Machine Learning Developments in ROOT

Sergei Gleyzer, Lorenzo Moneta
for the ROOT-TMVA Team

CHEP 2016, October 10, 2016

Outline

- **Status and Overview**
- **New TMVA Features**
  - **External Interfaces**
  - **Deep Learning, Jupyter, Parallelization**
- **Future Plans and Outlook**
- **Summary**

TMVA

Toolkit for Multivariate Analysis:

- HEP Machine Learning workhorse
- Part of ROOT
- In LHC experiments production
- Easy for beginners, powerful for experts
- 17 active contributors (5 GSoCs)

New TMVA version released in upcoming ROOT 6.0.8

New TMVA Features

New Features

- Modularity, External Interfaces, Updated SVMs
- Analyzer Tools: Variable Importance

Added in 2015

- Deep Learning CPU, GPU
- Parallelization with multithreading and GPUs
- Analyzer Tools: Cross-Validation, Hyper-Parameter Tuning
- Regression Loss Functions
- Jupyter: Interactive Training, Visualizations

Added in TMVA ROOT 6.0.8

- Unsupervised Learning
- Deep Autoencoders
- Multi-processing, Spark parallelization

Upcoming 2016

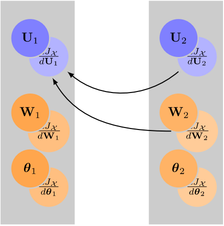
TMVA Interfaces

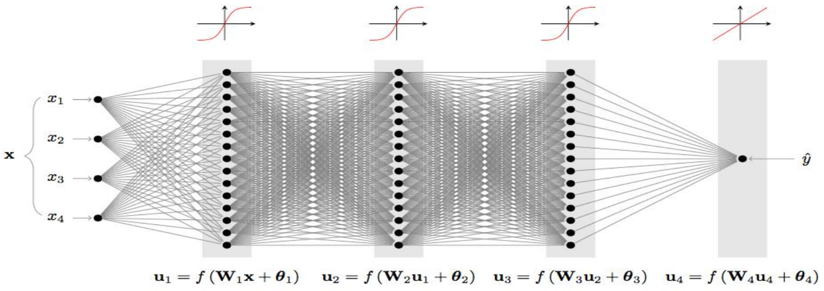
Interfaces to External ML Tools

- RMVA interface to R
- PyMVA interface to scikit-learn
- KMVA interface to Keras
  - High-level interface to Theano, TensorFlow deep-learning libraries

Deep Learning

Is a powerful Machine Learning method based on Deep Neural Networks (DNN) that achieves significant performance improvement in classification tasks

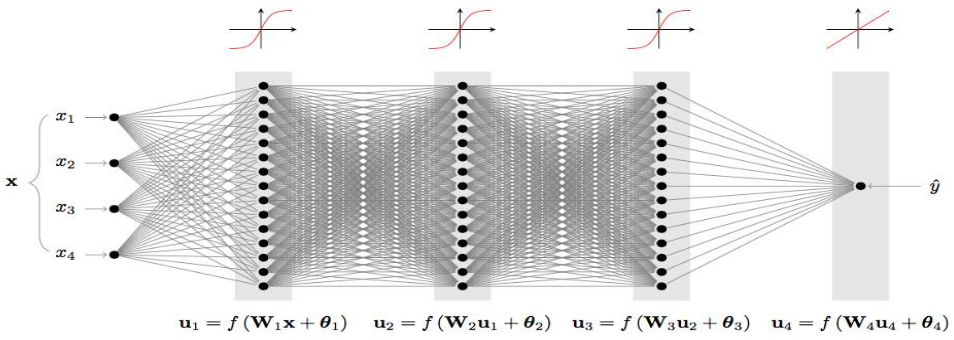




Deep Learning

New Deep-Learning Library in TMVA

- **GPU support**
  - **CUDA**
  - **OpenCL**



- **Excellent performance and high numerical throughput**

Deep Learning

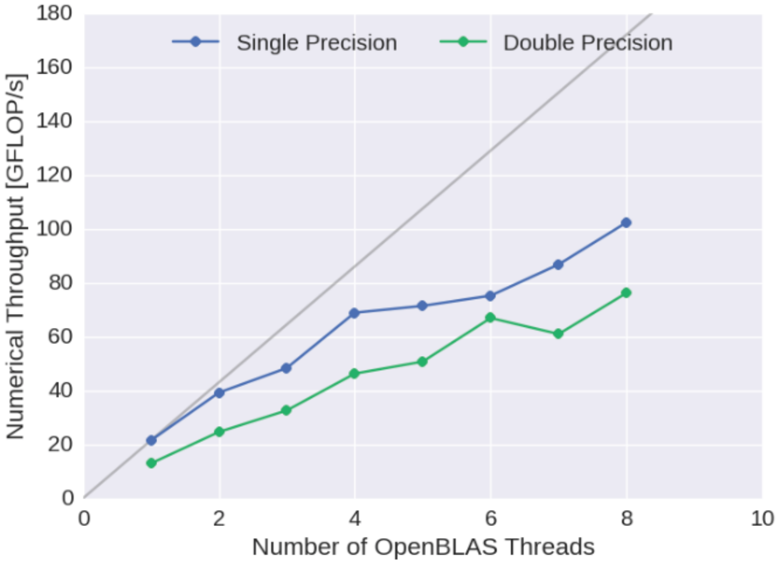
CPU Performance:

Implementation:

- OpenBLAS, TBB

Peak performance per core:

- 16 GFLOP/s
- Single, Double Precision



Deep Learning

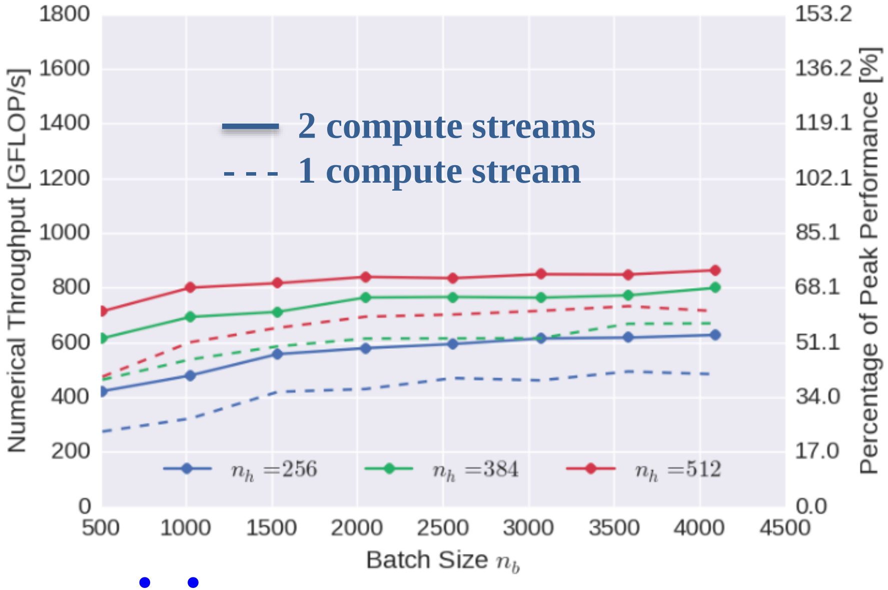
GPU Performance:

Network:

- 20 input nodes
- 5 hidden layers with n_h nodes each

Hardware:

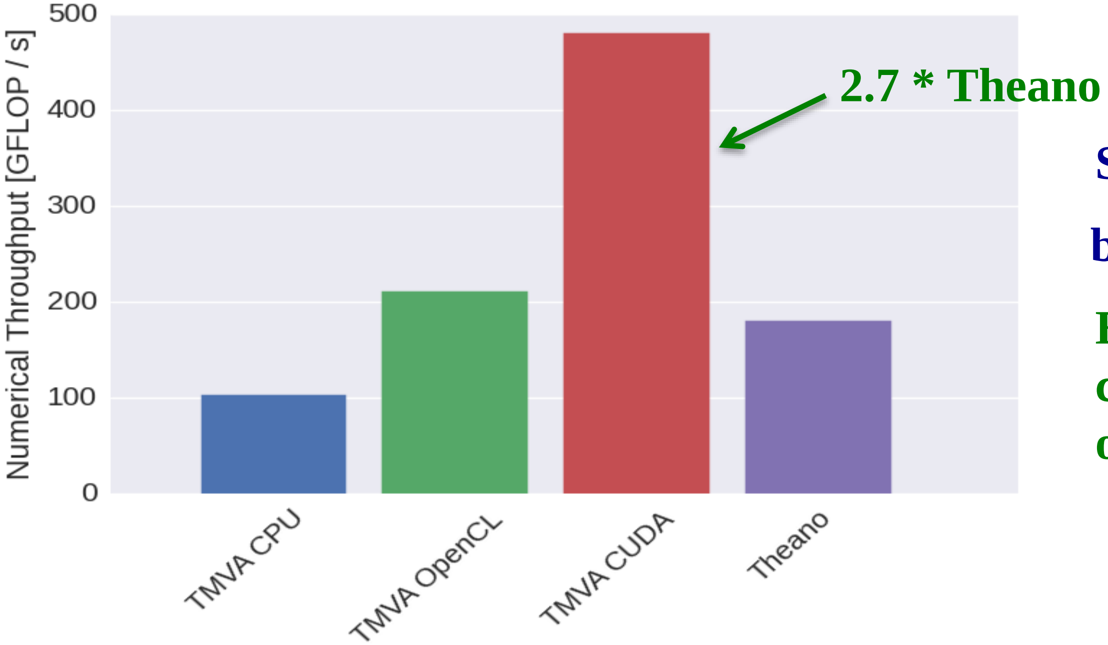
- NVIDIA Tesla K20
- 1.17 TFLOP/s peak performance @ double precision



Good Throughput

Deep Learning

Throughput Comparison

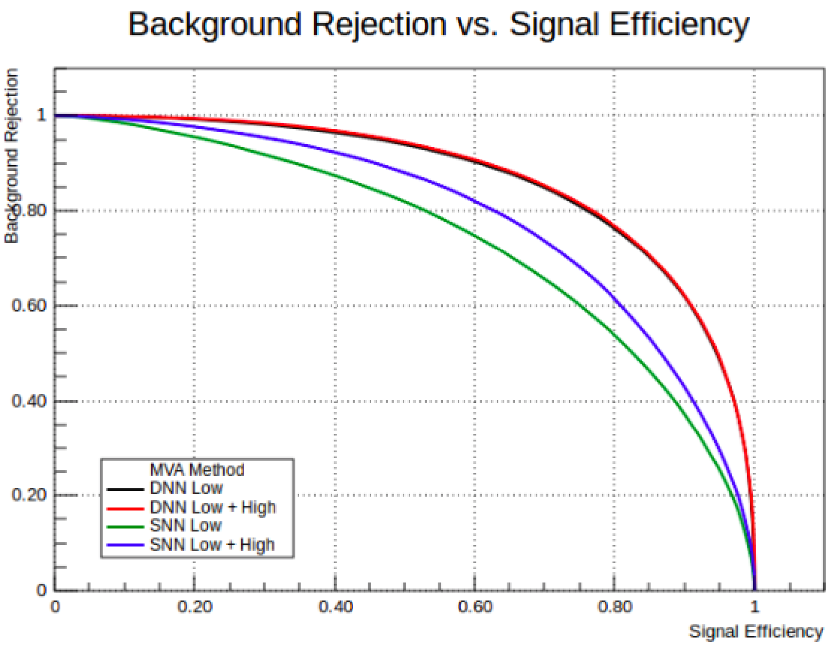


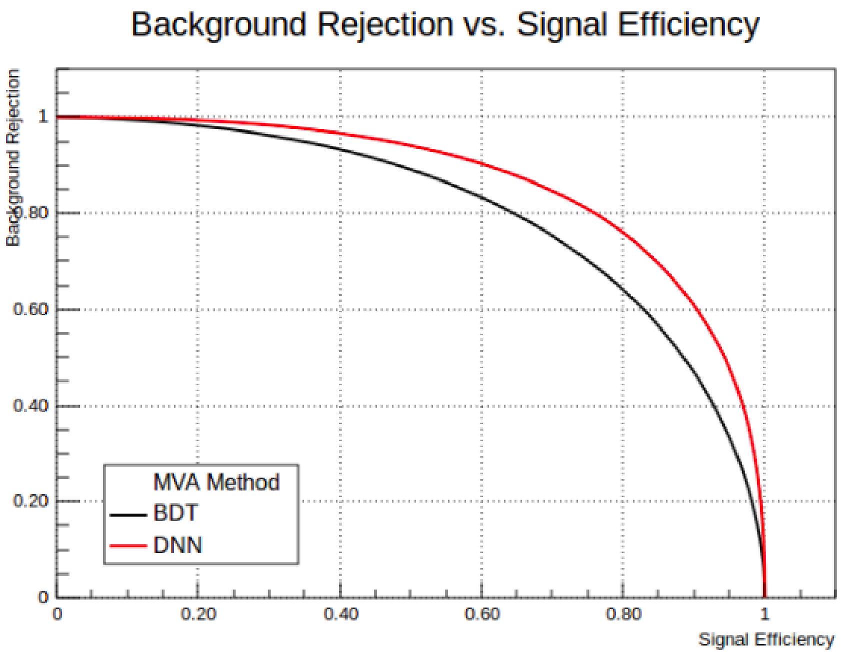
Single precision

batch size = 1024

Excellent throughput compared to Theano on same GPU

Deep Learning



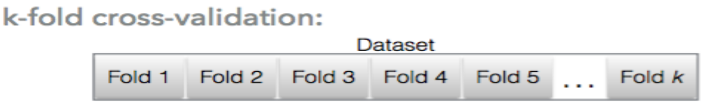


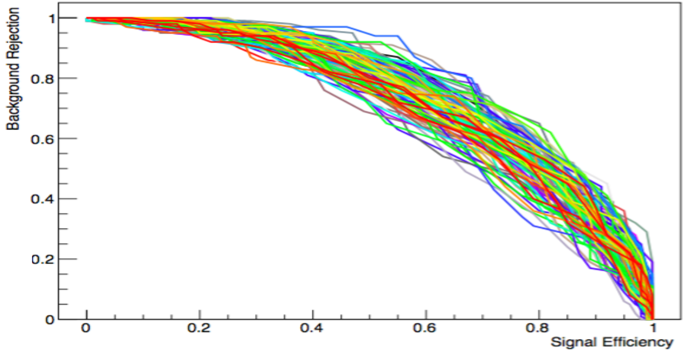
ROC Performance: significant improvements compared to shallow networks and boosted decision trees

Cross Validation

New features:

- **k-fold cross-validation**





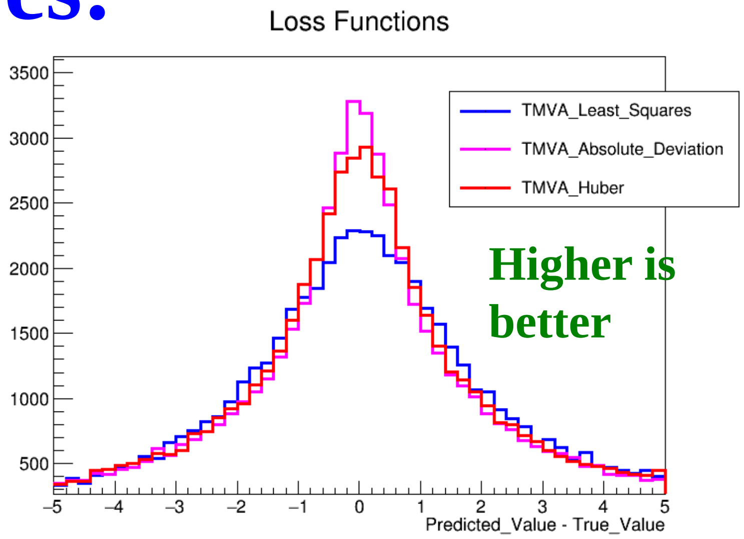
- **Hyper-parameter tuning**
  - **Find optimized parameters (SVM, BDT)**

Regression

New Regression Features:

Loss functions:

- Huber (default)
- Least Squares
- Absolute Deviation
- Custom Function



Higher is better

Important for regression performance

Jupyter Integration

Classifier output: Neural networks, decision trees

Simple neural network

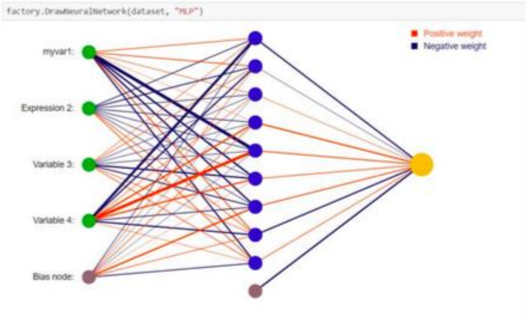
- Python function reads the network, converts to JSON; JS with d3js make the visualization from JSON
- Interactive: focusing connections, zooming, moving

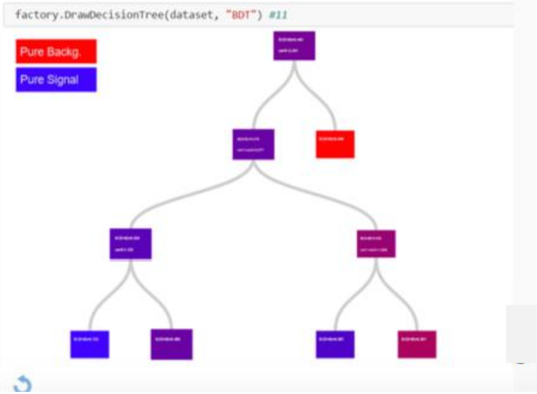
Deep neural network

- HTML5 Canvas visualization (speed)
- Less interactive: zooming, moving

Decision trees

- Ipywidgets: input field for selecting the tree
- Visualization from JSON with D3js
- Interactive: closing subtree, showing the path, focusing, moving, zooming, reset

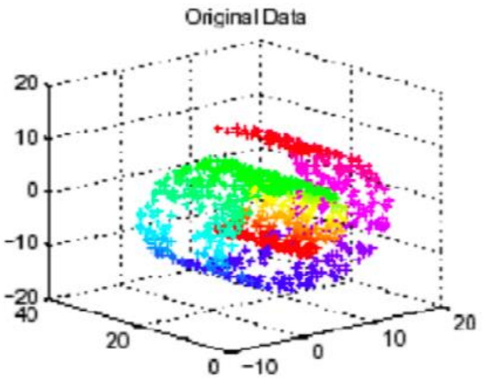


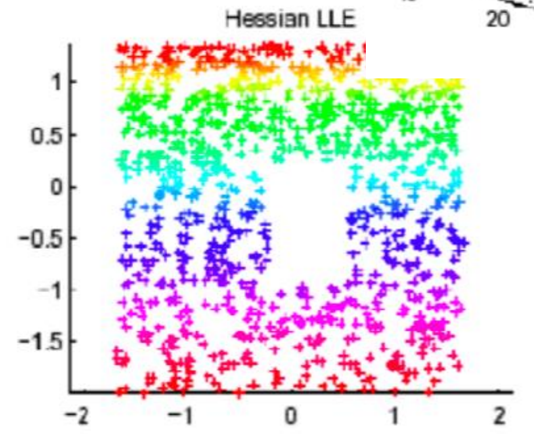


Pre-processing

New pre-processing features:

- Hessian Locally Linear Embedding
  - (Hessian LLE)
- Variance Threshold

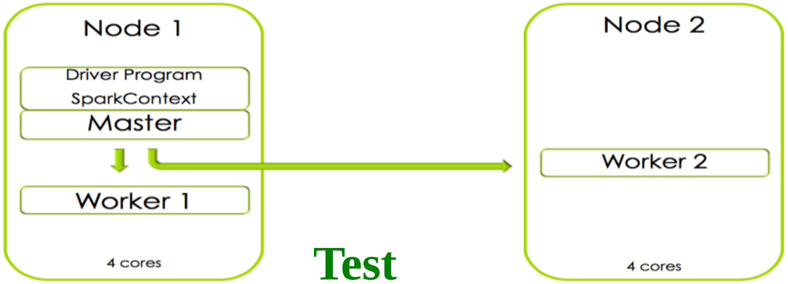




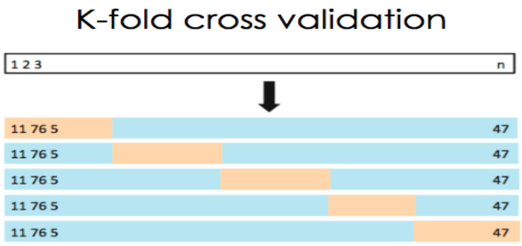
Some Upcoming Features

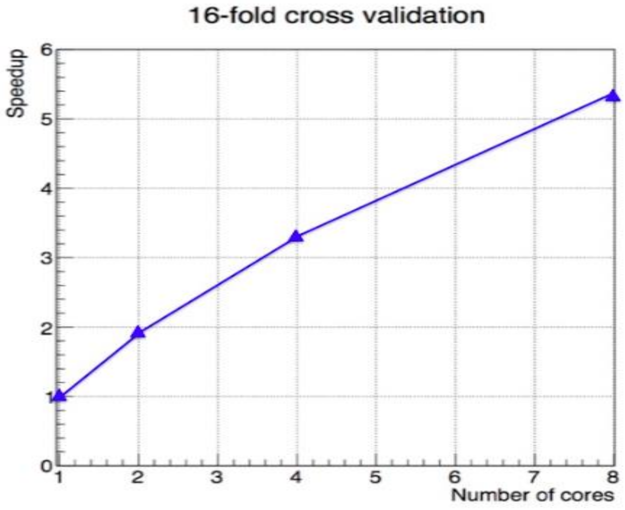
Spark TMVA

SPARK Parallelization



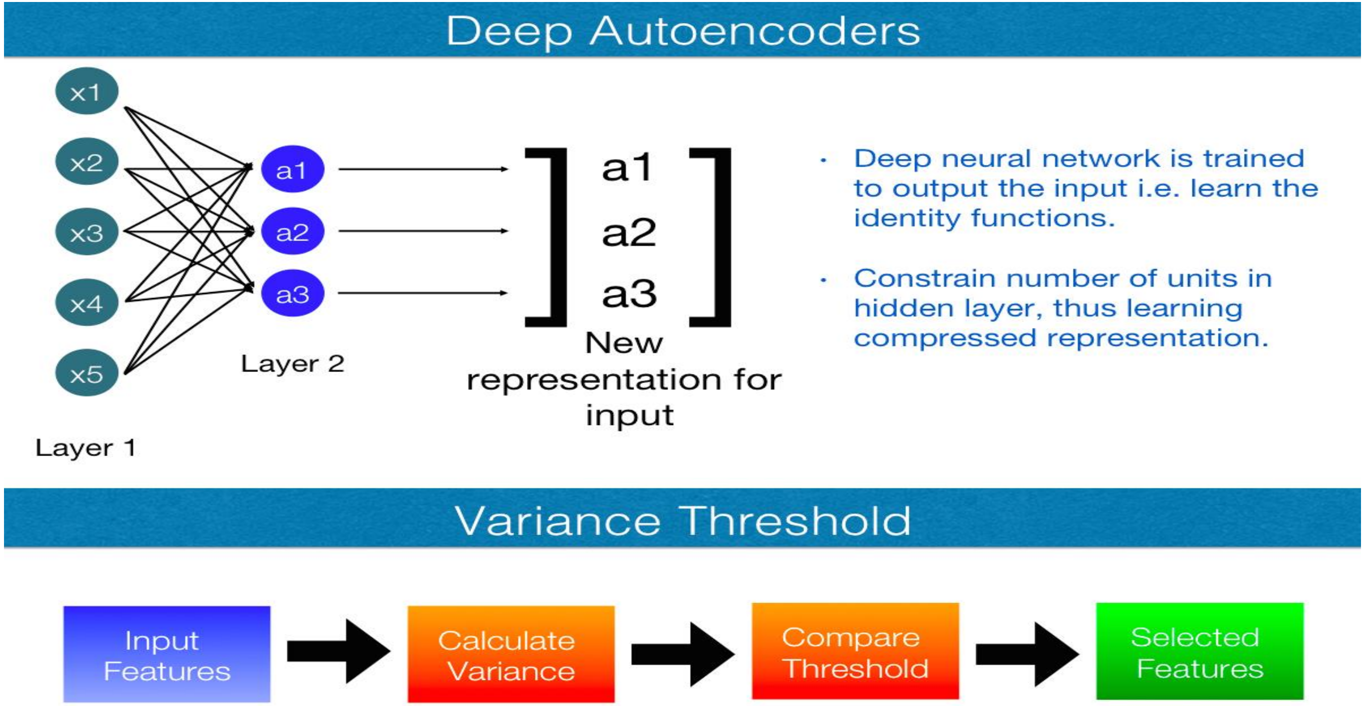
Test





Good speed-up in prototype R&D

Deep Autoencoder



Summary

- **Many new features in TMVA release upcoming in ROOT 6.0.8**
  - **Production-ready parallelized Deep Learning**
  - **Cross-validation, Hyper-parameter tuning**
  - **Jupyter integration**
  - **More pre-processing features**
  - **Regression updates**
- **Many contributions**
- **Feedback and further contributions welcome**

Feature Contributors

- Sergei Gleyzer — Analyzer Tools, Algorithm Development
- Lorenzo Moneta — Multi-threading, Multi-processing
- Omar Zapata Mesa — PyMVA, RMVA, Modularity, Parallelization
- Peter Speckmeyer — Deep-Learning CPU
- Simon Pfreundschuh — Deep-Learning CPU and GPU
- Adrian Bevan, Tom Stevenson — SVMs, Cross-Validation, Hyperparameter Tuning
- Attila Bagoly — Jupyter Integration, Visualization, Output
- Albulena Saliji — TMVA Output Transformation
- Stefan Wunsch — KERAS Interfance
- Pourya Vakilipourtakalou — Cross-Validation, Parallelization
- Abhinav Moudhil — Pre-processing, Deep Autoencoders
- Georgios Douzas — Spark, Cross-Validation, Hyperparameter Tuning
- Paul Seyfert — Performance optimization of MLP
- Andrew Carnes — Regression, Loss Functions, BDT Parallelization

Continued invaluable contributions from Andreas Hoecker, Helge Voss, Eckhard von Thorne, Jörg Stelzer, and key support from CERN EP-SFT Group

More Information

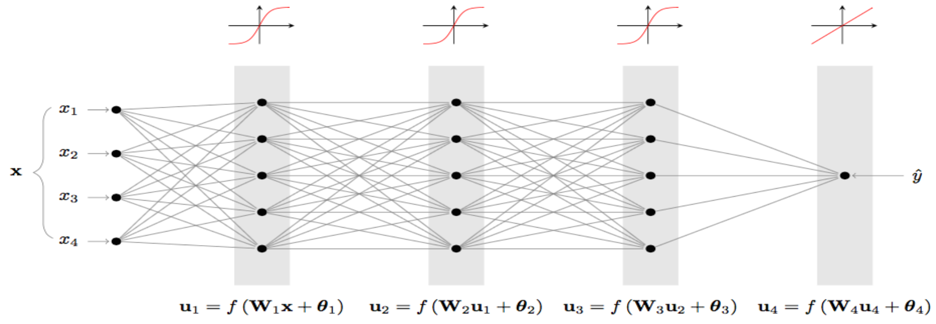
Websites: http://root.cern.ch
http://iml.cern.ch
http://oproject.org

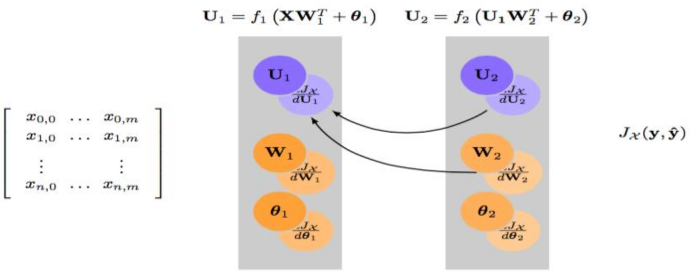
Inter-experimental LHC Machine Learning working group

- Exchange of HEP-ML expertise and experience among LHC experiments
- ML Forum
- ML software development and maintenance
- Exchange between HEP and ML communities
- Education (Tutorials)

Backup

TMVA Deep Learning





Design

[link]