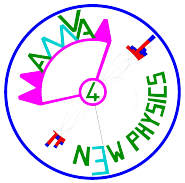
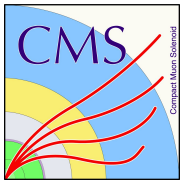






TÉCNICO LISBOA


LUMIN

A DATA SCIENCE AND DEEP LEARNING ECOSYSTEM FOR HIGH-ENERGY PHYSICS

Giles Strong

IML Workshop, CERN - 17/04/2019

giles.strong@outlook.com

twitter.com/Giles_C_Strong

Amva4newphysics.wordpress.com

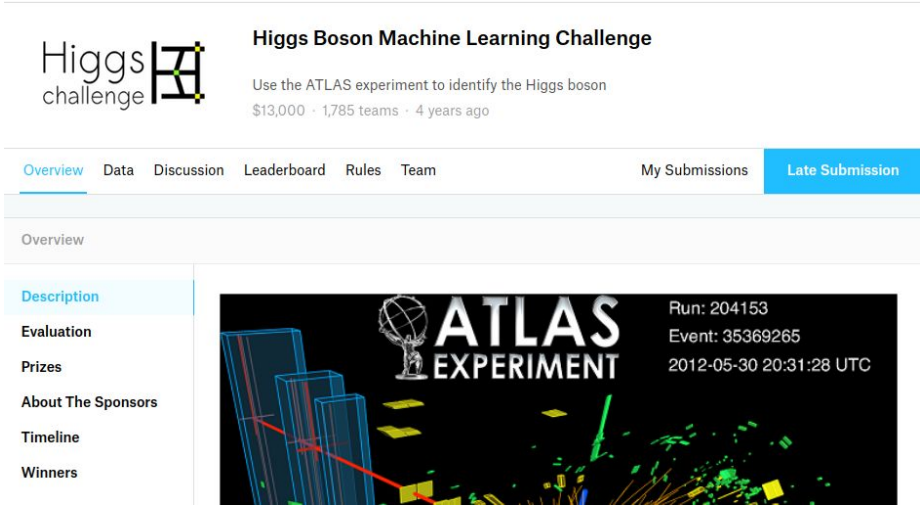
github.com/GilesStrong

CASE STUDY

2014 Higgs ML Kaggle Challenge

OVERVIEW

- Last year I spent quite a bit of time studying the 2014 Higgs ML Kaggle challenge
- The dataset as several nice properties:
  - Representative of typical high-energy physics (HEP) problem in terms of task and dataset size
  - Realistic performance metric - Approximate Median Significance (AMS)
  - Well studied = strong baselines to measure performance



RESULTS

- The aim was to test whether several recently developed deep neural network techniques could bring improvements in a HEP context
- Full study documented in AMVA4NewPhysics Deliverable 1.4
- Also reported at the last IML meeting of 2018
- Approach also used in CMS HL-LHC projection studies for CERN Yellow Report

AMVA4NewPhysics ITN

Work Package 1 - Deliverable 1.4

Final Activity Report: Classification and Regression Tools in Higgs Measurements

AMVA4NewPhysics authors

October 31, 2018

Abstract

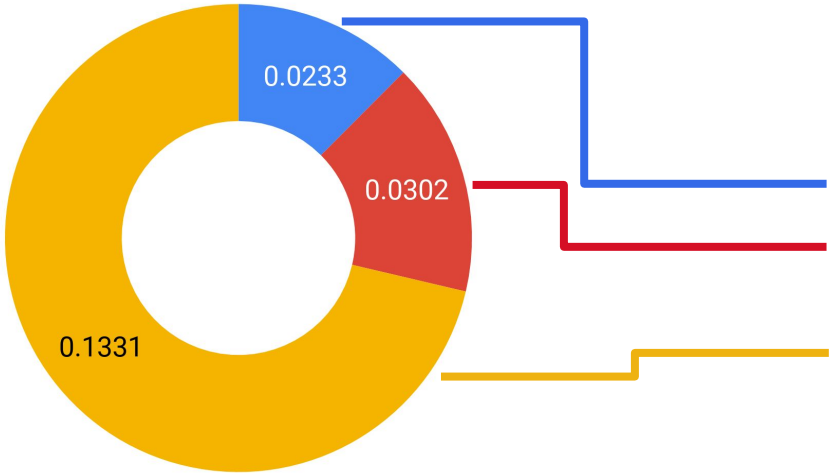
This document describes the performance of the optimized algorithms developed for application to the classification and regression problems of WP1.

RESULTS SUMMARY

- The study resulted in a method which:
  - Outperformed the winning solution
  - Trained 16 times quicker
  - Inferred 1.5 times quicker
  - Ran on a mid-budget laptop as opposed to a top-end graphics card

Solution	New	1st place
Method	10 DNNs	70 DNNs
Train time	1.5 hours	24 hours
Inference time	40 min	1 hour
Score	3.818	3.806
Hardware requirements	Intel i7-6500U <8 GB RAM (2016 laptop)	Titan GPU <24 GB RAM

IMPROVEMENT BREAKDOWN



- Initial model: ensemble of 10 ReLU based DNNs - score = 3.631
- Swish activation function → 3.654
- Cosine learning rate annealing with warm restarts → 3.6846
- Train-time/Test-time data augmentation → 3.818

SOFTWARE REQUIREMENTS

- The DNNs were implemented using Keras + Tensorflow
- However required functionality was missing, e.g.:
  - Swish activation function
  - Learning Rate finder
  - Learning rate schedules
  - HEP-specific data augmentation
  - Advanced ensembling
- The fastai library contains some of this functionality, but doesn't support sample weighting - necessary for HEP data

SOFTWARE REQUIREMENTS

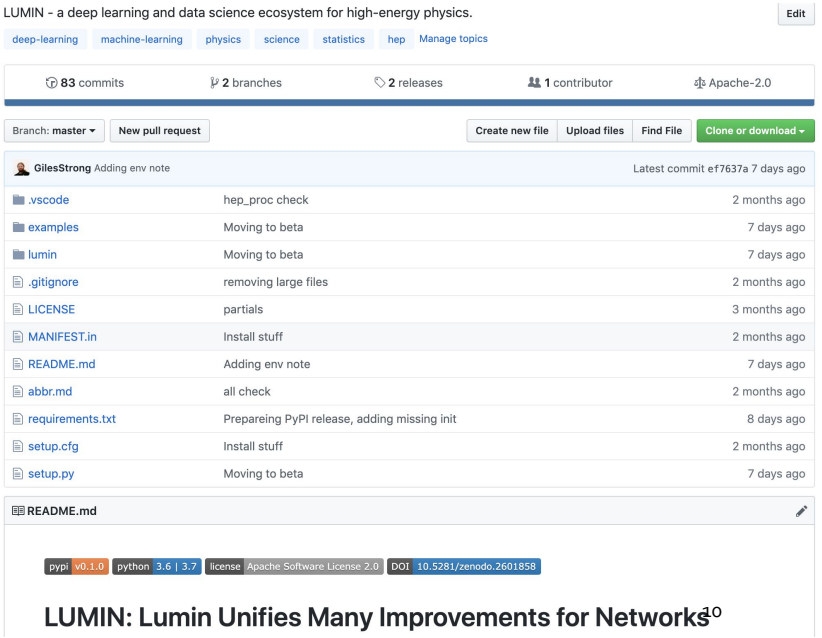
- A lot of extra code had to be written to provide the necessary functionality
- However this sometimes required working with Tensorflow, which Keras was meant to be abstracting
- Similarly, other Keras functions weren't being used as intended due to data augmentation and the ensembling techniques
- Afterward the study I rewrote the entire framework from scratch using PyTorch for the networks

LUMIN

Lumin Unifies Many Improvements to Networks

OVERVIEW

- At its heart LUMIN contains the required functionality to reimplement the Higgs ML solution
- But it does so in an adaptable way, meaning it can easily be applied to other problems and tasks
- On top of this, it provides useful tools for both:
  - Machine learning & data science
  - HEP-specific tasks and evaluations
- LUMIN aims to become an ecosystem for physicists to quickly apply the best approaches to their analysis work



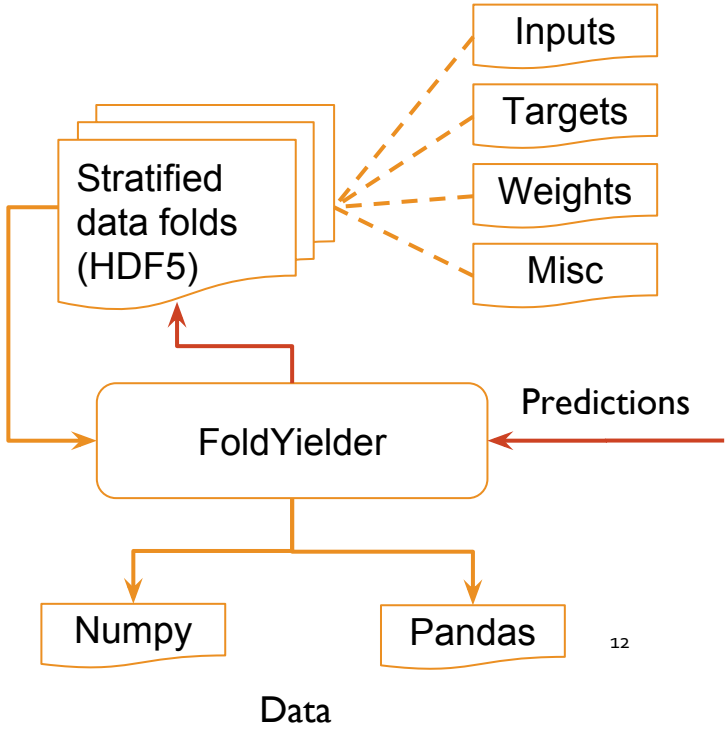
CAPABILITIES

- LUMIN can be used to train neural networks for supervised classification and regression tasks using columnar data (features in columns - events in rows)
- Many options available (full list), such as:
  - Learning rate & momentum schedules; e.g. cosine annealing, One-cycle
  - Advanced ensembling; e.g. Snapshots, Fast-Geometric, Stochastic Weight Averaging
  - Entity embedding of categorical features
  - See backup slides for summary of techniques
- Feature selection via importance, dependency, and dendrograms

Universal handling of sample weights

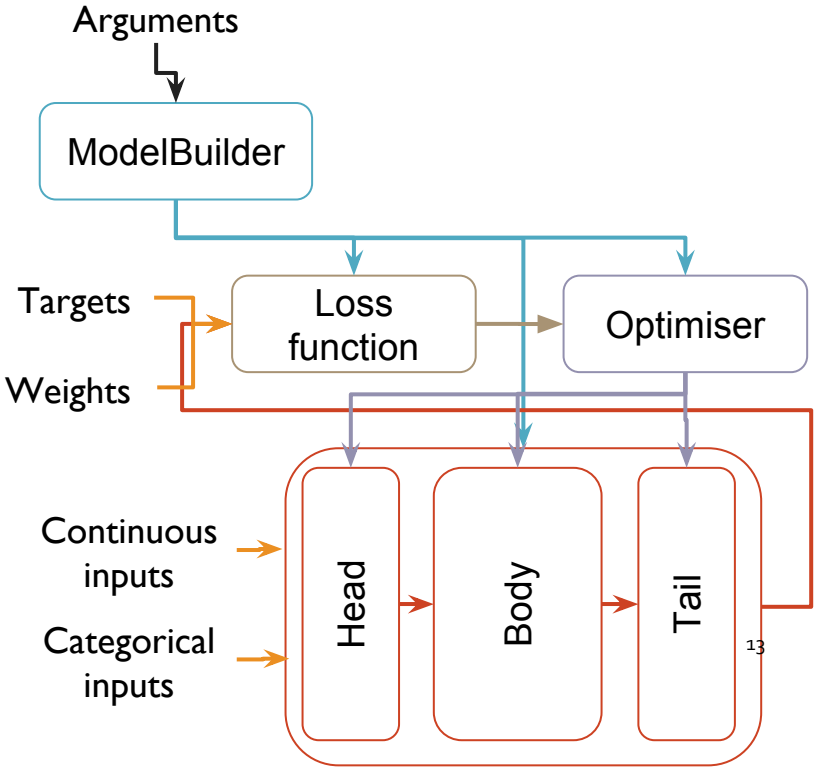
CENTRAL CLASSES: FoldYielder

- N-tuples extracted, processed, and saved to HDF5 file
  - General and HEP-specific pre-processing functions available
  - Data split into folds for ensembling and cross-validation (helper functions available)
- FoldYielder interfaces with HDF5 file to provide data on demand as: Numpy arrays or Pandas DataFrames
- Inheriting classes can provide data augmentation at train and test time
- Many LUMIN functions expect, or act differently on, FoldYielders
  - Memory overhead reduced
  - Averaging over folds



CENTRAL CLASSES: ModelBuilder

- ModelBuilder initialised with specification for the NN architecture and optimiser
- Once initialised, will yield NNs and optimisers on request
- NNs consist of three modular sections:
  - Head - takes continuous and categorical inputs and scales up the width
  - Body - provides most of the computation
  - Tail - scales down the body to match the output dimension and provides the final activation layer
- These can be swapped and configured as required



CENTRAL CLASSES: Model

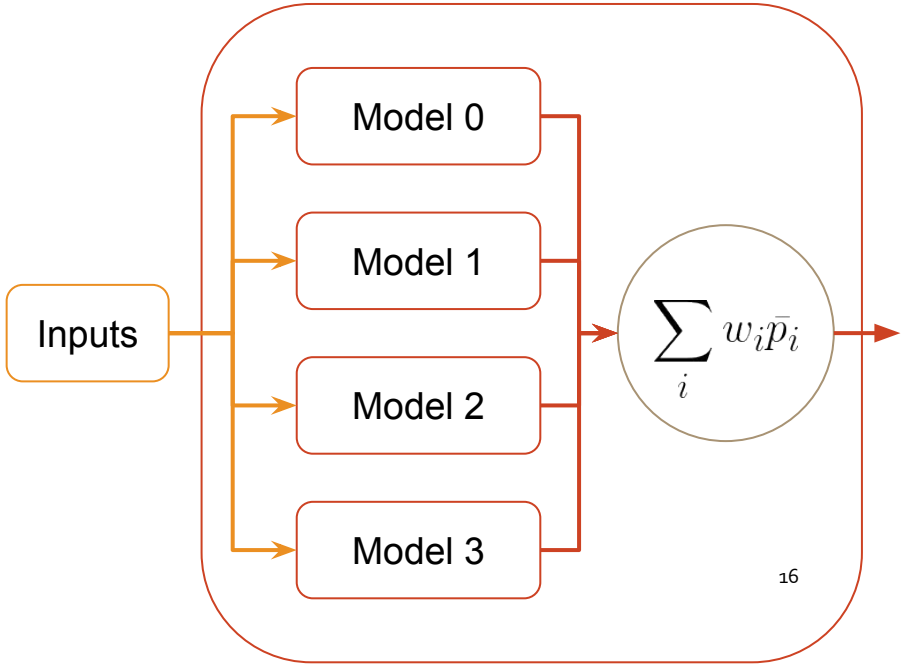
- Model is a wrapper class for the NNs created by ModelBuilders, providing methods for:
  - Fitting
  - Predicting
  - Evaluating
  - Loading/Saving/Exporting
- The recommended process for training is to use the fold_train_ensemble method (even for single models) to interface a FoldYielder with Model.fit
- Once finished, a new Model can be instantiated, and the weights saved during training can be loaded

CENTRAL CLASSES: Callback

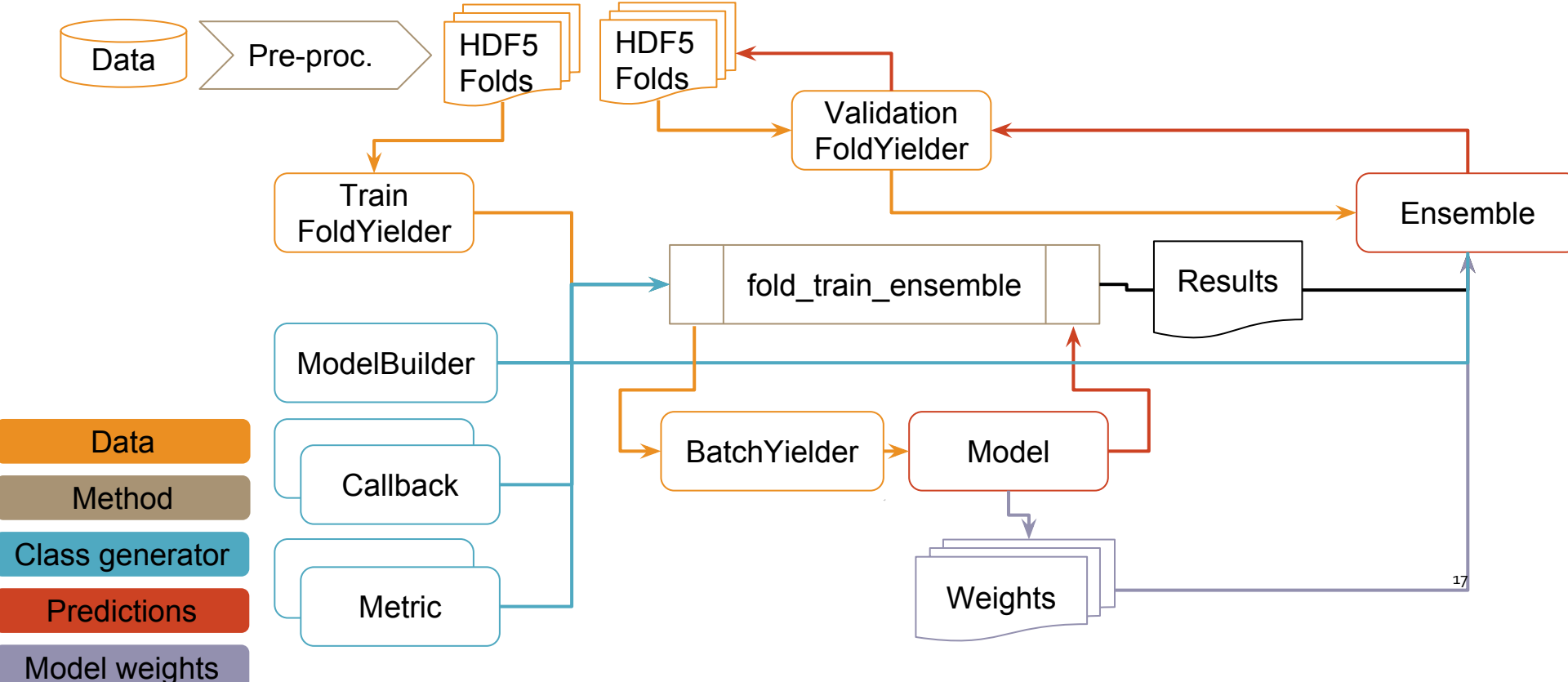
- Similar to Keras, the Callback class can be used to adjust the training procedure, model, et cetera whilst training is ongoing
- The fold_train_ensemble method looks for two special types:
  - Subclasses of AbsModelCallback with a get_loss method will affect the early stopping of training by considering the validation loss of any model variant the callback maybe maintaining, e.g. a Stochastic Weight Average of models
  - Subclasses of AbsCyclicalCallback, e.g. cosine annealing, will:
    - Change early-stopping patience from epochs without improvement to cycles without improvement
    - Save model weights after every cycle (e.g. for SSE or FGE)
    - Be passed to any subclasses of AbsModelCallback, e.g so model weights are only averaged at the end of a cycle

CENTRAL CLASSES: Ensemble

- The Ensemble class loads model trained by fold_train_ensemble and provides bulk methods for prediction, saving/loading/exporting, and feature importance evaluation
- Individual predictions of models can be weighted by some metric, e.g validation loss, or given equal weighting
- Can also build ensembles from (weighted) snapshots of models for SSE or FGE



CLASS INTERACTION



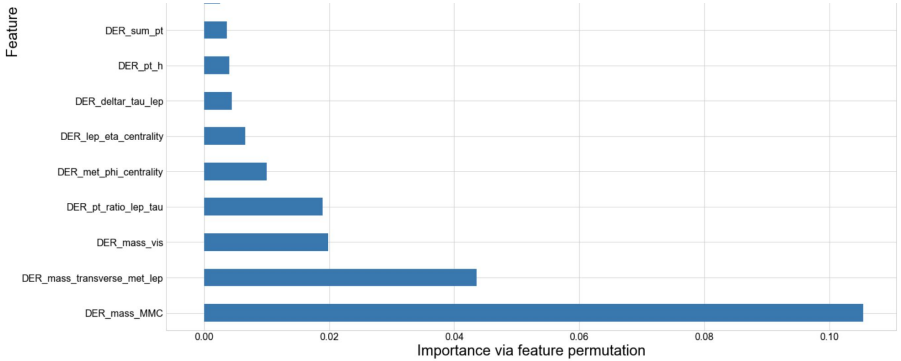
OTHER HIGHLIGHTS: SET DICRIMINATION

- Uses random forests to quickly see whether one's validation set is indistinguishable from one's training and testing sets
  - If not, highlights which features are most different
- Could also be used to spot mis-modelling of collider data in Monte Carlo samples

```
AUC for test-validation discrimination = 0.4998
Top 10 most important features are:
   index                 Feature  Importance
0      0           DER_mass_vis    0.001422
1      2     DER_prodeta_jet_jet    0.001204
2      3              PRI_lep_py    0.001204
3      4              PRI_lep_px    0.001204
4      1              PRI_tau_px    0.001204
5      5                DER_pt_h    0.001094
6      6              PRI_lep_pz    0.001094
7      7   PRI_jet_subleading_px    0.001094
8      8  DER_lep_eta_centrality    0.000985
9      9    DER_pt_ratio_lep_tau    0.000328
```

OTHER HIGHLIGHTS: FEATURE SELECTION

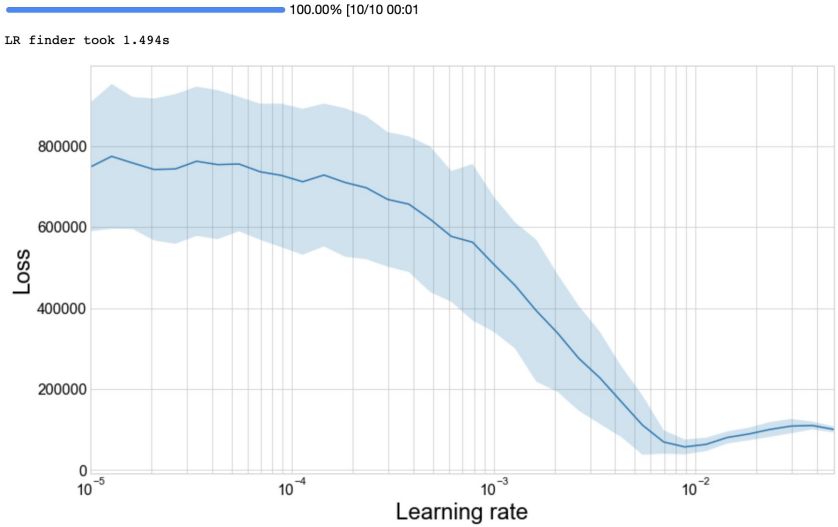
- Uses auto-optimising random forests to check permutation importance of features
  - Retrains on a reduced set of features to check for performance drop when low importance features are removed
  - Permutation importance also available for interpreting NNs and ensembles - allows for sanity checking
- Feature dependency (ease of regression of a feature using other features) also available via rfpimp package
  - Accounts for multicollinearities, which permutation importance would not pick up




```
12 features found with importance greater than 0.001:
 ['DER_mass_MMC', 'DER_mass_transverse_met_lep', 'DER_mass_vis', 'DER_pt_ratio_lep_tau', 'DER_met_phi_centrality', 'D
ER_lep_eta_centrality', 'DER_deltar_tau_lep', 'DER_pt_h', 'DER_sum_pt', 'DER_deltaeta_jet_jet', 'DER_mass_jet_jet',
'PRI_jet_num']

Optimising new RF

Total time: 00:09

Comparing RF scores, higher = better
All features:    0.83233
Top features:    0.83062
```

OTHER HIGHLIGHTS: LR FINDER

- The Smith LR range test allows one to quickly find optimal learning rates for a given architecture and dataset
- Passing a FoldYielder will show the mean and standard deviation for a range of trainings = smoother curve



STATE OF LUMIN

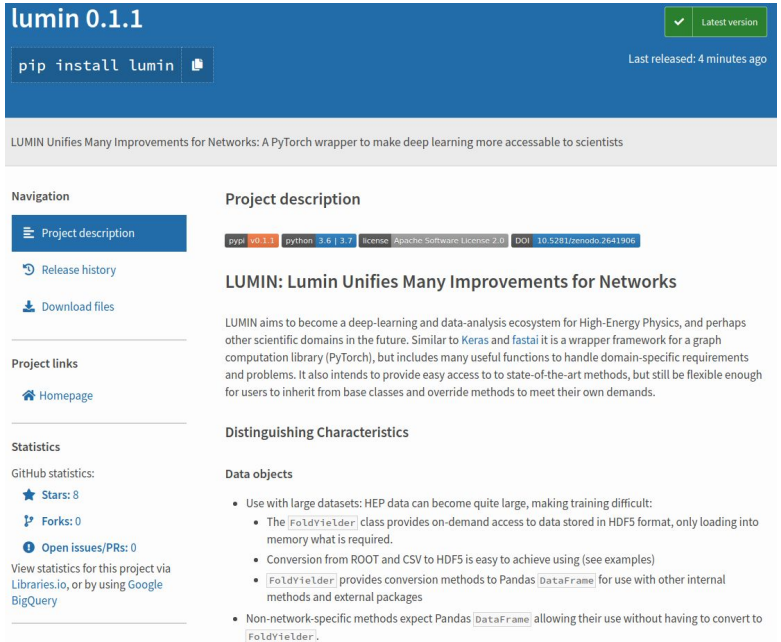
LUMIN ON HIGGS ML

- Currently reconfirming results from original study
- LUMIN appears to reproduce results, but averaging over many runs puts score on par with winning solution
- However, even greater speed up over original code
  - NB, change in test-time augmentation means inference time should timesed by 4 to compare to original times

Solution	LUMIN-GPU	LUMIN-CPU	1st place
Method	10 DNNs		70 DNNs
Train time	20 minutes	40 minutes	24 hours
Inference time	15 seconds	130 seconds	1 hour
Score	3.806±0.002		3.806
Hardware	Nvidia 1080 Ti GPU	Intel Core i7-8559U (MacBook Pro 2018)	Nvidia Titan GPU

CURRENT STATUS

- LUMIN is stored on a public Github repo: https://github.com/GilesStrong/lumin
- Installable from source or PIP: https://pypi.org/project/lumin/
  - Both methods require manual installation of additional, independent packages not on PIP
- Still in beta; latest release is v0.1.1
- OSX and Linux are supported
- No documentation or unit tests yet
- Four examples showing most of the capabilities:
  - Binary & multiclass classification
  - Single & multi target regression



FUTURE

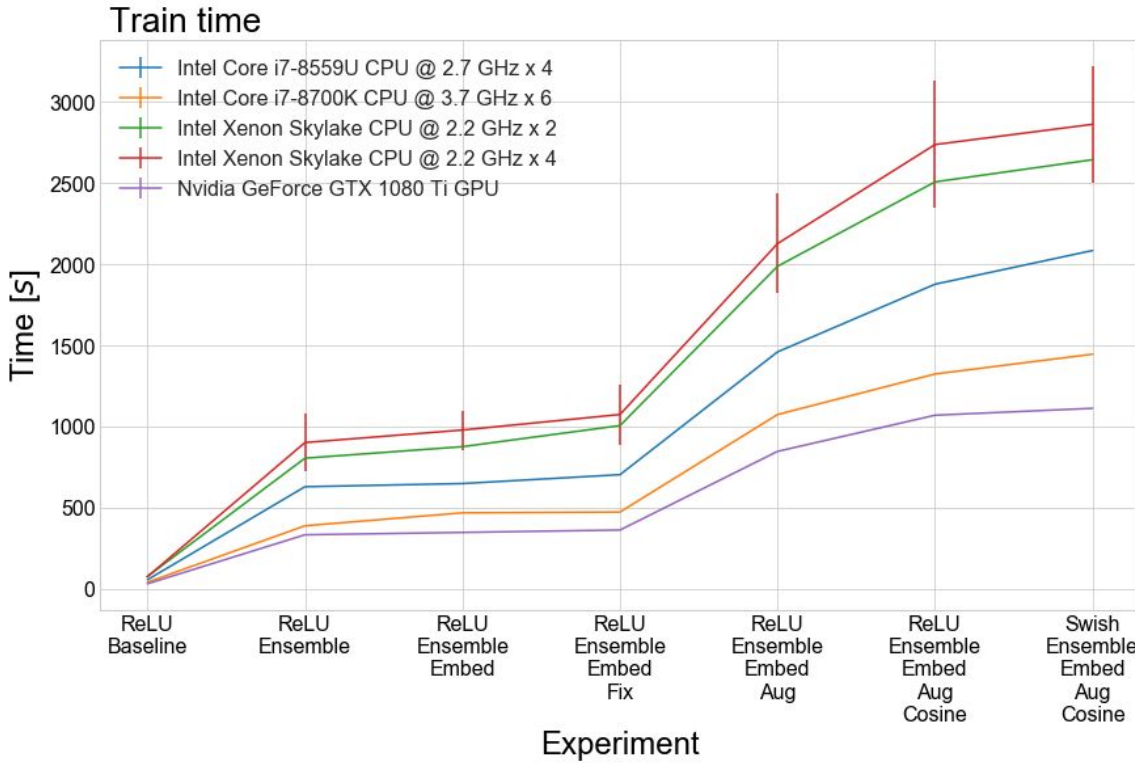
- Documentation is a necessary step
- As the number of users and contributors (hopefully) grows, tests will need to be added; currently the examples are doubling as tests.
- Really, though, the package needs people trying it out, playing around, and giving feedback on:
  - Bugs
  - Design & layout choices
  - General suggestions
- Contributions are most welcome: I'm hoping this can become a more general tool for the experimental-science community, but am only able to really cover my research areas

This Report is part of a project that has received funding from the **European Union's Horizon 2020 research and innovation programme under grant agreement Nº675440**

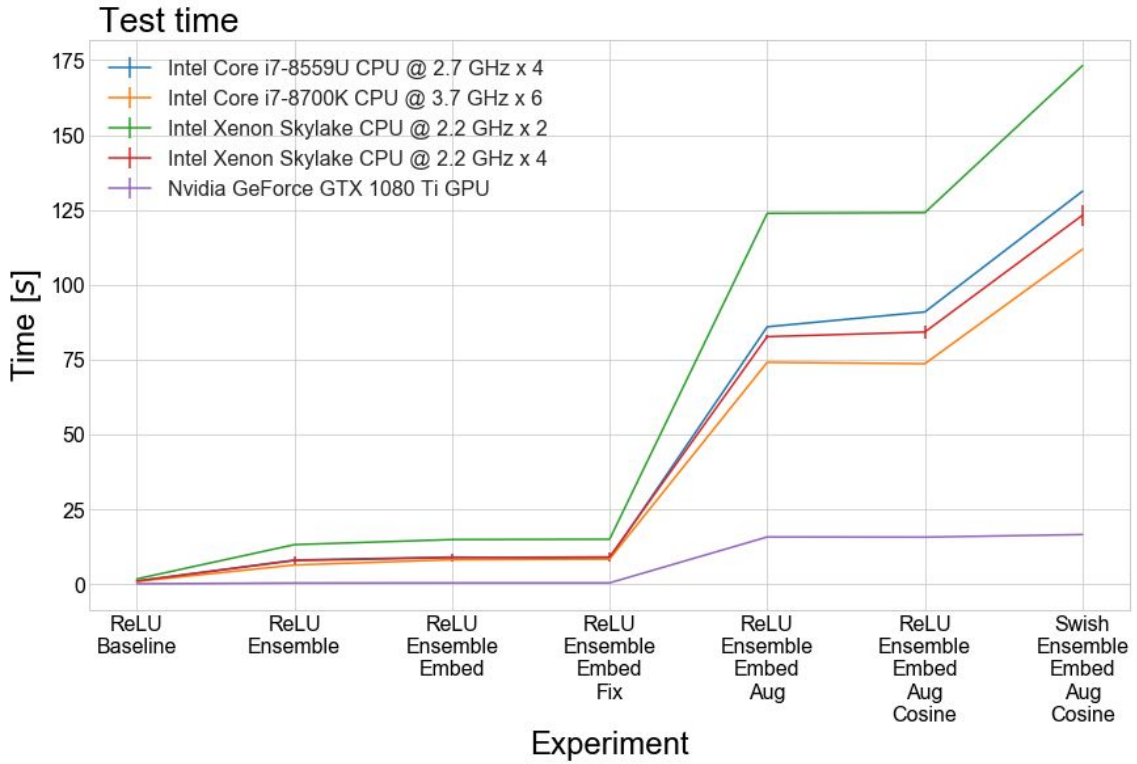
BACKUP SLIDES

LUMIN TIMING

TRAIN TIME

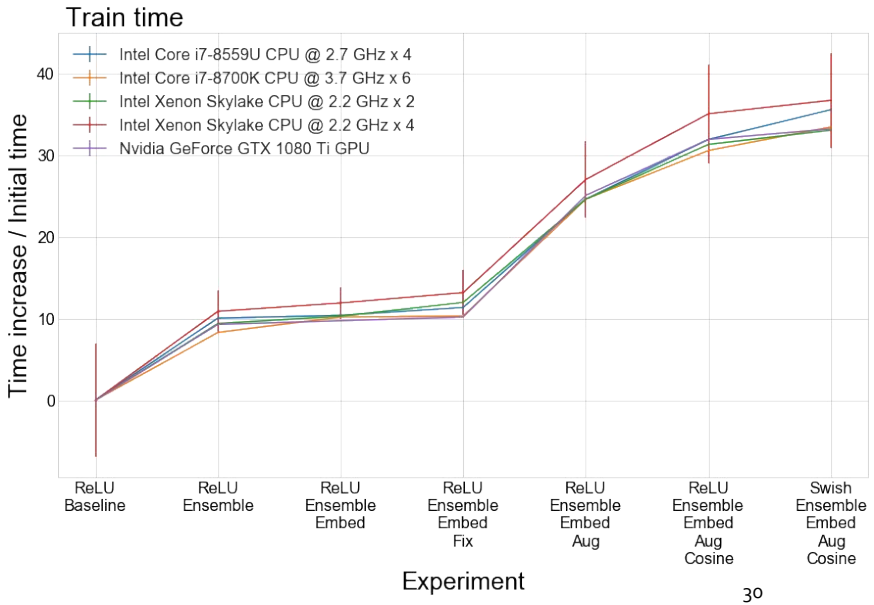

Train time
Intel Core i7-8559U CPU @ 2.7 GHz x 4
Intel Core i7-8700K CPU @ 3.7 GHz x 6
Intel Xenon Skylake CPU @ 2.2 GHz x 2
Intel Xenon Skylake CPU @ 2.2 GHz x 4
Nvidia GeForce GTX 1080 Ti GPU
Time [s]
0
500
1000
1500
2000
2500
3000
ReLU Baseline
ReLU Ensemble
ReLU Ensemble Embed
ReLU Ensemble Embed Fix
ReLU Ensemble Embed Aug
ReLU Ensemble Embed Aug Cosine
Swish Ensemble Embed Aug Cosine
Experiment

TEST TIME


Test time
Intel Core i7-8559U CPU @ 2.7 GHz x 4
Intel Core i7-8700K CPU @ 3.7 GHz x 6
Intel Xenon Skylake CPU @ 2.2 GHz x 2
Intel Xenon Skylake CPU @ 2.2 GHz x 4
Nvidia GeForce GTX 1080 Ti GPU
Time [s]
175
150
125
100
75
50
25
0
ReLU Baseline
ReLU Ensemble
ReLU Ensemble Embed
ReLU Ensemble Embed Fix
ReLU Ensemble Embed Aug
ReLU Ensemble Embed Aug Cosine
Swish Ensemble Embed Aug Cosine
Experiment

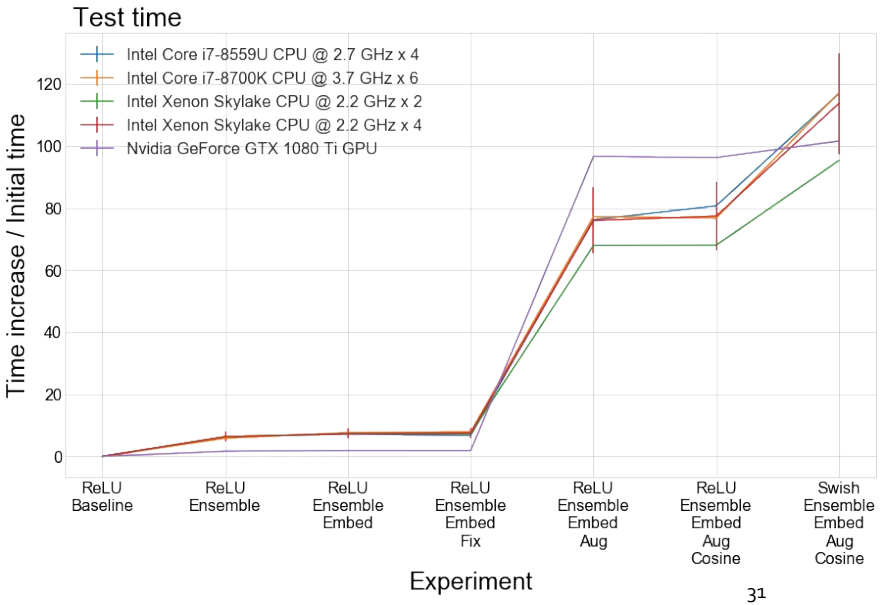
RELATIVE TRAIN-TIME INCREASE

- All additions bring about a 35 times increase in train time
- Accounting for ensemble training, 3.5 times increase



RELATIVE TEST-TIME INCREASE

- All additions bring about a 110 times increase in inference time
- Accounting for ensemble training, ~11 times increase
- Increases on par with expectation
  - Just under 10 times for ensembling
  - NB, timing includes time for data loading - hence why GPU appears to show super-sublinear scaling for ensembling
  - ~8 times for test-time augmentation (8 sets of augmentations are applied)
  - Increase for Swish due to exponential evaluation (and lack of JIT compilation?)



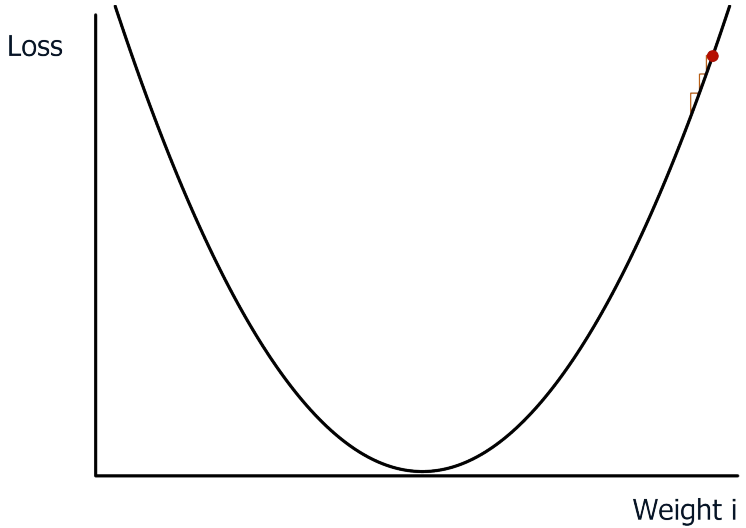
METHOD SUMMARIES

Learning rate finder

- "*[The Learning Rate] is often the single most important hyperparameter and one should always make sure that it has been tuned*" - Bengio, 2012
- Previously this required running several different trainings using a range of LRs
- The LR range test (Smith 2015 & 2018) can quickly find the optimum LR using a single epoch of training

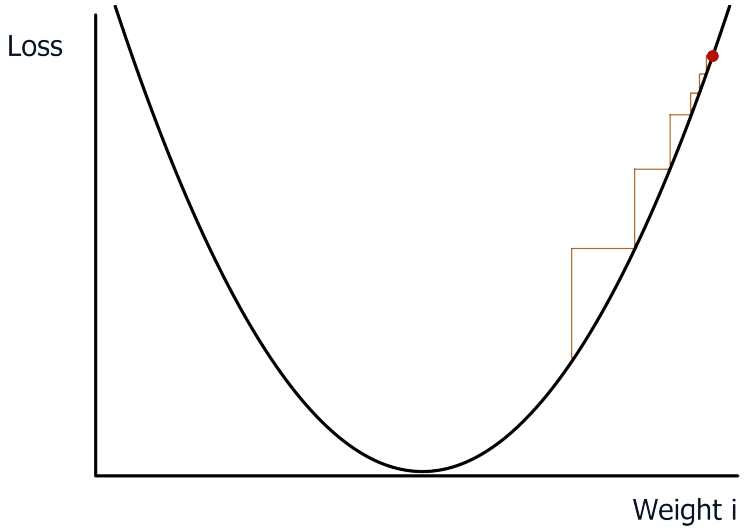
Learning rate finder

1. Starting from a tiny LR (~1e-7), the LR is gradually increased after each minibatch



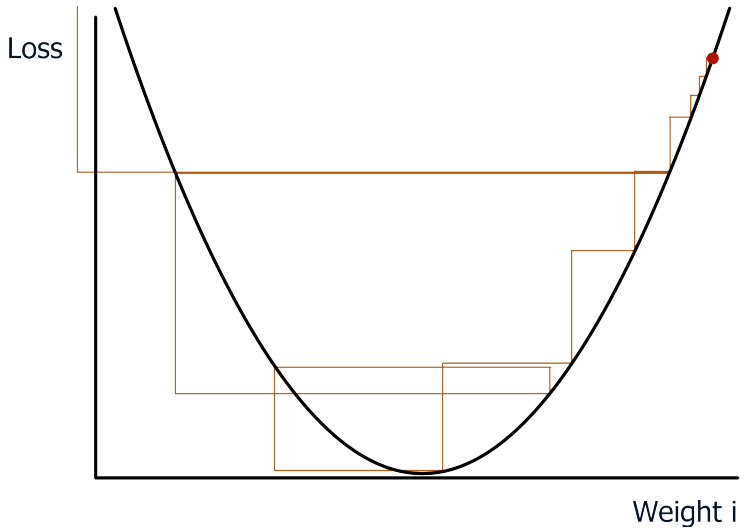
Learning rate finder

1. Starting from a tiny LR (~1e-7), the LR is gradually increased after each minibatch
2. Eventually the network starts training (loss decreases)



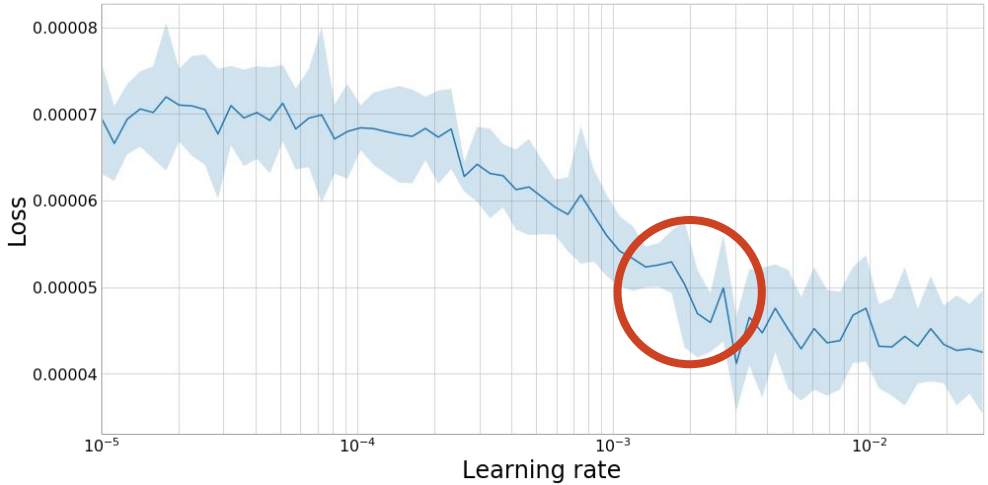
Learning rate finder

1. Starting from a tiny LR (~1e-7), the LR is gradually increased after each minibatch
2. Eventually the network starts training (loss decreases)
3. At a higher LR the network can no longer train (loss plateaus), and eventually the network diverges (loss increases)



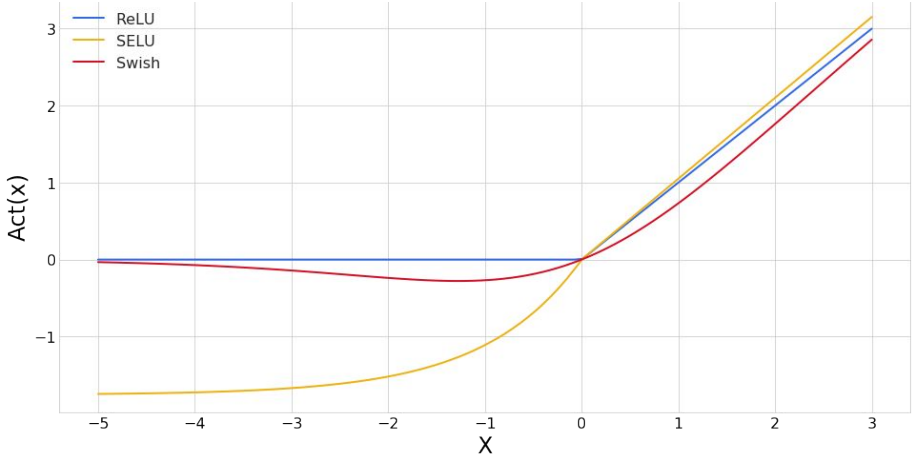
Learning rate finder

- The optimum LR is the highest LR at which the loss is still decreasing
- Further explanation in this lesson



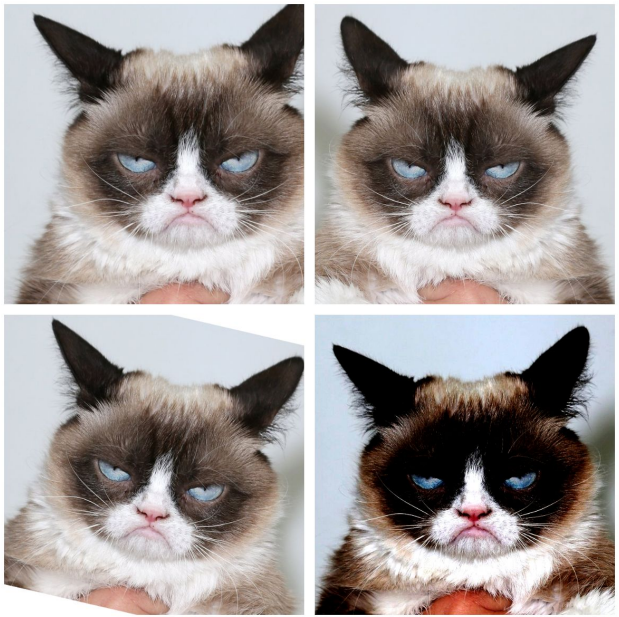
ACTIVATION FUNCTIONS

- Whilst ReLU is a common activation function, newer ones are continually being introduced
- SELU uses carefully derived scaling coefficients allow networks to self-normalise, removing any need for batch normalisation
  - SELU Example
- Swish, found via reinforcement learning, provides a region of negative gradient
  - Swish example



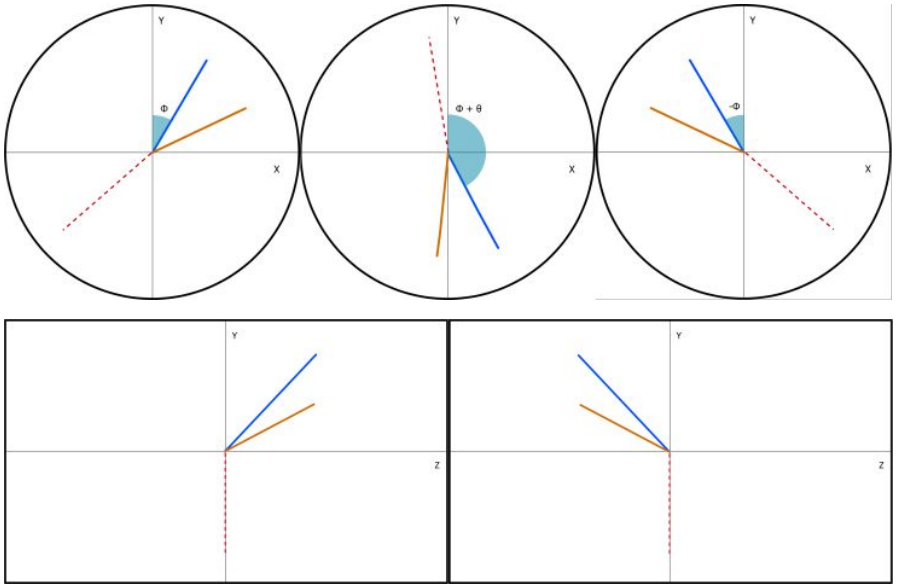
Data augmentation

- Data augmentation involves applying transformations to input data such that the a new data point is created, but the underlying class is unchanged
- This is well used in image classification to artificially increase the amount of training data (train-time augmentation), e.g Krizhevsky et al. 2012
- It can also be applied at test time by predicting the class of a range of augmented data and then taking an average of the predictions.



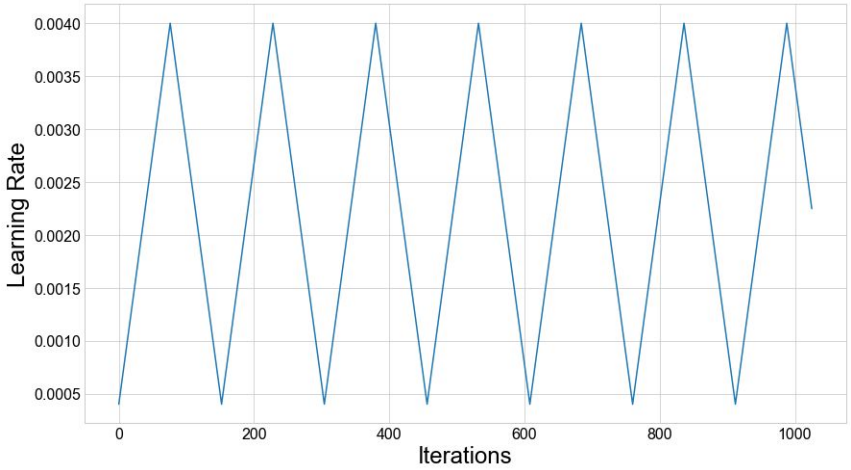
Data augmentation

- Correct application of augmentation relies on exploiting invariances within the data: domain specific
- At the CMS and ATLAS detectors, the initial transverse momentum is zero, therefore final states are produced isotropically in the transverse plane: the class of process is invariant to the rotation in azimuthal angle
- Similarly, the beams collide head on with equal energy: therefore final states are produced isotropically in Z-axis
- Alternative is to remove symmetries by setting common alignment for events
  - Data augmentation example
  - Data fixing example



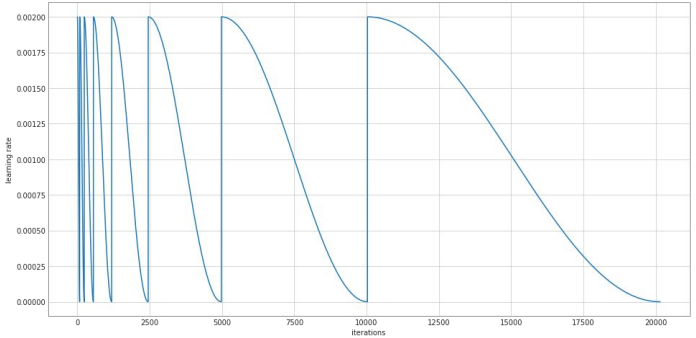
LINEAR CYCLING

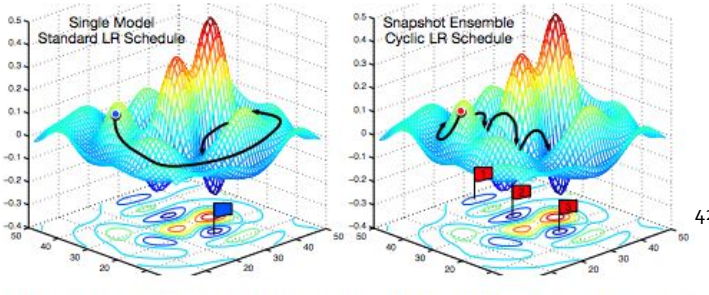
- Adjusting the LR during training is a common technique for achieving better performance
- Normally this involves decreasing the LR once the validation loss becomes flat
- Smith 2015 suggests instead to cycle the LR between high and low bounds
- Smith 2017 showed that the additional application of an out-of-phase schedule to the optimiser momentum/beta$_1$ coefficient can sometimes lead to *super convergence*
- Linear cycle example



COSINE ANNEALING

- Loshchilov and Hutter 2016 instead suggests that the LR should be decay as a cosine with the schedule restarting once the LR reaches zero
- Huang et al. 2017 later suggests that the discontinuity allows the network to discover multiple minima in the loss surface
- 2016 paper demonstrates on image and EEG classification
- Cosine annealing example

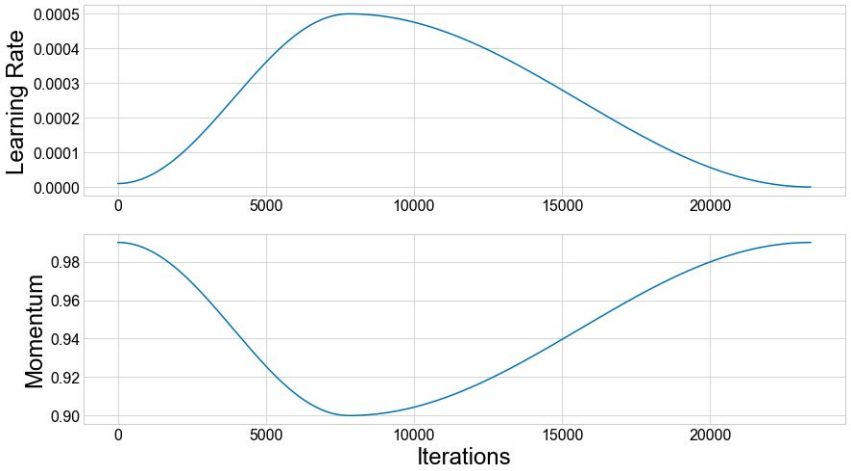




Lower figure - Huang et al., 2017, arXiv:1704.00109

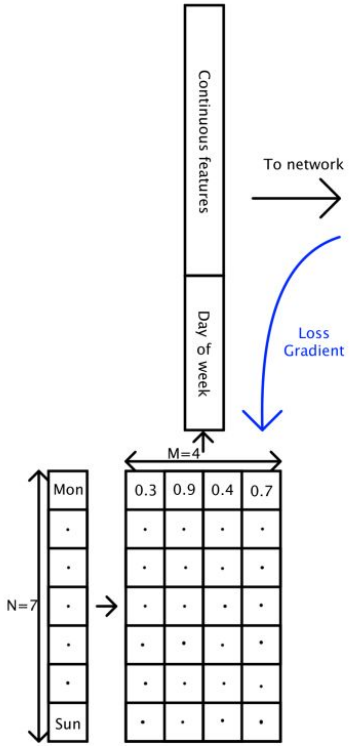
ONE CYCLING

- Smith 2018 introduces the 1cycle schedule which further improves the super convergence
- This involves running through a single cycle of increasing and then decreasing the lR, with a similar, inverted schedule applied to momentum/beta$_1$
- Original paper used linear interpolation
- FastAI found a cosine interpolation was better
- LUMIN includes both interpolations
- Onecycle example



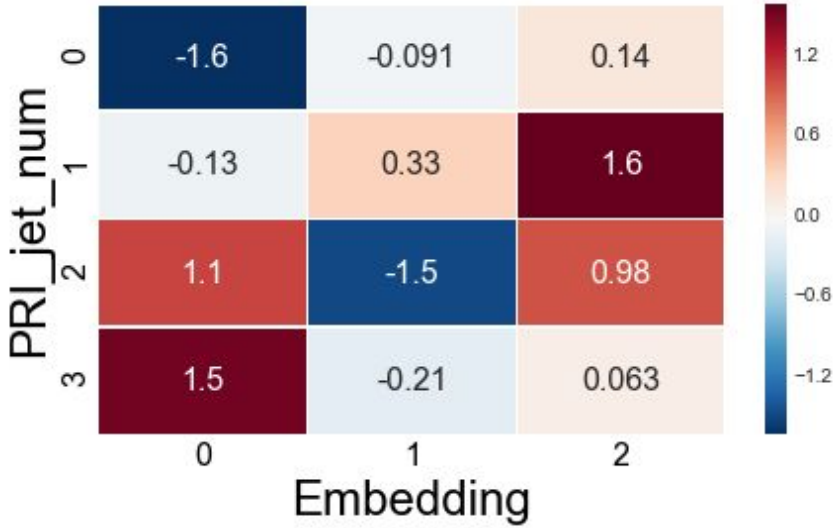
ENTITY EMBEDDING

- Categorical features = features with discrete values and no numerical comparison
- Normal to 1-hot encode as Boolean vector (Monday → 1000000)
- But potentially means a large number of extra inputs to NN (day of year = 365 inputs)
- Guo 2016 learns lookup tables which provide a compact, but rich, representation of categorical values as vector of floats (Monday → 0.3,0.9,0.4,0.7)



ENTITY EMBEDDING

- Embedding values start from random initialisation
- Receive gradient during backpropagation and are learnt just like any other network parameter
- Once learnt, embeddings can then be transferred to other tasks which require embedding the same, or similar, feature (better than random init.)
- Random init. Example
- Embedding loading example



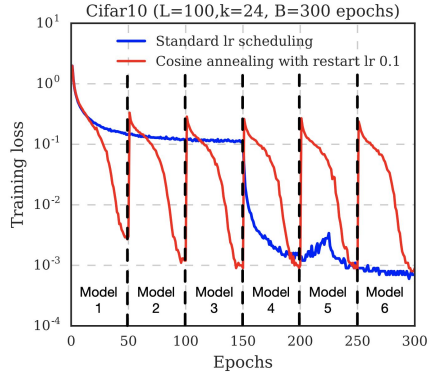
ENSEMBLING

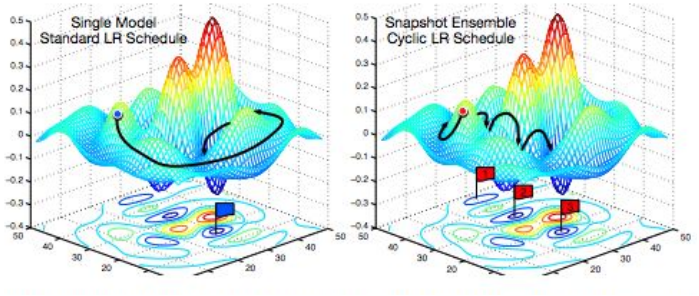
- Basic ensembling requires training multiple models, and then averaging over their predictions
- Advantages:
  - Greater generalisation to unseen data
  - Often a more powerful model
  - Provides resistance against possibility of bad training
- Disadvantages
  - Increases train time
  - Increases inference time

Basic ensembling example

SNAPSHOT ENSEMBLING

- SSE uses the idea that a warm-restarted LR will find multiple minima across the loss surface
- Just before the LR jump, when the network is in a minima, a snapshot of the model weights is saved
- The model then jumps out and begins converging to different minima
- This allows one to create an ensemble of models in a single training

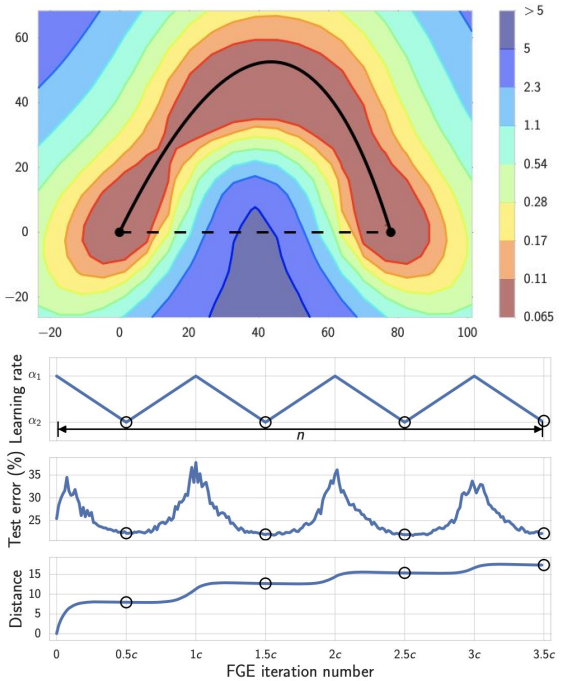




Figures - Huang et al., 2017, arXiv:1704.00109

FAST GEOMETRIC ENSEMBLING

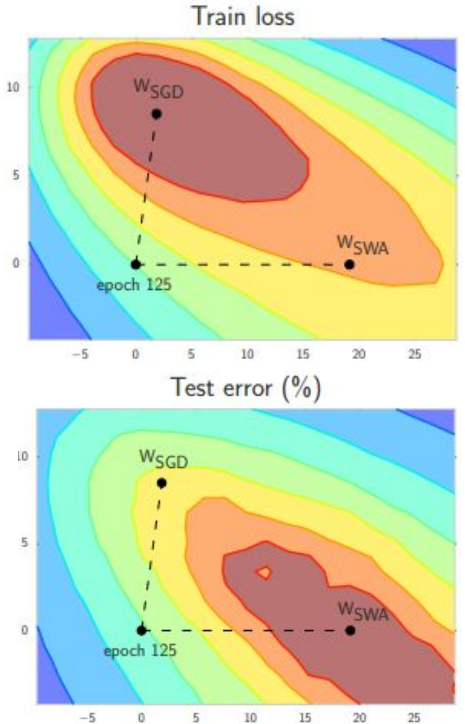
- FGE further improves on SSE by finding that loss minima are connected by curves of constant loss (rare to find true minima - almost certainly a saddlepoint/valley given dimensionality)
- Using a high-frequency linearly cycled LR it aims to direct the model along these curves, saving snapshots along the way
- FGE example



Figures - Garipov et al., Feb. 2018, arXiv:1802.10026

STOCHASTIC WEIGHT AVERAGING

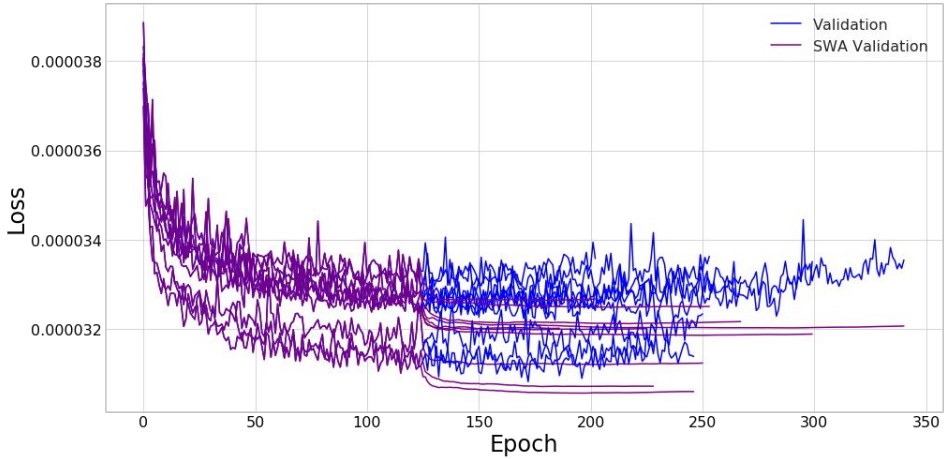
- Both SSE and FGE solve the problem of increased training time, but still incur an increased inference time
- SWA solves this problem by averaging in *weight space* rather than *model space*
- As the model is trained, a running average of the model parameters is kept
- Can be used with both constant, cycled, and annealed LR schedules
- SWA example



Figures - Izmailov et al., Mar. 2018, arXiv:1803.05407

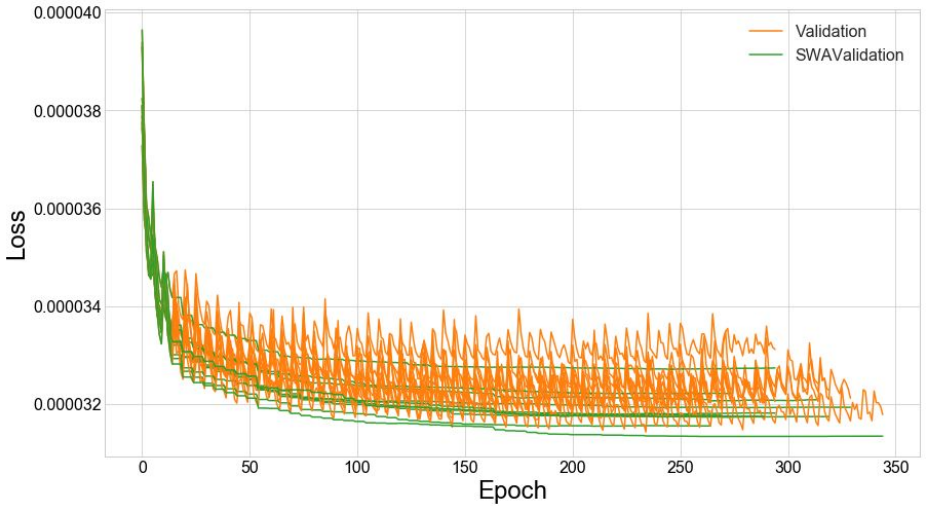
STOCHASTIC WEIGHT AVERAGING

- Published SWA requires setting a priori when to start averaging
  - Too early = spoilt by initial weights being bad
  - Too late = no exploration



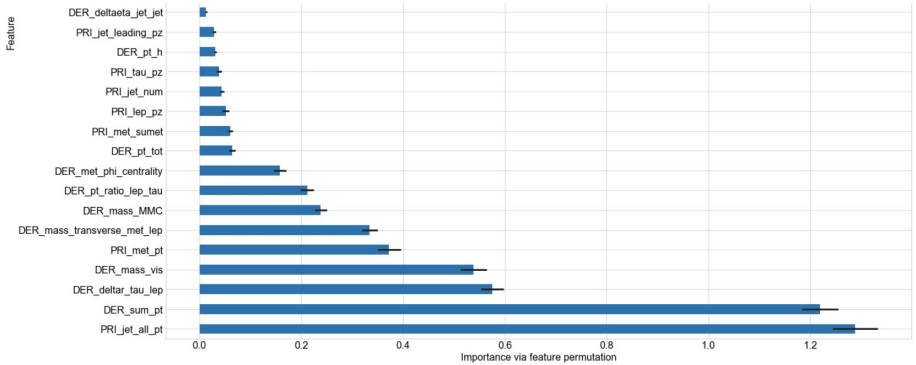
STOCHASTIC WEIGHT AVERAGING

- LUMIN's implementation can track multiple averages, replacing and restarting them if new averages would be better
- Slightly slower, but ensures you never need to train once beforehand to know when to start averaging



PERMUTATION IMPORTANCE

- Method to quantify the importance of each input feature
  a. Loss of trained mode evaluated on training data
  b. Copy of data made and one feature column is shuffled = info destroyed
  c. Loss re-evaluated
  d. Increase in loss corresponds to feature importance - Large change implies heavy reliance by model
- Can either be used interpret a trained model, or to reduce input feature-space
- Does not work for collinear features - model can recover information from another feature, so importance is reported to be lower than it actually is



FEATURE DEPENDENCE

- For data with collinear feature, feature dependence can be evaluated
- This involves training regressors to predict the value of a certain feature given the other features
- The more performant the regressor, the more information about that feature is carried by the other features
- Can be used to *carefully* remove training features
- See this for more information: https://explained.ai/rf-importance/index.html