
1. Simulating COVID-19 transmission under different testing and policy strategies on the Colorado School of Mines campus

[S] Laura Albrecht, Colorado School of Mines

We develop a data-driven model to simulate the spread of COVID-19 on the Colorado School of Mines campus. The model is useful to simulate different surveillance testing strategies and policy decisions which can be compared to minimize key metrics such as active cases by a certain date or the number of resident students in quarantine or isolation at one time. We adapted a stochastic compartmental epidemic model (SEIR) to represent the transmission of the virus through the student population. Notably, we have included compartments for individuals in the population that are in isolation, quarantine, or being tested and waiting for results. Our population is stratified into groups such as resident students, non-resident students, athletes, faculty, and staff. Some model parameters, such as contact rates between individuals, are uncertain and a key feature is to quantify how this uncertainty propagates through our model and into our predictions. Our initial estimates for these parameters come from fitting our model output to the observed COVID-19 case data on the Mines campus from the Fall 2020 semester. This model can then be used to simulate and compare different surveillance testing strategies and policy decisions to minimize key metrics such as active cases by a certain date or the number of resident students in quarantine or isolation at one time.

Joint work with Doug Nychka, Colorado School of Mines; Karin Leiderman, University of North Carolina Chapel Hill

2. Open World Dempster-Shafer using Complementary Sets

[S] Cassandra Armstrong, Los Alamos National Laboratory

We consider the Dempster-Shafer framework for reasoning with uncertainty. One assumption of Dempster-Shafer Theory is a closed-world, or the assumption that all propositions are known a priori. In this poster, we explore an alternative formulation of Dempster-Shafer that allows for the dynamic inclusion of new propositions. Specifically, we expand the framework to include the complement of every proposition as well as complementary sets of sets of propositions. This adjustment enables an open-world interpretation that can support unspecified and dynamic propositions as we learn about the problem space. We demonstrate our data fusion method on a Sentinel-2 land cover classification problem.

Joint work with Erik Skau, Los Alamos National Laboratory, David Gerts, Los Alamos National Laboratory, Kari Sentz, Los Alamos National Laboratory

3. Applications of Machine Learning for Laser Control

[S] Aasma Aslam, University of New Mexico

To configure a photoinjector to reproduce a given electron bunch with the desired characteristics, it is necessary to adjust the operating parameters with high precision. More or less, the fine tunability of the laser parameters are of extreme importance as we try to model further applications of the photoinjector. The laser pulse incident on the photocathode critically affects the electron bunch 3D phase space. Parameters such as the laser pulse transverse shape, total energy, and temporal profile must be controlled independently, any laser pulse variation over both short and long-time scales also requires correction. The ability to produce arbitrary laser intensity distributions enables better control of electron bunch transverse and longitudinal emittance by affecting the space-charge forces throughout the bunch. In an accelerator employing a photoinjector, electron optics in the beamline downstream are used to transport, manipulate, and characterize the electron bunch.

4. A Conversational Assistant for Democratization of Data Visualization

[S] Abari Bhattacharya, University of Illinois Chicago

Data visualization is an important aspect of exploratory data analysis which requires expertise, posing a challenge to many users. In this work we present a conversational system to make data visualization accessible, where users can generate visualizations of data by natural language conversational interaction with the system and make sense of complex data with ease. We also discuss the findings of the evaluation of the system conducted by assigning data exploration tasks to users.

Joint work with Veronica Grosso*, Barbara Di Eugenio*, Andrew Johnson* (*University of Illinois Chicago), Roderick Tabalba, Nurit Kirshenbaum, Jason Leigh (University of Hawaii at Manoa), Moira Zellner (Northeastern University)

5. Applying PCA to Random Forest Analysis to Tease Out Correlated Data When Predicting Bias in Integral Experiments*[S] Brian Bell, University of Arizona Mathematics and Los Alamos National Laboratory XCP-5*

Nuclear data are used as fundamental input data for neutron-transport simulations to answer questions related to various nuclear technologies. Sub-sets of nuclear data, encompassing as a whole >40,000 of data points, are validated with respect to 1000s of criticality experiments that represent various applications on a small scale. The explicit aim of validation with these experiments is to find errors in nuclear data. The key challenge here is that several 100s of nuclear data are used to simulate one integral value. Hence, one cannot clearly identify what nuclear data are leading to bias in criticality measurements. In fact, a mistake in one nuclear data observable can be compensated with an error in another, and the simulated criticality value would still be predicted in agreement with experimental data. Random forest (RF) was previously employed to predict bias in criticality measurements using sensitivities of simulated criticality experiments to nuclear data. The SHaply Additive exPlanations (SHAP) metric was then applied to attribute importance of each nuclear data experiment and observable to bias prediction. This, however, did not highlight what nuclear data were jointly related to predicting bias. This is important as it could inform us on where compensating errors in nuclear data could hide. We tackle this shortcoming here by first decomposing the nuclear data into principal components, using principle component projections to predict bias via the RF and SHAP, and then using SHAP values and principle components to reconstruct detailed SHAP values for each nuclear data observable. We demonstrate that these extended SHAP bias predictions are more robust, less noisy, more efficient and more readable for experts. In addition, we show that this approach accounts for co-variance in nuclear data sensitivities and automates identification of where compensating errors could hide in nuclear data. LA-UR-23-20862

Joint work with B.W. Bell, M.J. Grosskopf, J. Hutchinson, D. Neudecker

6. Data Analysis and Control of an MeV Ultrafast Electron Diffraction System using Machine Learning*[S] Trudy Bolin, University of New Mexico*

An MeV ultrafast electron diffraction (MUED) instrument such as the one located at the Accelerator Test Facility (ATF), Brookhaven National Laboratory, is a unique characterization technique used to study ultrafast processes in a variety of materials systems by a pump-probe method. This technology can be advanced further into a turnkey instrument by using data science and artificial intelligence (AI) mechanisms in conjunction with high-performance computing. This system can facilitate automated operation, data acquisition, and real-time or near-real-time processing. The AI-based system controls can provide real-time feedback on the electron beam, or provide virtual diagnostics of the beam. Deep learning can be applied to the MUED diffraction patterns to recover valuable information on subtle lattice variations that can lead to a greater understanding of a wide range of material systems. A data-science-enabled MUED facility will also facilitate the application of this technique, expand its user base, and provide a fully automated state-of-the-art instrument. Updates on research and development efforts for the MUED instrument in the Accelerator Test Facility of Brookhaven National Laboratory are presented.

Joint work with Salvador Sosa (UNM), Aasma Aslam (UNM, CBB), Sandra Biedron (UNM)

7. MCMC for Bayesian Parametric Galaxy Modeling*[P] James Buchanan, Lawrence Livermore National Laboratory*

We apply Markov Chain Monte Carlo (MCMC) to the problem of parametric galaxy modeling, estimating posterior distributions of galaxy properties such as ellipticity and brightness for more than 100,000 images of galaxies taken from DC2, a simulated LSST-like survey. The resulting posterior samples enable rigorous probabilistic inference of galaxy model parameters and their uncertainties. These posteriors are one key ingredient, along with probabilistic object detection, in a fully probabilistic description of galaxy catalogs, which can ultimately enable a refined Bayesian estimate of cosmological parameters. We examine the reliability of various point estimates of galaxy parameters, and of the posterior width as a measure of uncertainty, and we look at the additional insights enabled by correlated parameter modeling. We organize the probabilistic modeling and MCMC inference using the JIF (Joint Image Framework) tool, which we make freely available online.

Joint work with Michael Schneider, Robert Armstrong, Kerianne Pruett (LLNL)

8. Application of Machine Learning and Deep Learning Techniques to Magnetic Field Sensor Data Collected at HFIR*[S] Braden Burt, Air Force Institute of Technology*

The nuclear fuel cycle forms the basis for producing special nuclear materials used in nuclear weapons via a series of interdependent industrial operations. These industrial operations each produce characteristic emanations that can be gathered to ascertain signatures of facility operations. This work seeks to address nonproliferation concerns by focusing on analyzing signatures gathered at a nuclear reactor, which could be used to produce Pu. Machine learning and deep learning techniques were applied to time series magnetic field sensor data collected at the High Flux Isotope Reactor (HFIR) by the Complexity team led by UC Berkeley to assess the feasibility of determining the ON/OFF operational state of the reactor. When the data is transformed to the frequency domain, it was found that both machine and deep learning methods were able to classify the operational state to a balanced accuracy over 90%. This result suggests that the utilized methods have promise for use in the detection of proliferation activities with nuclear reactors. Additional effort is recommended to seek models and architectures that will more fully capitalize on the data's temporal nature by incorporating the magnetic field's time dependence to improve model robustness and classification performance.

Joint work with B. J. Borghetti, A.L. Franz, D.E. Holland, A.A. Bickley

9. Interpretability Methods for Deep Neural Networks as Applied to TePla Damage Calibration in Copper*[S] Skylar J Callis, Los Alamos National Laboratory XCP-8*

We present an application of convolutional neural networks (CNNs) for calibration of a tensile plasticity (TePla) damage model simulating spallation in copper under high-explosive shock loading. These CNNs are trained on images of a synthetic density field or radiograph of an idealized representation of a shock experiment in copper. The CNNs also take as input a scalar value of the high-explosive detonation velocity. Our models estimate three key TePla damage parameters along with a simulation time-stamp useful for matching synthetic and experimental data. Regardless of a network's ability to produce accurate inferences, application of machine-learning methods must be accompanied by an analysis of how they are making their inferences in order to build confidence in these predictions and to predict likely shortcomings in the technique. This poster will highlight the various interpretability methods that have been explored thus far for the trained CNNs. The CNN models make predictions by passing inputs through layers; each layer produces a set of features. The interpretability methods explored all center on directly extracting and analyzing features. Extracted features are compared to radiographic and hydrodynamic fields--both fields that the network has trained on and fields that remain unseen. Additionally, scalar cross-correlations are calculated between extracted features and properties of interest, including the synthetic radiograph, the hydrodynamic fields, and network predictions. These methods allow for an analysis of what the CNN identifies as the features most applicable to parameterizing the damage model. As a more in depth analysis, the derivative of the model predictions with respect to an internal feature is calculated using a twin model with an internal scaling factor. This aims to capture information about the sensitivity of model predictions to unseen internal model states. While existing sensitivity methods for CNNs often lack mathematical background, this derivative method is explored as a way to reasonably quantify model sensitivity.

10. Bayesian Projection Pursuit Regression*[S] Gavin Collins, Ohio State University, Los Alamos National Laboratory*

In projection pursuit regression (PPR), an unknown response function is approximated by the sum of M "ridge functions," which are flexible functions of one-dimensional projections of a multivariate input space. Traditionally, optimization routines are used to estimate the projection directions and ridge functions via a sequential algorithm, and M is typically chosen via cross-validation. We introduce a novel Bayesian version of PPR, which has the benefit of accurate uncertainty quantification. To learn the projection directions and ridge functions, we apply novel adaptations of methods used for the single ridge function case ($M=1$), called the Bayesian Single Index Model; then use reversible jump MCMC to learn the number of ridge functions M . We evaluate the predictive ability of our model in 20 simulation scenarios and for 23 real datasets, in a bake-off against an array of state-of-the-art regression methods. Its effective performance indicates that Bayesian Projection Pursuit Regression is a valuable addition to the existing regression toolbox.

Joint work with Devin Francom and Kellin Rumsey, Los Alamos National Laboratory

11. Deep Gaussian Processes for Surrogate Modeling with Categorical Data

[S] Andrew Cooper, Virginia Tech Department of Statistics

Many applications of experimental design produce categorical response data. Popular classifiers such as neural network models and support vector machines can provide high predictive accuracy for examples with large input dimension. However, these models require large amounts of data and offer poor uncertainty quantification (UQ). This provides a challenge for situations where available training data is sparse. Gaussian processes (GP's) are stochastic models that can be modified to handle categorical responses and capture uncertainty with little training data. However, these models often struggle with non-stationary behavior in the form of asymmetrical response surfaces and rigid boundaries between classes. Deep Gaussian processes (DGP's) are functional compositions of GP's, and have excelled in regression settings for their ability to handle non-stationary behavior by warping the input space. We introduce a fully Bayesian implementation of the DGP model for multiclass classification. We showcase our model's ability to handle non-stationarity and accurately perform UQ in small-data settings.

Joint work with Annie Sauer (Virginia Tech Department of Statistics), Robert Gramacy (Virginia Tech Department of Statistics)

12. Automatic Relevance Determination for Gaussian Processes with Functional Inputs

[S] Luis Damiano, Department of Statistics, Iowa State University

In the context of Gaussian process regression, it is common to treat functional inputs as a vector. The parameter space becomes prohibitively complex as the functional input definition increases, thus hindering automatic relevance determination. Generalizing work for time-varying inputs, we introduce the automatic dynamic relevance determination (ADRD) framework to enforce smoothness on the predictive relevance profile over the index space with only a limited number of parameters. Fully Bayesian estimation is carried out to identify relevant regions of the functional input space and validation is performed to benchmark against traditional vector-input model specifications. In a case study for surrogate modeling, we find that ADRD outperforms models with input dimension reduction via functional principal component analysis. Furthermore, the predictive power is comparable to high-dimensional models, in terms of both mean prediction and uncertainty, with 10 times fewer tuning parameters. Finally, ADRD rules out erratic patterns associated with vector-input models.

Joint work with Margaret Johnson (JPL, Caltech), Joaquim Teixeira (JPL, Caltech), Max D. Morris (ISU), and Jarad Niemi (ISU)

<https://doi.org/10.48550/arXiv.2209.00044>

13. Prediction of Impact Sensitivity, Heat of Formation and Heat of Explosion using Atomic Connectivity

[S] Jack V Davis, Los Alamos National Laboratory

A very large database of about 500 explosives and 135 descriptors were examined to develop a quick model of predicting impact sensitivity. In this quick model, only structural information and information that can be simply calculated from structural information is considered, such as, bond environments, molecular formula, functional groups, and oxygen balance among others. Using random forests, the number of descriptors was reduced to 18 important descriptors to describe impact sensitivity among all functional group types with similar accuracy to previously reported models ($R^2 = 0.788$ and $RSME = 0.312$). In addition to impact sensitivity, the model was found to accurately predict important, high explosive parameters, heat of formation and heat of explosion ($R^2 = 0.966, 0.916$ respectively) allowing for a fast screening of novel high explosives before they are made.

14. Demonstration of Transfer Learning using Machine Learning Techniques with Multiphenomenological Sensor Data to Determine a Nuclear Reactor's Operational State

[S] Preston Dicks, Air Force Institute of Technology

The threat of nuclear proliferation has grown with the rapid rate of technological development. One of the ways to combat this threat is to monitor locations using passive sensors that collect data from multiple phenomenologies. These signals can be exploited using machine learning (ML) techniques if the models can be trained on data from one facility and then work on data from other facilities, a process called transfer learning. ML models trained using magnetic and seismic data collected near the cooling fans of the High Flux Isotope Reactor (HFIR) were applied to data collected near the cooling fans of the McClellan Nuclear Research Center (MNRC) reactor to determine if the reactor was on or off. Using only the magnetic phenomenology, the ML model K-Means predicted the MNRC binary operational state with a balanced accuracy of 87.5%. In comparison, a modified one-shot learning model was developed which used both the magnetic and seismic phenomenologies and resulted in a 99.4% balanced accuracy. This application of transfer learning using multiphenomenological data within the nuclear fuel cycle demonstrates the viability of using ML in the field of nuclear proliferation detection.

Joint work with B. J. Borghetti, A.L. Franz, D.E. Holland, A.A. Bickley

15. Detecting Synthetic Opioids with NQR Spectroscopy and Complex-Valued Neural Networks*[S] Amber Day, The University of Texas at Austin, Los Alamos National Laboratory*

We are developing statistical methods to improve Nuclear Quadrupole Resonance (NQR) technology. Traditionally, NQR technology has been used to detect explosives and landmines. However, the advancement of this technology could allow for the creation of scanners that can detect fentanyl in unopened packages. Fentanyl is a synthetic opioid that is cheap and easy to produce, which has contributed to its widespread misuse and the opioid epidemic in the United States. It is also highly potent and frequently mixed with other drugs, making it a significant danger to users. In order to effectively combat the opioid crisis, it is crucial to intercept shipments of fentanyl before they reach their destination. Currently, packages must be flagged and opened to be analyzed, which is a slow and impractical process. The implementation of NQR scanners could significantly improve the efficiency of detecting and intercepting these shipments, potentially saving lives, and mitigating the impact of the opioid epidemic on individuals, families, and communities. NQR technology uses radio-frequency signals to detect whether certain chemicals are present in a package. However, the raw NQR measurements are often weak signals highly corrupted by noise. Current techniques for denoising the NQR signals often fail when the signal is weak. Therefore, we need new strategies for denoising the measurements from fentanyl. Since our measurements are complex-valued (CV), we researched the use of CV-NNs for these tasks. We compared CV and real-valued (RV) neural networks (NNs) for two tasks: signal denoising and signal detection. We investigated various deep learning architectures to capture the inherently complex-valued nature of NQR signals and found that the best performing ones were those that allowed the network to learn relationships between the real and imaginary components of the signal. This is because the true RV signal is recorded as a CV signal, where some information is captured in the real and imaginary components and some information is captured in the relationship between the two. We have shown that our deep learning-based approaches, Autoencoder (AE) and ConvTasNet (CTN), are more effective than three traditional methods (maximum likelihood, singular spectrum analysis, and wavelets) at denoising low signal-to-noise ratio (SNR) data. Typically, scientists in this field assume that it is not possible to accurately recover the true underlying signal when the SNR is very low, but our research suggests that it is possible with these approaches. This research offers a valuable new method for analyzing NQR data and represents an important first step towards the goal of improving NQR technology to the point where it is capable of detecting fentanyl.

16. Hydrodynamic parameter estimation using statistical machine learning for dynamic radiography*[P] Soumi De, Los Alamos National Laboratory*

Reliable characterization of hydrodynamic behavior and material properties of objects made to undergo strong deformations is an important task in national security, material science, and shock physics applications. We train neural networks with databases of simulations of an imploding shell and use them to map hydrodynamic features to physics parameter estimates -- characterizing the material involved in the implosion. Experiments such as those performed at Los Alamos National Laboratory's DARHT facility use high-powered x-rays to capture time sequences of radiographic images of evolution of materials in hydro tests. In this work, we are interested in using the aforementioned experimental radiographic data sets to infer properties of materials involved, as a long-term goal. However, in a real-world scenario, complications resulting from noise, scatter, etc. in the experiments prevent identification of underlying physics with sufficient confidence. Hence, in the developmental stage of our analysis architectures, we work with numerical simulations, which serve as models mimicking the physics in real experiments. Without the inherent presence of noise in these data sets, learning from simulations represent best-case scenarios of extracting physics from data. Such a setup indicates which kind of features in the data contain necessary and sufficient information for extracting the physics in question. Our machine learning architecture is a probabilistic network. We use it to study 1-dimensional and 2-dimensional simulations of imploding steel shells generating shock waves, which serve as our training and testing data. The probabilistic network predicts a "distribution of degenerate parameter solutions" capturing uncertainties propagated down from the training data. This combats one of the challenges encountered with standard (non-probabilistic) neural networks, which predict a "single point parameter solution" with no means of quantifying confidence in the solution. We show how well our probabilistic network recovers hydro, equation of state, and strength parameters. We discuss whether the network can be generalized to produce accurate predictions when tested in regions of the parameter space it has not seen before. Finally, we discuss future goals, as well as any shortcomings of the current architecture with plans of further developments to overcome them.

Joint work with Marc Klasky (Los Alamos National Laboratory), Oleg Korobkin (Los Alamos National Laboratory), Sidharth GS (Iowa State Univ.), Balu Nadiga (Los Alamos National Laboratory)

17. QuadConv: Quadrature-Based Convolutions with Applications to Non-Uniform Data Compression

[S] Kevin Doherty, Sandia National Laboratory

We present a new convolution layer for deep learning architectures which we call QuadConv --- an approximation to continuous convolution via quadrature. Our operator is developed explicitly for use on non-uniform data, and accomplishes this by learning a continuous kernel which facilitates evaluation at any point in the domain. When compressing partial differential equation simulation data, we show that a QuadConv-based autoencoder can match the performance of standard discrete convolutions on uniform grid data (i.e., autoencoding CNNs) and maintain this accuracy on non-uniform data. In the future we hope to explore preservation of quantities of interest at the expense of general reconstruction error.

Joint work with Cooper Simpson, Stephen Becker, Alireza Doostan, Daniel Dunlavy

18. 3D Reconstruction using Computer Vision and Machine Learning for Large Data

[S] Desiree Dominguez, Los Alamos National Laboratory

Scientists run simulations at high resolutions that contain terabytes of information and can generate extreme scale of data over hours or even days. Traditional scientific visualization tools, like Paraview [1], do not have the capability or I/O bandwidth to visualize and analyze such data, making it difficult for scientists to fully understand their simulations. Databases of image proxies, a 'screenshot' of the simulation from various perspectives and at various parametric values, have proven to be an effective way to visualize such data [2]. However, this results in several problems such as: determining how many images to capture, at what angles to capture the images to fully represent the data, and understanding how the camera angles must move as the data moves through space over time. In this poster, we take steps towards designing a framework that extracts features using scale-invariant feature transform (SIFT), A-KAZE (Accelerated-KAZE), KAZE, Oriented Fast and Rotated BRIEF (ORBS), Binary Robust Invariant Scalable Keypoints (BRISK), and low features from enhanced images to provide 3D image reconstruction. The information extracted from these algorithms and images will be fed into a deep learning model and a computer vision algorithm for 3D reconstruction. We then evaluate the results using statistical metrics to compare the results from both algorithms.

[1] Ahrens, James, Berk Geveci, and Charles Law. "Paraview: An end-user tool for large data visualization." The visualization handbook 717.8 (2005). [2] J. Ahrens, S. Jourdain, P. O'Leary, J. Patchett, D. H. Rogers and M. Petersen, "An Image-Based Approach to Extreme Scale in Situ Visualization and Analysis," SC '14: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, 2014, pp. 424-434, doi: 10.1109/SC.2014.40.

19. A Bayesian Record Linkage Approach to Tree Demography Using Overlapping Lidar Scans

[S] Lane Drew, Colorado State University

It has become increasingly common for data about individuals to be spread across multiple sources, making it necessary to identify which records refer to the same individual. The goal of record linkage is to identify these duplications in the data in the absence of a unique identifiable attribute. We present a Bayesian hierarchical record linkage model for marked spatial point processes motivated by estimation of population growth curves for forests. Understanding the growth characteristics of a forest allows practitioners to assess forest health in light of changing climates and to estimate potential timber yield. The spatial data is comprised of overlapping lidar scans taken at regular time intervals and incorporates environmental covariates relevant to the biological mechanisms of tree growth. Each scan is post-processed to obtain the locations of the tree crowns and estimates of tree canopy volume. Subsequently, annual tree growth functions are estimated, dependent upon correctly identifying unique trees across scans without a unique identifier. Application of the model resolves the unique individuals while quantifying the uncertainty in the linkage process and incorporating it into the inference on tree growth. We discuss the model formulation, including data and process models, and assess performance on simulated data and scans of the Upper Gunnison Watershed provided by the Rocky Mountain Biological Laboratory. A joint model formulation for simultaneous spatial record linkage and inference on growth shows promising results for improved coverage in the covariate parameters as well as improved ability to recover the correct linkage structure for varying stand densities.

Joint work with Andee Kaplan (Colorado State University), Ian Breckheimer (Rocky Mountain Biological Laboratory)

20. Fast Gaussian Process Posterior Mean Prediction via Local Cross-Validation and Precomputation

[P] Alec M. Dunton, Lawrence Livermore National Laboratory

Gaussian processes (GPs) are Bayesian non-parametric models useful in a myriad of applications. Despite their popularity, the cost of GP predictions (quadratic storage and cubic complexity with respect to the number of training points) remains a hurdle in applying GPs to large data. We present a fast posterior mean prediction algorithm called FastMuyGPs to address this shortcoming. FastMuyGPs is based upon the MuyGPs hyperparameter estimation algorithm and utilizes a combination of leave-one-out cross-validation, batching, nearest neighbors sparsification, and precomputation to provide scalable, fast GP prediction. We demonstrate several benchmarks wherein FastMuyGPs prediction attains superior accuracy and competitive or superior runtime to both deep neural networks and state-of-the-art scalable GP algorithms.

Joint work with Benjamin W. Priest, Lawrence Livermore National Laboratory; Amanda Muyskens, Lawrence Livermore National Laboratory

21. Characterization of the Point Spread Functions in Pulse Powered X-ray Radiography

[P] Nicholas Eisenberg, NNSS

In pulse power X-ray radiography, an accurate characterization of the point spread function (PSF) is not often straightforward. Radiographers rely on a combination of radiographic calibration objects and axially symmetric regression models to estimate the PSF. The classic methodology performs an unconstrained optimization; accepting any candidate solution that sufficiently minimizes the usual loss model. While this approach is sufficient when characterizing an imaging system with minimal shot-to-shot variations, attempting to quantify changes to the PSF from the unconstrained model alone is impractical. Further, recent work has demonstrated that high-quality image restorations are possible by decoupling X-ray spot source and detector blurs. Herein we propose a technique to address both situations. We develop a composite PSF model that first establishes a stationary detector blur, then utilizes a model regressor comprised of compactly-supported radial basis functions (RBFs) to approximate the source's contribution to the blur. While the optimization method itself remains unconstrained, the RBFs share a spatial dilation which should force all corresponding coefficients to converge uniquely, up to uncertainty. The result is a trackable time series of spatial scale-correlated datapoints, tracking the spot blur from shot to shot.

Joint work with Sean Breckling

22. Deep Learning Surrogate for Radiative Heat Transfer in High Temperature Flows

[S] Joey Farmer, University of Notre Dame

Surrogate models can play a crucial role in the development of complex multiphysics simulations by mitigating physical, computational, and theoretical barriers. One area where this is particularly true is in the coupling of radiative transfer and molecular transport. While both phenomena are explicitly represented in the conservation of energy equation, radiative transfer is often phenomenologically at odds with molecular transport, especially in the context of a computational fluid dynamics simulation. The local nature of molecular transport enables energy balances on infinitesimal volumes and can be described by partial differential equations of up to four variables (space and time). On the other hand, the nonlocal nature of radiative transfer requires an integral formulation of up to seven variables (space, time, direction, and wavelength) which considers the entire domain volume. These factors contribute to a dichotomy of modeling methodologies that has typically made coupling radiation physics in computational fluid dynamics packages a cumbersome task. Nevertheless, over the past decade, finite volume Monte Carlo-based solvers have become an intriguing option for resolving radiative transfer in high temperature flows with participating species. By pre-tabulating the absorption and emission coefficients of various species at various thermodynamic gas states, detailed line-by-line simulations can be had at the cost of gray calculations. However, the amount of data stored from the radiative spectra can easily exceed $O(10)$ gigabytes. This is amplified for thermal radiation in nonequilibrium applications, where the state of the gas is described by multiple temperatures and the range of observed states may be broader. To address these challenges, this work presents a deep learning-based surrogate model that can accurately simulate radiative energy transfer and spectra for gases in either equilibrium or nonequilibrium states. The model is trained by simulating representative distributions of gas states via a finite volume Monte Carlo solver. The surrogate model takes as input the thermodynamic state of the gas and outputs the total radiative energy transfer per finite volume and the total radiative spectrum. When tested, the model achieves respectable accuracy as compared to the Monte Carlo-based solver throughout the flow time. In addition, the surrogate model drastically reduces the total computational cost. For one simulation, the total time spent by the Monte Carlo solver was approximately thirty minutes while the surrogate model computes the radiation from the entire flow through in less than five seconds.

Joint work with Ryan McClarren

23. Understanding System Resilience via Simple Multilayer Network Models*[S] Samuel Gailliot, Sandia National Laboratories*

Multilayer network models for high consequence facilities and critical assets security have been proposed to better capture the complexity, dynamism, and interdependencies of current—and anticipated—security operations. Resilience, the ability for a system to absorb, adapt to and overcome a shock or targeted attack, is a critical aspect of security systems. Multilayer network models readily provide tools for studying system resilience. Specifically, much work has been done modeling resilience of critical infrastructure and ecological networks, though it has been mostly limited to single layer cases or interdependent networks with significant simplifying assumptions. In response, we propose a novel method for analyzing the absorptive capacity of complex systems—like security for high consequence facilities and critical assets—by modeling them as multilayer networks which permit representation as a supra-adjacency matrix. Using several established network metrics we compare the absorptive capacity of multilayer networks composed of various permutations of common network models (e.g., small-world or preferential attachment) and examine which aspects of the multilayer network topology inherently impact resulting absorptive capacity. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

24. Combined Data and Deep Learning Model Form Uncertainties: An Application to the Measurement of Fuel Regression Rate*[P] Georgios Georgalis, Data Intensive Studies Center, Tufts University, Medford MA 02155*

“Data” used in the model definition and/or validation is often the result of complicated processing itself involving denoising processes often using careful statistical and ML based models. As an example, experimental images from combustion experiments are typically noisy and challenging to segment their pixels with a CNN model, but it is a necessary process to estimate the regression rate, i.e. the rate that the fuel recedes over the course of a burn. The regression rate is a quantity of interest in hybrid rockets since it defines the geometry and performance of the motor. Characterizing the uncertainty in these data sets and the CNN models used in preparing them is essential to the overall goal of predictive simulations using ML and physics models. In previous work, we trained a U-net with such combustion experimental image data to replace the manual process of segmenting the fuel masks and the U-net performed adequately for the task. However, a mean prediction is not enough to justify an expectation for the regression rate. To capture the model form uncertainty (i.e. how confident the U-net model form is for each predicted pixel in the segmentation masks) we used Monte-Carlo Dropout to generate an uncertainty map for each predicted segmentation mask. As a next step, we characterized any uncertainty/error sources possible for the image data including: a) optical distortions from the camera, b) the non-zero angle placement of the fuel specimen, and c) the variability from the manually segmented images used for training it the CNN model. In this poster, we show a forward propagation uncertainty quantification (UQ) process to produce a probabilistic distribution for the observed regression rate, by combining both the data and model form uncertainty sources. The main contribution of this work is the investigation and inclusion of some of the experimental image data uncertainties involved and how they combine with the model form uncertainty of the deep network. We show results from 7 case studies on combinations of these uncertainty sources with the model form uncertainty and show that their effects combine: a right-shift in the model form uncertainty distribution caused by the additive effect of the manual segmentation uncertainty, a moderating effect from the non-zero angle uncertainty caused by the effect of randomness of the fuel placement, and the overall added variability throughout the model form uncertainty distribution caused from the distortion uncertainty.

Joint work with Kolos Retfalvi, Paul DesJardin, Abani Patra

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25. Practical Path Kernels : Approximating Neural Networks as Kernel Machines*[S] Michael Geyer, Los Alamos National Laboratory, University of Texas at San Antonio*

This study investigates the relationship between kernel machines and deep neural networks. A theory of the neural path kernel has been proposed by integrating tangent kernels as a means of studying deep neural networks through the lens of kernel machines. The neural tangent kernel is a well established method which represents training gradients as a kernel method. The path kernel extends this comparison by directly constructing a kernel machine approximation of the neural network by integrating tangent kernels. This would allow researchers to leverage many of the powerful tools and techniques developed for kernel machines to analyze and interpret the behavior of deep neural networks. Unfortunately, this path kernel is a complex object which is prohibitively expensive to compute and requires additional justification to guarantee that it indeed approximates a neural network well. By studying the geometric properties of the neural path kernel we are able to provide performance guarantees of path kernels relative to the neural networks they approximate. Our results demonstrate the potential for using the path kernel to study deep neural networks and provide a foundation for further research in this area. In addition, we study methods of approximating this true path kernel to reduce computation costs while maintaining these useful properties. Our findings demonstrate that the essential properties of the neural path kernel can be replicated by a simple linear interpolation in parameter space for artificial neural networks. This linear path kernel would provide a computationally tractable kernel for studying deep neural networks. This would allow many useful techniques from kernel machines to be applied to the study of deep neural networks, such as sample importance, differential privacy analysis and vulnerability to inversion attacks, to name a few. This study has important implications for the advancement of machine learning and artificial intelligence by bridging the gap between kernel machines and deep neural networks.

Joint work with Brian Bell University of Arizona, Juston Moore Los Alamos National Laboratory, Amanda Fernandez University of Texas at San Antonio

26. Exploring the relationships between environmental conditions and the fungal disease blastomycosis in the midwestern United States*[S] Andrew Greene, Los Alamos National Laboratory*

Blastomycosis is a potentially serious fungal infection commonly caused by inhalation of the fungi *Blastomyces dermatitidis* or *Blastomyces gilchristii*. The disease is endemic to the midwestern and southeastern US, as well as Manitoba and Ontario, Canada. The annual incidence of blastomycosis is approximately one to two cases per 100,000 people in the endemic area. About 50% of those who inhale *Blastomyces* spp. will become symptomatic. The disease is often initially misdiagnosed as pneumonia or other common pulmonary diseases. Because *Blastomyces* spp. are difficult to culture from the environment, the epidemiology of the disease is poorly understood. We examined the relationships between reported cases of blastomycosis in Wisconsin, Michigan, and Minnesota and environmental factors such as temperature, precipitation, snow melt, and soil moisture, as well as soil minerals. We also quantified and visualized the connection between disease cases and land surface characteristics of the counties where the cases were reported. These characteristics include the relative prevalence of forests and bodies of water, which have both been suggested to contribute to the ecological niche of *Blastomyces* and have been attributed to high endemicity. Finally, we observe the seasonality of blastomycosis and characterize the different trends in each state to demonstrate the need for closer and more consistent testing and reporting across the entire endemic region.

Joint work with Kim Kaufeld - Los Alamos National Laboratory, Morgan Gorris - Los Alamos National Laboratory

27. AToMS: Author-Topic Manifold Summarization for Interpretable Author-Collaboration Forecasting*[S] Conrad D. Hougén, University of Michigan*

In nuclear nonproliferation, models of author behavior critically reveal how information sharing and information propagation occur within the nuclear science community. In particular, longitudinal topic models provide insights into time-evolutionary topic trends within specific document corpora. By combining such longitudinal document-topic models with related author-topic models, we present a novel approach to the problem of co-authorship prediction. Our approach makes clear the benefits of using topic modeling to forecast author behavior, providing a richer interpretation than standard methods in bibliographic link prediction. Specifically, our model predicts the existence and topic of unobserved author collaborations, while generating visualizations of topic trajectories. We demonstrate that our model is scalable due to the usage of fast similarity search for manifold learning. We apply our method to several article databases, both for comparison and to generate insights relevant to nuclear nonproliferation. Furthermore, we provide encouraging quantitative comparisons between our approach and known methods in bibliographic link prediction.

Joint work with Karl T. Pazdernik (Pacific Northwest National Laboratory), Alfred O. Hero III (University of Michigan)

[1] Wang, Y., Hougén, C., Oselio, B., Dempsey, W., & Hero, A. "A Geometry-Driven Longitudinal Topic Model." *Harvard Data Science Review* (2021).

28. Fast Emulation and Modular Calibration for Simulators with Functional Response*[S] Grant Hutchings, Los Alamos National Laboratory, Simon Fraser University*

Scalable surrogate models facilitate computationally tractable emulation of computer models (or simulators) when large ensembles of runs are available. Gaussian Process (GP) models are commonly used for computer model emulation; however they cannot scale to truly large datasets. Dense functional output such as spatial or time-series data adds an additional layer of complexity that must be handled carefully for fast emulation. In this work we develop a highly scalable emulator for functional data motivated by Kennedy and O'Hagan (2001) and Higdon et al. (2008), but built upon Local Approximate Gaussian Process (Gramacy, 2016). We apply our emulator to model calibration using global GP lengthscale parameter estimates to scale the input space, which dramatically increases the speed of MCMC. We show that our fast approximation based emulator can be a suitable alternative to the methods in Higdon et al. (2008) for functional response at a fraction of the computational cost.

*Joint work with Derek Bingham, SFU***29. Analyses of Lossy Compression of Seismic data using zfp floating point compression***[S] Abdul Hafiz Issah, Applied Math and Stats Department, Colorado School of Mines*

Distributed Acoustic Sensing allows seismic data to be gathered at close sensor spacing and a high sampling rate in time. This can be done over long periods of time with little requirement for instrument maintenance. This enables a high-resolution study of various sources of seismic noise over long periods of time. However, this method produces large amounts of data and as a consequence, high storage and computation requirements. Zfp presents an algorithm for compressing floating point data. It provides a lossless compression mode and other modes to specify preferred levels of lossy compression. We will present some analysis of compressed data with emphasis on the connection of the norm of errors introduced in the lossy-compressed data to errors in seismic processing and subsequent errors in processing goals such as detection and location of seismic events. We summarise these errors in illustrations such as confusion matrices indicating which events were missed or falsely classified and bloxplots to indicate shifts in detection times. This serves as a preliminary study of the amount of compression attainable and the suitability of zfp for compressing seismic data. Our computational experiments show an increase in the range of errors in detection times for earthquakes through template matching as compression rate increases with median remaining close to zero. We will provide updates on this research and the analysis of other computational experiments. The data used here was recorded during an experiment in 2016 at the geothermal field at Brady Hot Springs, Nevada. This data is composed of both active and passive seismic data that can be analyzed separately to study compression effects on different seismic data.

*Joint work with Eileen R. Martin***30. Multi-stage Multi-fidelity (M2GP) Gaussian Process Modeling and Designs, with an Application in Heavy-ion Collisions***[S] Irene Ji, Department of Statistical Science, Duke University*

In an era where scientific experimentation is often costly, multi-fidelity emulation provides a powerful tool for predictive scientific computing. While there has been notable work on multi-fidelity modeling, existing models do not incorporate an important multi-stage property of multi-fidelity simulators, where multiple fidelity parameters control for accuracy at different experimental stages. Such multi-stage simulators are widely encountered in complex nuclear physics and astrophysics problems. We thus propose a new Multi-stage Multi-fidelity Gaussian Process (M2GP) model, which embeds this multi-stage structure within a novel non-stationary covariance function. We show that the M2GP model can capture prior knowledge on the numerical convergence of multi-stage simulators, which allows for cost-efficient emulation of multi-fidelity systems. We also develop a COst-cOnstrained muLti-stage (COOL) designs framework for the M2GP model, which generates a set of multi-fidelity design points under certain budget constraint. We demonstrate the improved predictive performance of the M2GP model and COOL designs over state-of-the-art methods in a simulation study and an application for emulating the evolution of the quark-gluon plasma, which was theorized to have filled the Universe shortly after the Big Bang.

Joint work with Henry Shaowu Yuchi (Georgia Institute of Technology), Derek Soeder (Duke University), J.-F. Paquet (Vanderbilt University), Steffen A. Bass (Duke University), V. Roshan Joseph (Georgia Institute of Technology), C. F. Jeff Wu (Georgia Institute of Technology), Simon Mak (Duke University)

31. The correlation between accessible DNA and the epigenetic tag H3K27ac varies significantly by chromosome*[S] Vanessa Job, Los Alamos National Laboratory - HPC Design*

All of one's cells typically contain the same DNA, but the type of the cell, whether it is a heart cell or a lung cell, or whether the cell is normal or cancerous, depends on the conformation of the DNA. The conformation (shape) of the DNA allows different genes to be accessed for transcription and hence allows different genes to be expressed. DNA along with other proteins are packaged into a structure called chromatin, where the other proteins serve as scaffolding for the DNA. This scaffolding facilitates the rolling and unrolling of DNA, exposing different genes and making them accessible for transcription. As part of chromatin, proteins called histones act as spools around which DNA is rolled (or unrolled) depending on whether that piece of DNA is being used for transcription. The conformation of chromatin is dynamic: different pieces of chromatin may be exposed (open) depending on the cell type and what is currently going on in the cell. For instance, different clock genes are activated at different stages of the circadian cycle. Small chemical tags called epigenetic tags can attach to the histone spools. These tags are sometimes inherited and their presence or absence can be influenced by factors such as diet and exercise. They do not change the DNA itself; they influence how tightly the DNA is wrapped around the histones, and thus which genes are accessible. The approximate location of epigenetic tags can be determined by an assay called ChIP-seq (Chromatin immunoprecipitation followed by sequencing). Another assay, ATAC-seq (Assay for Transposase-Accessible Chromatin using sequencing), indicates which pieces of chromatin are accessible and hence which genes are available to be expressed. The goal of our research is to relate the structure of chromatin to epigenetic tags. We use the well-studied A549 cell line. We focus on the epigenetic tag H3K27ac, a tag which is associated with open chromatin. It is widely believed that this tag acts similarly in all chromosomes. Hence, we expect high correlation between ATAC-seq assay data and ChIP-seq assay data for H3K27ac. We also expect that the correlation between ATAC-seq assay data and ChIP-seq data for H3K27ac should be roughly the same for every chromosome. In this work, we show that the correlation between ATAC-seq and ChIP-seq for H3K27ac varies significantly by chromosome. We discuss reasons that this may be the case and discuss factors that are not the cause of the difference. Additionally, we show that if we restrict our attention to regions around ATAC-seq peaks, the correlations between ATAC-seq and H3K27ac assay data are similar over all chromosomes. LA-UR-23-20899

32. Vision Transformer based Approach for Post-Flood Damage Assessment*[S] Nancy Joseph, Los Alamos National Laboratory*

Natural disasters are one of the leading causes of human displacement and economic downturn. As past events (e.g., Hurricanes Katrina and Harvey) have shown, making decisions and allocating resources in an emergency environment is a challenging task with high consequences for those affected. This highlights the need for quick and accurate damage assessment, as it enables disaster response teams to better evaluate the situation for the prioritization of emergency and recovery efforts. When dealing with damage assessment, emergency management agencies could use overhead imagery that lends itself to machine learning for automated image analysis. However, application of machine learning in real-world post-disaster environment to assess damage poses important challenges. This is consequence of the need to localize and recognize different damage types that depend on the type of disaster, the disaster's location, season, and climate. Unmanned aerial vehicles (UAV) have been increasingly used to assess damaged areas in recent years. This addresses a gap in satellite imagery as the visible spectra depends on acquisition and weather conditions (e.g., cloud coverage), and spatial resolution of satellite imagery may not have sufficient fidelity to reliably identify small objects like vehicles and debris. FloodNet, a high resolution annotated UAV image dataset created after Hurricane Harvey, provides a good benchmark for two important machine learning tasks for flood damage assessment: image classification and semantic image segmentation. For image classification, the images are classified into Flooded and Non-Flooded categories. Semantic segmentation aims to categorize pixels (the smallest units in a digital image) of an image into nine types of objects, including: Flooded and Non-Flooded Buildings; Flooded and Non-Flooded Roads; Water; Tree; Vehicle; and Pool. In this work, we examine the application of vision transformer for UAV image classification and semantic segmentation tasks. Vision transformer models outperform conventional convolutional neural networks, advancing the state-of-the-art for image classification and segmentation tasks. Specifically, we use a lightweight neural network model with the reduced computational complexity of self-attention called the SegFormer. The results demonstrated a clear performance gain of the SegFormer over baseline on FloodNet dataset. Specifically, the SegFormer-based segmentation achieved a higher mean Intersection over Union (mIoU) value, where mIoU score represents how well the bounding boxes around the detected objects of interest (e.g., flooded buildings) match the ground truth bounding boxes. We present details of the SegFormer-based approach, its evaluation, and discuss the implications of this for emergency management as well as the directions for future research.

Joint work with Alexei Skurikhin (Los Alamos National Laboratory), Kari Sentz (Los Alamos National Laboratory)

33. Detecting nuclear effluent signatures at FluxNet ecological monitoring stations*[P] Vachel Kraklow, Los Alamos National Laboratory*

Detection, location, characterization, and compliance determination of nuclear facilities is typically accomplished through remotely sensed data from satellites and aircrafts or through on-site inspections and deployed equipment. Both methods are limited temporally, making it challenging to detect potential attempts to perform short-term nefarious operations or release effluents outside of treaty compliance monitoring times. Additionally, the second method requires facility access and can only operate under the owner's supervision. Here, we present a case study investigating a novel approach to remotely detect nuclear proliferation utilizing publicly available data from Fluxnet. Fluxnet is a global ecosystem monitoring network with >900 stations that continuously measure physical, chemical and biological signatures of natural ecosystem function and human activities at distances 1-100km from measurement towers. Specifically, we aim to determine whether facility operational status and can be detected from thermal energy fluxes, and whether atmospheric releases of chemical effluents can be detected. Preliminary results investigating abnormal events from the Salem and Columbia Nuclear Power Plants show that Fluxnet towers may be able to detect thermal and chemical effluent signatures. The overall aim of this project is to provide a novel method for proliferation detection that can broaden surveillance capabilities and treaty compliance verification in limited access scenarios, as well as fill spatiotemporal gaps in other key global proliferation detection sensor networks.

Joint work with Turin Dickman (Los Alamos National Laboratory), Sanna Sevanto (Los Alamos National Laboratory), Emily Casleton (Los Alamos National Laboratory), Ann Junghans (Los Alamos National Laboratory)

34. Tail dependence as a measure of teleconnected warm and cold extremes of North American wintertime temperatures*[P] Mitchell Krock, Argonne National Laboratory*

Current models for spatial extremes are concerned with the joint upper (or lower) tail of the distribution at two or more locations. Such models cannot account for teleconnection patterns of two-meter surface air temperature (T_{2m}) in North America, where very low temperatures in the contiguous United States may coincide with very high temperatures in Alaska in the wintertime. This dependence between warm and cold extremes motivates the need for a model with opposite-tail dependence in spatial extremes. This work develops a statistical modeling framework which has flexible behavior in all four pairings of high and low extremes at pairs of locations. In particular, we use a mixture of rotations of common Archimedean copulas to capture various combinations of four-corner tail dependence. We study teleconnected T_{2m} extremes using ERA5 reanalysis of daily average two-meter temperature during the boreal winter. The estimated mixture model quantifies the strength of opposite-tail dependence between warm temperatures in Alaska and cold temperatures in the midlatitudes of North America, as well as the reverse pattern. These dependence patterns are shown to correspond to blocked and zonal patterns of mid-tropospheric flow. This analysis extends the classical notion of correlation-based teleconnections to considering dependence in higher quantiles. We also investigate the ability of normalizing flows, a technique from machine learning, to model opposite-tail dependence in the general multivariate setting.

35. Multi-scale feature prediction for additive manufacturing*[S] William Kunkel, University of Wisconsin-Madison, department of Mechanical Engineering*

Additive manufacturing (AM) techniques provide novel opportunities for the fabrication of advanced materials and multi-functional properties of complex geometries with fewer steps than conventional manufacturing techniques. However, the ability to define and predict these responses within the processing-structure-property (PSP) relationships is not mature. AM presents a unique hurdle to understanding PSP relationships due to numerous process variables and the large sample size needed to understand the effect of each. In this study, we present a machine learning (ML) approach that can be used to identify both macro and micro-scale PSP relationships of 316L stainless steel components manufactured using directed energy deposition (DED). This enables, at an accelerated rate, predictive processing strategies for AM. At present, build height, dendrite arm spacing (DAS), and hardness were used to represent the PSP linkages. In total, 35 cubes were manufactured under a range of process conditions. A dimensionless number was utilized for the design of experiments, and a combination of high throughput (HT) processing and low throughput (LT) characterization methods were used. Sample build height was collected both in situ and post-synthesis in all samples, and the DAS and hardness were investigated in a select number of samples. The data from this analysis was then used in three ways: 1) develop an analytical model to explain the relationship between build height and process parameters, 2) develop a relationship between layer height and hardness, and 3) train ML models to predict build height, DAS, and hardness from process parameters. Results show that hardness, DAS, and build height can all be predicted as a function of the processing conditions for DED. Furthermore, this investigation serves as an outline for ML-aided multi-objective design of experiments for AM techniques and can be expanded upon to include more PSP relationships of interest.

Joint work with Phalgun Nelaturu, Dan Thoma, department of Material Science and Engineering

36. malbacR: A package for comparing batch correction methods for small molecule omics data

[P] Damon Leach, Pacific Northwest National Laboratory

Due to the nature of experiments within the fields of metabolomics and lipidomics, samples from the same experiment are often ran over the course of multiple batches. Batches of samples ran at different times of day, in different laboratories, by different technicians, separated in runtime by months, etc. can lead to possible variations). These seemingly small variations can lead to large differences between batches called batch effects. Without adjusting for these batch effects, inaccurate conclusions may be drawn if biological differences are obscured by batch-related differences. Within R, many batch correction methods are available. Because these methods are often implemented by different research teams, these algorithms are available in separate R packages with each one with different formats for the data input and data returned. To simplify this process for users, we have created the malbacR package. This new R package consolidates eleven common batch effect correction methods for small molecule omics data into one location for easy use and comparison. The eleven methods we include span from scaling methods (pareto scaling, power scaling, range scaling), methods involving quality control samples (QC-RLSC, TIGER, SERRF), methods utilizing negative controls/internal standards (NOMIS, RUV-random), to other commonly used methods (ComBat, EigenMS, WavelCA2.0). This package is compatible with the psmartR package, which was designed to assist users in the entire omics analyses from preprocessing to statistical results. By enabling users to stick with a single data format for the entire analysis pipeline, we have streamlined analysis and made possible the comparison of different batch effect correction methods.

Joint work with Joint work at Pacific Northwest National Laboratory with Kelly Stratton, Jan Irvahn, Rachel Richardson, Bobbie-Jo Webb-Robertson, Lisa Bramer

37. Machine Learning Driven Detection of Nuclear Material Storage Container Anomalies

[S] Ross Lee, Los Alamos National Laboratory

As a condition of use, nuclear material storage containers at US DOE sites must meet requirements outlined in Manual 441.1-1 to ensure safety to the worker, public, and environment. To satisfy these standards, workers routinely inspect containers in high radiation field environments which limits the surveillance frequency of these packages. Moreover, these are human-intensive inspections that require greater-than-familiarity knowledge. The tools currently in use lack the ability to record observations of all anomalies—such as corrosion, dents, or scratches—during and between these human-intensive inspections. While region-based convolutional neural network architectures (such as Mask R-CNN and detectron2) offer significant discriminating performance (AUROC scores $> \sim 0.95$), supervised models fail to detect anomalous instances omitted in the training process. Unsupervised detection models are one potential way to remediate this problem. A subset of these, which can train on pristine objects of interest and identify deviations from the “ground truth” data, provide the most robust approach to reducing false negatives encountered by supervised models. In this study, we evaluate the improvements to surveillance of nuclear material storage containers by implementing a package called PaDiM (Patch Distribution Modeling) on container anomalies such as denting, corrosion, or other features of concern. The combination of both supervised and unsupervised approaches offers a more robust detection scheme that outperforms more traditional object recognition techniques and approaches subject matter expert accuracy.

Joint work with Steven Lukow, Joseph Hafen, David Grow, Jonathan Gigax

38. Continuous Representations of Heterogeneous Data

[P] David Lenz, Argonne National Laboratory

Analyzing heterogeneous data from multiple sources is necessary in many scientific domains, but representing, comparing, and learning from such data is challenging. For example, data produced from weather simulations and data assembled from meteorological measurements frequently need to be analyzed in concert with one another. However, these data sets may possess different data models, resolutions, or even different scientific observables, all of which complicate efforts to visualize or explore the full picture. Here, we present research into a continuous representation of heterogeneous data, which is a technique that can enhance analysis and visualization tasks by unifying disparate data sets with a common model. Our framework translates structured or unstructured data sets into a meshless, functional representation that can be queried, differentiated, and integrated anywhere. Specifically, this approach fits a tensor-product B-spline function to the data and then utilizes the function directly for downstream analysis tasks. In addition, this fitting process can be controlled to achieve a user-defined accuracy by adding and shifting parameters that define the B-spline function. Finally, we will highlight how these B-spline representations can be applied to multivariate data, where some variables are closely related (e.g. individual components of a velocity vector) while others are not (e.g. humidity, air quality, and temperature). In such cases, the user can “couple” some variable models together by re-using degrees of freedom, while simultaneously “decoupling” others that would benefit from a different set of degrees of freedom.

Joint work with Tom Peterka (Argonne National Laboratory)

39. Neural network denoising of high-energy-density x-ray images*[P] Joseph M. Levesque, Los Alamos National Laboratory*

Noise is a significant problem for x-ray transmission images of High-Energy-Density (HED) experiments and reduces the accuracy of inferring quantitative physical properties from these images. We consider experiments which image the x-ray attenuation of a thin layer of material to observe its hydrodynamic evolution. The spatial variance of the x-ray transmission across the system due to changing opacity serves as an analog for measuring density in this evolving layer. However, the noise in these images significantly reduces the accuracy of inferring density and other physical quantities, particularly at small spatial scales. Denoising these images is thus necessary to improve our quantitative analysis, but any denoising method also affects the underlying information in the image. We present a method for denoising HED x-ray images via a Deep Convolutional Neural Network (CNN) model with a modified DenseNet architecture. In our denoising framework, we estimate the noise present in the real (data) images of interest and apply the inferred noise distribution to a set of natural images. These synthetic noisy images are then used to train a neural network model to recognize and remove noise of that character. We show that our trained networks significantly reduce the noise in our experimental images.

40. Use-case Examples of Feature-based Geospatial Change Detection*[S] Maxwell Low, Sandia National Laboratories*

Detecting changes in an object's position within a geographic region allow analysts to make informed decisions about these objects and their behavior within an area of interest. We use a feature-based approach for determining when a change occurs among a collection of distinct objects. Given a geographic region of a few square miles, the location of every object is recorded in discrete timesteps. The motion of vehicles is of particular interest and the focus of this proof of concept. Between timesteps the configuration may change. Changes to the collection of vehicles may include quantity, type, translation, stretch, or rotation to some or to all the objects. The goal is to identify if any changes occur and to allow the detection of changes to be filtered based on user defined importance. We generate example use-cases as a proof of concept of a feature-based change detection approach. Each object will represent a vehicle, in our case an ice cream truck. We use ice cream trucks as non-sensitive proxies for mission datasets. Their stationary periods, frequent movement, and territory-based patterns make them excellent candidates for change detection. The position of each truck is known at every discrete timestep. The general area of activity for study is referred to as a "site". Data is collected at a site for each relevant object and for every timestep. Objects may enter or exit the site. The collection of objects at a site for a discrete timestep is referred to as a "cluster". Pertinent spatial relations in a cluster are synthesized into a feature vector. By using features to represent clusters the approach is scalable to a large number of objects in a cluster, and detection will occur even when only a handful of objects are out of place. Feature effectiveness was demonstrated by using synthetically generated configuration changes.

41. Design and analysis for placement of RFID tags on nuclear material containers in a mockup test environment*[S] Will McDermott, Los Alamos National Laboratory*

Radio Frequency Identification (RFID) tags have seen frequent use in commercial applications for inventory management. Their employment in nuclear material accounting has the potential benefit of faster active inventory identification, improved daily administrative checks, plant alignment verification, fewer people on inventory task and lower person-dose. RFID tags viability for nuclear material operations is largely unexplored. In addition to properties of the sensors (e.g., read range, radiation pattern), the complex interaction of radio frequency (RF) waves around metallic nuclear material containers and inside gloveboxes necessitates an understanding of any inaccuracies in accounting RFID tags. We investigate how placement of RFID tags on nuclear material containers impacts both the probability of detecting tags for objects of interest and false detection probability for a fixed RFID reader configuration. Using formal design of experiment principles, we explore various tag locations, modeling how these placements interact with the spatial configuration of random sets of variable-sized containers to impact tagging performance.

42. A Proxy-Labeling Method for Data in the Absence of Ground Truth with Domain Adaptation*[S] Zachary McGuire, University of California - Berkeley*

Nuclear reactors produce clean energy and radioisotopes essential to modern medicine, but their use imposes an inherent proliferation risk as they can be misused to produce weapons grade material. Common problems handled by traditional machine learning methods, such as classification, with domain adaptation techniques fail for non-proliferation applications. Reactor plant specifics such as reactor type, cooling tower type, local weather, etc., can vary from plant to plant making classification with domain adaptation a difficult task. Here, a method for domain adaptation to enable the application of traditional machine learning methods is presented. To do this, a nested-binary cluster-then-label process is proposed using data from inexpensive, non-radiological multi-sensors with a three-class label scheme. Data from the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory, and the TRIGA reactor at the McClellan Nuclear Research Center (MNRC) were collected and are treated as the testbed and target respectively. Data from sensors at both reactors' cooling towers is separated by class in binary layers. For example, given three classes, Full Power Ext., Low Power, and Off, layer one would separate Full Power Ext. from Not Full Power Ext. (i.e. Low Power and Off) and layer two, Low Power and Not Low Power. The separation is achieved via the application of an augmented implementation of the DBSCAN algorithm which combines resultant clusters based on proximity to most populous cluster centroids. Using the HFIR data, the performance of this classification is optimized, and the optimal clustering parameters are transferred directly to the target where the process is repeated. At the testbed, a Matthew's Correlation Coefficient (MCC) of 0.88 is achieved in layer one, and when corresponding parameters are transferred to the target, an MCC of 0.61 is achieved. Layer two performance has been poor, indicating that new data spaces on which to cluster are necessary for improved performance. Results for the entire process are limited by the performance achieved in the first layer. This nested binary process could potentially be applied to additional non-proliferation tasks beyond reactor power monitoring but other applications using data collected by the multi-sensors remain to be explored.

Joint work with Goldblum, B.L., Stewart, C. L., Whetzel, J.

43. Neural Operator Models for Accelerating Particle-Resolved Direct Numerical Simulations*[P] Mohammad Atif, Brookhaven National Lab*

We will present our work on the use of operator learning methods for the purpose of accelerating numerical simulations driven by partial differential equations. More precisely, we work with a particle-resolved direct numerical simulation method designed to study cloud microphysics. The dynamical model consists of two main components, namely, a set of fluid dynamics equations for air velocity, temperature, and humidity, coupled with a set of equations for particle (i.e., cloud droplet) tracing. The model is solved numerically in a Eulerian-Lagrangian framework. Rather than attempting to replace the original numerical solution method in its entirety with a machine learning (ML) method, we consider developing a hybrid approach wherein we exploit the potential of neural operator learning to yield fast and accurate surrogate models, develop such surrogates for select components of the fluid dynamics model, and integrate the resulting ML surrogates into the original numerical solution framework. We will discuss results from numerical experiments designed to assess the performance of different ML architectures under consideration as well as their suitability for capturing dynamical systems behavior of interest. This work is supported by Laboratory Directed Research and Development program at Brookhaven National Laboratory, which is sponsored by the US Department of Energy, Office of Science, under Contract Number DE-SC0012704.

Joint work with Vanessa López-Marrero, Tao Zhang, Lingda Li, Fan Yang, Yangang Liu, Meifeng Lin

44. Using Ecological Versus Geopolitical Regions to Explore Climate-Disease Connections: The Case of West Nile Virus in the United States*[S] S. Kane Moser, Genomics and Bioanalytics, Los Alamos National Laboratory*

In infectious disease forecasting, issues of scale and resolution present obstacles for effective modeling. Technological advances have made more finely detailed spatial and temporal input data accessible; however, the conceptual problem of determining the appropriate resolution and scope for a given model cannot be solved through increased computational power. For vector-borne diseases such as West Nile virus, complex vector biology and transmission dynamics make geographical scaling particularly difficult. Most infectious disease forecasting models in the United States (US) are built with data partitioned into geopolitically classified regions as opposed to regions defined by natural ecosystem characteristics, largely because human-made borders are the basis for collecting and analyzing epidemiologic data through established public health departments and disease reporting systems. Disease systems are ecologically driven, and as such, geopolitical regions that span multiple ecosystems are likely to have variable disease risk, and ecological processes important to disease transmission could potentially be masked. Many models use statistical relationships between climate conditions and disease cases reported at the county level to infer regional disease risk across ecosystems. This can lead to conflicting climate-disease signals and can compound errors when scaled to even broader political or administrative scopes. Our goal was to draw attention to the potential for differences in statistical power between predictive models scaled to geopolitical versus ecological regions using West Nile virus in the US as a case study. We compared correlations among historical temperature, precipitation, and West Nile neuroinvasive disease (WNND) case data from 2005 to 2019 between two different regional geographical classification systems of the continental US: geopolitically classified climate regions defined by the National Oceanic and Atmospheric Administration (NOAA), and ecologically classified Level 1 Ecoregions defined by the Environmental Protection Agency (EPA). We found that the sets of correlation coefficients varied substantially in both direction and magnitude. These results demonstrate that meaningful climate-disease connections emerge when unique ecosystems spanning various geopolitical regions are used to scale model input data, and indicate that ecosystem-level processes important to disease transmission can be obscured or difficult to interpret when input data is scaled according to geopolitical classifications alone. Using more ecologically informed geographical boundaries such as ecoregions for spatiotemporal analysis could not only enhance the predictive power of disease forecasts at different scales, but also reveal underlying biological mechanisms for disease dynamics that may inform better surveillance and prevention efforts.

Joint work with Morgan Gorris (Information Systems and Modeling, Los Alamos National Laboratory), Julie Spencer (Information Systems and Modeling, Los Alamos National Laboratory), Martha Barnard (Division of Biostatistics, University of Minnesota), James Hyman (Tulane University), Carrie Manore (Theoretical Biology and Biophysics, Los Alamos National Laboratory)

45. Tensor Decompositions using Stochastic and Deterministic Optimization*[S] Jeremy M. Myers, Sandia National Laboratories*

Low-rank tensor decompositions in general, and canonical polyadic (CP) tensor decompositions specifically, are now ubiquitous in the area of multi-way data analysis. Recent research in developing efficient methods for computing CP tensor decompositions via maximum likelihood estimation reflects an emergent dichotomy in numerical linear algebra: deterministic versus randomized algorithms. CP Alternating Poisson Regression (CPAPR) is a deterministic CP tensor decomposition method that alternates over a sequence of convex Poisson loss subproblems iteratively. Generalized CP (GCP) tensor decompositions extend previous work on CP decompositions to incorporate general loss functions and stochastic optimization methods. Previously, in [1], we showed that CPAPR is performant and can compute accurate maximum likelihood estimator approximations with a higher probability than GCP. Here we explore a hybrid method for computing CP tensor decompositions that leverages GCP for scalability and CPAPR for performance and accuracy [2].

Joint work with Daniel M. Dunlavy, Sandia National Laboratories

[1] Using Computation Effectively for Scalable Poisson Tensor Factorization: Comparing Methods Beyond Computational Efficiency, J.M. Myers and D.M. Dunlavy, in IEEE High Performance Extreme Computing Conference, 2020. <https://doi.org/10.1109/HPEC49654.2021.9622795> [2] A Hybrid Method for Tensor Decompositions that Leverages Stochastic and Deterministic Optimization, J.M. Myers, D.M. Dunlavy, arXiv:2207.14341, July 2022. <https://arxiv.org/abs/2207.14341>

46. Methodology for Determining Optimal Transuranic Waste Packing Limits

[S] Kate O'Connor, Los Alamos National Laboratory

Transuranic waste can only be shipped and stored at the Waste Isolation Pilot Plant (WIPP) in Carlsbad, New Mexico, and to do so the waste must meet strict requirements. These requirements are outlined in the WIPP Waste Acceptance Criteria (WAC), and include a limit on the Pu-239 fissile gram equivalent (FGE) of a drum, which is an overall measurement of radioactivity. Most 55-gallon drums have a 200 FGE limit. Each drum is measured independently by both Los Alamos National Laboratory (Los Alamos National Laboratory) and the Central Characterization Program (CCP), an independent DOE contractor, before shipment to ensure compliance. Consistent differences between these values resulted in Los Alamos National Laboratory applying an internal packing limit of 150 FGE to prevent CCP's measurement from exceeding the WIPP WAC limit. This internal packing limit reduces the amount of waste that can be shipped in an individual drum and increases costs related to number of shipments and number of drums needed, so stakeholders at the National Nuclear Security Administration are interested in optimizing this limit. Here we present a methodology for optimizing Los Alamos National Laboratory's packing limit by quantifying the likelihood of a container exceeding the WIPP WAC packing limit and applying a cost-minimization model. These results are easily generalizable to sub-populations of transuranic waste drums.

Joint work with Neal Martin (Los Alamos National Laboratory), Benjamin Fisher (Los Alamos National Laboratory)

47. Developing a Profile of Medium- and Heavy- Duty Electric Fleet Adopters with Text Mining and Machine Learning

[S] Fletcher Ouren, Colorado State University

The transportation sector must rapidly decarbonize to meet its emissions reduction targets. Medium- and heavy-duty decarbonization is lagging the light-duty sector due to technical and operational challenges and the choices made by medium- and heavy-duty fleet operators. Research investigating the procurement considerations of fleets has relied heavily on interviews and surveys, but many of these studies suffer low rates of participation and are difficult to generalize. To model fleet operators' decision-making priorities, we apply a robust text analysis approach based on latent Dirichlet allocation (LDA) to a broad corpus of fleet adoption studies. We find operational compatibility to be the most salient factor, followed by long-term economics, technological familiarity, and perceived reliability. Our presentation focuses on the statistical and text mining tools pertinent to the investigation. After taking the traditional text-mining pre-processing steps of stop-word removal, lemmatization, and n-gram searching, we focus on ways to increase the interpretability and repeatability of our work. We use a manual synonymizing process coupled with ensemble parameter tuning to stabilize model results. Finally, we employ a saliency (rather than coherency) metric to rank our categories. Using saliency as the final scoring metric leverages the detailed outcomes of LDA while still considering more generic word distribution metrics. Our application of LDA as the basis for saliency scores in medium- and heavy-duty electric vehicle adoption perceptions is a novel approach that applies key concepts in data science and allows us to provide insights that can accelerate the electrification process.

Joint work with David Trinko, Timothy Coburn, Steven Simske, Thomas H. Bradley

48. Generalized Foldover Designs: A Class of Designs for Irregular Fractional 3^k Factorial Experiments with Bias Protection Properties

[S] Vinny Paris, Iowa State University

Fractional factorial experiments are often used when the total number of runs in the full factorial experiment is too large. This introduces bias if higher order interaction effects are unaccounted for in the model. The original foldover method proposed by Box and Wilson (1951) allows for complete dealiasing of main effects from unaccounted for second order interactions in fractional 2^k factorial experiments. A new class of designs for irregular fractional 3^k experiments based on a generalization of the foldover method will be presented. By restricting the design space, this new class of designs can dealias main effects from a subset of unaccounted for second order interactions. A construction technique for this class is also introduced and a small simulation study will be presented.

Joint work with Max D. Morris, Iowa State University

G.E.P. Box and K.B. Wilson. On The Experimental Attainment of Optimum Conditions. Journal of the Royal Statistical Society Series B (Methodological), 13:1–45, 1951

49. A Spatially Varying Bayesian Approach to Solving Inverse Problems: Applications to Deblurring Cygnus Radiographs

[P] Jordan Pillow, Nevada National Security Site

Many scientific experiments such as those found in astronomy, geology, microbiology, and X-ray radiography require the use of high-energy instruments to capture images. Since blur and noise are inevitably present in any imaging system, the images must be “deblurred” to extract the full information content. Mathematically, image deblurring is an ill-posed inverse problem that requires regularization. The regularization, in turn, has a large effect on the deblurred image: different regularization strengths, and types, lead to drastically different reconstructions. Moreover, many images contain a mixture of smooth and sharp features which suggests the use of multi-regularization, i.e., varying the type of regularization (e.g., Tikhonov or total variation) across the image. We address these issues by formulating the image deblurring problem within a hierarchical Bayesian framework in which we spatially adapt the strength of the regularization across the image. In this way, the image itself, along with corresponding regularization strength at each pixel, are described jointly by a posterior distribution which we can sample by Markov chain Monte Carlo (MCMC) methods. We illustrate our techniques on simplified test problems and apply them to high-energy X-ray images taken at the Nevada National Security Site. Numerical tests show that our new method is robustly applicable and increases the quality of the image reconstruction when compared to other (Bayesian) methods.

Joint work with Eric Machorro, Pacific Northwest National Laboratory

50. The Evaluation and Calibration of Epistemic Uncertainty Estimates

[S] Christopher Qian, University of Illinois

Recently, a surge of interest has been given to quantifying epistemic uncertainty (EU), the reducible portion of uncertainty due to lack of data. However, few studies attempt to directly evaluate the quality of EU estimates. We adopt the definition of EU as the difference in accuracy between the optimal prediction and the current prediction at a given point, and we propose to evaluate the quality of EU estimates based on how well they agree with the observed accuracy gain when more data is added. Our proposed evaluation procedure also gives rise to a way of improving EU estimates by learning a calibration mapping. We demonstrate our evaluation and calibration method on real and simulated datasets, where we assess and compare the quality of two standard EU estimators obtained from a Gaussian process classifier.

51. Identifying behaviors in executable binaries with Deep Learning

[S] Sophie Quynn, Sandia National Labs

Abstract: Cybersecurity analysts aim to recognize and categorize novel malware to identify zero-day threats and track malware family lineage. Novel malware can be characterized by the combination of behaviors it displays when executed, which provide an understanding of the activity and purpose of a suspicious file. My poster will review the background and motivation for using large datasets of executable binaries to train deep learning models to identify behaviors in malware. Additionally, I will dive into the results of the Sandia project MalGen’s behavior identification model. MalGen extends the Malconv model, that predicts if a binary is malicious or benign, to include generative machine learning techniques that create additional training data based on specific behaviors. SAND No.SAND2023-11720A

Joint work with Mike Smith, Sandia National Labs

52. A Data-Driven Method for the Analysis of BEV Operational Inconvenience and Causal Factors

[S] Aaron I Rabinowitz, Colorado State University

As governments and the automotive industry push toward total electrification of the transportation sector, it becomes increasingly critical to address factors that influence individual car buying decisions. Evidence suggests that operational inconvenience, or the perception thereof, plays a large role in consumer decisions concerning acquisition of battery electric vehicles (BEVs). BEV ownership inconvenience and its causal factors have been relatively understudied, leading to a lack of reliable information that renders mitigating such issues difficult. This presentation describes a statistical method for producing an empirical equation that relates operational inconvenience to charging location and other electric vehicle support infrastructure (EVSE) factors. It also demonstrates how the equation can be employed in a geo-spatial context that may facilitate more effective EVSE infrastructure development and deployment policies. Finally, it discusses current data limitations and future information needs. The proposed methodology and analytical results suggest that potential investment in EVSE infrastructure should be largely tied to BEV operational inconvenience associated with charging.

Joint work with Timothy C Coburn, Colorado State University, John G Smart, Idaho National Laboratory, Thomas H Bradley, Colorado State University

53. Augmenting System Assurance with Component Assurance Tests*[S] Jace Ritchie, Brigham Young University*

In order to successfully determine if a system meets some reliability standard, typically assurance tests are conducted on the full system. This proven approach is extremely effective. However, it can be cost prohibitive when full system tests are expensive. Previous work has incorporated component and subsystem data to supplement the priors before a full system assurance test. While this can be helpful, we propose an additional advance of allowing component and subsystem tests as part of the assurance test. We show that by augmenting full system tests with component and subsystem tests, in some cases, we can reduce the cost of the assurance test. For a system that can be decomposed into independent series and parallel parts the theory works perfectly. In the case where we cannot accurately classify parts using the series or parallel structure we add a generalization that works for systems which are “almost-series” or “almost-parallel.”

54. A Parametric Approach for Learning Long-Term Stable Surrogates of Dynamical Systems with Multiple Time Scales*[P] Daniel Serino, Los Alamos National Laboratory*

Direct simulations in fusion energy sciences and climate modeling often involve resolving multiple time scales and can be prohibitively slow for tasks such as high-fidelity prediction and optimization. Reduced order models (ROM)s can provide significant speed-up compared to direct numerical simulations, however, they typically lack accuracy and stability for long-time predictions. We propose a structure-preserving neural ODE architecture to promote long-term stability. The network is parameterized so that any choice of weights results in a fast-slow dynamical system where the linearized dynamics are dissipative. This is achieved by using a general Schur-based parameterization for the linear portion of the neural ODE and ensuring that the eigenvalues lie on or to the left of imaginary axis. The split between the fast and slow eigenvalues is controlled through the use of a (known) physical parameter. The architecture is asymptotic-preserving in the limit of this parameter approaching zero. It is shown that the a slow manifold exists when the parameter is sufficiently small. Using the Schur-based parameterization of the linear term, an efficient IMEX scheme is developed for integrating the stiff neural ODE system forward in time and a fast adjoint-based method is utilized to estimate gradients with respect to the tunable weights. It will be demonstrated that the asymptotic behavior is preserved in the limit of the physical parameter approaching zero and that the model can robustly integrated to longer times beyond the training interval. Potential future applications of the proposed architecture include fusion modeling, accelerator physics, and weather prediction, where long time dynamics can be of great interest.

Joint work with Joshua Burby (Los Alamos National Laboratory), Qi Tang (Los Alamos National Laboratory)

55. Veins of the Earth: A Flexible Framework for Mapping, Modeling, and Monitoring the Earth's River Networks*[P] Jemma Stachelek, Los Alamos National Laboratory*

The tandem rise in satellite-based observations and computing power has changed the way we (can) see rivers across the Earth's surface. Global datasets of river and river network characteristics at unprecedented resolutions are becoming common enough that the sheer amount of available information presents a challenge. Fully exploiting this new knowledge requires linking these geospatial datasets to each other within the context of a river network. In order to cope with this wealth of information, we are developing Veins of the Earth (VotE), a flexible system designed to synthesize knowledge about rivers, lakes, and their networks into an adaptable and readily-usable form. VotE is not itself a dataset, but rather a toolset linking the relationships between existing datasets to allow for rapid comparison and exports of river networks at arbitrary resolutions. Current applications include comparisons of global river widths, LSTM-based global metamodels for streamflow prediction, and hydrologic referencing of real-time information on lake occurrences.

Joint work with Schwenk, Jon; Bennett, Katrina; Prior, Elizabeth; Zussman, Tal; Rowland, Joel [Earth and Environmental Sciences, Los Alamos National Laboratory]

56. Systematic Evaluation of Environmental Sample Interpretation Methods: Characterizing Reactor Operations Under Realistic Challenges*[S] Jordan Stomps, Oak Ridge National Laboratory*

Recent advances in multiphysics reactor modeling are simultaneously increasing the fidelity and volume of data that may be generated. Results from reactor simulations may be used to develop machine learning models to aid analysis and interpretation of environmental samples collected around reactors and other nuclear fuel cycle facilities. However, not all models are appropriate for all analyses, nor are all simulated data sufficiently transferable to real-world measurements. Developing effective analyses requires careful testing to evaluate a realistic expectation of deployment performance. To this end, a testing framework developed here provides a model agnostic tool for systematic testing, using defensible quantitative metrics, that compares algorithms and identifies their sensitivity to challenge scenarios. Data from several high-fidelity reactor simulations are used to train and test several multivariable data analytic methods and compare their performance to canonical analyses. In these initial results, multivariable methods exhibit less bias in estimates and smaller associated variance by virtue of ingesting multiple nuclides to reduce sensitivity to the spatial variation of isotopic composition throughout the reactor core. In addition, a model's performance is improved by averaging over multiple specimens per sample, which avoids the influence of spatially dependent physical characteristics. However, this tacitly assumes a representative sample of specimens randomly distributed across a reactor core. The testing framework also highlights this weakness by generating samples with nonrepresentative sampling to assess and quantify the effect on analysis performance. Moreover, the age or cooling time of samples must be assessed in real-world samples, and the interaction between sample age, burnup, and sample analysis is complex, requiring systematic testing to resolve competing effects. Overall, the testing framework allows each of these properties to be compared, which can enhance or guide the use of these data analysis techniques for a variety of applications.

Joint work with B. Phathanapirom (ORNL), J. Hite (ORNL), K. Dayman (ORNL), A. Conant (ORNL), R. Kapsimalis (ORNL)

57. Transfer Learning for Explosion Detection on Smartphones*[S] Samuel "Kei" Takazawa, University of Hawai'i*

Prompt detection is key in explosion monitoring. This can be achieved through a smartphone network equipped with a machine learning (ML) model trained for blast detection. To create a model, we utilized ~400 acoustic explosion signals collected on smartphones along with the ESC-50 (Dataset for Environmental Sound Classification) as our training data and used transfer learning methods with Yet Another Mobile Network (YAMNet). The explosion data was collected in collaboration with INL and NNSS over a two-year period with data ranging in yield from 7 grams to 1.8 kilotons TNT equivalent yield over a distance ranging from 160 meters to 110 kilometers. Our final model had a 98% accuracy in detecting explosions with a lower false positive rate compared to previous iterations.

Joint work with Milton Garces, Luis Ocampo Giraldo, Jay Hix, David Chichester, Cleat Zeiler

58. Data-Driven Automatic Calibration (DDAC) Routine for High-Energy-Resolution X-ray Emission Spectroscopy*[P] Emily S. Teti, Los Alamos National Laboratory, NEN-1*

High-energy-resolution x-ray emission spectroscopy presents a challenging problem in nonlinear energy calibration. Pulses from multiple pixels are aggregated to create a high-statistics spectrum, with an arbitrary domain that has a monotonic, nonlinear relationship to the energy range of the spectrum. Calibration requires identifying known emission peaks and features in the spectrum and uses a spline or polynomial interpolation between features to map response to energy. Manual energy calibration requires a nontrivial amount of time and effort by subject matter experts (SMEs). This presents a serious bottleneck in processing data from next-generation spectrometers with high throughput. We have developed a data-driven, automatic calibration (DDAC) routine based on pattern-matching of multiple peaks from an individual element using a database of expected emission lines. DDAC's parameters are optimized using gradient descent to determine the combination of peak descriptors to most accurately identify key features in the spectra. We present the results of DDAC on a set of spectra withheld during development, benchmarked against an SME's calibration. Some of the test spectra are measured from similar samples using the same detector as the development set, while others contain elements not included in the development set and measured on a different detector. DDAC produces a calibrated spectrum with comparatively more identified features than the SME can reasonably identify and a list of elements automatically identified in the spectrum to aid in further analysis.

Joint work with Matthew Carpenter

59. Uncertainty quantification for image segmentation of uranium ore concentrates*[P] Cole Thompson, Los Alamos National Laboratory*

One focus of nuclear forensic efforts is to determine the origin and processing pathway of nuclear material. Imaging with scanning electron microscopy (SEM) of nuclear material and subsequent statistical analysis is one data path to support determination of origin and/or pathway. Morphology, or the analysis of shape and distribution of particles, is emerging as an important approach to the characterization of nuclear materials with the potential of providing signatures of process history. The Morphological Analysis for Material Attribution (MAMA) software developed at Los Alamos National Laboratory is a human assisted machine learning toolkit for morphological analysis. Expert MAMA users perform segmentation of material particles from images from which statistical information can be derived to develop signatures. The information from segmentation is useful to the forensic mission, the challenge of image segmentation is that it is a time-consuming for the user and requires many decisions on which particles to segment within the image and for which edges to use when segmenting a specific particle. This work looks at potential signals in human segmentation of images to understand why a particular segmentation is chosen from many potential segmentations. We are using SEM imagery of uranium ore concentrates that has been segmented by experts to understand different kinds of signals from the grey level co-occurrence matrix within segmented particles, the area surrounding the segmented particle, the extracted image patch with the segmented particle and surrounding area, and the edge of the segmented particle. This data will be used to develop a characterization of the uncertainty for the edges of a segmented particle and the discriminability of a segmented particles compared to particle surroundings.

Joint work with Kari Sentz (Los Alamos National Laboratory), Reid Porter

60. A Tensor-Train Approach for 1D Boltzmann Neutron Transport Equations*[P] Duc P. Truong, Los Alamos National Laboratory*

The time-independent Boltzmann neutron transport equation is an integro-differential equation for the neutron angular flux describing the location in space, energy, and direction of neutrons in a physical system of interest such as a nuclear reactor. Discretization of the neutron transport equation is driven by the physics of neutron interactions in matter, and in most cases of interest to nuclear engineers, generates large linear systems of equations. Recently, tensor train (TT) technique is shown to provide a useful low-rank approximation framework for high dimensional problems. Here we present a new approach to solve the time-independent Boltzmann neutron transport equation in Cartesian geometry using the TT representation of the governing equations. The TT representation is explicitly constructed from a matrix formalism of the discretization of the governing equations using diamond differencing in space, multigroup-in-energy, and discrete ordinate collocation in angle. The proposed methodology is verified/validated by solving two canonical examples of the one-dimensional (1D) neutron problem. The first example treats the k -effective eigenvalue neutron transport equation in one-dimensional slab geometry with isotropic scattering, and the second example considers the external source problem for 1D slab geometry. Analysis of the matrix formalism, and boundary conditions, for both examples, are presented, along with the derivation of corresponding TT representations. Solutions strategies, and boundary condition treatments are presented and discussed. We also compare and contrast accuracy and time complexity benchmark results obtained using the proposed TT approach to results obtained from existing state-of-the-art numerical solvers. We will discuss their merits, together with their limitations and also discuss various challenges and decisions that were made along the way.

Joint work with Mario Ortega, Ismael Boureima, Boian Alexandrov

61. Elastic Partial Functional Principal Component Regression with Unmatched Boundaries*[S] Xiaoxia Champon, Sandia National Laboratories*

We propose the elastic partial functional principal component regression, where functional predictors indicate not only both phase and amplitude variability but also have unmatched boundaries. Current literature of scalar on functional regression assumes functions are well aligned without phase variability and have fixed matching boundaries. We extend elastic partial matching and develop a elastic partial regression to accommodate the previous restrictions. Utilizing the group structure of a diffeomorphism allows registering the partial curves, and a joint functional principal component analysis integrates amplitude, time scaling, and time warping all together. This framework utilizes the square-root velocity functions which provides a proper metric which are invariant random warping. Finite sample properties are investigated through simulations under different conditions. This work is motivated by the COVID-19 pandemic study and applied to a public available COVID-19 data set to assess the predictability of the average excess deaths from COVID-19 rate curves. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

Joint work with J. Derek Tucker (Sandia National Laboratories)

62. Bayesian Optimization with Gaussian Processes for Inertial Confinement Fusion Target Design*[P] N.N. Vazirani, Los Alamos National Laboratory*

One of the “grand challenges” of society is to produce energy via controlled fusion reactions on Earth. Following the recent record-breaking inertial confinement fusion (ICF) ignition shot [1], realizing self-sustaining fusion-based power systems feels closer than ever to providing humans with access to secure, renewable energy. Progress towards such energy has focused on carrying out ICF experiments at large laser facilities such as the National Ignition Facility (US) or Laser Mega-Joule (France). The high cost per shot and limited number of shots that are possible per year makes it prohibitive to perform large numbers of experiments. As such, experimental design relies heavily on complex predictive physics simulations for high fidelity “pre shot” analysis. These multi-dimensional, multi-physics, high-fidelity simulations have to account for controlling many free parameters as well as modeling the extreme conditions (pressures and densities) present at ignition. Such simulations (especially in 3-D) can become computationally prohibitive to turn around for each ICF experiment. In this work, we explore using Bayesian optimization with Gaussian processes (GPs) to find optimal designs for ICF double shell targets [2, 3], while keeping computational costs to manageable levels. These double shell targets have an inner shell that grades from beryllium on the outer surface to a higher Z material on the inside in order to create more stable implosions. We describe our results for “capsule-only” xRAGE [4] simulations to study the physics between different capsule designs, inner shell materials, and energy sources on the capsule.

Joint work with R. Sacks, B.M. Haines, M.J. Grosskopf, D.J. Stark, P.A. Bradley

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63. The Collection of Image Segmentation Datasets for Glove Box Domains*[S] Shivansh Sharma, University of Texas at Austin*

Glove box work is arduous and ergonomically taxing; however, the application of human-robot collaboration (HRC) may reduce the amount of time workers spend in gloves and alleviate ergonomic pain by sharing in the workers’ labor. We take actionable steps toward achieving this technology for the DOE by developing an image segmentation dataset for predicting hands and gloves within diverse, cluttered glove box configurations. Prior datasets published for hand segmentation tasks include biases, low variable variation, little to no documentation, and are not aligned with DOE domain relevant tasks, e.g., glove box work. We address these gaps by providing a supervised dataset for collaborative assembly within a glove box of roughly 100 videos. This work improves upon the shortcomings of prior work (Sajedi, 2022), by increasing racial and gender diversity within the dataset and collecting data on out-of-distribution scenarios. Our data collection includes diversity across skin tones, arm orientations, task activities, and introduces noise via green screen manipulations. During the experiments, participants were tasked with dismantling toolboxes and stacking Jenga towers while glovebox clutter configurations were permuted between trials. Included within the dataset is a datasheet which documents the motivation, process of collection, and uses of this dataset (Geburu et al., 2018). We supplement the dataset by providing UNet segmentation models trained with deep bayesian neural network baselines, e.g., deep ensembles and monte carlo dropout sampling on the hand segmentation task for in distribution and out of distribution scenarios. Thus contributing toward robustness of computer vision systems for safety-critical, HRC tasks.

Joint work with Mathew Huang (University of Texas at Austin), Sanat Nair (University of Texas at Austin), Alan Wen (University of Texas at Austin), Christina Petlowany (University of Texas at Austin), Selma Wanna (Los Alamos National Laboratory, University of Texas at Austin), Mitch Pryor (University of Texas at Austin)

- S. Sajedi, W. Liu, K. Eltoumy, S. Behdad, M. Zheng and X. Liang, “Uncertainty-Assisted Image-Processing for Human-Robot Close Collaboration,” in *IEEE Robotics and Automation Letters*, vol. 7, no. 2, pp. 4236-4243, April 2022, doi: 10.1109/LRA.2022.3150487. Timnit Geburu, Jamie Morgenstern, Briana Vecchione, Jennifer Wortman Vaughan, Hanna Wallach, Hal Daumé III, and Kate Crawford. 2021. Datasheets for datasets. *Commun. ACM* 64, 12 (December 2021), 86–92. <https://doi.org/10.1145/3458723>

64. Convolutional Non-homogeneous Poisson Process with Application to Wildfire Risk Quantification for Power Delivery Networks*[S] Guanzhou Wei, Department of Industrial Engineering, University of Arkansas*

The current projection shows that much of the continental U.S. will have significantly hotter and drier days in the following decades, leading to more wildfire hazards and threatening the safety and reliability of the power grid. Unfortunately, the U.S. power industry is not well prepared and still predominantly relies on empirically calculated fire danger indices, which do not consider the full spectrum of factors and dynamic information, leading to ineffective mitigation actions. This paper proposes a new spatio-temporal point process model known as the Convolutional Non-homogeneous Poisson Process (cNHPP) to quantify wildfire risks for power delivery networks. The proposed model captures (i) the current effects on wildfire risks due to the key environmental covariate information, (ii) the cumulative long-term effects that explain how historical covariate information affect current wildfire risks, and (iii) the spatio-temporal dependency among different segments within the power delivery network. The computation and interpretation of the intensity functions are thoroughly investigated, and a connection between the proposed cNHPP and Recurrent Neural Network (RNN) is also discussed. Finally, we apply the proposed approach to model and predict wildfire risks on major transmission lines in California, utilizing historical fire incident data, meteorological and vegetation data obtained from the National Oceanic and Atmospheric Administration (NOAA) and National Aeronautics and Space Administration (NASA). Comparison studies are performed to show the applicability and predictive capability of the proposed approach. Useful insights are obtained that potentially enhance power grid resilience against wildfires. Computer code is made available on GitHub.

Joint work with Feng Qiu (Argonne National Lab), Xiao Liu (University of Arkansas).

Wei, Guanzhou, Feng Qiu, and Xiao Liu. "Convolutional Non-homogeneous Poisson Process with Application to Wildfire Risk Quantification for Power Delivery Networks." arXiv preprint arXiv:2301.00067 (2022).

65. Calibration of a slip-twinning model for beryllium strength*[P] Laura J Wendelberger, Lawrence Livermore National Laboratory*

Metal strength models predict a stress response based on physical mechanisms, with the models exhibiting a wide range of behaviors depending on both simulated conditions and model calibration parameters. These models must balance accuracy and fidelity to the experimental data against simplicity and computational expense. We propose and explore the behavior of a simple model that incorporates competition between deformation mechanisms, twinning and slip, to predict flow stress in metals with hexagonal close-packed (HCP) crystal structure undergoing deformation at high strain rates. Data were collected using Kolsky bar type experiments under a variety of strain rate and temperature conditions. We take a hierarchical Bayesian approach to fit the slip-twinning model to the Kolsky bar data for the HCP metal Beryllium. The new model is then compared to existing common strength models fit in the same Bayesian hierarchical paradigm. These initial calibrations assume shared material parameters, which is favorable for generalizability of the model, but neglects to explicitly account for the nonlinear effects of material parameter variability among samples. Therefore, we further investigate the inclusion of sample-specific effects on parameters in the slip-twinning model and its impact on uncertainty attribution.

*Joint work with Kathleen L Schmidt, Will J. Schill, Matt D Nelms, Nathan R. Barton***66. Detecting Changepoints in Globally-Indexed Functional Time Series***[P] Drew Yarger, Sandia National Laboratories*

In environmental and climate data, there is often an interest in determining if and when a change occurs in a system. In the presence of a sudden change in a data-generating process, stationary statistical models are inadequate. We consider a statistical changepoint problem in the context of functional time series, where one observes a function for each year specifying the behavior of a climate variable like temperature over the course of that year. Furthermore, such data may be measured at many spatial locations on Earth, which motivates considering sets of functional time series that are spatially-indexed on a sphere. In this setting, a change may also occur at different times for different locations, and inferring these changes simultaneously is a challenging problem. We propose test statistics for detecting these changepoints, and we demonstrate our approach on simulations and climate data. The developed methodology is used to evaluate changes in historical climate reanalysis data of surface temperature, stratospheric temperature, and aerosol optical depth. Changes in these variables may be associated with the eruption of Mt. Pinatubo in 1991. We also discuss multiple testing approaches that allow for simultaneous detection of changepoints at multiple locations with statistical error control. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

Joint work with J. Derek Tucker, Sandia National Laboratories, Lyndsay Shand, Sandia National Laboratories

67. Transferring Properties of Analogous Datasets Through Data-Informed Latent Spaces Using Heterogeneous Metaphoric Data Fusion

[P] Tian Yu Yen, Sandia National Laboratories

In recent years, the fields of optimization, uncertainty quantification and machine learning have all been gravitating towards developing algorithms and models that can enable the capacity to incorporate, or fuse, data from disparate sources or fidelities. One approach to perform heterogeneous data fusion is to find a common latent space between two analogous datasets. In metaphoric data fusion, a common latent space can be found by independently training two autoencoders where the encoders project the two datasets to hidden layers with the same number of nodes. Decoders can then be swapped so that representations of each dataset can be projected—or decoded—into the space of the analogous dataset. However, without placing additional restrictions on the two independent autoencoders, information transfer between these autoencoders is at best random and marginally informative. At worst, such an unrestricted approach may lead to severe negative transfer learning. We discuss approaches to generate and organize meaningful properties of the latent space learned by autoencoders in the context of metaphoric data fusion and some of the challenges involved in these forms of transfer learning. Computational results with both positive and negative transfer are illustrated and discussed.

Joint work with Timothy Wildey

68. Using Neural Networks to Identify Mixture Components in Hyperspectral Reflectance Data

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Neural networks have been employed to identify materials of interest from hyperspectral data (generally imagery) based on their unique spectral signatures. Traditionally, the output of these neural networks is a series of probabilities that identify the most likely candidates. One of the assumptions of this approach is that there is a single material that is standing out from the image background that will be identified by the network. However, in reality there are a number of complicating factors. For example, depending on the spatial resolution of a given image, it is likely that more than one material is in a particular pixel. A “material of interest” may itself be a mixture of multiple materials to begin with and if that specific mixture is not in the network’s spectral library it may not be identified. As such, the first goal of our work is to develop a neural network that can identify multiple components of a mixture simultaneously. We have adapted a neural network designed to identify mixture components from Raman spectra to work with our reflectance data. The second goal of our work is related to enhancing the spectral library being used by the network to identify mixture components. It takes a great deal of work in the laboratory to identify, make, and measure all potential mixtures of interest. Given this, researchers will often calculate synthetic spectra using algorithms with various degrees of fidelity to the actual physics that results in natural mixture spectra. These algorithms vary from a simple linear combination to using full radiative transfer models. We tested our neural network using synthetically mixed spectra calculated with three of these algorithms to determine the level of physics-fidelity needed for the network to properly identify real mixture components with a high success rate.

Joint work with Eric Flynn (Los Alamos National Laboratory)