Machine Learning at Argonne National Laboratory

March 14 – March 15, 2017
Building 446
APCF Auditorium

Tuesday, March 14, 2017

9:00 a.m.	**Welcome** *Paul Kearns*
9:15 a.m.	**Orientation** *Rick Stevens* • Describing Machine Learning • Machine Learning Impacting the World
10:45 a.m.	**Morning Break**
11:00 a.m.	**Overview Mathematical Methods** *Prasanna Balaprakash*
11:30 a.m.	**Overview of Hardware** *Kalyan Kumaran*
12:00 p.m.	**Working Lunch**
1:00 p.m.	**Cancer: Predicting Tumor Cell Response to Drug Treatments** *Fangfang Xia*
1:30 p.m.	**Optimization and Unsupervised Learning on X-Ray Fluorescence Data** *Sven Leyffer*
2:00 p.m.	**Materials Properties Prediction** *Subramanian Sankaranarayanan*
2:30 p.m.	**Cosmology Lensing: Machine Learning and Automated Analysis of Gravitational Lensing** *Nan Li*
3:00 p.m.	**Afternoon Break**
3:15 p.m.	**Vehicle Technology: Leveraging Machine Learning to Estimate the Effectiveness Potential of Advanced Vehicle Technologies** *Aymeric Rousseau*
3:45 p.m.	**Computer Science: Application Performance Prediction on HPC Systems** *Prasanna Balaprakash*
4:15 p.m.	**Uncertainty of Thermodynamic Properties: Humans and Machines** *Marius Stan*
4:45 p.m.	**Reception**

Wednesday, March 15, 2017

9:00 a.m. **Machine Learning Tutorials Overview**
Tom Brettin

9:15 a.m. **Run First Example**
Prasanna Balaprakash

9:30 a.m. **Iterating with More Complicated Examples**
Prasanna Balaprakash
- Meta map of all machine learning
- Supervised learning example
- Unsupervised learning example

10:15 a.m. **Morning Break**

10:30 a.m. **Examples of Ensemble Learning**
Jim Davis
- Random Forest
- Ada Boost
- XG Boost

11:00 a.m. **Feature Importance and Extraction**
Jim Davis

11:30 a.m. **Neural Networks**
Fangfang Xia
- Unsupervised learning
- Supervised Learning

12:00 p.m. **Working Lunch**

1:00 p.m. **Validation**
Hal Finkel
- Cross-validation
- ROC, AUROC
- Confusion Matrix

1:30 p.m. **Dealing with Unbalanced Data**
Tom Brettin
- Undersampling – Random, TOMEK
- Oversampling – SMOTE

2:00 p.m. **Lab Strategy on Machine Learning**
Rick Stevens
- Machine Learning and Argonne Science
- Next steps

Session Presenters

Prasanna Balaprakash	Assistant Computer Scientist, MCS/ALCF
Tom Brettin	Strategic Program Manager, CELS
James Davis	Computational Scientist, CELS
Hal Finkel	Lead Compiler Technology and Programming Languages, ALCF
Paul Kearns	Interim Laboratory Director
Kalyan Kumaran	DD of Science, Advanced Technologies, ALCF
Sven Leyffer	Project Leader/Sr. Computational Mathematician, MCS
Nan Li	Joint Appointment, HEP
Robert Ross	Interim Division Director, MCS
Aymeric Rousseau	Section Manager, Systems Modeling and Control, ES
Subramanian Sankaranarayanan	Scientist, NST
Marius Stan	Sr. Computational Energy Scientist, GSS
Rick Stevens	Associate Laboratory Director, CELS
Venkat Vishwanath	Data Sciences and Workflows Team Lead, ALCF
Fangfang Xia	Computer Scientist, CELS

Workshop Goal

The predictive power of machine learning has increasingly made it a go-to method across the scientific domains. This gives rise to new challenges and new opportunities as researchers explore various approaches and drive changes in data production, data usage, and scientific understanding in their field.

The Machine Learning at Argonne Workshop will dive into the wide-range use of machine learning across the Lab, highlighting opportunities for cross-disciplinary discussion and collaboration. The workshop will also offer an introductory hands-on tutorial session for researchers of all backgrounds on using machine learning for their research.

Registration for the first day is limited to 100 participants. Refreshments will be provided. To maximize your experience, the tutorial session on the second day will be limited to 30 participants. Register now! Seats are reserved on a first-come, first-served basis.

Registration

https://www.surveymonkey.com/r/MachineLearningWorkshop2017