ML as a Service for HEP

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CMS R&D, IML meetings

Machine Learning as a Service

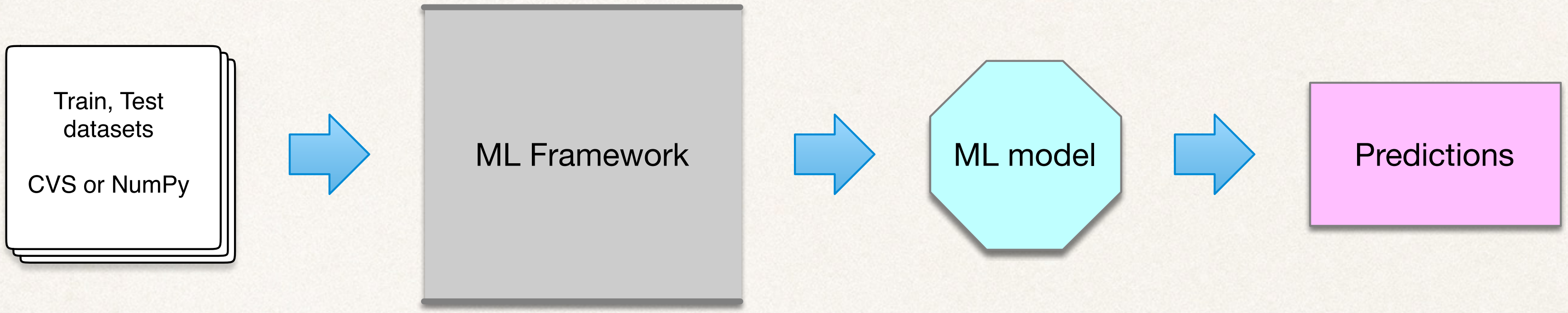
CLOUD MACHINE LEARNING SERVICES COMPARISON

	Amazon ML	Amazon SageMaker*	Azure ML Studio	Google Prediction API	Google ML Engine**
Classification	✓	✓	✓	✓	✓
Regression	✓	✓	✓	✓	✓
Clustering	✗	✓	✓	✗	✓
Anomaly detection	✗	✓	✓	✗	✓
Recommendation	✗	✓	✓	✗	✓
Ranking	✗	✓	✓	✗	✓
Algorithms	unknown	10 built-in + custom available	100+ algorithms and modules	unknown	TensorFlow-based
Frameworks	✗	TensorFlow, MXNet	✗	✗	TensorFlow
Graphical interface	✗	✗	✓	✗	✗
Automation level	high	medium	low	high	low

- MLaaS is a set of tools and services service providers offer to clients to perform various ML tasks, e.g. classification, regression, DeepLearning, etc.
- Tools and services include: data visualization, pre-processing, model training and evaluation, serving predictions, etc.
- Major tech companies (Goolge, Amazon, Microsoft, IBM, etc.) and plethora of start-ups provide different types of MLaaS services.

Can we use existing MLaaS in HEP?

Traditional ML workflow



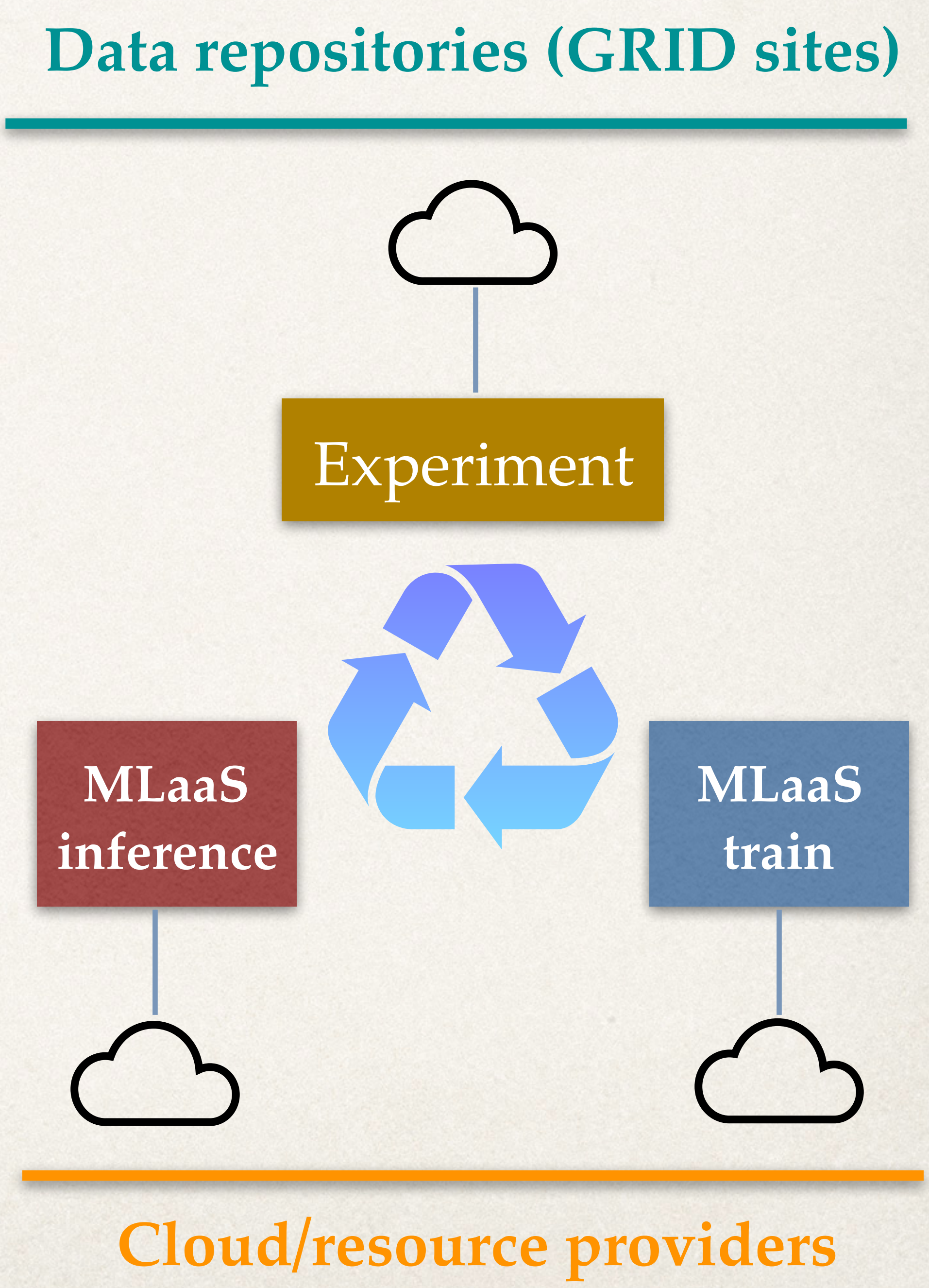
- Traditional ML workflow consists of the following components
  - obtain train, test, validation datasets in tabular (row-wise) data-format, most of the cases ML deal with either CSV or NumPy arrays representing tabular data
  - train ML model and for inference (separation leads towards MLaaS concept)
- Input datasets are usually small, < O(GB) and should fit into RAM of the training node
- HEP datasets may be quite large, at PB scale, they are stored in ROOT data-format, and can be distributed across the GRID nodes
  - **Traditional ML frameworks can't read HEP data in ROOT data-format**
  - **it creates a gap between CS, ML and HEP communities**

ML in HEP

- Training phase:
  - we transform our data from ROOT data-format to CSV/NumPy for training purposes
    - other pre-processing steps can be done at this phase
  - we train our ML models using available ML frameworks, e.g. Python+Keras, TF, PyTorch
  - **we don't use ROOT data directly in ML frameworks**
- Inference phase:
  - we access trained ML models via external libraries integrated into our frameworks, e.g. CMS CMSSW-DNN, ATLAS LTNN libraries, etc.
    - R&D for specialized solutions to speed-up inference on FPGAs, e.g. HLS4ML, SonicCMS, etc.
  - **Resource utilization constrained by run-time, can't be used outside framework language (C++)**
- **Does these approaches sufficient?**

Step towards MLasS for HEP

- MLaaS for HEP should provide the following:
  - **natively read HEP data,** e.g. be able to read ROOT files from local or remote distributed data-sources
  - **utilize heterogeneous resources**, local CPU, GPUs, farms, cloud resources, etc.
  - **use different ML frameworks** (TF, PyTorch, etc.)
  - **minimize infrastructure changes**, should be able to use it in different frameworks, inside or outside framework boundaries
  - **serve pre-trained HEP models**, à la model repository, and access it easily from any place, any code, any framework



ML as a Service for HEP R&D

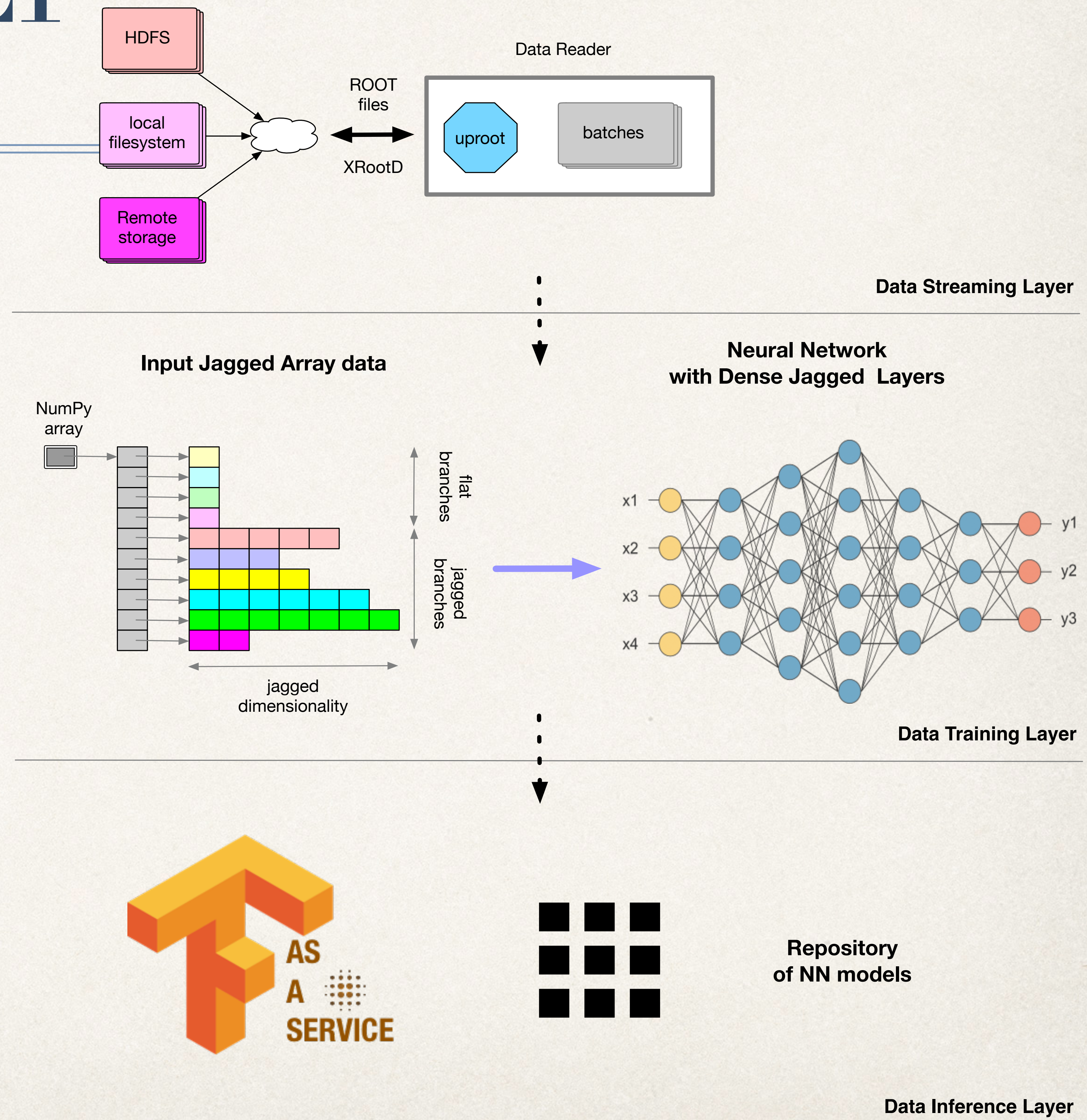
- Data streaming and training tools: github.com/vkuznet/MLaaS4HEP
- Data inference tools: github.com/vkuznet/TFaaS

Goal:

- *be able to read arbitrary size dataset(s) from ROOT files*
- *be able to plug ROOT data into existing ML frameworks*
- *be able to access pre-trained models anywhere*

MLaaS for HEP

- **Data Streaming Layer** is responsible for local or remote data access of HEP ROOT files
- **Data Training Layer** is responsible for feeding HEP ROOT data into existing ML frameworks
- **Data Inference Layer** provides access to pre-trained HEP model for HEP users
- All three layers are independent from each other and allow independent resource allocation



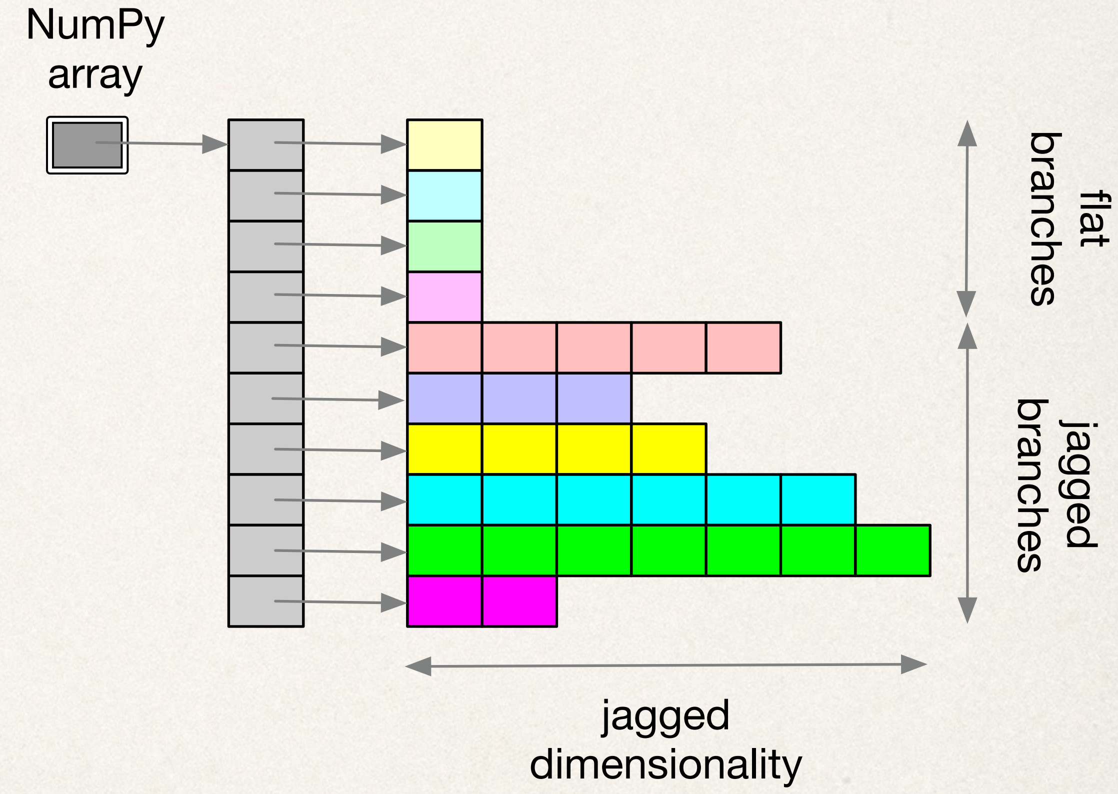
Data Streaming Layer

BETA

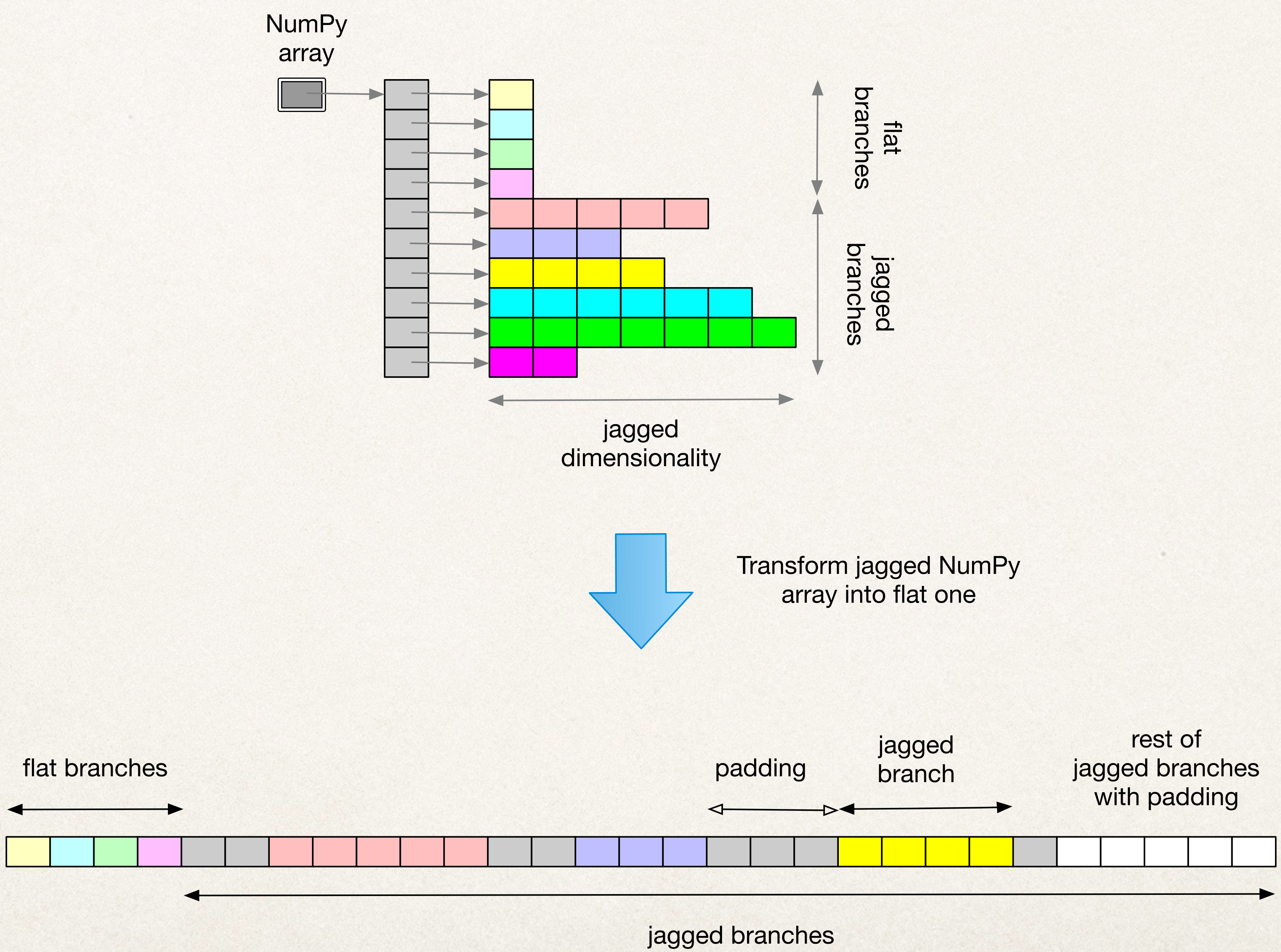
- Recent development of DIANA-HEP uproot ROOT I/O library provides ability to read ROOT data in Python, access them as NumPy arrays, and implements XrootD access
- Now we're able to access ROOT files via XrootD protocol in C++, Python and Go
- MLaaS4HEP extends uproot library and provide APIs to read local and remote distributed ROOT files and feed them into existing ML frameworks
  - the DataReader and DataGenerator wrappers were created to read local or remote ROOT files and deliver them upstream as batches
    - random reads from multiple files are also supported (data shuffle mode)
  - the ROOT data are read and represented as Jagged Arrays
    - we explored both vector and matrix representations, see next slides

Data Training Layer, part I **R&D**

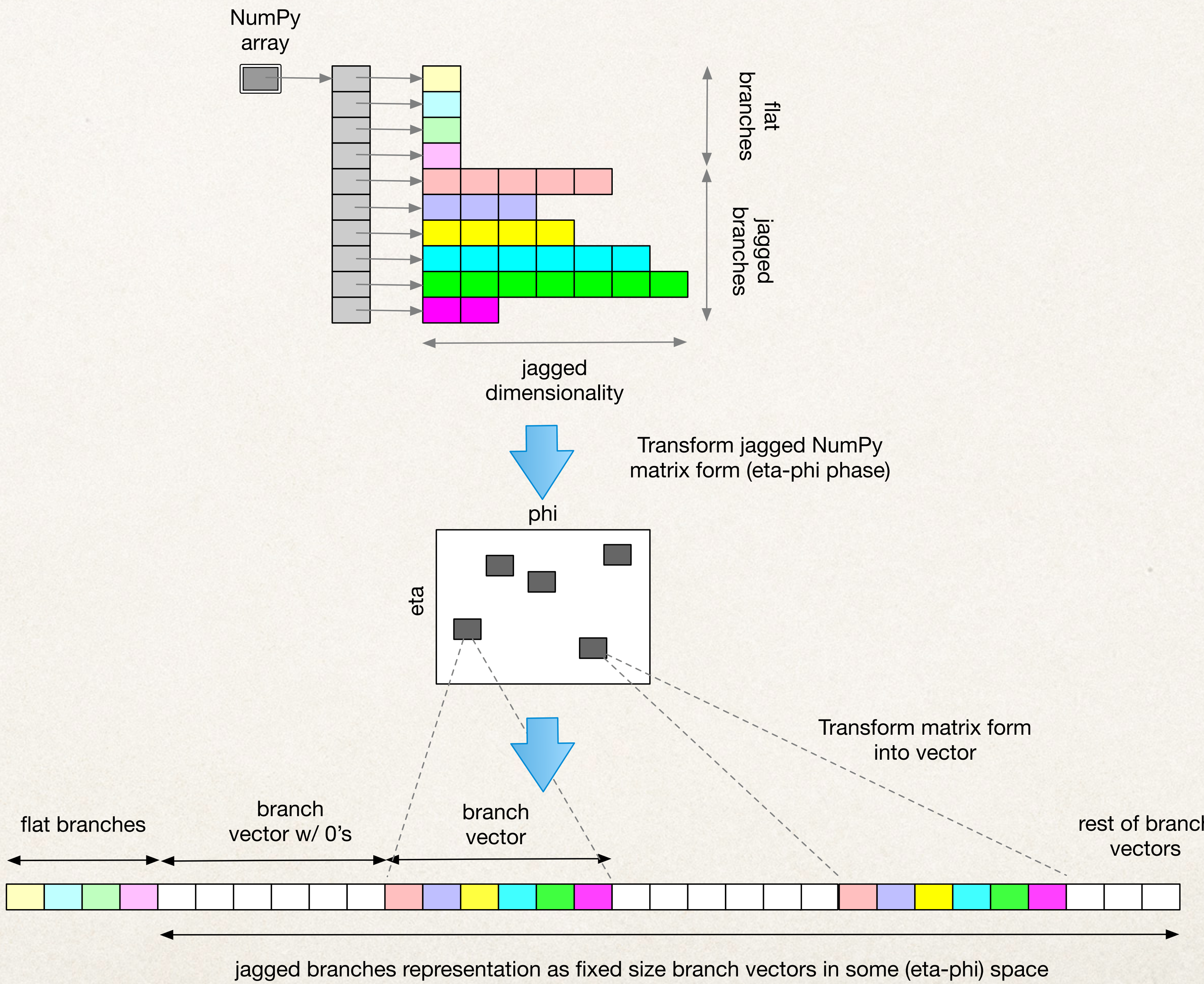
- We can read ROOT files via uproot
- Each event is a composition of flat and jagged arrays
- Usually flat arrays size is less then jagged ones
- Such data representation is not directly suitable for ML (dynamic dimension of jagged arrays across events) and should be flatten to fixed size inputs
- To feed these data into ML two-step procedure is required:
    - obtain dimensionality of jagged arrays
    - flatten jagged array into fixed size array



Data transformation (vector wise)



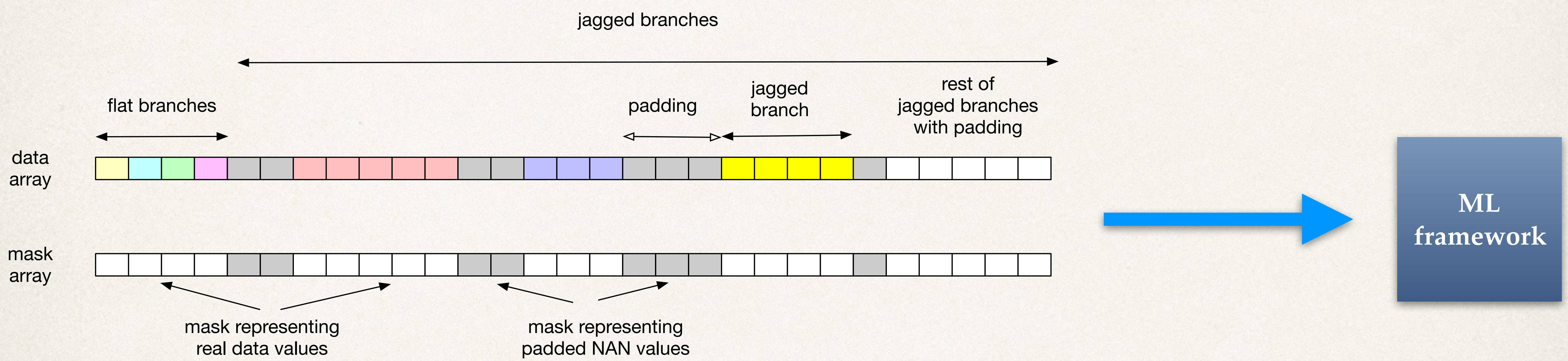
Data transformation (matrix wise)



ML and Jagged Arrays

- In order to use ML we need to resolve how to treat Jagged Array input
  - as array with padding values via vector-wise transformation
    - need to know up-front dimensionality of every jagged array attribute (pre-processing step)
    - padding values should be assigned as NANs since all other numerical values can represent attribute spectrum
  - as a large sparse array via matrix-wise transformation
    - need to choose granularity of matrix cells
    - need to choose a view transformation (X-Y, eta-phi, etc.)
    - it is possible to have collisions in a cell from different jagged array attributes which happen to have the same cell coordinate (can be resolve via multi-dimensional matrix representation, e.g. combining X-Y, Y-Z and Z-X views)

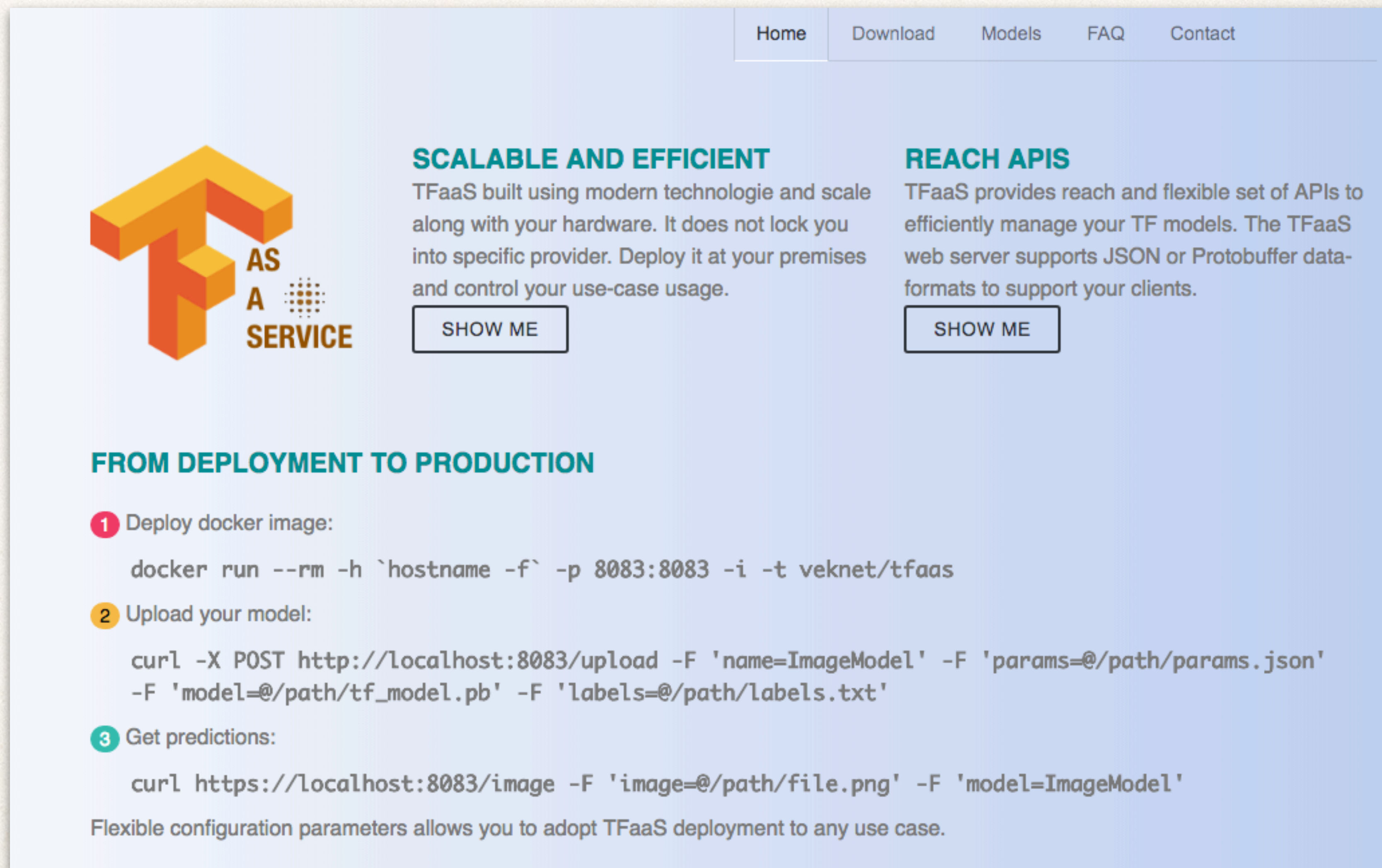
Data Training Layer, part II R&D



- Keep data array with paddings (NaNs) and mask array with their locations
  - mask array may be useful when training AutoEncoder type models where we can use mask array to cast padded values after the decoding the data
- Either adjust ML framework or handle data accordingly for existing ML frameworks
  - write a wrapper for existing ML framework to deal with two input arrays, e.g. for training NN models we can assign NaNs to zeros to handle **W**x**X** multiplications

Data Inference Layer

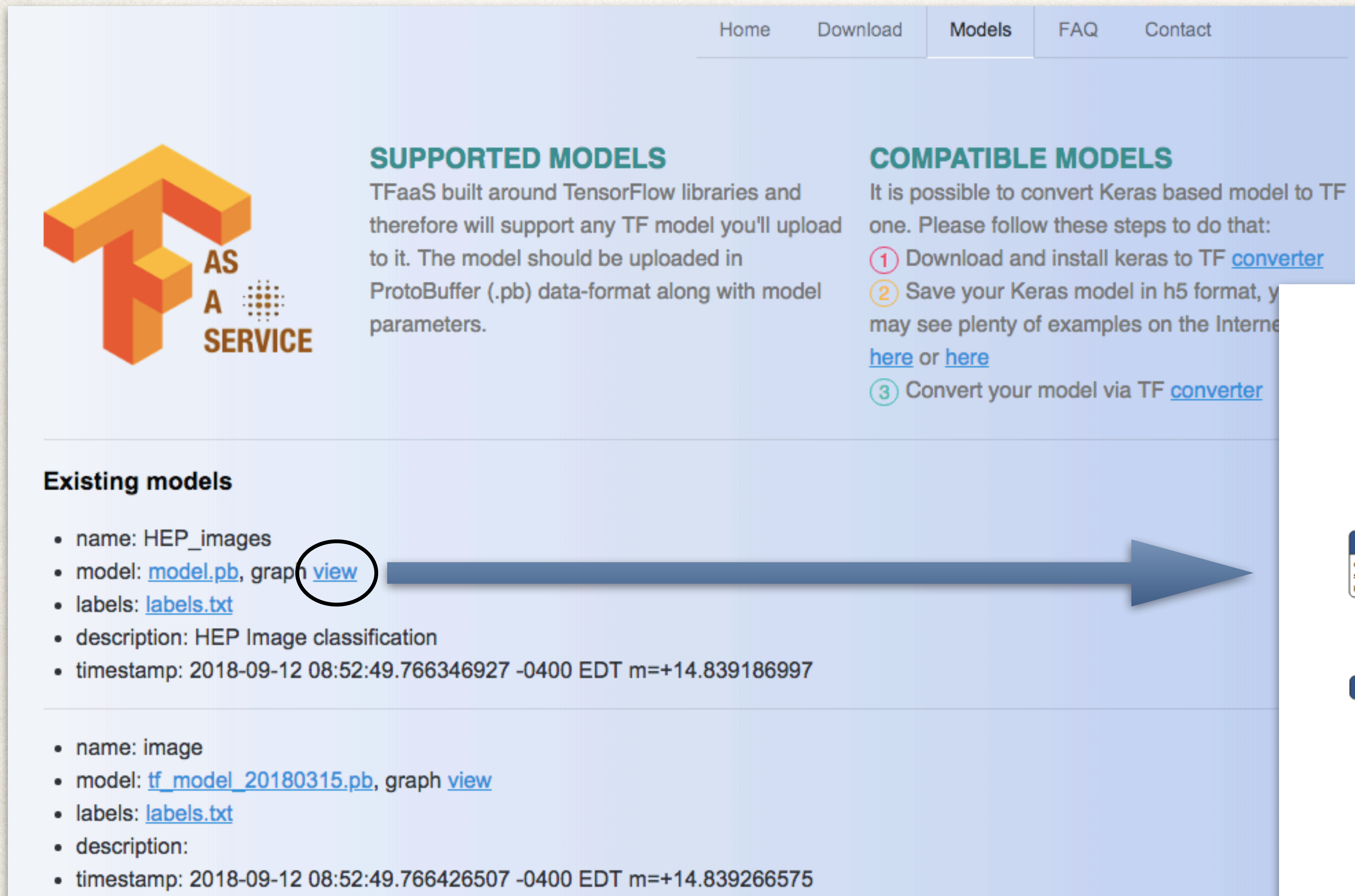
- Data Inference Layer is implemented as TensorFlow as a Service (TFaaS)
- Capable of serving any TensorFlow models
- Can be used as global repository of pre-trained HEP models
- Can be deployed everywhere
  - Docker image and Kubernetes files are provided
  - TFaaS is available as part of DODAS (Dynamic On Demand Analysis Service)



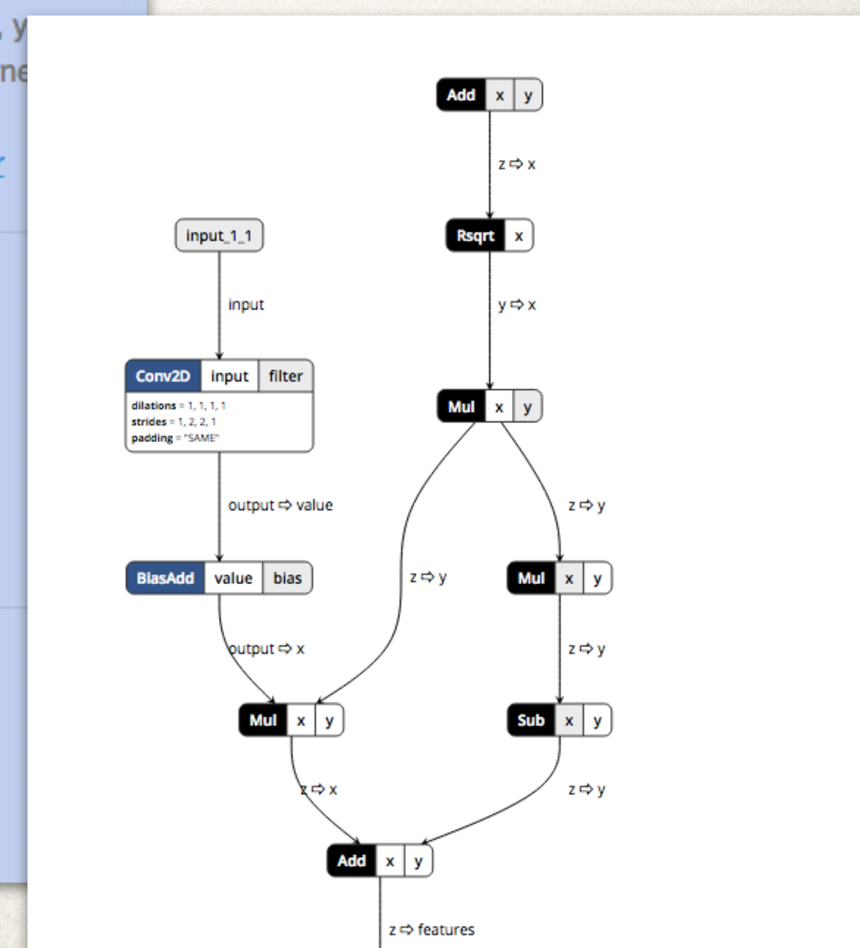
TFaaS features

- HTTP server written in Go to serve **arbitrary** TF model(s) using Google Go TF APIs
  - users may upload **any number** of TF models, models are stored on local filesystem and cached within TFaaS server
  - TFaaS repository provides instructions/tools to convert Keras models to TF
  - TFaaS supports JSON and ProtoBuffer data-formats
- Any client supporting HTTP protocol, ***e.g. curl, C++ (via curl library or TFaaS C++ client), Python***, can talk to TFaaS via HTTP end-points
  - C++ client library talks to TFaaS using ProtoBuffer data-format, all others use JSON
- Benchmarks: 200 concurrent calls, throughput **500 req/sec** for TF model with 1024x1024 hidden layers
  - performance are similar to JSON and ProtoBuffer clients

Model inspection



Integrated Netron model viewer



TFaaS HTTP end-points

- **/json**: handles data send to TFaaS in JSON data-format, e.g. you'll use this API to fetch predictions for your vector of parameters presented in JSON data-format (used by Python client)
- **/proto**: handlers data send to TFaaS in ProtoBuffer data-format (user by C++ client)
- **/image**: handles images (png and jpg) and yields predictions for given image and model name
- **/upload**: upload your TF model to TFaaS
- **/delete**: delete TF model on TFaaS server
- **/models**: return list of existing TF models on TFaaS
- **/params**: return list of parameters of TF model
- **/status**: return status of TFaaS server

Python client

- **upload** API lets you upload your model and model parameter files to TFaaS

```
tfaas_client.py --url=url --upload=upload.json # upload.json contains model parameters
```

- **models** API lets you list existing models on TFaas server

```
tfaas_client.py --url=url --models
```

- **delete** API lets you delete given model on TFaaS server

```
tfaas_client.py --url=url --delete=ModelName
```

- **predict** API lets you get prediction from your model and your given set of input parameters

```
# input.json: {"keys":["attr1", "attr2", …], "values": [1,2,…]}
tfaas_client.py --url=url --predict=input.json
```

- **image** API provides predictions for image classification (supports jpg or png data-formats)

```
tfaas_client.py --url=url --image=/path/file.png --model=HEPImageModel
```

C++ client

CMS BuildFile.xml

```
<use name="protobuf"/>
<lib name="curl"/>
<lib name=“protobuf"/>
```

```cpp
#include <iostream>
#include <vector>
#include <sstream>
#include “TFClient.h”                                   // part of TFaaS repository

int main() {                                            // main function
    std::vector<std::string> attrs;                     // define vector of attributes
    std::vector<float> values;                          // define vector of values
    auto url = “http://localhost:8083/proto”;          // define your TFaaS server URL
    auto model = “MyModel";                             // name of your model in TFaaS

    // fill out your data
    for(int i=0; i<42; i++) {                           // the model I tested had 42 parameters
        values.push_back(i);                            // create your vector values
        std::ostringstream oss;
        oss << i;
        attrs.push_back(oss.str());                     // create your vector headers
    }

    // make prediction call
    auto res = predict(url, model, attrs, values); // get predictions from TFaaS server
    for(int i=0; i<res.prediction_size(); i++) {
        auto p = res.prediction(i);                     // fetch and print model predictions
        std::cout << "class: " << p.label() << " probability: " << p.probability() << std::endl;
    }
}
```

TFaaS: use cases

- TFaaS provides access to TF models independently from framework and infrastructure
  - easy to integrate into existing workflow, e.g. Python or C++ or any other (via HTTP protocol)
  - C++ client library can be used to integrate within C++ framework, based on curl and protobuf libraries
- Rapid development or continuous training of TF models and their validation
  - clients can test multiple TF models at the same time
- TFaaS can be used as repository of pre-trained HEP TF models
- TFaaS deployment is trivial (via docker) and you can setup your TFaaS server at your premises, e.g. on your local hardware or at a cloud provider (tested with DODAS) or as k8s deployment
- Can be used in distributed environment, i.e. clients can connect to TFaaS server(s) via HTTP

MLaaS for HEP proof-of-concept

- Train toy models in PyTorch and TF (via Keras) using CMS NANOAOD data
  - run code locally on laptop, lxplus and GPU node
  - access data from local or remote ROOT files
- Serve model in TFaaS server deployed at CERN k8s cluster

MLaaS workflow w/ user models

PyTorch example

```python
from jarray.pytorch import JaggedArrayLinear
import torch

def model(idim):
    "Simple PyTorch model for testing purposes"
    model = torch.nn.Sequential(
        JaggedArrayLinear(idim, 5),
        torch.nn.ReLU(),
        torch.nn.Linear(5, 1),
    )
    return model
```

Keras/TF example

```python
from keras.models import Sequential
from keras.layers import Dense, Activation

def model(idim):
    "Simple Keras model for testing purposes"

    model = Sequential([
        Dense(32, input_shape=(idim,)),
        Activation('relu'),
        Dense(2),
        Activation('softmax'),
    ])
    model.compile(optimizer='adam',
                  loss='categorical_crossentropy',
                  metrics=['accuracy'])
    return model
```

```
./workflow.py —files=files.txt —model=<model.py> —params=params.json
```

MLaaS workflow | **Input ROOT files** | **User model** | **MLaaS parameters**

Read remote ROOT file **Init ML model** **Perform train cycle**

```
<__main__.DataGenerator object at 0x1137c85d0> [09/Oct/2018:15:21:06] 1539112866.0
model parameters: {"hist": "pdfs", "verbose": 1, "exclude_branches": "", "batch_size": 256, "selected_branches": "", "ep
ochs": 50, "branch": "Events", "chunk_size": 1000, "nevts": 3000, "redirector": "root://cms-xrd-global.cern.ch"}
Reading root://cms-xrd-global.cern.ch//store/data/Run2018C/Tau/NANOAOD/14Sep2018_ver3-v1/60000/6FA4CC7C-8982-DE4C-BEED-C
90413312B35.root
+++ first pass: 2877108 events, (720-flat, 232-jagged) branches, 2560 attrs
<reader.DataReader object at 0x116e97490> init is complete in 0.00181102752686 sec
init DataReader in 21.474189043 sec

TFaaS read from 0 to 1000
# 1000 entries, 955 branches, 3.8979845047 MB, 33.7647099495 sec, 0.115445520205 MB/sec, 85.2105054154 kHz
### input data: 2560
Sequential(
  (0): JaggedArrayLinear(in_features=2560, out_features=5, bias=True)
  (1): ReLU()
  (2): Linear(in_features=5, out_features=1, bias=True)
)
x_train chunk of (1000, 2560) shape
x_mask chunk of (1000, 2560) shape
preds chunk of (1000, 1) shape

TFaaS read from 1000 to 2000
# 1000 entries, 955 branches, 3.87852573395 MB, 93.1551561356 sec, 0.0416351160241 MB/sec, 30.8851181121 kHz
x_train chunk of (1000, 2560) shape
x_mask chunk of (1000, 2560) shape
preds chunk of (1000, 1) shape

TFaaS read from 2000 to 3000
# 1000 entries, 955 branches, 3.90627861023 MB, 24.3904368877 sec, 0.1601561558 MB/sec, 117.96049465 kHz
x_train chunk of (1000, 2560) shape
x_mask chunk of (1000, 2560) shape
preds chunk of (1000, 1) shape
```

Read another ROOT file

```
Reading root://cms-xrd-global.cern.ch//store/data/Run2018C/Tau/NANOAOD/14Sep2018_ver3-v1/60000/282E0083-6B41-1F42-B665-9
73DF8805DE3.root
+++ first pass: 368951 events, (720-flat, 232-jagged) branches, 2560 attrs
<reader.DataReader object at 0x1182cfd50> init is complete in 0.00151491165161 sec
init DataReader in 6.09789299965 sec
```

Perform another train cycle

```
TFaaS read from 1000 to 2000
# 1000 entries, 955 branches, 4.16557407379 MB, 61.9209740162 sec, 0.0672724248928 MB/sec, 5.9584172546 kHz
x_train chunk of (1000, 2560) shape
x_mask chunk of (1000, 2560) shape
preds chunk of (1000, 1) shape
```

Benefits of MLaaS approach

- Clear separation of streaming, training and inference layers
  - dynamically and independently scale resources for training and inference layers
- Hide complexity of data transformation from ROOT I/O to ML
  - user data-transformation can be dynamically loaded using user based functions
- Ability to use ML framework of your choice
  - R&D work towards model transformation from one framework to another
- Inference results can accessible via HTTP protocol
  - new models can be uploaded and used immediately without changes of existing infrastructure
  - can be used as a global repository of HEP pre-trained models shared across experiment boundaries

Summary: MLaaS training

- MLaaS training layer is capable of reading remote ROOT files
- Data transformation from Jagged Array representation to vector form
- Random reads from multiple files (data shuffle mode)
- Customization: total number of events to read; data read chunk size; select or exclude branches to read, choice of XrootD redirector
- Dynamically load user based models
- **Planning:** dynamically load user based pre-processing functions; visual inspection of ROOT file content (via go-hep/groot); possible graphical UI to build full workflow pipeline (via go-hep/groot); perform tests as part of DODAS infrastructure

Summary: TFaaS inference

- TFaaS server natively supports concurrency, it organizes TF models in hierarchical structure on local file system, and it uses cache to serve TF models to end-users
    - no integration is required to include TFaaS into your infrastructure, i.e. clients talks to TFaaS server via HTTP protocol (python and C++ clients are available)
    - allow separation TF models from experiment framework, do not use experiment framework run-time resources, dedicated resources can be used to scale TFaaS
    - can be used as model repository, TFaaS architecture allows to implement model versioning, tagging, …
- TFaaS server was tested with concurrent clients, we obtained 500 req/sec throughput for mid-size model inference (subject of TF model complexity)
- TFaaS docker image and k8s deployment files are available

Summary

- MLaaS for HEP is a feasible and we demonstrated fully functional proof-of-concept workflow
- MLaaS4HEP repository:
  - **Data Streaming Layer** responsible for remote access to distributed ROOT files and capable of streaming ROOT data via uproot ROOT I/O to upstream layers
  - **Data Training Layer** provides necessary data transformation and batch streaming to existing ML frameworks. The main problem is understanding how to deal with Jagged Array in context of ML framework
- TFaaS repository (non HEP specific):
  - **Data Inference Layer**: serves TF models via Go HTTP server and Google TF Go APIs
    - ready to use (docker or k8s), provides basic TF model repository functionality

Collaboration is welcome

https://arxiv.org/abs/1811.04492

R&D topics

- Model conversion: PyTorch, fast.ai, etc. to TensorFlow
- Model repository: implement persistent model storage, look-up, versioning, tagging, etc.
- MLaaS/TFaaS scalability: explore kubernetes, auto-scaling, resource provisioning (FPGAs, GPUs, TPUs, etc.)
- Real model training model with distributed data (MLaaS with DODAS)