech.stanford.edu
https://www.pnas.org/cgi/doi/10.1073/pnas.1915768117
Genomics is enabling a revolution in many fields like personal healthcare, disease association studies. There is a huge disparity in that about 80% of the population studied is of European ancestry. In order to bring the positive effects of such studies to other populations, there is a need to identify and annotate the ancestry of an individual along the genome. This is the problem of local ancestry inference. With the advent of machine learning and AI, there can be an algorithmic solution to this problem. In our work, we build a tree-based algorithm that consists of 2 layers: a windowed ancestry estimator and a smoothing layer. After obtaining motivating results on datasets with limited global coverage, we are currently studying more powerful neural models on datasets with a whole-world coverage to not only predict ancestry, but also to regress global coordinates of the ancestry. This gives a better picture of an individual's ancestral makeup.

This research is in collaboration with Alexander Ioannidis and Bustamante Lab, Stanford University.

Arvind is a first year masters student in Data Science in ICME. His interests lie in developing machine learning and AI tools. He is also interested in applying them to scientific disciplines like genomics, natural language understanding and social sciences.

Relevant Links:
https://documentcloud.adobe.com/link/track?uri=urn:aaid:scds:US:5fb5c84a-0b6f-4602-b3cf-c0651c5a376e

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In population genetics, patterns of the migration between populations is essential in studying the population structures in nature. Directly measuring the patterns of migration between populations is usually impossible. Therefore, it is of interest to infer migration patterns from the genetic compositional differences between populations, often summarized in pairwise FST statistics. One of the well-known results under the two-population model suggests that pairwise FST is proportional to migration rates under several assumptions, but their relationship in a network of more than two populations remains unclear. In this project, we studied problems of whether multi-population migration patterns can be inferred from pairwise FST measures, whether a similar proportional relationship holds between them even under ideal assumptions, and whether the information in pairwise FST is sufficient to uniquely determine the pair-wise migration rates. By analyzing the system of inferring migration from pairwise FST, we investigated the conditions for which migration is identifiable, and the extent to which pairwise FST can be interpreted as being proportional to migration in the multi-population network. Our results suggest a lack of identifiability in the inference of migration from pairwise FST under the multi-population model, which highlights a problem in the common interpretation of pairwise FST being an indicator proportional to the underlying migration.

Xiran is a second year PhD student in ICME. He is working with Professor Noah Rosenberg from the Biology department. His current research interest is mathematical and computational biology and application of computational methods in biomedical sciences.
Neural networks have become state-of-the-art models in numerous machine learning tasks and strong empirical performance is often achieved by deeper networks. One landmark example is the residual network (ResNet). To better understand the success of ResNet, we take a limit of the depth of ResNet to infinity and obtained a continuous ODE limit. From the ODE limit, we explore the power of this analysis from three aspects, modeling, optimization and inferencing. This project include works published at ICML2018, ICLR2019, NeurIPS2019 and works submitted to ICML2020.

Yiping Lu is a first year PhD student in the Institute for Computational and Mathematical Engineering at Stanford. His work borrows idea from differential equation, control theory and statistics to make machine learning systems, especially deep learning systems, more robust and reliable. He is also working on nonparametric statistics and robustness of machine learning systems.

Relevant Links:
https://documentcloud.adobe.com/link/track?uri=urn:aaid:scds:US:e556e1ce-9fa3-47e9-ad7f-16f6a91e4aba

Yiping Lu
ICME PhD Student

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For my research I am accelerating and extending a path-planning based patient-specific modeling method commonly used for anatomic model creation for cardiovascular fluid dynamics simulations. I am also addressing a longstanding open question of how realistic patient-specific model geometry variability influences simulation output uncertainty. I accelerate model building using recently developed deep learning methods and convolutional neural networks to automatically generate vessel surfaces from image data. I have further enabled the quantification of simulation output uncertainty due to geometry variation by modeling the probability distribution of vessel surfaces using convolutional Bayesian dropout networks.

Gabriel Maher is a PhD student at the Institute for Computational and Mathematical Engineering at Stanford University and works with Dr. Alison Marsden at the Cardiovascular Biomechanics Computation Lab. For his research Gabriel is applying Deep Learning to the problem of blood vessel detection in volumetric MR and CT medical images. He has further extended these methods to quantify the effects of geometry uncertainty on cardiovascular fluid dynamics simulations using Bayesian dropout networks.
Quantitative science has been successfully applied in public equity investing space by hedge funds and other systematic investment managers but little progress has been recorded in the private markets. Of particular interest has been the application of reinforcement learning to optimal trade order execution, market making, hedging derivatives and portfolio allocation problems. The private market space is still more of a relationship market but increased digitalisation and availability of rich data sets, especially for PE and VC firms with many portfolio companies has seen many investors turning their attention to data science to complement their work. In this work, I examine the application of reinforcement learning algorithms to source investment deals and manage portfolio companies to enhance value creation. Specifically, I try to answer the optimal exit timing problem in a portfolio company, and hence determine whether to exit and if not, how much follow-on investment to make in portfolio companies to create maximum value.

Andrew Matangaidze is a final year dual MS/MBA degree candidate at Stanford Graduate School of Business (GSB) and ICME. In the MS program at ICME, he focuses on Data Science and Computational Finance, with special interests on the application of Machine Learning to problems in finance and business/commerce. He spent the last two summers at Goldman Sachs in NYC and Cisco after working for more than 7 years as an investor before coming to Stanford.
My current research is focused on using topological structure for computations and data analysis. Recently, with Anjan Dwaraknath and Gunnar Carlsson, I have developed a framework for matrix factorizations on quiver representations to compute algebraic invariants of diagrams of topological spaces. I have also recently shown how geometric complexes parameterized by covers of a data set can be used to reduce the size of computations, and encode known structure in the data. Finally, I have generalized a topological model for image patches (small squares of pixels sampled from an image) to higher dimensional images, and used this to understand the topology of image patches in 3-dimensional image data sets. I am currently working on applying topological data analysis to different applications, and developing theory and computational tools that bring together applied topology and other areas of applied mathematics and data analysis.

Brad Nelson is a graduating ICME PhD student working in applied and computational topology. He has a BA in mathematics from Dartmouth, previously worked at Epic developing medical record software, has done internships at Ayasdi and Lawrence Livermore National Lab while at Stanford, and worked with the Neutrino group at SLAC developing deep learning algorithms for particle detection. At ICME, he has taught short courses on Python, Julia, and libraries for scientific computing. After graduation, he is headed to the Department of Statistics in the University of Chicago as a Kruskal Instructor.
Precise splice junction calls are currently unavailable in scRNA-seq pipelines such as the 10x Chromium platform but are critical for understanding single-cell biology. Here, we introduce SICILIAN, a new method that assigns statistical confidence to splice junctions from a spliced aligner to improve precision. SICILIAN’s precise splice detection achieves high accuracy on simulated data, improves concordance between matched single-cell and bulk datasets, increases agreement between biological replicates, and reliably detects unannotated splicing in single cells, enabling the discovery of novel splicing regulation.

Julia Olivieri is a fourth year PhD student in ICME interested in the statistics of single cell RNA sequencing.

Point-set registration is a classical image processing problem that looks for the optimal transformation between two sets of points. In this work, we analyze the impact of outliers when finding the optimal rotation between two point clouds. The presence of outliers motivates the use of least unsquared deviation, which is a non-smooth minimization problem over non-convex domain. We compare approaches based on non-convex optimization over special orthogonal group and convex relaxations. We show that if the fraction of outliers is larger than a certain threshold, any naive convex relaxation fails to recover the ground truth rotation regardless of the sample size and dimension. In contrast, minimizing the least unsquared deviation directly over the special orthogonal group exactly recovers the ground truth rotation for any level of corruption as long as the sample size is large enough. These theoretical findings are supported by numerical simulations. https://arxiv.org/abs/2004.08772

Cindy Orozco Bohorquez is a fifth year PhD student working on the intersection of numerical analysis and machine learning. She holds a BS in mathematics and civil engineering from Universidad de los Andes, Colombia and master's in applied mathematics from King Abdullah University of Science and Technology (KAUST), Saudi Arabia. Cindy is passionate about diversity and math education.

Relevant Links:
Before coming to Stanford, I worked on GAMs (Global Autoregressive Models), which combine an autoregressive component with a log-linear component, allowing the use of global a priori features to compensate for lack of data. We also derived different approaches for approximating the normalized distribution given by GAMs, for fast inference.

During the rotation program at Stanford, I worked with Professor Eric Darve in deriving bounds on the number of neurons and layers of Relu NN necessary for approximate any analytic function arbitrarily close. During the winter quarter, I worked with Professor Lexing Ying on defining Hamiltonian layerwise for NN and using them to approach the delayed gradient problem to decouple layers during the backpropagation.

Tetiana Parshakova is a PhD student in ICME. Previously, she obtained a bachelor's and a master’s degree at KAIST.

Relevant Links:

Nearshore bathymetry, the topography of ocean floor in coastal zones, has played a vital role in prediction of surf zone hydrodynamics and route planning for avoidance of subsurface features. Hence, it becomes increasingly important in a wide variety of applications including shipping operations, coastal management and risk assessment. However, direct high resolution surveys of nearshore bathymetry are rarely performed due to budget constraints and logistical restrictions. One possible alternative when only sparse observations are available is to use Gaussian processes regression, or Kriging. However, it is often difficult for traditional methods to recognize patterns with sharp gradients like those found around sand bars or submerged objects, especially when observations are sparse. In this work, we present several deep learning based techniques to estimate nearshore bathymetry with sparse, multi-scale measurements. We develop a deep neural network to directly compute posterior estimates of nearshore bathymetry, as well as a conditional Generative Adversarial Network (cGAN) that samples from the posterior distribution. We train our neural networks based on synthetic data generated from nearshore surveys provided by the U.S. Army Corps of Engineer Field Research Facility (FRF) in Duck, North Carolina. We compare our methods with Kriging on real surveys as well as ones with artificially added patterns of sharp gradient. Results show that both direct estimations and sampling by DNN give better predictions than Kriging. Finally, we propose a novel method which combines deep learning based models with Kriging, and shows further improvement of the posterior estimates.

Yizhou Qian is a second-year PhD student in ICME at Stanford University, where he is advised by Eric Darve from Department of Mechanical Engineering. His main research interests include physics-based learning, data assimilation, task-based runtime systems and parallel computing. Before joining Stanford, he obtained his bachelor's and master's degree (2014-2018) in mathematics at University of California, Los Angeles.
IMPACT OF DATA SOURCES ON MULTI-TASK LEARNING

In collaboration with Ranjay Krishna, as part of the CS231N course (Convolutional Neural Networks for Image Recognition). We investigate the relative performance of a multi-task computer vision model that is trained on a single data source (containing annotations for each target task per image) against a model that is trained on disjoint data sources, where each target task has a dedicated source. We want to understand whether having a single data source can act as a regularizer and improve the model's ability to generalize to unseen data. The results of this investigation can guide researchers on how to develop multi-task datasets and train models.

Abhinav Rangarajan is a first-year master's student in ICME. He is interested in machine learning applications in finance. Abhinav has a BA in mathematics and computer science from Cornell University, and has worked in the finance industry for three years, most recently as a software engineer at Bloomberg.

Arvind S. Kumar is a first year master's student at ICME. His research interest lies in developing AI and machine learning tools to solve problems in areas such as genomics, computer vision and language understanding.

Nicolas Aagnes is a first year master's student in the ICME Data Science track. He received his Bachelor’s degree in Mathematical Engineering from Politecnico di Milano.

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Decommissioning internal combustion engine vehicles (ICE) and replacing them with electric vehicles constitute one of the main challenges engineers and scientists have to face in order to reduce the emissions from the ICE vehicles. The design of equitable policies to decommission ICE vehicles requires a traffic flow model that allows the effective prediction of traffic flow and corresponding emissions on critical commute/transportation routes. In my research, I’m interested in developing a new traffic flow PDE (Partial Differential Equation) based model, calibrated on Sonoma County and Santa Cruz County. My model will extend those found in the literature by incorporating features such as the shape of the road, carpool lanes and randomness. The goal of these extensions is to achieve more realistic results.

Nadim Saad is a second year PhD student in ICME advised by Professor Margot Gerritsen. His interests lie broadly in Numerical Partial Differential Equations (PDEs) and Optimization. He’s currently working on PDE based traffic flow models. Nadim is originally from Lebanon and speaks English, French and Arabic.
We develop a new class of quantum stabilizer codes by associating stabilizers to faces of a closed 2-cell graph embedding on a closed 2-dimensional manifold. All such codes can be reduced to the case where the graph embedding has only degree 3 or degree 4 vertices, using a canonical construction that I will describe. These codes come in two distinct classes --- ones that are checkerboardable, and ones that are not. Checkerboardable means that the faces can be colored using 2 colors (say black and white) such that around every vertex, no adjacent sectors have the same color. We prove that the checkerboardable codes are exactly the toric codes (first introduced by Kitaev). The non-checkerboardable codes contain many existing code families like the triangular surface code, the rotated surface code, etc, and some others that are new. We derive the number of encoded qubits by these code families (which is the easy part), but also derive bounds on the distance (which is harder). It will be shown that computing the distances for the checkerboardable codes can be done exactly in polynomial time, while a factor 1/2 approximation of the distance can be computed efficiently for the non-checkerboardable case. A particular code, that we call the cyclic toric code, is explored in some detail where we have been able to prove the distances exactly.

This is joint work with Ted Yoder, IBM Research, Yorktown Heights

Rahul Sarkar is a PhD student in ICME, advised by professors Biondo Biondi and András Vasy. Rahul holds a BS and MS degree from Indian Institute of Technology Kharagpur, India, as well as an MS degree from ICME at Stanford University. His current projects include computational inverse problems, quantum error correcting codes, and mathematical analysis.

Relevant Links:

The classes in classification tasks are often composed of finer-grained subclasses. Models trained using only the coarse-grained class labels tend to exhibit highly variable performance across different subclasses. Moreover, the subclasses are often unknown ahead of time, making it difficult to identify and reduce such performance gaps. This "hidden stratification" problem can be critical in applications such as medical imaging and algorithmic fairness, where the costs of different types of mistakes are not equal. We propose a framework to address hidden stratification that combines representation learning, unsupervised clustering, and robust optimization to automatically identify the subclasses and train models with better worst-case subclass performance—without requiring prior knowledge of the subclasses. In this way, our framework allows machine learning practitioners to find poorly performing subclasses and improve performance on them, without needing to resort to expensive relabeling of the data.

Nimit Sharad Sohoni is a fourth-year ICME PhD student, advised by Professor Christopher Ré. He is broadly interested in the theoretical and practical development of optimization methods for machine learning. Nimit earned his bachelor’s degrees in mathematics and computer science at Cornell University.

Relevant Links:
Research into geographic modeling -- using remote sensing and image processing -- on healthcare outcomes can facilitate policy making, which can contribute to providing systematic and targeted care in a developing country. As data on healthcare outcomes is scarce in developing countries, recent research (Jean et al. 2016; Perez et al. 2017; Xie et al. 2016) have provided strong evidence for the fusion of machine learning with satellite data to extract information about socioeconomic variables with respect to geography. This work has shown that we can use techniques like transfer learning to develop maps of several healthcare outcomes in Nigeria, using satellite images taken over a period of time, such as Landsat data which goes as far back as 1970. We aim to use the approach of transfer learning in a closely related field: socioeconomics, specifically the geospatial distribution of assets, or wealth, in Pakistan. Searching for an accurate model for predicting the distribution of assets could have vast applications. With the knowledge of socioeconomic outcomes, like wealth, over a period of time, we can gain a better understanding of past policy effects on the population, and inform more efficacious future policy.

Veer Shah is a first year master's student in ICME, in the data science track. His areas of study revolve around statistics, data science, and machine learning, particularly to applications in economics, healthcare, climate change, and other high impact problem spaces.
The project is part of Stanford's Smart Primer project, and aims to use deep reinforcement learning and NLP techniques to generate hints for middle school children. The research focuses on teaching children simple geometry by using their current performance and messages with a chatbot-style functionality. The first phase of the research involves building a children simulation openAI gym environment.

William Steenbergen is a first year master's student in the data science track in ICME. He is focused on reinforcement learning and federated machine learning.

Relevant Links: https://hci.stanford.edu/research/smartprimer/
The US Preventive Services Task Force recommends lung cancer screening for high risk individuals aged 55-80 with at least 30 pack-years (a metric quantifying smoking exposure), and no more than 15 years since smoking cessation. Many other risk factors are associated with lung cancer incidence, yet screening eligibility is solely based on age and smoking history, leading to sub-optimal screening strategies. We propose a partially observable Markov decision process (POMDP) that provides individualized optimal screening strategies for current and former smokers. Decisions are made based on the risk of the individuals accounting for previous screening results and changes in individuals’ smoking behavior.

Iakovos Toumazis is a postdoctoral fellow in the Department of Biomedical Data Science at Stanford. He is a member of the NCI-sponsored Cancer Intervention and Surveillance Modeling Network (CISNET). He received his PhD in Industrial Engineering from the State University of New York at Buffalo. Part of his doctoral dissertation received the Best Graduate Student Paper award from the Society for Health Systems of the Institute of Industrial & Systems Engineers (2015). In 2017, he received the Ruth L. Kirschstein National Research Service Award (NRSA) Individual Postdoctoral Fellowship (Parent F32) from the National Institutes of Health. His research interests include sequential decision making under uncertainty, applications of Operations Research in healthcare, simulation systems, robust optimization, and cost-effectiveness analysis of cancer interventions.
A MODEL TO ESTIMATE BED DEMAND FOR COVID-19 RELATED HOSPITALIZATION

As of March 23, 2020 there have been over 354,000 confirmed cases of coronavirus disease 2019 (COVID-19) in over 180 countries, the World Health Organization characterized COVID-19 as a pandemic, and the United States (US) announced a national state of emergency. In parts of China and Italy the demand for intensive care unit (ICU) beds was higher than the number of available beds. We sought to build an accessible interactive model that could facilitate hospital capacity planning in the presence of significant uncertainty about the proportion of the population that is COVID-19+ and the rate at which COVID-19 is spreading in the population. Our approach was to design a tool with parameters that hospital leaders could adjust to reflect their local data and easily modify to conduct sensitivity analyses. We developed a model to facilitate hospital planning with estimates of the number of Intensive Care Unit (ICU) beds, Acute Care (AC) beds, and ventilators necessary to accommodate patients who require hospitalization for COVID-19 and how these compare to the available resources. Inputs to the model include estimates of the characteristics of the patient population and hospital capacity. We deployed this model as an interactive online tool. The model is implemented in R 3.5, RStudio, RShiny 1.4.0 and Python 3.7.

Jin Xie is a fourth-year PhD student in ICME, advised by Professors Peter Glynn and Jose Blanchet. Her research mainly focuses on healthcare data analysis, artificial intelligence algorithm design, and application of stochastic optimization in statistics and finance. She is interested in using mathematical tools to solve real-world problems in healthcare and finance. Before joining Stanford, Jin studied mathematics at Peking University.

Linying Yang is a 2nd year master's student in ICME. Her research interests include applied Bayesian statistics and simulation.

Teng Zhang is a fourth year PhD student in Management Science and Engineering. He studies stochastic models and simulation, with application in machine learning and healthcare.

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https://surf.stanford.edu/covid-19-tools/covid-19/
PHYSICS CONSTRAINED LEARNING

Deep neural networks (DNNs) have been demonstrated effective for approximating complex and high dimensional functions. In the data-driven inverse modeling, we use DNNs to substitute unknown physical relations, such as constitutive relations, in a physical system described by partial differential equations (PDEs). The coupled system of DNNs and PDEs enables describing complex physical relations while satisfying the physics to the largest extent. However, training the DNNs embedded in PDEs is challenging because input-output pairs of DNNs may not be available, and the physical system may be highly nonlinear, leading to an implicit numerical scheme. We propose an approach, physics constrained learning, to train the DNNs from sparse observations data that are not necessarily input-output pairs of DNNs while enforcing the PDE constraints numerically. Particularly, we present an efficient automatic differentiation based technique that differentiates through implicit PDE solvers. We demonstrate the effectiveness of our method on various problems in solid mechanics and fluid dynamics. Our PCL method enables learning a neural-network-based physical relation from any observations that are interlinked with DNNs through PDEs.

Kailai Xu is a fourth-year PhD student diving deep into the intersection of machine learning and scientific computing. He obtained his BS degree in mathematics from Peking University. His current research interest centers on physics-based machine learning for inverse problems in scientific computing. He developed the open-source software ADCME.jl in Julia and C++ for high-performance inverse modeling using automatic differentiation. Specifically, he has researched novel physics-based machine learning methods and developed software packages based on ADCME.jl for solving inverse problems in stochastic processes, solid mechanics, geophysics and fluid dynamics. One highlight of his research is combining neural networks with numerical solvers for Partial Differential Equations (PDEs), which enables data-driven modeling with physics knowledge.

Relevant Links:
https://documentcloud.adobe.com/link/track?uri=urn:aaid:scds:US:5c69500c-49b7-49be-a75a-ecf94909d77b

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We investigate algorithms for anomaly detection with deep generative models. Previous anomaly detection methods focus on modeling the distribution of non-anomalous data provided during training. However, this does not necessarily ensure the correct detection of anomalous data. We propose a new Regularized Cycle Consistent Generative Adversarial Network (RCGAN) in which deep neural networks are adversarially trained to better recognize anomalous samples. This approach is based on leveraging a penalty distribution with a new definition of the loss function and novel use of discriminator networks. It is based on a solid mathematical foundation, and proofs show that our approach has stronger guarantees for detecting anomalous examples compared to the current state-of-the-art. Experimental results on both real-world and synthetic data show that our model leads to significant and consistent improvements on previous anomaly detection benchmarks. Notably, RCGAN improves on the state-of-the-art on the KDDCUP, Arrhythmia, Thyroid, Musk and CIFAR10 datasets.

Ziyi Yang is a fourth year PhD student from the Mechanical Engineering department advised by Professor Eric Darve. His research interest includes anomaly detection with deep learning and natural language processing. He obtained his MS In EE from Stanford and BS in physics from Nanjing University.

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In this work, we study the continuous-time limit of quasi-Newton methods, one of the most widely used family of iterative algorithms for solving medium to large scale nonlinear equations $g(x) = 0$. The key idea is to utilize the secant conditions for identifying the correct scaling of the approximate Jacobian update equations. Focusing on the Broyden’s method, we study its connection with the continuous-time Newton’s method, and elucidate the caveat that prevents the (local or global) existence of its trajectories. We then propose some stabilization tricks motivated by momentum methods, and establish some preliminary theory on global convergence using a Lyapunov argument. This is a joint work with Junzi Zhang and Professor Stephen P. Boyd.

Honglin Yuan is a 3rd year PhD student from Stanford ICME advised by Professor Tengyu Ma. His research interest lies in Machine Learning Theory, in particular Deep Learning and Optimization Theory. His research is supported by a TOTAL fellowship.
We study a new reinforcement learning algorithm designed to explore and generalize efficiently via linearly parameterized value functions. The algorithm achieves exploration through the injection of noise in the learned data, and is provably sample and computational efficient. Furthermore, the algorithmic structure is easily generalizable to more complex architectures than linear predictors.

Andrea Zanette is a PhD candidate in the Institute for Computational and Mathematical Engineering at Stanford University advised by professors Emma Brunskill and Mykel J. Kochenderfer. His research focuses on provably efficient methods for Reinforcement Learning, in particular, he develops agents capable of autonomous exploration. His research is currently supported by Total.

Relevant Links:
https://nips.cc/Conferences/2019/ScheduleMultitrack?event=13690
Adaptive experiments can result in considerable cost savings in multi-armed trials by enabling analysts to quickly focus on the most promising alternatives. Most existing work on adaptive experiments (which include multi-armed bandits) has focused maximizing the speed at which the analyst can identify the optimal arm and/or minimizing the number of draws from sub-optimal arms. In many scientific settings, however, it is not only of interest to identify the optimal arm, but also to perform a statistical analysis of the data collected from the experiment. Naive approaches to statistical inference with adaptive inference fail because many commonly used statistics (such as sample means or inverse propensity weighting) do not have an asymptotically Gaussian limiting distribution centered on the estimate, and so confidence intervals constructed from these statistics do not have correct coverage. But, as shown in this paper, carefully designed data-adaptive weighting schemes can be used to overcome this issue and restore a relevant central limit theorem, enabling hypothesis testing. We validate the accuracy of the resulting confidence intervals in numerical experiments. This is joint work with Vitor Hadad, David A. Hirshberg, Stefan Wager, Susan Athey, posted on https://arxiv.org/abs/1911.02768.

Ruohan is a third-year ICME student advised by Professor Susan Athey. Her research mainly focuses on causal inference, statistics and machine learning. She is particularly excited about policy evaluation and experimental design.

Relevant Links:
https://www.gsb.stanford.edu/faculty-research/centers-initiatives/sil
https://documentcloud.adobe.com/link/track?uri=urn:aaid:scds:US:a7aa6f32-d5a4-40a4-8d6b-bf6789f41727
A2DR: OPEN-SOURCE PYTHON SOLVER FOR PROX-AFFINE DISTRIBUTED CONVEX OPTIMIZATION

We consider the problem of finite-sum non-smooth convex optimization with general linear constraints, where the objective function summands are only accessible through their proximal operators. This problem arises in many different fields such as statistical learning, computational imaging, telecommunications, and optimal control. To solve it, we propose an Anderson accelerated Douglas-Rachford splitting (A2DR) algorithm, which combines the scalability of Douglas-Rachford splitting and the fast convergence of Anderson acceleration. In particular, A2DR exploits the block separable structure in the objective and partially decouples so that its steps may be carried out in parallel, and is hence fast and scalable to multiple processors. We show that A2DR either globally converges or provides a certificate of infeasibility/unboundedness under very mild conditions. We describe an open-source implementation (cf. https://github.com/cvxgrp/a2dr and https://pypi.org/project/a2dr/) and demonstrate its outstanding performance on a wide range of examples. This is joint work with Anqi Fu and Professor Stephen Boyd.

Junzi Zhang is a fifth-year PhD student in ICME, advised by Professor Stephen P. Boyd from the Department of Electrical Engineering. Before coming to Stanford, he obtained his BS degree in applied mathematics from School of Mathematical Sciences, Peking University, where he conducted his undergraduate research under the supervision of Professors Zaiwen Wen and Pingwen Zhang. His current research is focused on the design and analysis of optimization algorithms and software, as well as the applications in the fields of machine learning, causal inference, and decision-making systems (especially reinforcement learning). His current research is partly supported by Stanford Graduate Fellowship. He has also been the co-president of Association of Chinese Students and Scholars at Stanford (ACSSS), and had contributed to enhance the cooperation between the Chinese community and the Stanford school authority, as well as boosting the influence of the Chinese culture in the community of international students.

Relevant Links:
https://arxiv.org/abs/1908.11482