Machine Learning for Columnar High Energy Physics Analysis

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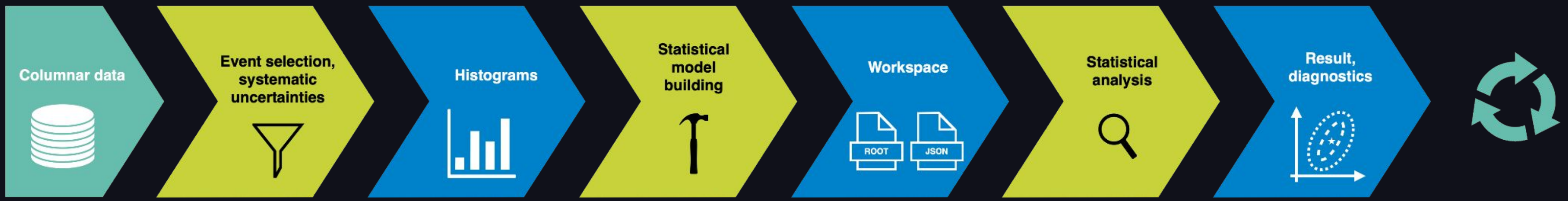
Outline

1. Analysis Grand Challenge Overview
2. Strategy for Integrating Machine Learning
3. Training Pipeline
4. Inference Pipeline

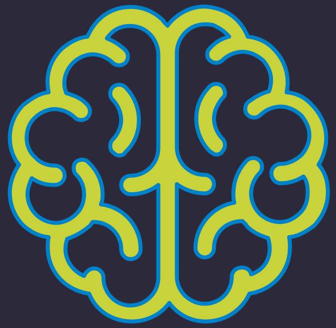
Analysis Grand Challenge

- ➔ Demonstrate **realistic analysis workflow** in anticipation of HL-LHC requirements
- ➔ Task: ttbar cross-section measurement using **2015 CMS Open Data**
  - ◆ Interactive and accessible user interface
  - ◆ **Open Data** – everyone can participate!
- ➔ Include all aspects of typical LHC analysis
  - ◆ Data access
  - ◆ Event selection
  - ◆ Histogramming
  - ◆ Statistical model building / fitting
  - ◆ Analysis preservation

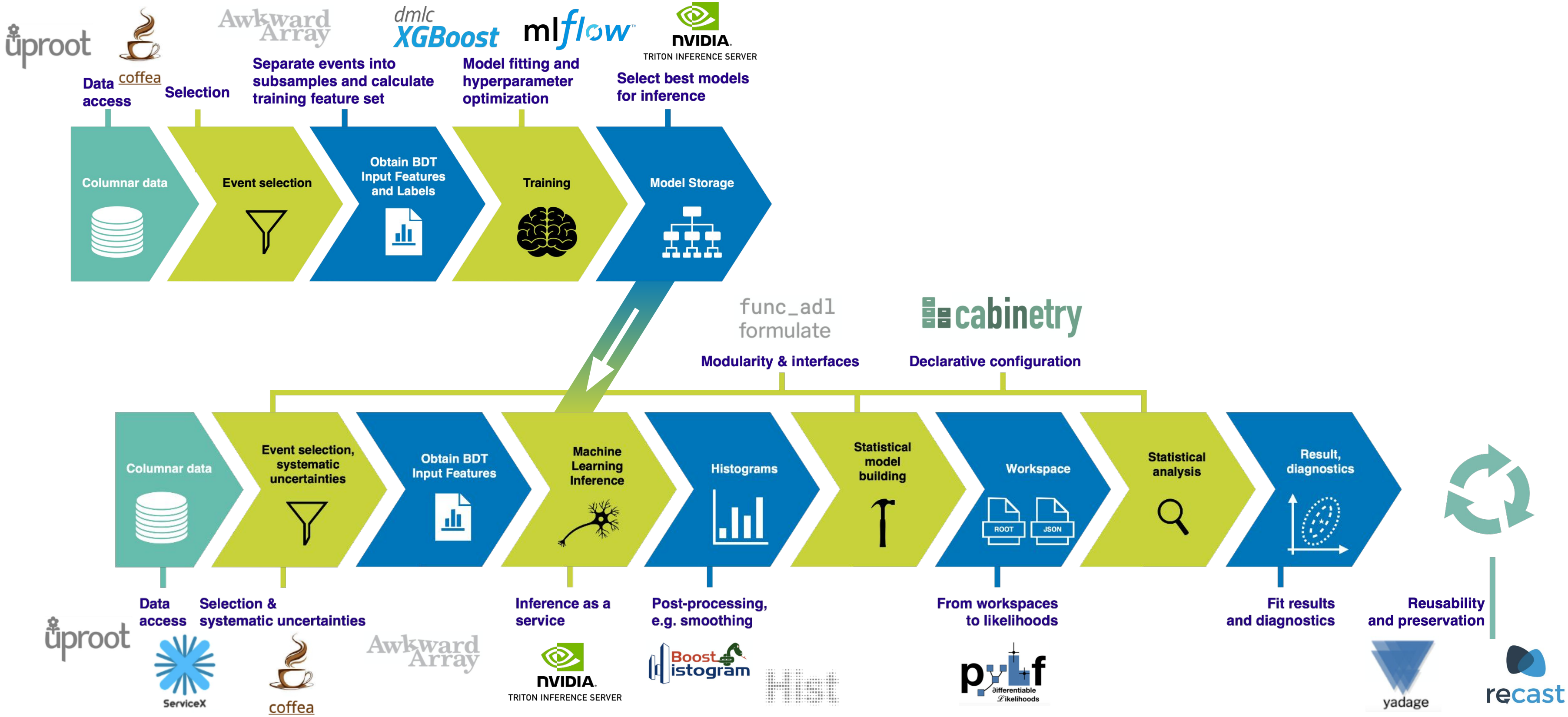


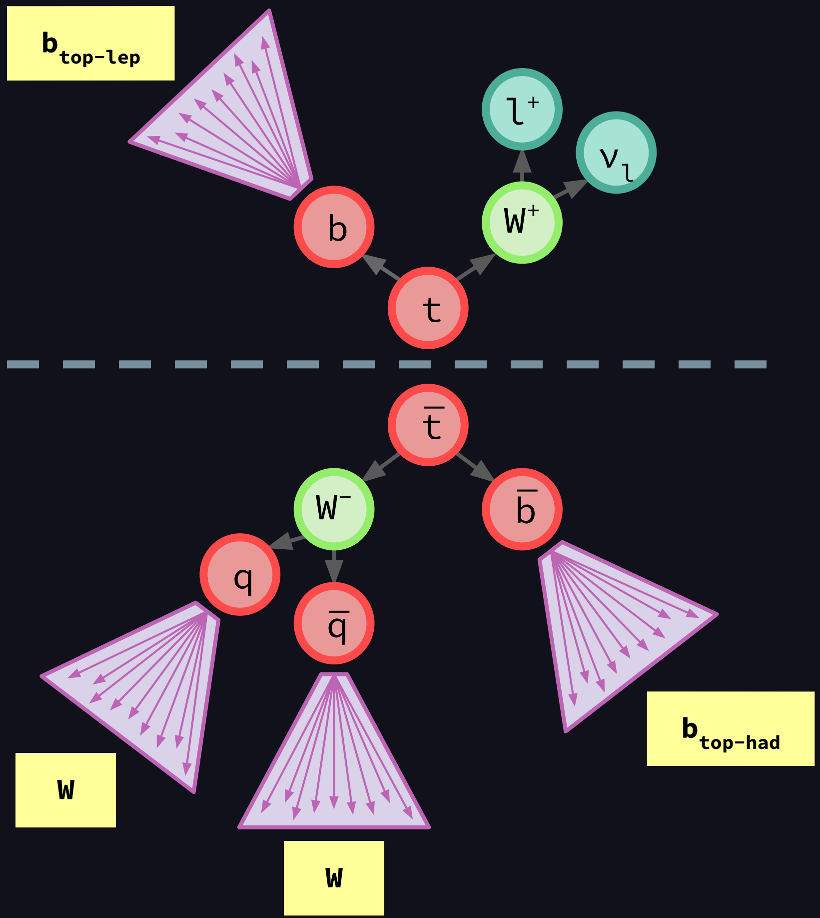
Machine Learning in HEP Analysis

- What is needed for HL-LHC?
  - Improvement in **algorithm performance**
  - Better utilization of **computational resources**
- Machine learning (especially deep learning) can help with this!
- Add ML task to AGC pipeline to reflect developments in HEP analysis



Analysis Grand Challenge + ML



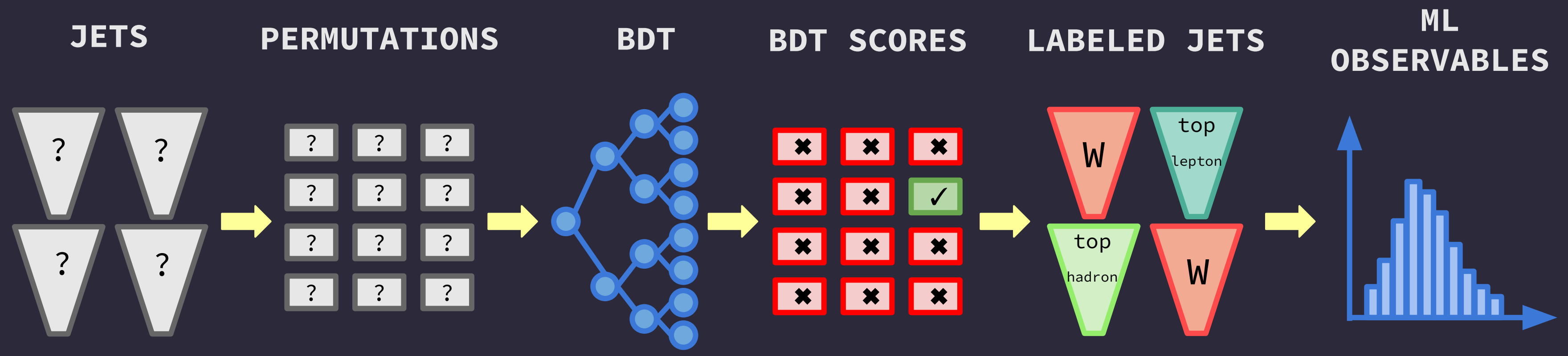


Machine Learning Task

- Assign jets to their parent partons
- Allows us to approximate observables such as
  - Mass of top quark (combined mass of $b_{top\text{-}had}$ and two W jets)
  - Angle between top_{lepton} jet and lepton ($\Delta\phi$)

Approach to ML Task

1. Consider **leading N jets** in each event
2. Find **all possible permutations** of parton assignments of these N jets (two W, one $b_{top\text{-}had}$, one $b_{top\text{-}lep}$)
3. **Calculate features** for each set of permutations and **feed into BDT**
4. Select permutation with **highest BDT score**
5. Use selection to **label jets**
6. Calculate **ML observables**



Training

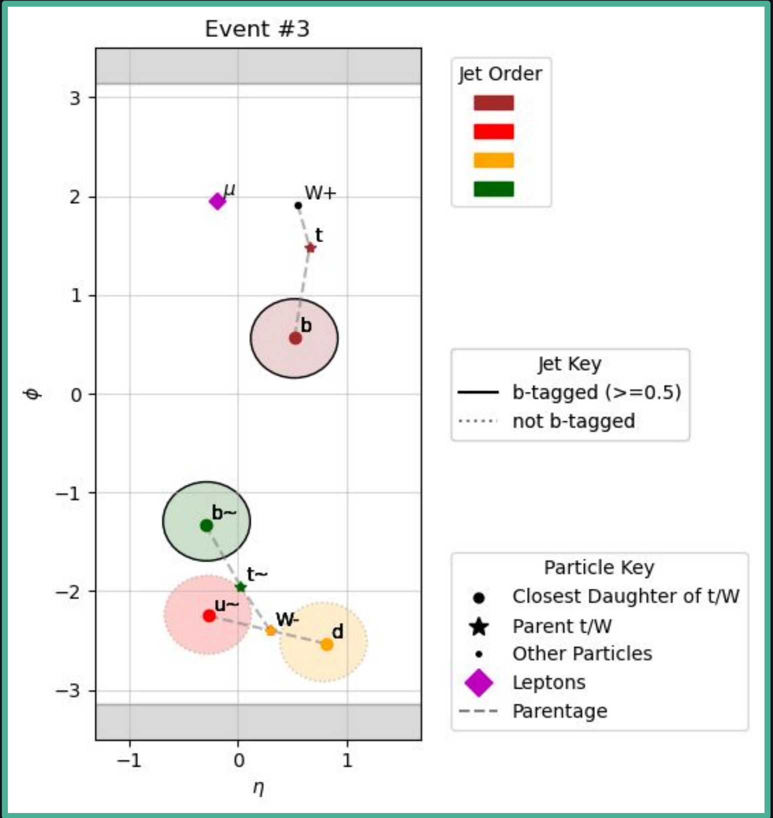

Columnar data
Event selection
Obtain Training Features
Training
Model Storage

Training: Event Selection

Example Event

- ➔ Only look at ttbar MC events
- ➔ Match jets to particles using ΔR matching
- ➔ Find parent particle (either W or top quark)
- ➔ Keep events which are 100% reconstructable

```
nearest_genpart = jets.nearest(genparts, threshold=0.4)
nearest_parent = nearest_genpart.distinctParent  # parent of matched particle
parent_pdgid = nearest_parent.pdgId  # pdgId of parent particle
```



Training: Obtaining Training Features

Python HEP libraries utilized:

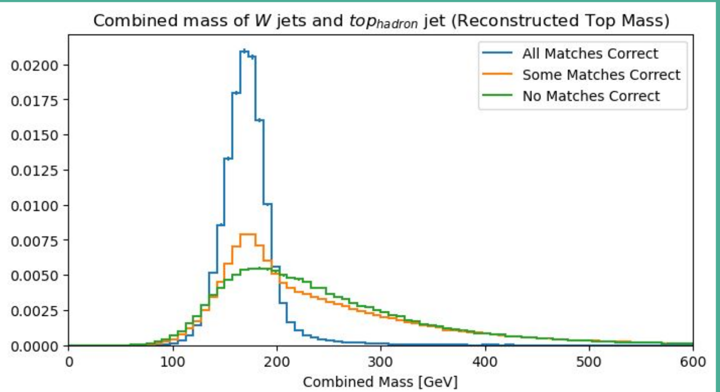
- uproot
- coffea
- awkward

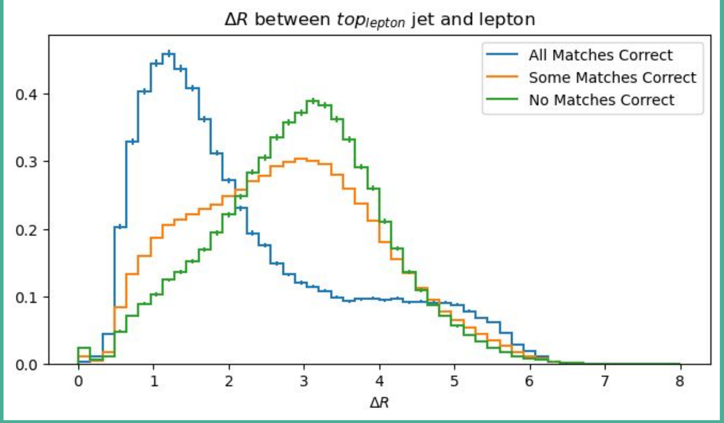
coffea processor with
coffea.nanoevents.NanoAODSchema

use awkward to calculate features

coffea.processor.column_accumulator objects

EXAMPLE FEATURES





Training: Hyperparameter Optimization

mlflow

Set up mlflow on dask workers

Map jobs to workers (each job trains models for each hyperparameter selection)

Number of times to split dataset for cross-validation

```
client = utils.get_client()
client.run(initialize_mlflow)

futures = client.map(fit_model,
                     samples_even,
                     features=features_even,
                     labels=labels_even,
                     evaluation_matrix=evaluation_matrix,
                     n_folds=N_FOLD,
                     mlflowclient=mlflowclient,
                     use_mlflow=USE_MLFLOW,
                     log_models=MODEL_LOGGING)

res = client.gather(futures)
```

Track input hyperparameters

```
mlflowclient.log_param(run_id, param, np.average(value))
```

Track training scores

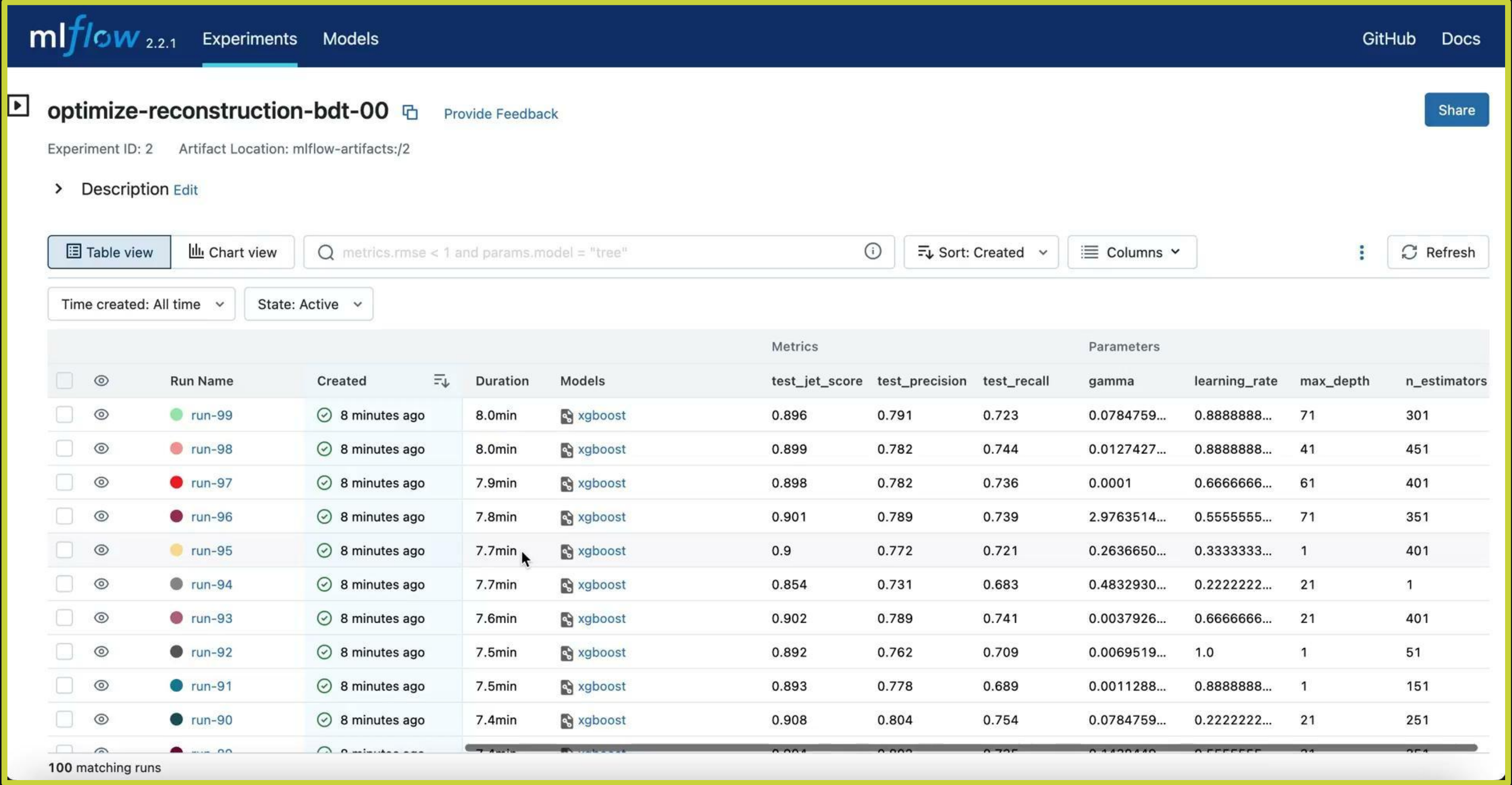
```
mlflowclient.log_metric(run_id, metric, np.average(value))
```

Log resulting model

```
with mlflow.start_run(run_id=run_id, nested=True) as run:
    mlflow.xgboost.log_model(result["model"], "model", signature=signature)
```

For each trial

Training: Hyperparameter Optimization



mlflow 2.2.1 Experiments Models GitHub Docs

optimize-reconstruction-bdt-00 Provide Feedback Share

Experiment ID: 2 Artifact Location: mlflow-artifacts:/2

Description Edit

Table view Chart view metrics.rmse < 1 and params.model = "tree" Sort: Created Columns Refresh

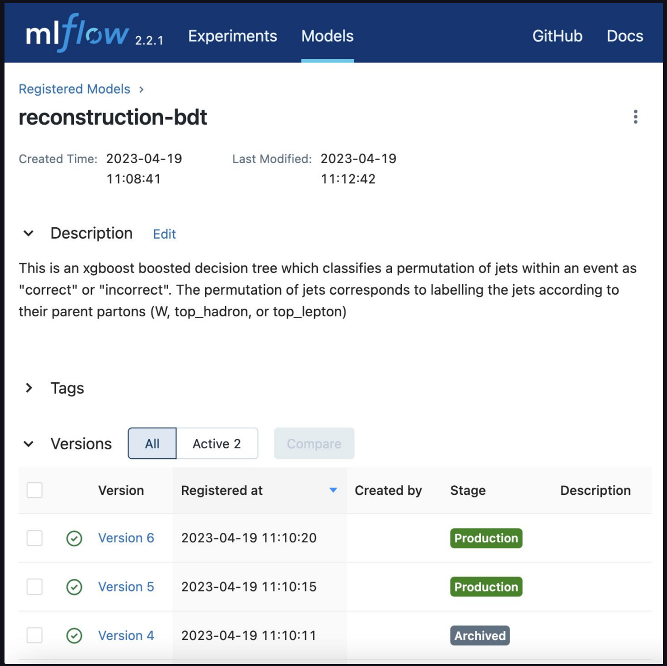
Time created: All time State: Active

				Metrics			Parameters			
Run Name	Created	Duration	Models	test_jet_score	test_precision	test_recall	gamma	learning_rate	max_depth	n_estimators
run-99	8 minutes ago	8.0min	xgboost	0.896	0.791	0.723	0.0784759...	0.8888888...	71	301
run-98	8 minutes ago	8.0min	xgboost	0.899	0.782	0.744	0.0127427...	0.8888888...	41	451
run-97	8 minutes ago	7.9min	xgboost	0.898	0.782	0.736	0.0001	0.6666666...	61	401
run-96	8 minutes ago	7.8min	xgboost	0.901	0.789	0.739	2.9763514...	0.5555555...	71	351
run-95	8 minutes ago	7.7min	xgboost	0.9	0.772	0.721	0.2636650...	0.3333333...	1	401
run-94	8 minutes ago	7.7min	xgboost	0.854	0.731	0.683	0.4832930...	0.2222222...	21	1
run-93	8 minutes ago	7.6min	xgboost	0.902	0.789	0.741	0.0037926...	0.6666666...	21	401
run-92	8 minutes ago	7.5min	xgboost	0.892	0.762	0.709	0.0069519...	1.0	1	51
run-91	8 minutes ago	7.5min	xgboost	0.893	0.778	0.689	0.0011288...	0.8888888...	1	151
run-90	8 minutes ago	7.4min	xgboost	0.908	0.804	0.754	0.0784759...	0.2222222...	21	251

100 matching runs

Training: Model Storage

```python
best_model_path = f'runs:/{best_run_id}/model'
best_model = mlflow.xgboost.load_model(best_model_path)  # load model locally
result = mlflow.register_model(best_model_path, "reconstruction-bdt")  # register best model in mlflow model repository
```



NVIDIA
TRITON INFERENCE SERVER

Training: Model Storage

NVIDIA
TRITON INFERENCE SERVER

```
model_name
├── 1
│   └── xgboost.model
└── config.pbtxt
```

```
name: "reconstruction_bdt_xgb"
backend: "fil"
max_batch_size: 50000000
input [
 {
    name: "input__0"
    data_type: TYPE_FP32
    dims: [ 20 ]
  }
]
output [
 {
    name: "output__0"
    data_type: TYPE_FP32
    dims: [ 2 ]
  }
]
instance_group [{ kind: KIND_GPU }]
parameters [
  {
    key: "model_type"
    value: { string_value: "xgboost" }
  },
  {
    key: "predict_proba"
    value: { string_value: "true" }
  },
]
version_policy: { all { }}
dynamic_batching { }
```

Inference

Columnar data
Event selection, systematic uncertainties
Obtain BDT Input Features
Machine Learning Inference
Histograms
Statistical model building
Workspace
ROOT
JSON
Statistical analysis
Result, diagnostics

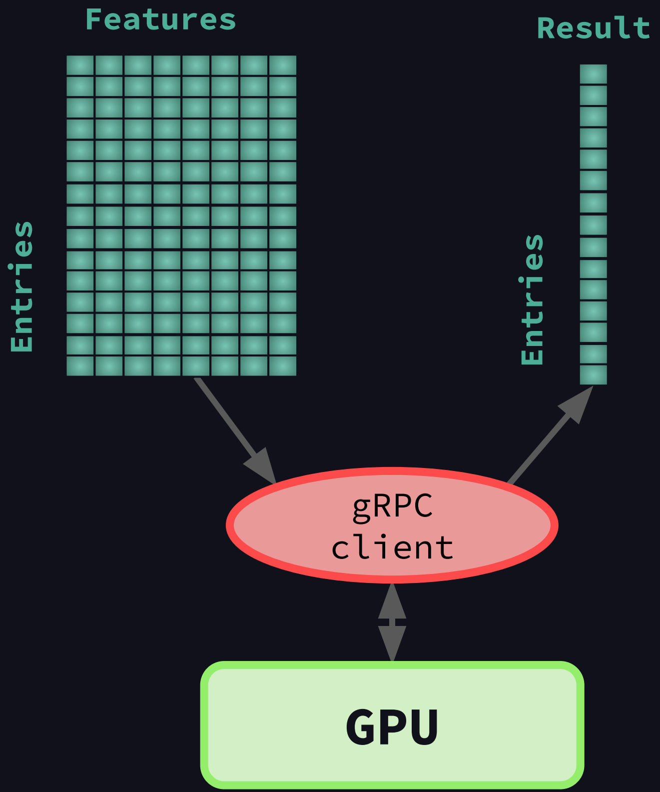
Inference: Machine Learning Inference

1. Set up Triton gRPC client
2. Perform inference request:

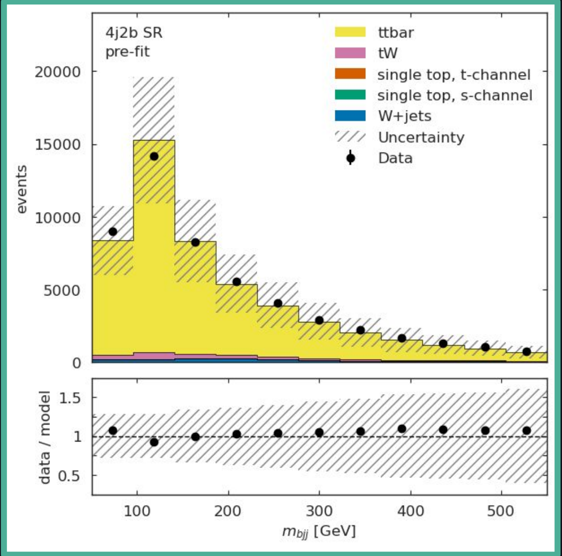
```
output = grpcclient.InferRequestedOutput(output_name)

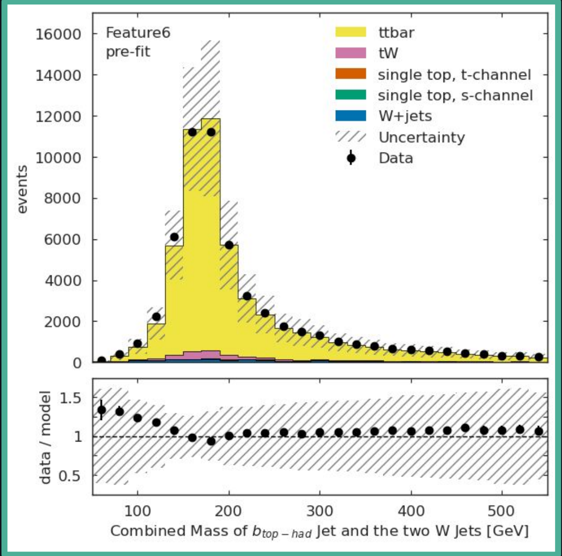
inpt = [grpcclient.InferInput(input_name, features.shape, dtype)]
inpt[0].set_data_from_numpy(features)

results[even_perm]=triton_client.infer(
    model_name=self.model_name,
    model_version=self.model_vers_odd,
    inputs=inpt,
    outputs=[output]
).as_numpy(output_name)[:, 1]
```



Inference: Result, diagnostics





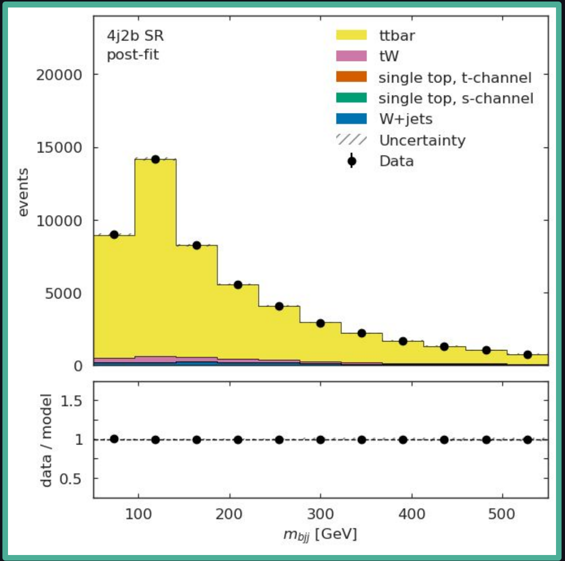
Python HEP libraries utilized:

- cabinetry
- hist

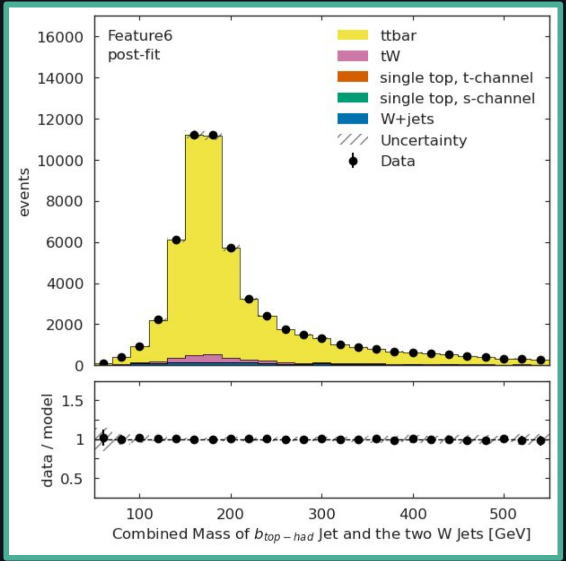
```
model_prediction = cabinetry.model_utils.prediction(model_ml)
fit_results_mod = cabinetry.model_utils.match_fit_results(model_ml, fit_results)
model_prediction_postfit = cabinetry.model_utils.prediction(model_ml, fit_results=fit_results_mod)
```

Inference: Result, diagnostics

Statistical model fit from non-ML approach



Apply fit results to model with ML observables



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model_prediction_postfit = cabinetry.model_utils.prediction(model_ml, fit_results=fit_results_mod)
```

Future Goals

- ➔ Explore more complex ML models
  - ◆ Now that we have the infrastructure in place, we can extend to deep learning approaches
  - ◆ Triton inference server will help a lot here!
- ➔ Benchmarking

Learn more about AGC!

AGC Documentation

Try it yourself!

- Coffea-casa @ UNL
- Elastic Analysis Facility @ Fermilab
- Local Setup

See other AGC talks!

- Physics analysis for the HL-LHC: concepts and pipelines in practice with the Analysis Grand Challenge (Alexander Held)
- Coffea-Casa: Building composable analysis facilities for the HL-LHC (Oksana Shadura)
- Analysis Grand Challenge benchmarking tests on selected sites (David Koch)
- First implementation and results of the Analysis Grand Challenge with a fully Pythonic RDataFrame (Vincenzo Eduardo Padulano)
- I/O performance studies of analysis workloads on production and dedicated resources at CERN (Andrea Sciabà)

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