Google Summer of Code Project

Integrating Machine Learning in Jupyter Notebooks

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ROOT Data Analysis Framework

jupyter

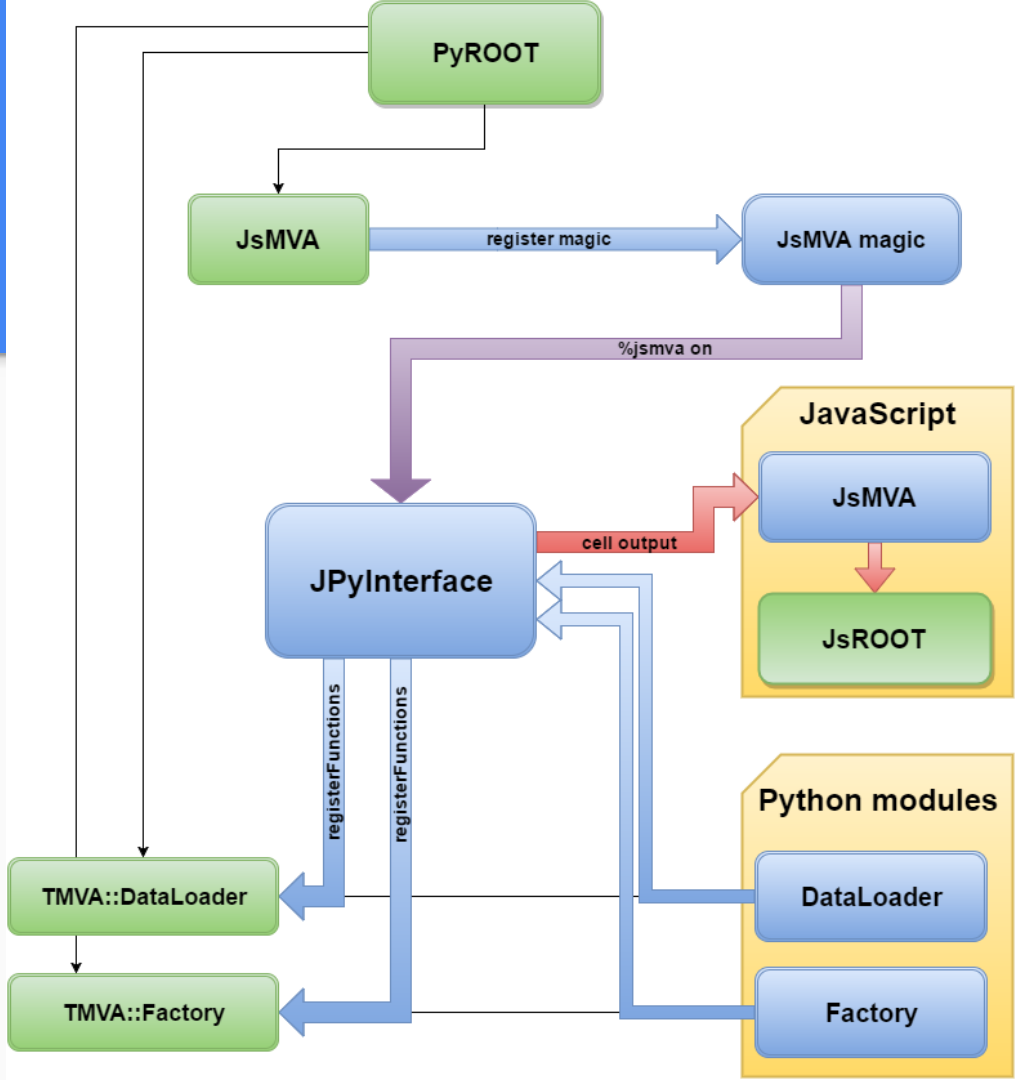
TMVA

Motivation

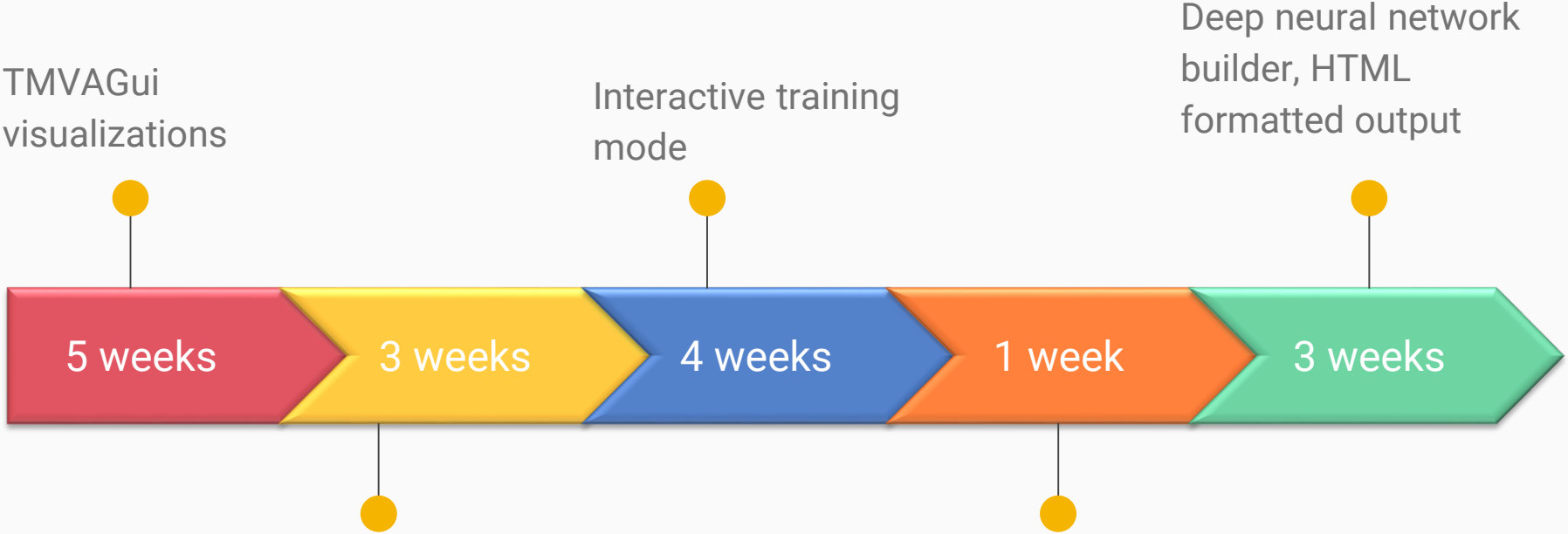
- Jupyter notebook:
  - Interactive coding
  - Document: HTML, Markdown support
  - Shareable: SWAN, nbviewer, binder
- Current status of TMVA:
  - We can’t use TMVAGui
  - We can read back the classifier outputs and we can make visualizations.
  - BUT users don’t want to spend time with making visualizations
- Integrating TMVA in Jupyter:
  - Support for TMVAGui in notebooks
  - New visualizations
  - Pythonic interface for a bunch of functions
  - Interaction: changes modify the state of TMVA
  - HTML formatted output

Code structure

- Importing ROOT will import JsMVA, this will register jsmva magic
- %jsmva on: JPyInterface inserts new methods to TMVA.DataLoader and TMVA.Factory, overloads some functions with a wrapper, register HTML transformer function
- New methods: inserting HTML to cell output, with JavaScript call for JsMVA.js
- JsMVA.js using JsROOT to create JavaScript plots

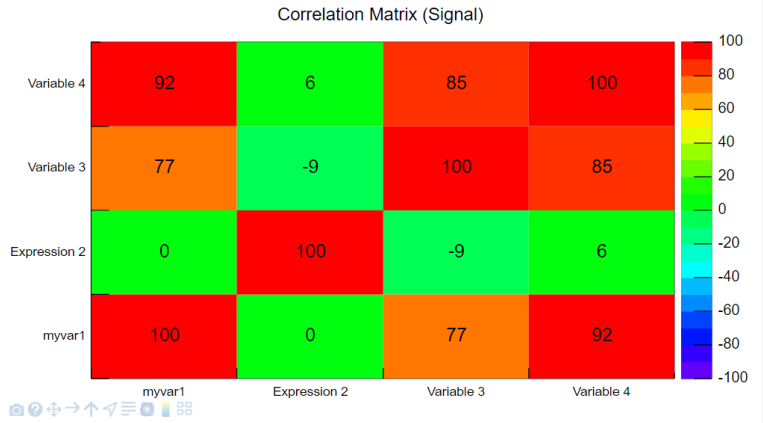


Timeline


TMVAGui visualizations
Interactive training mode
Deep neural network builder, HTML formatted output
5 weeks
3 weeks
4 weeks
1 week
3 weeks
Neural network, deep network, decision tree visualizations
New user interface, documentation, tutorials

TMVAGui visualizations

```
loader.DrawCorrelationMatrix("Signal")
```



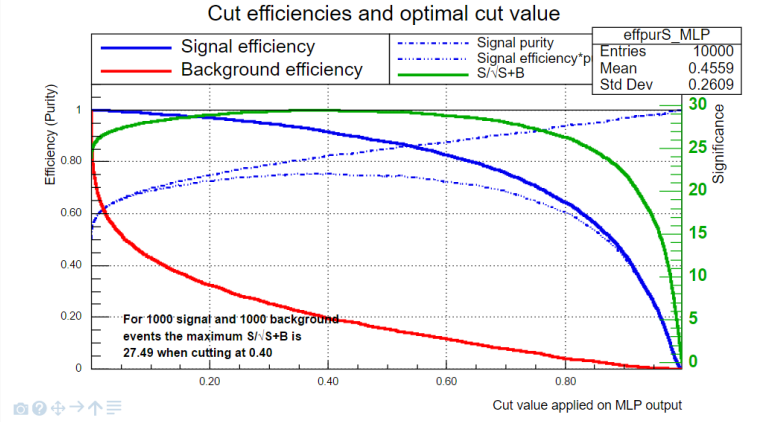
Visualizations related to input variables

- Correlation matrix
- Input variables
- Transform input variables & show

Visualizations related to classifier outputs

- ROC curve
- Output distributions
- Cut efficiencies

```
factory.DrawCutEfficiencies(dataset, "MLP")
```



Go back

Classifier output: Neural networks, decision trees

Simple neural network

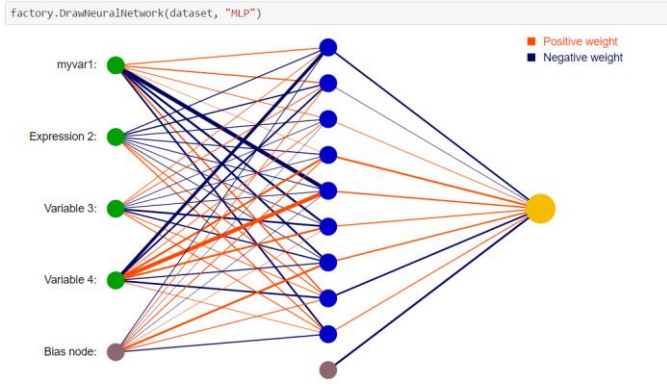
- Python function reads the network, converts to JSON; JS with d3js make the visualization from JSON
- Interactive: focusing connections, zooming, moving

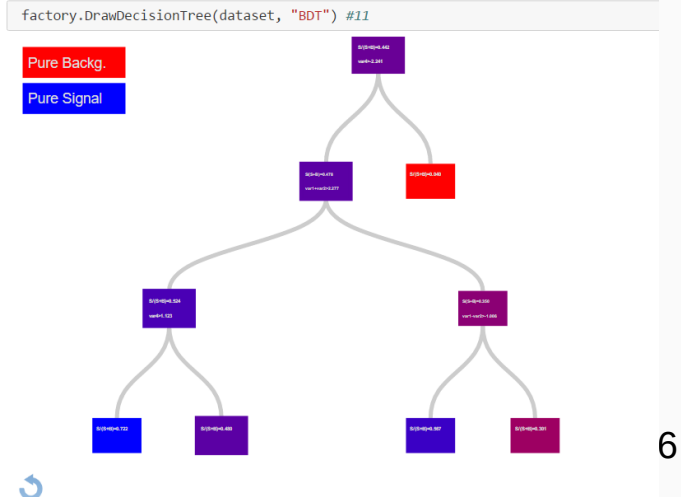
Deep neural network

- 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





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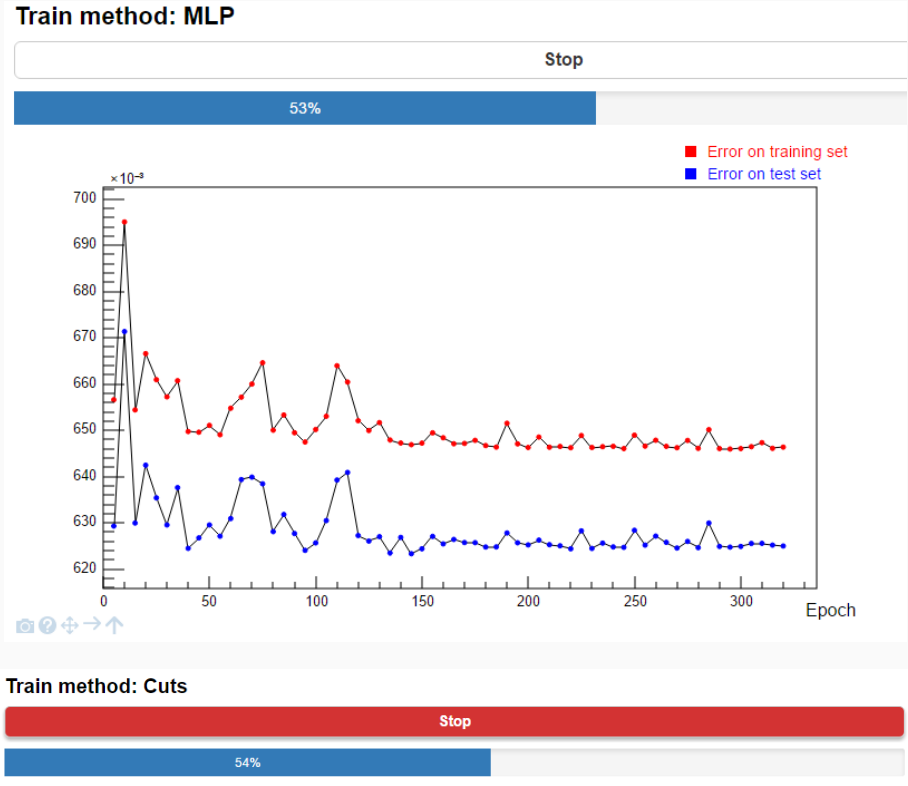
Interactive training mode

- C++ interface for tracking/stopping the training
- New thread for training
- Main thread periodically refreshes the plot (inserts small JS script, which removes itself)
- Error plots supported for MLP, DNN, BDT methods
- Progress bar for a bunch of methods
- Stop button: by clicking on it the main thread will send stop message for training loop (just the loop, no interfere with saving the net, or other data)



Go back

Pythonic user interface, tutorial notebooks, documentation

```
factory = TMVA.Factory(JobName="TMVAClassification", TargetFile=outputFile,
                       V=False, Color=True, DrawProgressBar=True, Transformations=["I", "D", "P", "G", "D"],
                       AnalysisType="Classification")
```

New interface

- Option strings not very nice, we can do better in python
- Bunch of functions use option string
- Wrapper functions for them, with jsmva magic these functions are replaced with corresponding wrapper function
- The settings can be passed by named arguments: V=True,Transformations=[“I”,“D”] will be translated to “!V:Transformations=I,D”

Arguments of constructor: The options string can contain the following options:

Keyword	Can be used as positional argument	Default	Predefined values	Description
JobName	yes, 1.	not optional	-	Name of job
TargetFile	yes, 2.	If not passed histograms won't be saved	-	File to write control and performance histograms histograms
V	no	False	-	Verbose flag
Color	no	True	-	Flag for colored output
Transformations	no	""	-	List of transformations to test. For example with "I;D;P;U;G" string identity, decorrelation, PCA, uniform and Gaussian transformations will be applied
Silent	no	False	-	Batch mode: boolean silent flag inhibiting any output from TMVA after the creation of the factory class object
DrawProgressBar	no	True	-	Draw progress bar to display training, testing and evaluation schedule (default: True)
AnalysisType	no	Auto	Classification, Regression, Multiclass, Auto	Set the analysis type

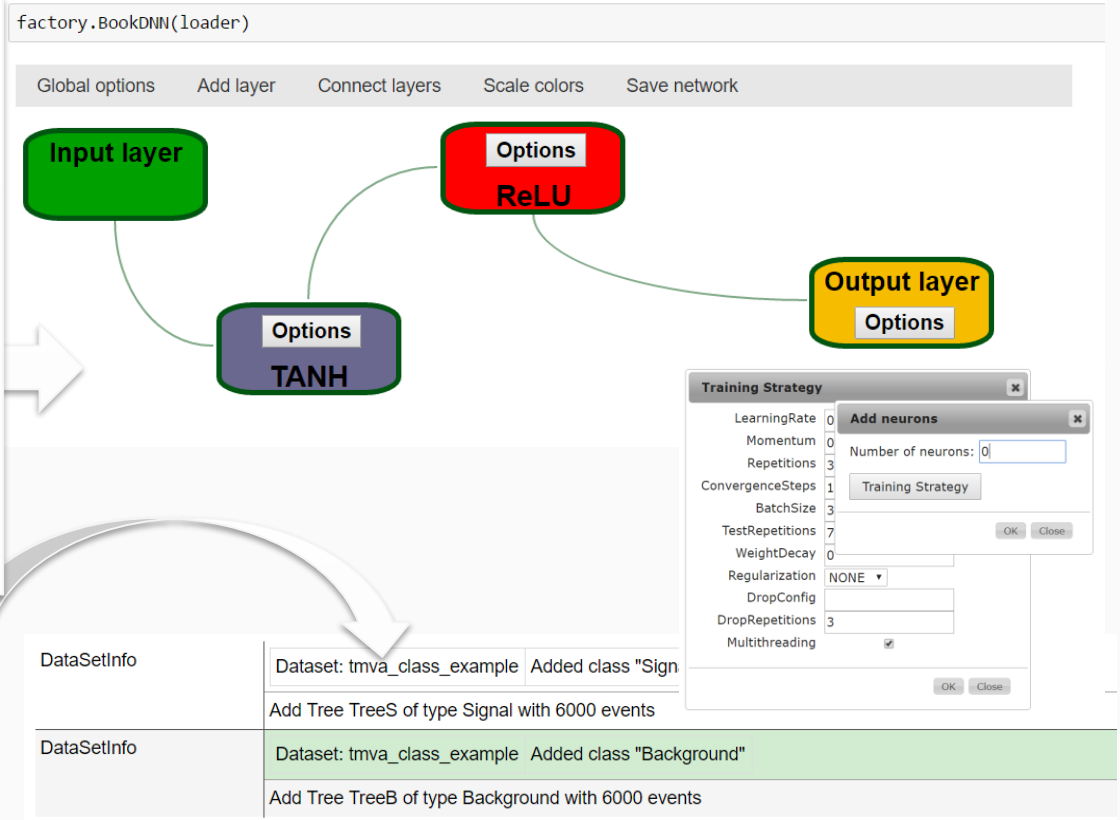
Tutorial, documentation links on

GitHub.com/qati/GSOC16

Go back

Deep neural network builder, HTML formatted output

- Booking DNN confusing: lot of settings, everybody forgets the exact names
- Graphical interface: booking DNN with pleasure
- We can add different types of layers
- Specify the neuron number and training strategy for layer
- Connect the layers: building the network
- Save network: transform the graphical representation to option string and books the method



- jsmva magic register output transformer function, inserts CSS to notebook
- Structures the data to CSS formatted HTML table

Go back

Notebooks

Everything on GitHub:

https://github.com/qati/GSOC16

Notebooks on nbviewer (static, rendered):

http://nbviewer.jupyter.org/github/qati/GSOC16/blob/master/index.ipynb

Notebooks on binder (interactive):

www.mybinder.org/repo/qati/GSOC16

Or you can download:

https://github.com/qati/GSOC16/tree/master/notebooks

Thank you!