

Data Quality in ML Pipelines





Agenda



- Defining the problem of Data Quality
- What can we do about it?
- What have we done about it?
- What still remains?

Data Quality: An Analogy

To have a smooth and safe trip,
all travelers must have:

- Identifying documents
- Boarding Pass with group
- Go through security
- Stay with their traveling party



Implementation by Analogy

Physical World	Machine Learning
A trip	ML Pipeline
Passport	Example Identifier + value of feature
Boarding Group	Split
Population Demographics	Statistics (The Shadow)
Description of traveling party	Schema
Traveling Party	Example
Luggage Tag	DQ Features
Security Check	The Prism
Check in	Transformed Features
Population	Entire Dataset (The Sun)
Sub-population	Subset (The beam)



UUID
FR201066781985627

Data Quality Challenges in ML Pipelines

- The data is in the pipeline. We are outside the pipeline.
- The data can be very large and messy
- Variety of formats to deal with at different stages
- Hard to see connection between data and its effect on models
- Good data is hard to find: > 85% of the effort/code is not actually machine learning, it is data processing

How Beam can help

Beam speaks a thousand formats. No data is outside of Beam's reach.

Beam + TFX reduce the surface area of skills required to do professional grade machine learning.

Beam, with its ability to execute user defined functions (UDFs) on behalf of the user, can reduce the burden of data processing at scale while abstracting the complexity away.

TFX, with its component architecture, can manage the end-to-end trip, using Beam wherever distributed computation is appropriate.

ML Metadata helps us open up the pipeline, without spilling a drop of data. Squeaky clean!

How Beam Can Help with Data Quality for ML

Step	How Beam Helps	Specifics
Pre-Ingestion	Determine Schema for Data	Schema Generator
Data Splitting & Identification	Deterministic Data Splitting at Scale	PartitionDoFn
Data Ingestion	Encoding Data at scale	ExampleGen (Standard)
Data Profile	Statistics	StatisticsGen (Standard)
Data Exploration	Produce JSON from TFRecord	JSONSampler
Non-graph intended feature injection	Apply Arbitrary Python UDFs	PreTransform
Filter	Remove examples which do not meet DQ requirements	FilterUDF

Schema aware PCollections simplify data processing and quality greatly.

Computing a schema, using all of the data, can be computationally difficult

With beam python sdk, you can process each element as a string, and use functions such as `yaml.safe_load(element)` to determine type of element

You can then compute a rough schema that you can tune

```
(2, [('str', 100001)])
(3, [('float', 97924), ('int', 2076), ('str', 1)])
(5, [('NoneType', 1), ('str', 1), ('int', 2082), ('float', 97917)])
(1, [('str', 1), ('int', 16213), ('float', 83787)])
(0, [('datetime.datetime', 100000), ('str', 1)])
(7, [('str', 1), ('int', 100000)])
(4, [('float', 97935), ('str', 1), ('int', 2065)])
(6, [('str', 1), ('NoneType', 1), ('int', 2065), ('float', 97934)])
(3, {'name': ['pickup_longitude'], 'schema': [('float', False)]})
(6, {'name': ['dropoff_latitude'], 'schema': [('float', True)]})
(7, {'name': ['passenger_count'], 'schema': [('int', False)]})
(0, {'name': ['key'], 'schema': [('datetime.datetime', False)]})
(1, {'name': ['fare_amount'], 'schema': [('float', False)]})
(5, {'name': ['dropoff_longitude'], 'schema': [('float', True)]})
(2, {'name': ['pickup_datetime'], 'schema': [('str', False)]})
(4, {'name': ['pickup_latitude'], 'schema': [('float', False)]})
from typing import NamedTuple, Optional
import datetime
class MyRecord(NamedTuple):
    key: datetime.datetime
    fare_amount: float
    pickup_datetime: str
    pickup_longitude: float
    pickup_latitude: float
    dropoff_longitude: Optional[float]
    dropoff_longitude_missing: float
    dropoff_latitude: Optional[float]
    dropoff_latitude_missing: float
    passenger_count: int
```


Data Splitting & Identification

For non time series data, you can do deterministic splitting using hashing algorithms if applicable.

For temporal data, you can use spans in ExampleGen in TFX

Or, you can use beam.Partition

You can use a DoFn if you want to add in other information, such as a deterministic UUID, missing feature indicators, split information

Ideally, the uuid integrates split information.

Here we do beam based approximate quantiles unless user provides split point. Use a compiled language like Go to determine split point under a minute.

```
split_point_object = MyRecordWithUUID(
    key=datetime.datetime(
        2012, 6, 2, 20, 43, tzinfo=datetime.timezone.utc),
    fare_amount=15.7, pickup_datetime='2012-06-01 14:23:00 UTC',
    pickup_longitude=-73.988975, pickup_latitude=40.750348,
    dropoff_longitude=-73.96391, dropoff_longitude_missing=0.0,
    dropoff_latitude=40.799752, dropoff_latitude_missing=0.0,
    passenger_count=1, internal_sequence=1338560580,
    uuid='85bb164805a8658d5e548513143aaea4')
data_split = (
    parsed_timestamped_pcollection
    | "PartitionData" >> beam.ParDo(
        PartitionDoFn(fixed_threshold=split_point_object),
        threshold_from_side_input=split_threshold_side_input_view
    ).with_outputs('train', 'eval')
)

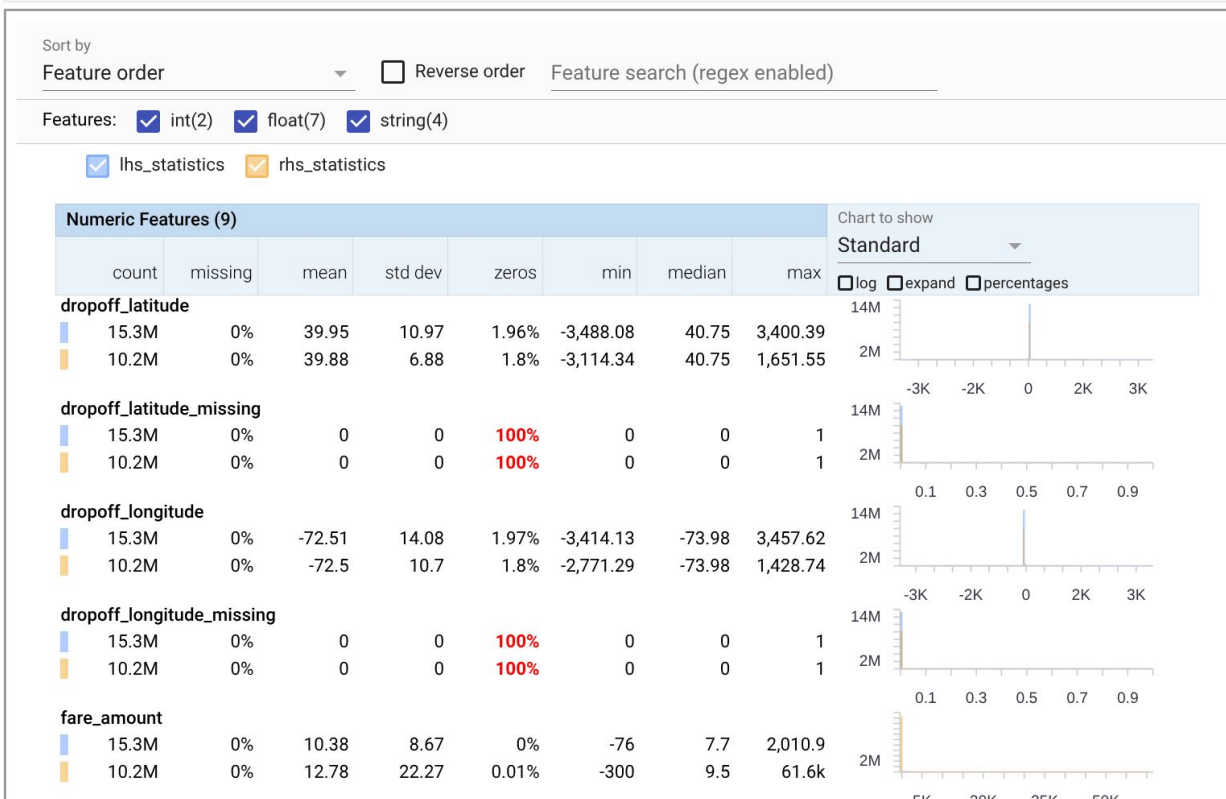
def _generate_uuid(data_dict: dict, keys_for_hashing: list) -> str:
    hasher = hashlib.sha1()
    for k in sorted(keys_for_hashing):
        field_val_str = str(data_dict.get(k, ''))
        hasher.update(field_val_str.encode('utf-8'))
    return uuid.UUID(bytes=hasher.digest()[:16]).hex
```

```
example_uuid = _generate_uuid(converted_dict,
                               original_keys_in_obj)
return obj(**converted_dict), example_uuid
```

real	13m14.998s
user	242m20.128s
sys	1m29.149s

Data Exploration: The Shadow

```
display_statistics(oldest_statistics)
```



Data Exploration: The Beam

The statistics are the shadow, and the talk is about data quality “in” ML pipelines. We have to go inside the pipeline.

This means going from `tf.train.Examples` to JSON or similar, and possibly sampling.

We can use the schema computed in the TFX pipeline to create a `NamedTuple` object dynamically, and plug in to Schema Aware PCollections. This is the heart of the `Executor` in `JSONSampler`

The json versions come from `tf.train.Examples`, and are fully tracked from an ML Metadata perspective

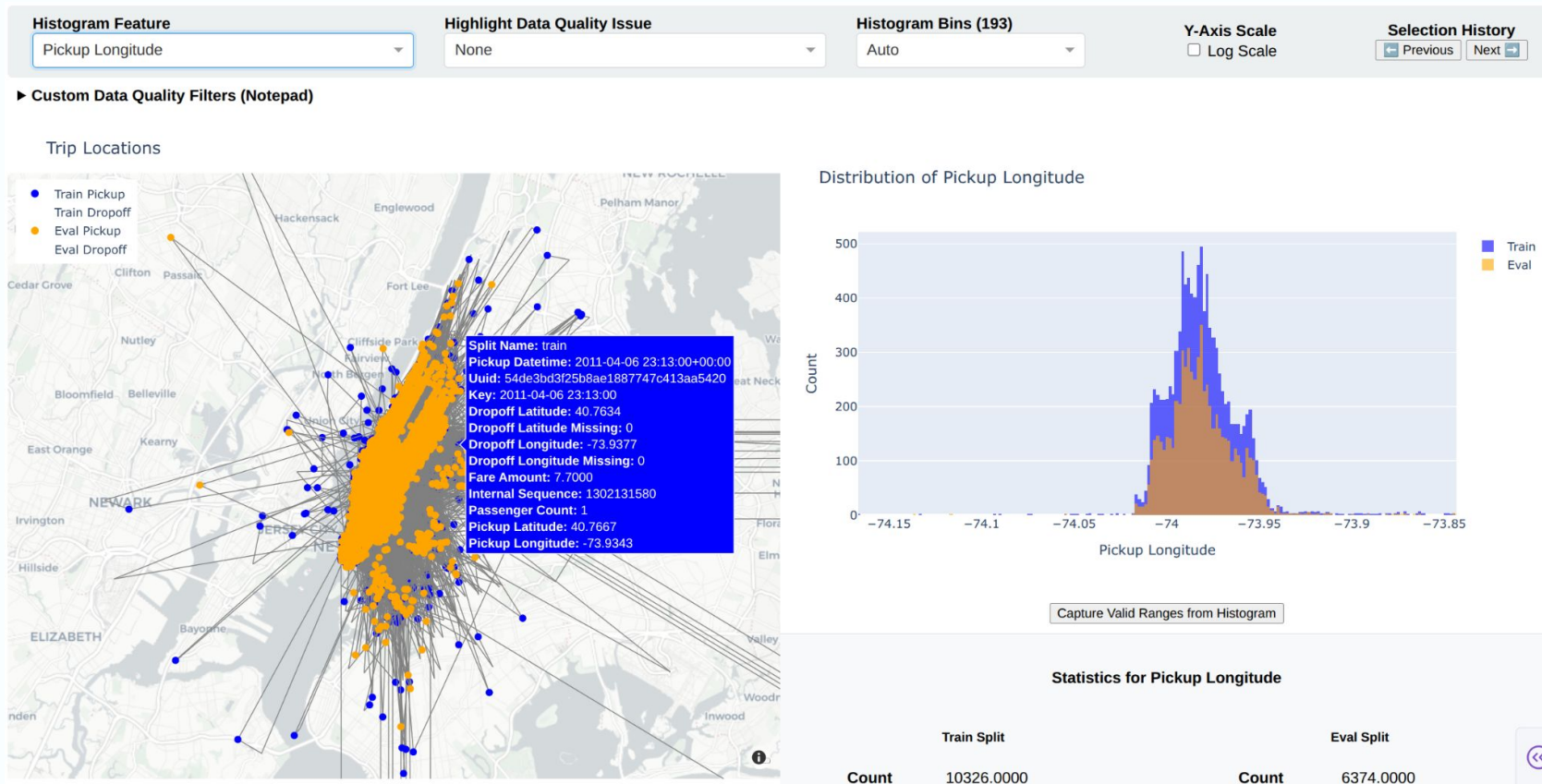
```
json_sampler = JSONSampler(examples=example_gen.outputs['examples'],
                           schema=schema_gen.outputs['schema'],
                           statistics=statistics_gen.outputs['statistics'],
                           sample_percent=0.25)

local_component_list = [
    example_gen,
    statistics_gen,
    schema_gen,
    example_validator,
    json_sampler,
]

from typing import NamedTuple
def NamedTupleGenerator(class_name, schema):
    name_type_tuples = [(f.name, f.type) for f in schema.feature]
    proto_dictionary = {}
    for feature_name, feature_type_int in name_type_tuples:
        if feature_type_int == 3:
            proto_dictionary[feature_name] = 1.0
        elif feature_type_int == 2:
            proto_dictionary[feature_name] = 1
        elif feature_type_int == 1:
            proto_dictionary[feature_name] = ""
        else:
            raise NotImplementedError
    TupleClass = NamedTuple(class_name, [(k, type(v)) for k, v in proto_dictionary.items()])
    return TupleClass
NTObject = NamedTupleGenerator("NTObject", schema)
beam.coders.registry.register_coder(NTObject, beam.coders.RowCoder)

[utM] In [21]: [j.uri for j in store.get_artifacts_by_type('JSONSampler')]
Out[21]:
['/home/pdodeja/experiments/fareamount_original/pipeline/JSONSampler/json_sampler/5',
 '/home/pdodeja/experiments/fareamount_original/pipeline/JSONSampler/json_sampler/11',
 '/home/pdodeja/experiments/fareamount_original/pipeline/JSONSampler/json_sampler/18']
```

Data Exploration: The Beam and the Shadow



We inject data quality indicators, `_dq` features, by interacting with statistics & sample data

Data Exploration: Designing the Prism

▼ Custom Data Quality Filters (Notepad)

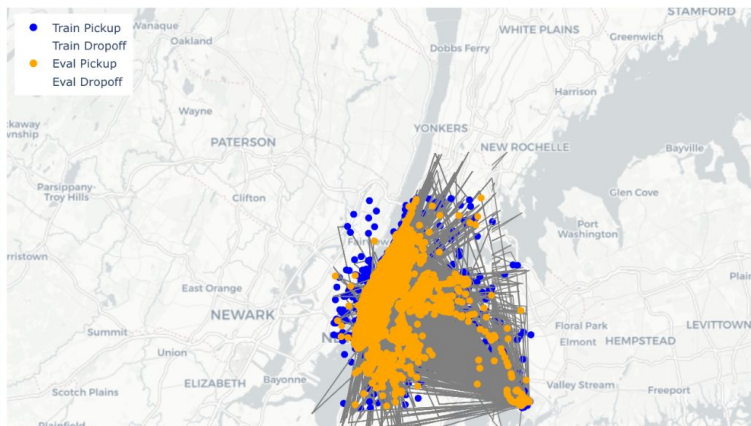
Get Python Equivalent

```
new_element['dropoff_latitude_dq'] = int(40.58639144897461 <= element['dropoff_latitude'] <= 40.9129753112793)
new_element['dropoff_longitude_dq'] = int(-74.0776596069336 <= element['dropoff_longitude'] <= -73.7736587524414)
new_element['fare_amount_dq'] = int(2.5 <= element['fare_amount'] <= 101)
new_element['pickup_latitude_dq'] = int(40.637603759765625 <= element['pickup_latitude'] <= 40.858280181884766)
new_element['pickup_longitude_dq'] = int(-74.0463638305664 <= element['pickup_longitude'] <= -73.77411651611328)
```

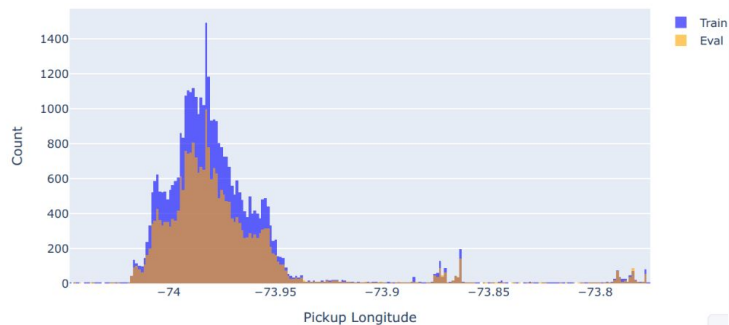
Copy

Dropoff Latitude	40.58639144897461	40.9129753112793	<input checked="" type="checkbox"/> Enable Filter
Dropoff Longitude	-74.0776596069336	-73.7736587524414	<input checked="" type="checkbox"/> Enable Filter
Fare Amount	2.5	101	<input checked="" type="checkbox"/> Enable Filter
Internal Sequence	Min	Max	<input type="checkbox"/> Enable Filter
Passenger Count	1	6	<input type="checkbox"/> Enable Filter
Pickup Latitude	40.637603759765625	40.858280181884766	<input checked="" type="checkbox"/> Enable Filter
Pickup Longitude	-74.0463638305664	-73.77411651611328	<input checked="" type="checkbox"/> Enable Filter

Trip Locations



Distribution of Pickup Longitude



Data PreTransform: Implementing the Prism

PreTransform takes in examples, a schema, and a module file. The module file contains our data quality contracts we got from the last step. It transforms the examples to native python equivalents using the schema, applies the provided function, and re-packs them back to TFRecords. We place StatisticsGen, SchemaGen, and JSONSampler to further verify data quality downstream. Because it can do arbitrary python functions, we could have created a polygon and evaluated data quality geographically (e.g. avoid slivers of the river that may not be possible using ranges)

```
pre_transform_module_file = os.path.join(REPO_PROJECT_ROOT, 'pre_transform_module.py')
pre_transform = PreTransform(
    examples=examples_cached_pre_transform.outputs['examples'],
    schema=import_schema_gen.outputs['schema'],
    module_file=pre_transform_module_file,
)
```

```
4 def transform_dict(element):
5     new_element = {}
6     for k in sorted(element.keys()):
7         new_element[k] = element[k]
8     new_element['dropoff_latitude_dq'] = int(
9         40.576972961142578 <= element['dropoff_latitude'] <= 40.95429611206055)
10    new_element['dropoff_longitude_dq'] = int(
11        -74.04652404785156 <= element['dropoff_longitude'] <= -73.76942443847656)
12    new_element['passenger_count_dq'] = int(
13        0.7438825448613378 <= element['passenger_count'] <= 6)
14    new_element['pickup_latitude_dq'] = int(
15        40.61164093017578 <= element['pickup_latitude'] <= 40.90285110473633)
16    new_element['pickup_longitude_dq'] = int(
17        -74.0501480102539 <= element['pickup_longitude'] <= -73.77628326416016)
18    return new_element
```

```
stats_options = tfdv.StatsOptions(label_feature=LABEL_KEY, num_histogram_buckets=NUM_HISTOGRAM_BUCKETS)
statistics_gen = StatisticsGen(examples=pre_transform.outputs['output_examples'], stats_options=stats_options)
schema_gen = SchemaGen(statistics=statistics_gen.outputs['statistics'], infer_feature_shape=True)
json_sampler = JSONSampler(examples=pre_transform.outputs['output_examples'], schema=schema_gen.outputs['schema'], statistics=statistics_gen.outputs['statistics'], sample_percent=25)
local_component_list = [
    examples_cached_pre_transform,
    import_schema_gen,
    pre_transform,
    statistics_gen,
    schema_gen,
    json_sampler,
]
```

Data PreTransform Scaling: Parallel Beams

Surprisingly, although there are no matrix or gradient operations, PreTransform processes allocate memory on the GPUs, and show a lot of parallelism (44 pids in nvidia-smi pmon). This likely has to do with the unpacking and packing of tf.train.Examples by the workers using beam. These workers execute work on both GPUs and use all CPU cores. Twenty five million examples processed in ~57 minutes, ~0.438 million examples/minute -> 7.3K data quality feature injections per second. It does as many in a few seconds as we are capable of visualizing. 20x wall clock performance on DirectRunner.

```
top - 04:48:37 up 10:56, 14 users, load average: 25.05, 23.85, 15.98
Tasks: 1095 total, 1 running, 1094 sleeping, 0 stopped, 0 zombie
%Cpu(s): 98.2 us, 0.7 sy, 0.0 ni, 0.3 id, 0.0 wa, 0.8 hi, 0.0 si, 0.0 st
MiB Mem : 128611.8 total, 40625.1 free, 63230.3 used, 53502.1 buff/cache
MiB Swap: 0.0 total, 0.0 free, 0.0 used. 65381.4 avail Mem
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
675519	pdodeja	20	0	20.5g	1.0g	556748	S	99.3	0.8	14:57.14	python
675543	pdodeja	20	0	20.5g	1.0g	556596	S	99.3	0.8	14:57.18	python
675553	pdodeja	20	0	20.5g	1.0g	556128	S	99.3	0.8	14:56.39	python
675580	pdodeja	20	0	20.5g	1.0g	560728	S	99.3	0.8	14:55.25	python
675511	pdodeja	20	0	20.5g	1.0g	554596	S	99.0	0.8	14:57.29	python
675524	pdodeja	20	0	20.5g	1.0g	554316	S	99.0	0.8	14:56.46	python
675536	pdodeja	20	0	20.5g	1.0g	556196	S	99.0	0.8	14:55.02	python
675547	pdodeja	20	0	20.5g	1.0g	561828	S	99.0	0.8	14:55.23	python
675557	pdodeja	20	0	20.5g	1.0g	560984	S	99.0	0.8	14:58.91	python
675560	pdodeja	20	0	20.5g	1.0g	560620	S	99.0	0.8	14:56.07	python
675562	pdodeja	20	0	20.5g	1.0g	560512	S	99.0	0.8	14:55.12	python
675574	pdodeja	20	0	20.5g	1.0g	558852	S	99.0	0.8	14:56.32	python
675522	pdodeja	20	0	20.5g	1.0g	560104	S	98.7	0.8	14:58.78	python
675528	pdodeja	20	0	20.5g	1.0g	562192	S	98.7	0.8	14:54.60	python
675566	pdodeja	20	0	20.5g	1.0g	557240	S	98.7	0.8	14:56.82	python
675506	pdodeja	20	0	20.5g	1.0g	561092	S	98.3	0.8	14:55.95	python
675509	pdodeja	20	0	20.5g	1.0g	557816	S	98.0	0.8	14:56.74	python
675571	pdodeja	20	0	20.5g	1.0g	561460	S	98.0	0.8	14:59.85	python
675545	pdodeja	20	0	20.5g	1.0g	557004	S	97.7	0.8	14:54.98	python
675531	pdodeja	20	0	20.5g	1.0g	558444	S	97.4	0.8	14:58.34	python
675540	pdodeja	20	0	20.5g	1.0g	561308	S	95.4	0.8	14:55.05	python
675577	pdodeja	20	0	20.5g	1.0g	559480	S	95.0	0.8	14:55.16	python
675533	pdodeja	20	0	20.5g	1.0g	557108	S	93.7	0.8	14:59.11	python
675516	pdodeja	20	0	20.5g	1.0g	561992	S	93.4	0.8	14:55.12	python
675260	pdodeja	20	0	4299804	1.0g	357524	S	9.9	0.8	1:44.09	python

NVIDIA-SMI 570.144		Driver Version: 570.144		CUDA Version: 12.8	
GPU	Name	Persistence-M	Bus-Id	DisSp.A	Volatile Uncorr. ECC
Fan	Temp	Pwr:Usage/Cap	Memory-Usage	GPU-Util	Compute M.
0	NVIDIA GeForce RTX 3060	Off	00000000:01:00:0	Off	N/A
36%	36C	P8	7W / 170W	2718MiB / 12288MiB	0%
1	NVIDIA GeForce RTX 3090	Off	00000000:05:00:0	Off	N/A
0%	34C	P8	9W / 350W	6300MiB / 24576MiB	0%

Processes:					
GPU	GI	CI	PID	Type	Process name
ID	ID	ID			
0	N/A	N/A	1863	G	/usr/libexec/Xorg
0	N/A	N/A	3579	C+G	.../c/gnome-remote-desktop-daemon
0	N/A	N/A	675506	C	.../versions/txf115/bin/python
0	N/A	N/A	675509	C	.../versions/txf115/bin/python
0	N/A	N/A	675511	C	.../versions/txf115/bin/python
0	N/A	N/A	675516	C	.../versions/txf115/bin/python
0	N/A	N/A	675519	C	.../versions/txf115/bin/python
0	N/A	N/A	675522	C	.../versions/txf115/bin/python
0	N/A	N/A	675524	C	.../versions/txf115/bin/python
0	N/A	N/A	675528	C	.../versions/txf115/bin/python
0	N/A	N/A	675531	C	.../versions/txf115/bin/python
0	N/A	N/A	675533	C	.../versions/txf115/bin/python
0	N/A	N/A	675536	C	.../versions/txf115/bin/python
0	N/A	N/A	675540	C	.../versions/txf115/bin/python
0	N/A	N/A	675543	C	.../versions/txf115/bin/python
0	N/A	N/A	675545	C	.../versions/txf115/bin/python
0	N/A	N/A	675547	C	.../versions/txf115/bin/python
0	N/A	N/A	675553	C	.../versions/txf115/bin/python
0	N/A	N/A	675557	C	.../versions/txf115/bin/python
0	N/A	N/A	675560	C	.../versions/txf115/bin/python
0	N/A	N/A	675562	C	.../versions/txf115/bin/python
0	N/A	N/A	675566	C	.../versions/txf115/bin/python
0	N/A	N/A	675571	C	.../versions/txf115/bin/python
0	N/A	N/A	675574	C	.../versions/txf115/bin/python
0	N/A	N/A	675577	C	.../versions/txf115/bin/python
0	N/A	N/A	675580	C	.../versions/txf115/bin/python
1	N/A	N/A	675506	C	.../versions/txf115/bin/python
1	N/A	N/A	675509	C	.../versions/txf115/bin/python

```
real 56m33.018s
user 1170m32.700s
sys 5m11.067s
```

Data Filtration: Beams Filtered through Prism

FilterUDF takes in examples, a schema, statistics (currently unused), and a module file. We construct our `_dq` indicators from the schema, which results in only data that passes all of our data quality checks to be passed through to the next stage.

```
filter_gen = FilterUDF(
    examples=examples_cached_pre_transform.outputs['examples'],
    schema=import_schema_gen.outputs['schema'],
    statistics=statistics_cached.outputs['result'],
    module_file=filter_module_file,
)
```

```
def filterfn(schema_dict, example):
    features = tf.io.parse_single_example(example, schema_dict.feature_spec)
    filter_features = [f for f in schema_dict.feature_spec.keys() if '_dq' in f]
    good_data = True
    for feature in filter_features:
        good_data = good_data and (features[feature].numpy()[0] > 0)
    return good_data
```

```
local_component_list = [
    examples_cached_pre_transform,
    statistics_cached,
    filter_gen,
    import_schema_gen,
    statistics_gen_filter,
    schema_gen_filter,
    json_sampler,
]
```

real	35m34.102s
user	689m10.120s
sys	4m29.607s

Exploring Filtered Data

Histogram Feature

Fare Amount Dq

Highlight Data Quality Issue

None

Histogram Bins (20)

Auto

Y-Axis Scale

☐ Log Scale

Selection History

Previous

Next

Custom Data Quality Filters (Notepad)

Trip Locations

Train Pickup

Train Dropoff

Eval Pickup

Eval Dropoff

Distribution of Fare Amount Dq

Fare Amount Dq Range	Train Count	Eval Count
0.5 - 1.0	0	~50,000
1.0 - 1.5	~20,000	0

Capture Valid Ranges from Histogram

Statistics for Fare Amount Dq

	Train Split		Eval Split
Count	74022.0000	Count	49766.0000
Min	1	Min	1
Max	1	Max	1
Mean	1.0000	Mean	1.0000

Downstream Pipeline Components

Now that our data is filtered, we can enrich (feature engineer) it, with `tf.Transform`.

real	58m22.517s
user	174m0.728s
sys	8m54.994s

We can place our `JSONSampler` to receive JSON versions of `TFTransform`'ed Examples.

As features are sometimes higher dimensional, we would need to enhance our conversion process (currently only python primitives).

Since we have UUIDs and split information, we can have fine grained tracing of the impact of each example on the training process (e.g. Analyze `BulkInferer` protocol buffers, re-inject back into visualization after sampling).

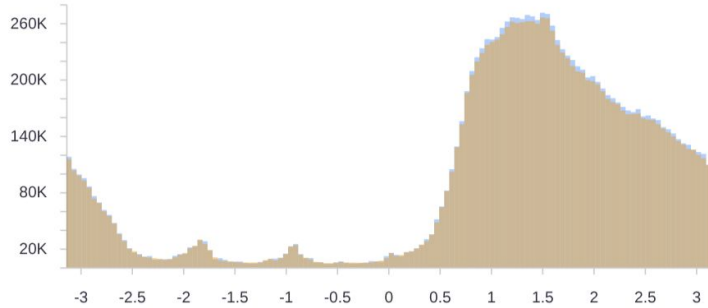
Models trained on the filtered data have lower validation loss (both train and val are filtered) than those on unfiltered data (no filtering on either split)

ML Metadata is what allows us to open up the pipeline, and re-seal it back together. An end-to-end hermetically sealed pipeline is not optimized for data quality, it is optimized for scaling and reproducibility.

Transformed Statistics

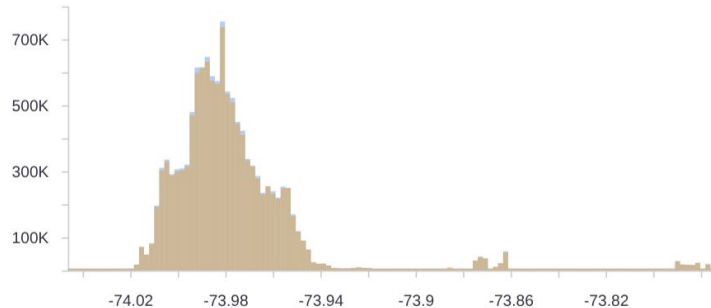
level_3_atan2

12.1M	0%	1.21	1.5	0%	-3.14	1.49	3.14
11.8M	0%	1.21	1.5	0%	-3.14	1.49	3.14



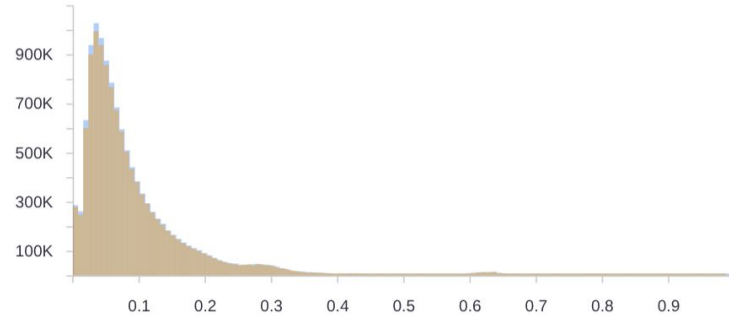
level_0_pickup_longitude

12.1M	0%	-73.98	0.03	0%	-74.05	-73.98	-73.77
11.8M	0%	-73.98	0.03	0%	-74.05	-73.98	-73.77



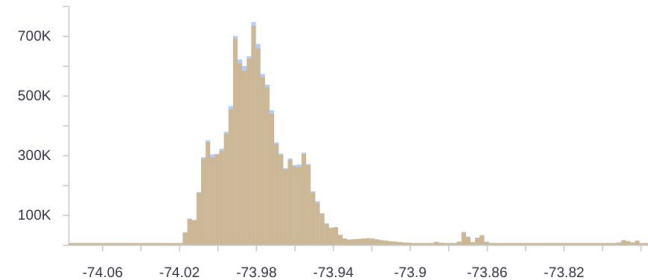
level_2_haverstein_distance_scaled

12.1M	0%	0.1	0.1	1.22%	0	0.07	1
11.8M	0%	0.1	0.1	1.22%	0	0.07	0.99



level_0_dropoff_longitude

12.1M	0%	-73.97	0.03	0%	-74.08	-73.98	-73.77
11.8M	0%	-73.97	0.03	0%	-74.08	-73.98	-73.77



How can we make it better?

Step	How Beam Helps	How we can improve?
Pre-Ingestion	Determine Schema for Data	Utility code for schema generation, integrate uuids better Use more scalable runner than DirectRunner (overall)
Data Splitting & Identification	Deterministic Data Splitting at Scale	Manage split point in metadata, splits in data Generate UUID post-split Component for temporal data (not just managing split points, also sequences/time series)
Data Exploration	Produce JSON from TFRecord	Multi-dimensional support (temporal, geo) Figure out scaling visualization (e.g. infinite zoom using “James Webb” feature.)
Non-graph intended feature injection	Apply Arbitrary Python UDFs	Support polygon generation from visualization, auto generate UDF
Filter	Remove examples which do not meet DQ requirements	Store filtered data as a managed artifact, filter individual examples
Post Transform	Evaluator, BulkInference	Integrate output into ML loop

Demo (Time/Conditions Permitting)

Capabilities:

How can we assign passports to our data? - Windowing/UUID

How can we attach luggage tags? - Inject Data Quality Indicators

How can we filter bad data at scale? - FilterUDFs

How can we manage the boarding process? - Data Quality Post Transform (Future)

How can we manage, and possibly avoid, turbulence? - BulkInference/Evaluator Integration (Future)

Call to action

- If you know Beam, you are more than halfway there for large scale machine learning.
- Follow <https://github.com/tensorflow/tfx> to keep up with the improvements in large scale ML.
- Try to understand TFX component architecture for a Beam based component. Three parts: component, with children component spec, and executor. I can provide book recommendations.
- Help me get these components into TFX!



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QUESTIONS?

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