datatonic

Effective sampling methods within TensorFlow input functions

Will Fletcher & Laxmi Prajapat

TensorFlow World - 31st October 2019 

Hello!

MChem Chemistry 🧪
Oxford, 2010-2014

MSc Computational Statistics & Machine Learning 👨‍💻
UCL, 2016-2017

Learning to walk 🤖
ZOA Robotics, 2017-2018

Researcher & Lecturer 📚
Oxford, 2014-2016

Joined Datatonic
London, 2018

Research Analyst
esa 2014

MSci Astrophysics 🚀
UCL, 2011-2015

Data Scientist 🔮
Barclays, 2015-2017

datatonic

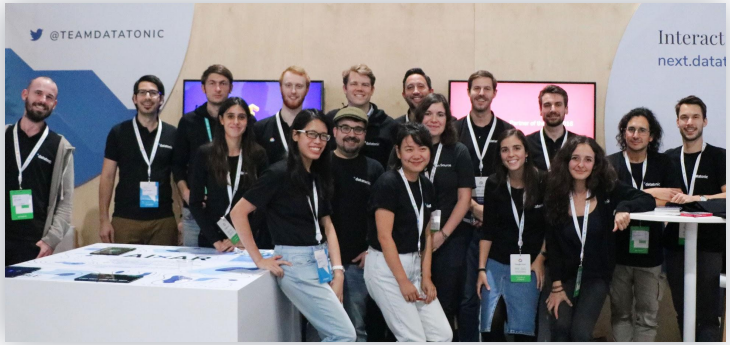
About Datatonic

EXPERTISE

MACHINE LEARNING

ANALYTICS

DATA ENGINEERING



TECHNOLOGY

Google Cloud · TensorFlow · Apache Spark · beam · looker

CLIENTS

sky · John Lewis & Partners · Transport for London – Every Journey Matters · BBC · ao.com

Premier Partner
Google Cloud
Machine Learning

Premier Partner
Google Cloud
Marketing Analytics

2018
Partner of the Year
Google Cloud

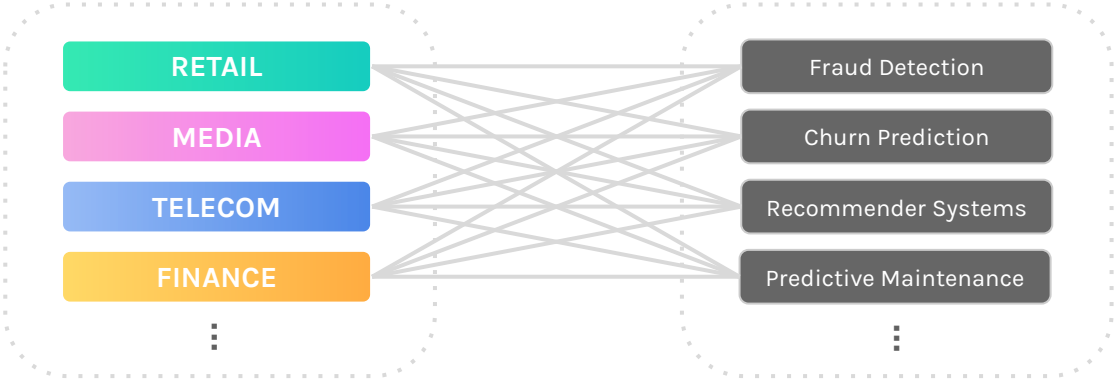
About the ML team

We use Google Cloud...

to accelerate Machine Learning workloads...

in a scalable way.

We work with imbalanced datasets very often...

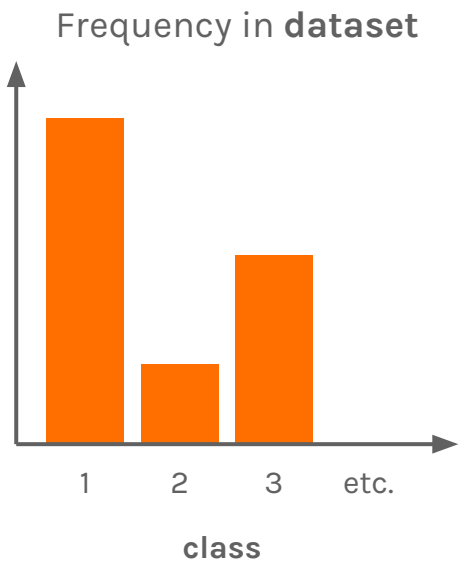


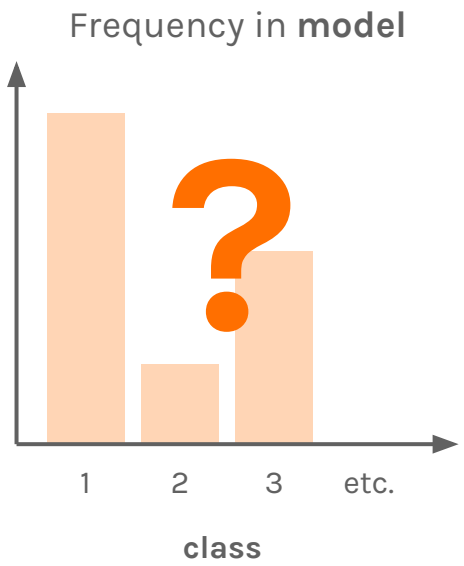
We are going to talk about...

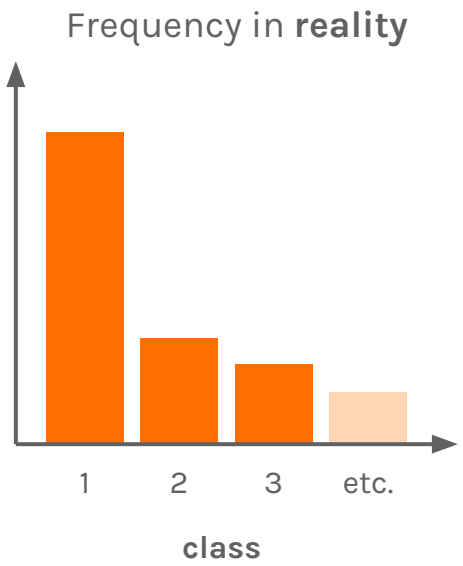
- Theory: **Why sample?**
- Tooling: **`tf.data` / `tf.estimator`**
- Examples: **The simple stuff**
- Our usage: **More advanced cases**

Why sample?

Dataset distributions







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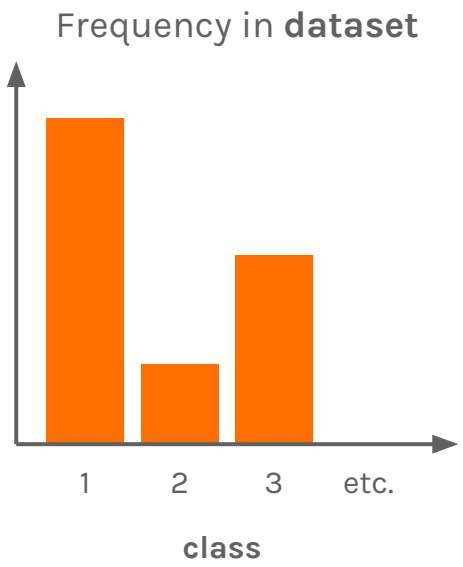

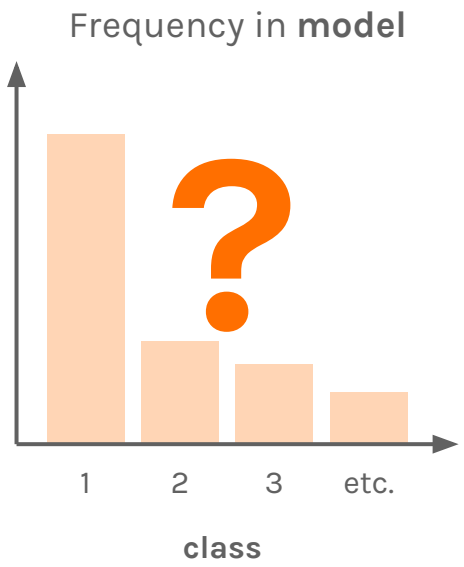

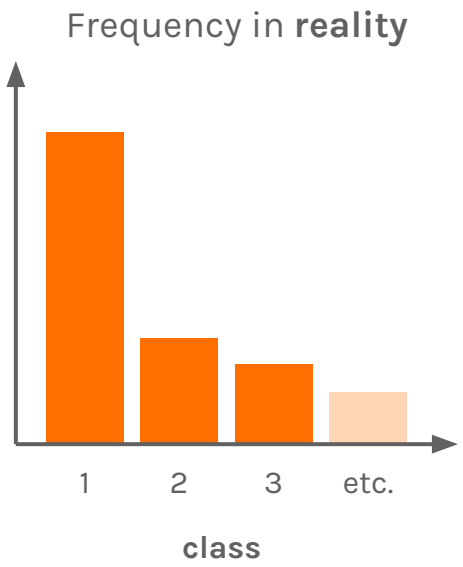

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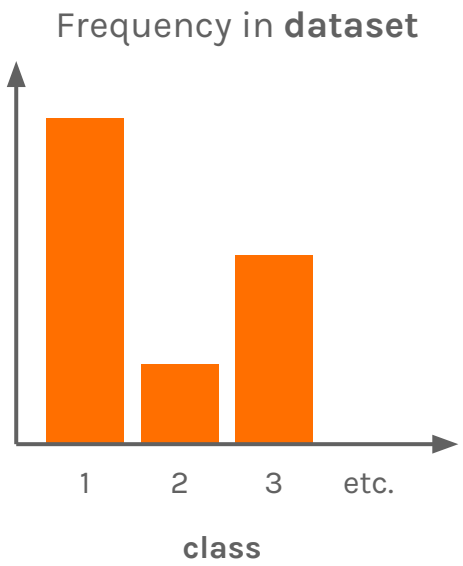
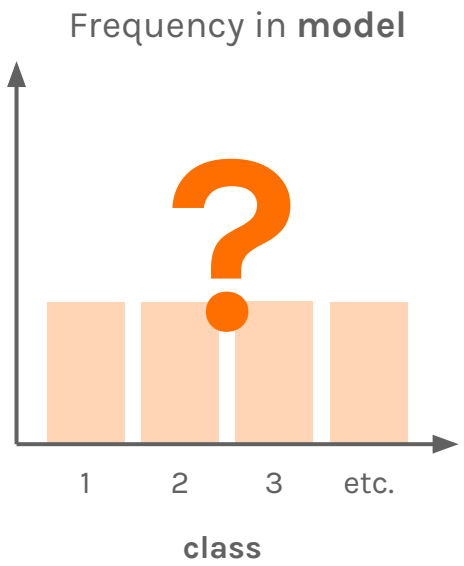
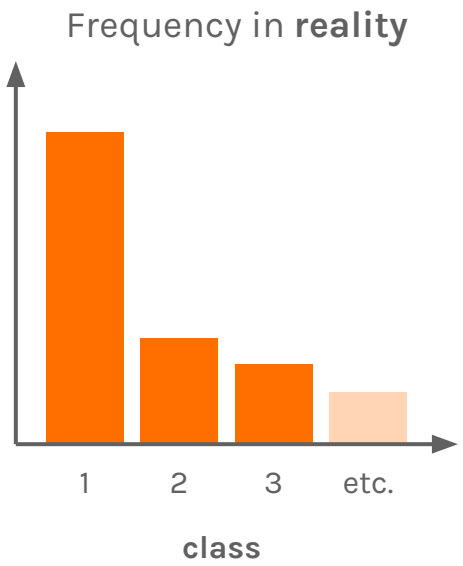


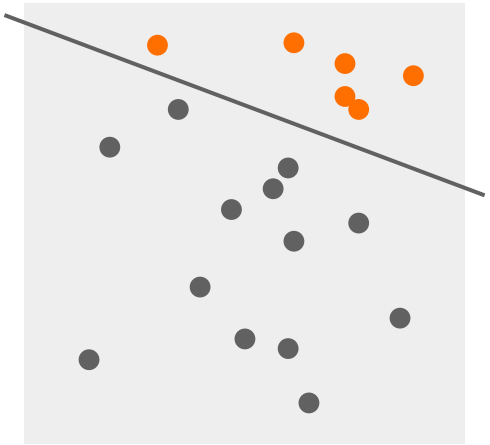




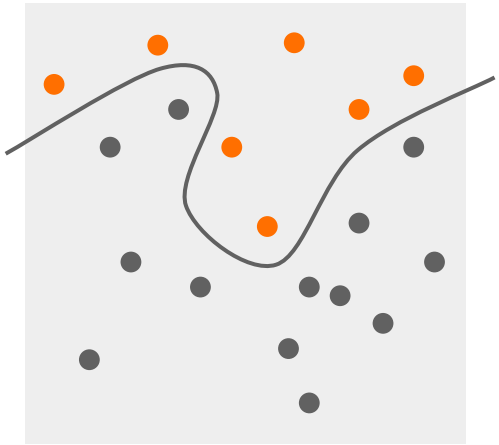
Learning from imbalanced data

In a classification problem, our task is to find the **boundary** between classes

linear



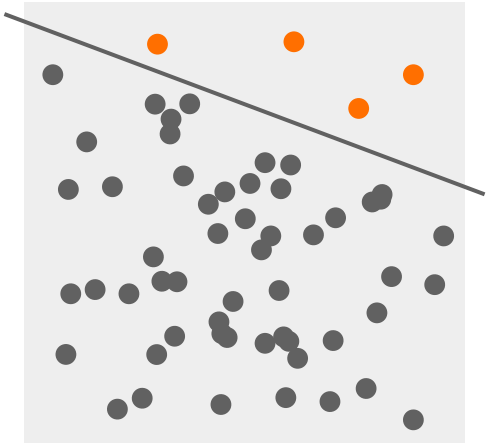
non-linear



Learning from imbalanced data

The solution is **independent** of the number of examples shown (if they are informative enough)

linear



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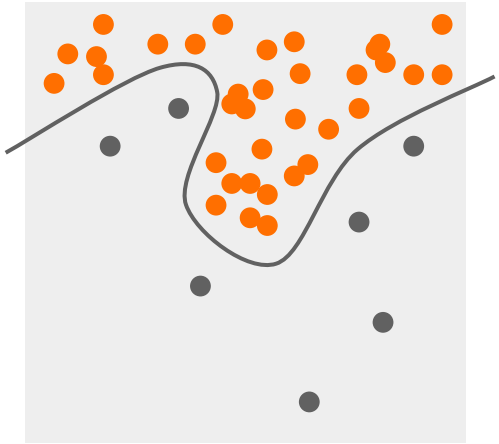

Learning from imbalanced data

… but there are side effects

1. **More examples ⇒ more computation**
   a. i/o 
   b. model updates ⚙️

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   a. solution quality may suffer 🚧
   b. more variance (overfitting) likely 🎯

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3. **Different distribution ⇒ different output probabilities**
   a. will not reflect probability of future examples 🎲

Learning from imbalanced data

What is the best learning environment?

Learning from imbalanced data

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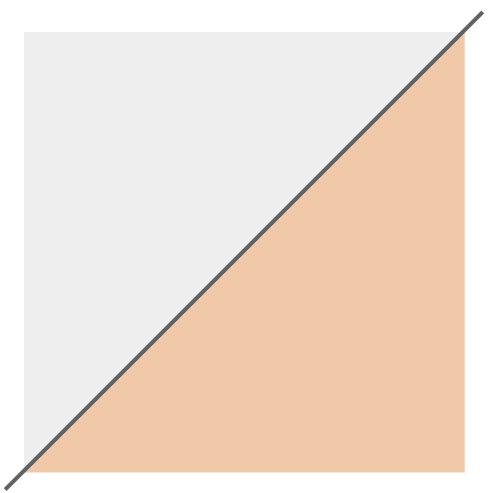


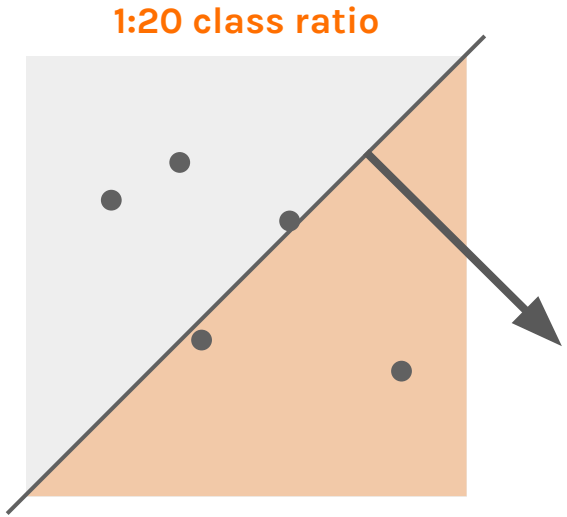
random initialization

Consider the
incremental updates

Learning from imbalanced data

What is the best learning environment?

Consider the incremental updates

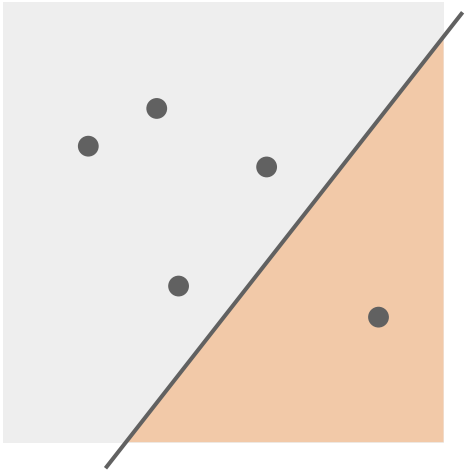


Learning from imbalanced data

What is the best learning environment?

Consider the incremental updates

1:20 class ratio



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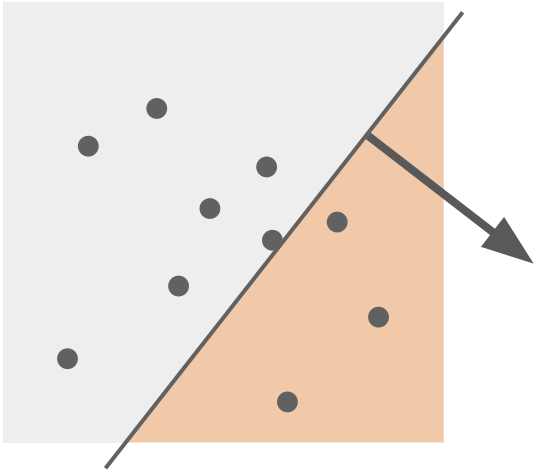

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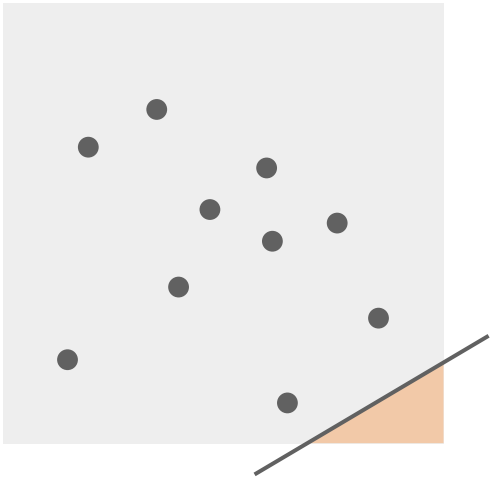

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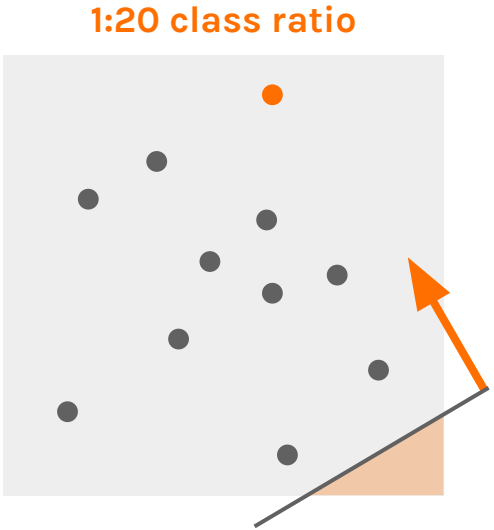

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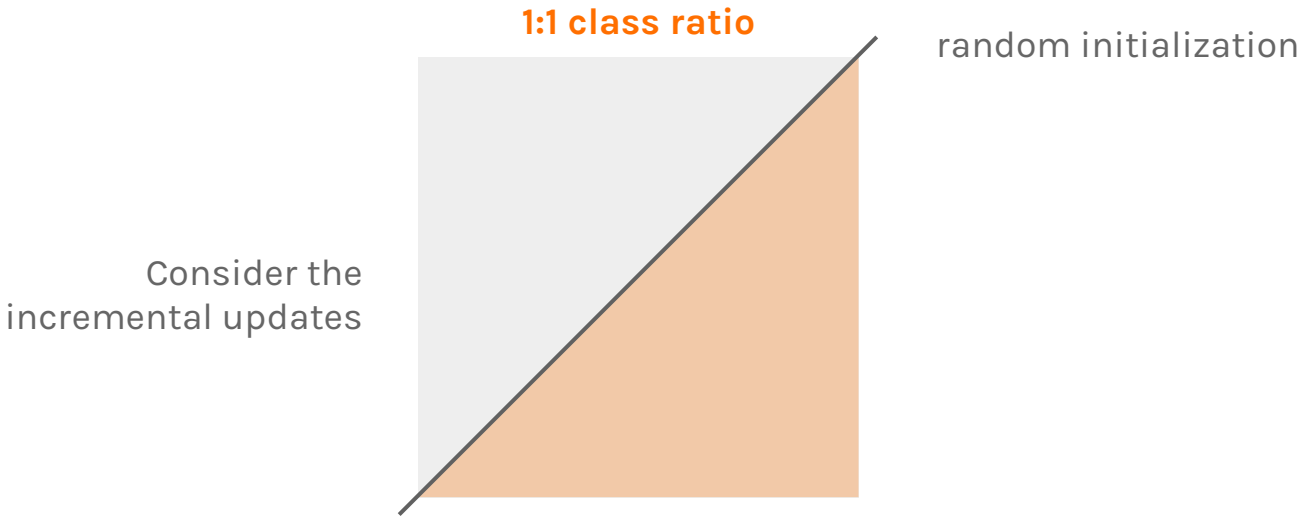

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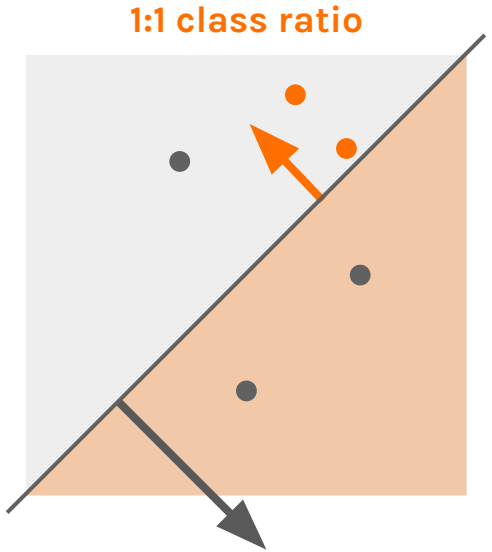

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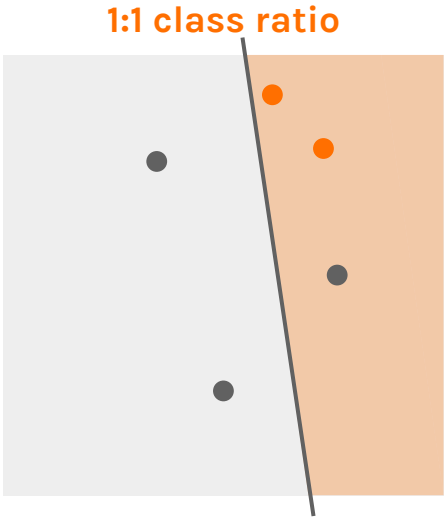

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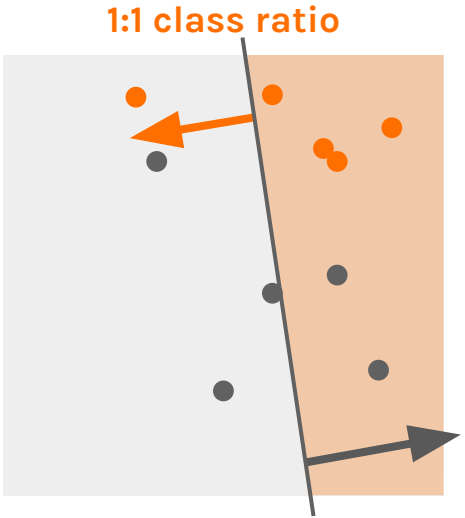

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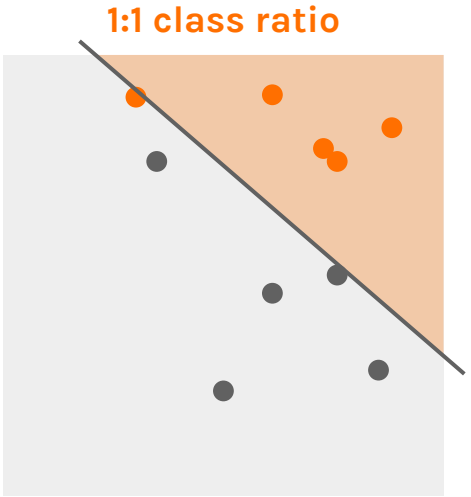
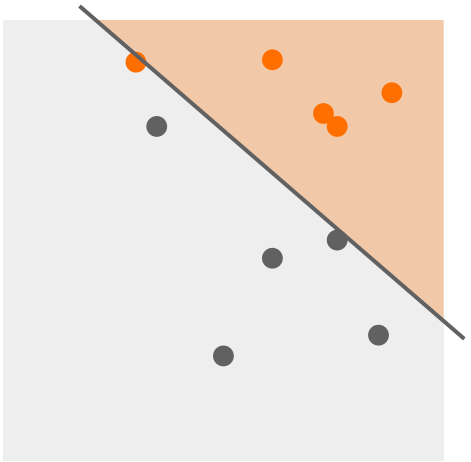


Learning from imbalanced data

What is the best learning environment?

More balanced batches give more information.



Learning from imbalanced data

Another technique – **example weighting**

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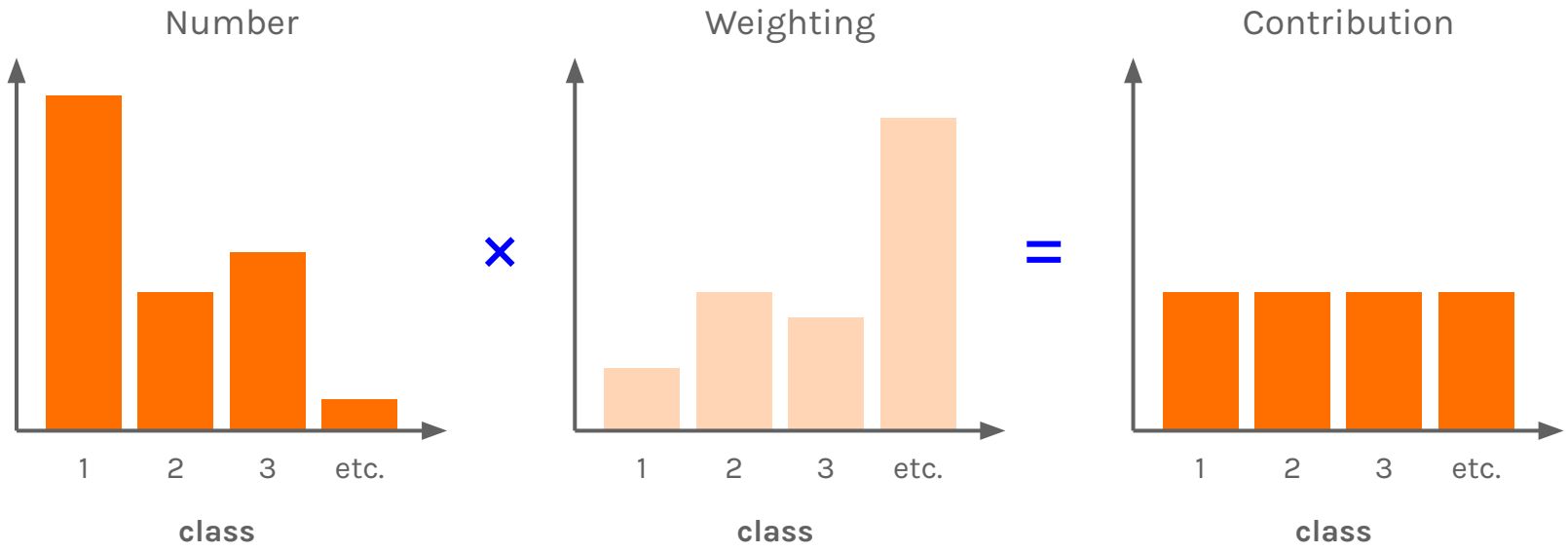

Learning from imbalanced data

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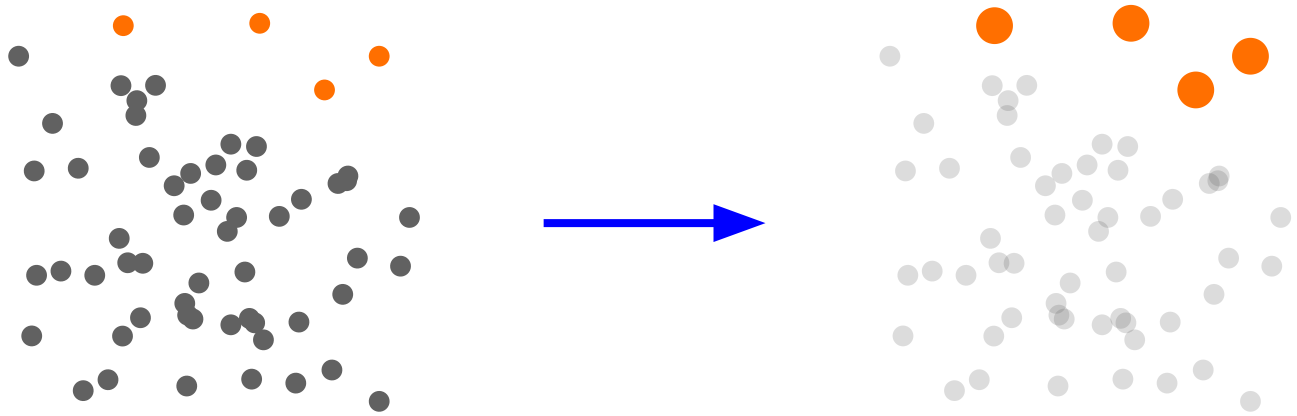

Learning from imbalanced data

Another technique – **example weighting**

The following training environments give **equivalent solutions** (with sufficient data):

Sample balance	Weighting	Threshold
true ratio **1:x**	equal **1:1**	true probability $(1+x)^{-1}$
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easiest to learn

Learning from imbalanced data

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easiest to learn

calibrated

Learning from imbalanced data

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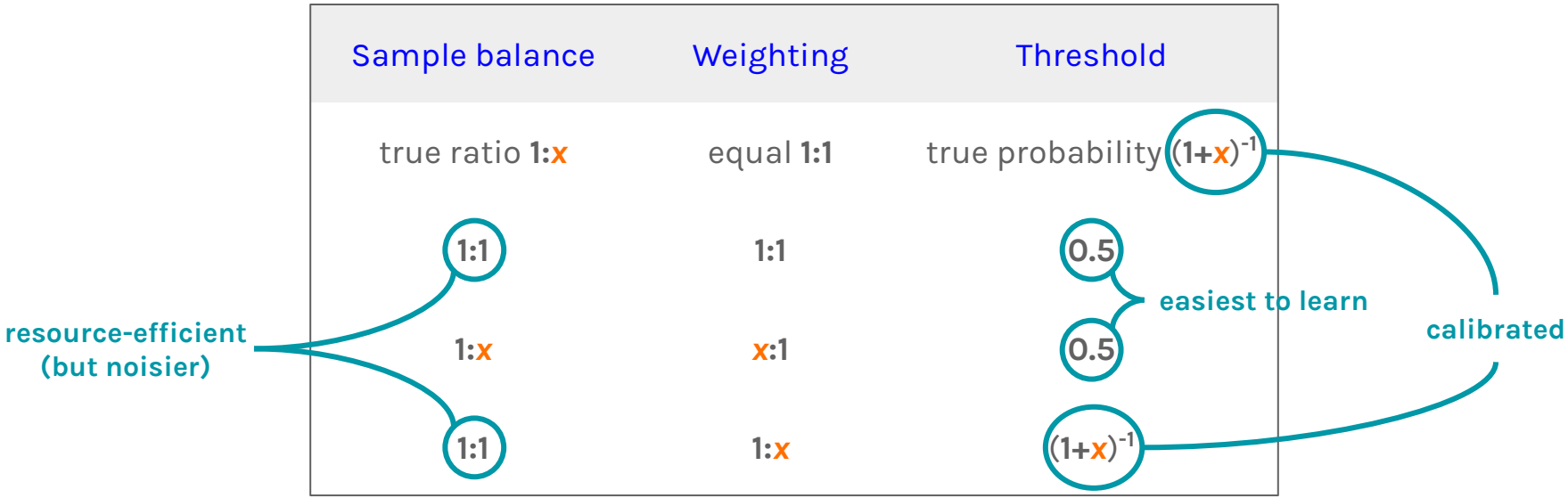

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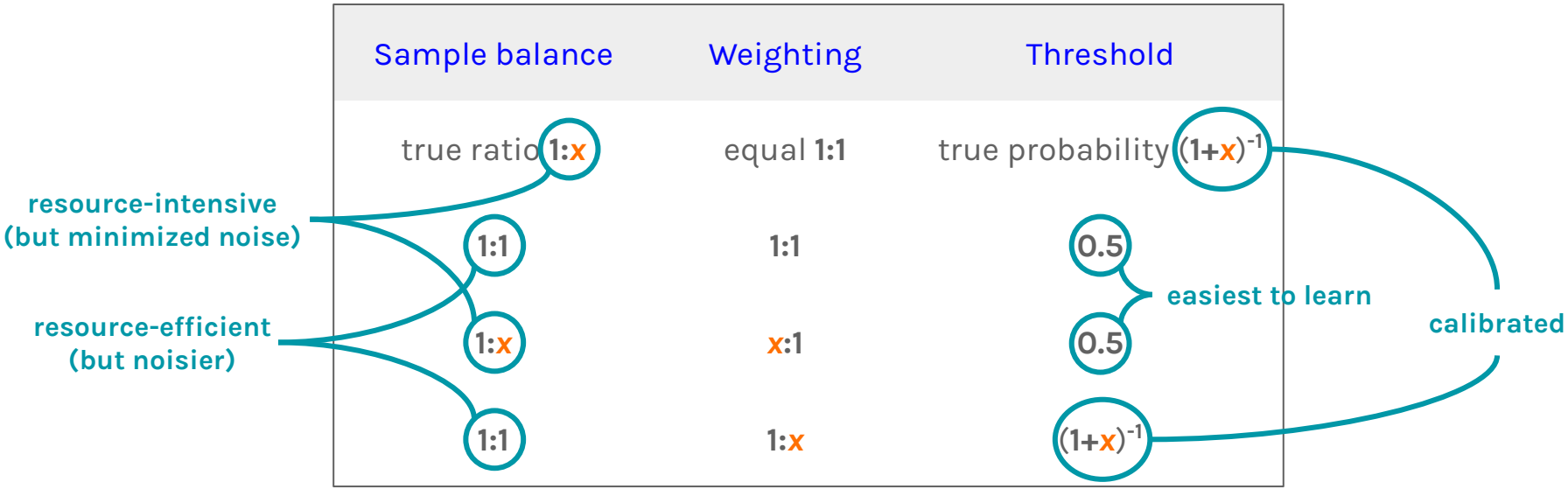

Learning from imbalanced data

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3. **Sampling** trades signal–noise ratio for fewer operations 🐝

Learning from imbalanced data

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Learning from imbalanced data

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1. Nothing fundamentally prevents a good solution from imbalanced data ⛳
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3. **Sampling** trades signal–noise ratio for fewer operations 🐝
4. The probabilities output by a model reflect the distribution of data fed in 🎲
5. **Sampling and weighting together** can give speedup without compromising interpretation of outputs as probabilities 🤝

Learning from imbalanced data

Not covered

- Cost-sensitive models / loss functions
- Data augmentation techniques e.g. SMOTE
- Imbalance-robust algorithms

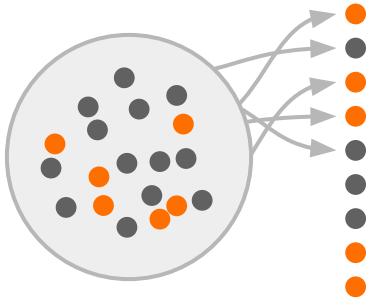
But...

But... real data lives in files

This changes **everything** 

Sampling from files

A file is a **fixed** collection of examples



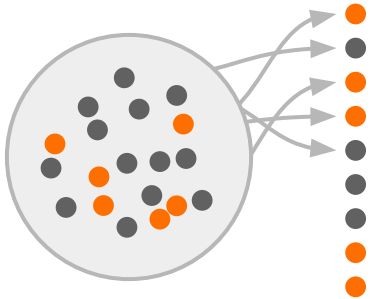
Reading is **sequential**

Sampling is **random**

Sampling from files

A file is a **fixed** collection of examples

Reading is **sequential**



easy in RAM!

Sampling is **random**

Sampling from files

How do we sample the data when reading from file?

Option 1

Load all the data into memory and use **`imbalanced-learn`** 

Option 2

Prepare a **one-off** random sampling of the data and **save to file** 

Option 3

Stream the data into memory and sample on the fly 🎶

Data input pipelines in TensorFlow

`tf.data`

tf.data

a layer between **sources** and **inputs**

tf.data > queues > feed_dict

We can build flexible input pipelines with the TensorFlow Dataset API (**tf.data**).

Extract

Read from in-memory or out-of-memory datasets

Transform

Apply preprocessing operations

Load

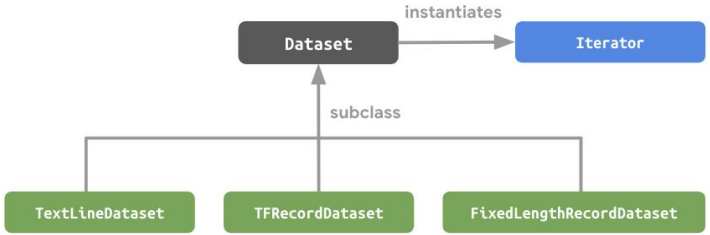
Load batched examples onto the accelerator ready for processing

Methods to create a Dataset object from a data source:

- `tf.data.Dataset.from_tensor_slices`
- `tf.data.Dataset.from_generator`
- `tf.data.TFRecordDataset`
- `tf.data.TextLineDataset`
- ...

Methods to transform a Dataset:

- `tf.data.Dataset.batch`
- `tf.data.Dataset.shuffle`
- `tf.data.Dataset.map`
- `tf.data.Dataset.repeat`
- ...



Prefetch elements from the input Dataset ahead of the time they are requested by calling the `tf.data.Dataset.prefetch` method.

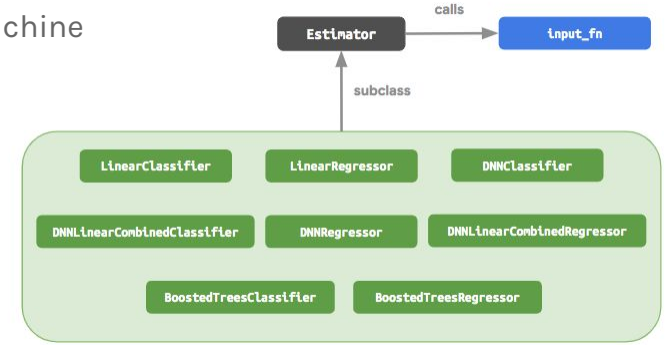
This transformation overlaps the work of a *producer* and *consumer*.

Estimators

Estimators (**`tf.estimator`**) is a high-level TensorFlow API that simplifies the machine learning process.

The `Estimator` class is an abstraction containing the necessary code to…

- run a training or evaluation loop
- predict using a trained model
- export a prediction model for use in production



The Estimator API enables us to build TensorFlow machine learning models in two ways:

CANNED

"users who want to use common models"

- Common machine learning algorithms made accessible
- Robust with best practices encoded
- A number of configuration options are exposed, including the ability to specify input structure using feature columns
- Provide built-in evaluation metrics
- Create summaries to be visualised in TensorBoard

CUSTOM

"users who want to build custom machine learning models"

- Flexibility to implement innovative algorithms
- Fine-grained control
- Model function (`model_fn`) method that build graphs for train/evaluate/predict must be written anew
- Model can be defined in Keras and converted into an `Estimator` (`tf.keras.estimator.model_to_estimator`)

Getting data from A to B

Data for training, evaluation and prediction must be supplied through **input functions** when working with the TensorFlow Estimator API (**tf.estimator**).

```
estimator.train(input_fn)
```

A valid input_fn takes no arguments, returning either a tuple (features, labels) or a **Dataset** generating such tuples:

- **features** – Tensor of features, or dictionary of Tensors keyed by feature name
- **labels** – Tensor of labels, or dictionary of labels keyed by label name

```
def input_fn():
    Read data and create Dataset object
    Apply transformations
    Create Iterator
return features, labels
```

In **keras.fit()**, this is done without the function wrapper.

And if you want to get batches **manually**, the final step is creating an **Iterator** object to retrieve them from the Dataset in sequence:

- tf.data.Dataset.make_one_shot_iterator
- tf.data.Dataset.make_initializable_iterator
- ...

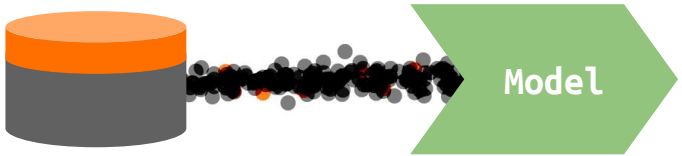
For example, a **one_shot_iterator** yields elements with every call of its **get_next()** method, until the Dataset is exhausted.

Typical pipeline

```
def make_examples(file_list):
    filenames = tf.data.Dataset.from_tensor_slices(file_list)
    filenames.shuffle(len(file_list))

    examples = filenames.interleave(
        lambda f: tf.data.TextLineDataset(f)
    )
    examples.shuffle(10**5)
    return examples
```

→→→ batch
→→→ parse
→→→ cache
→→→ repeat
→→→ prefetch



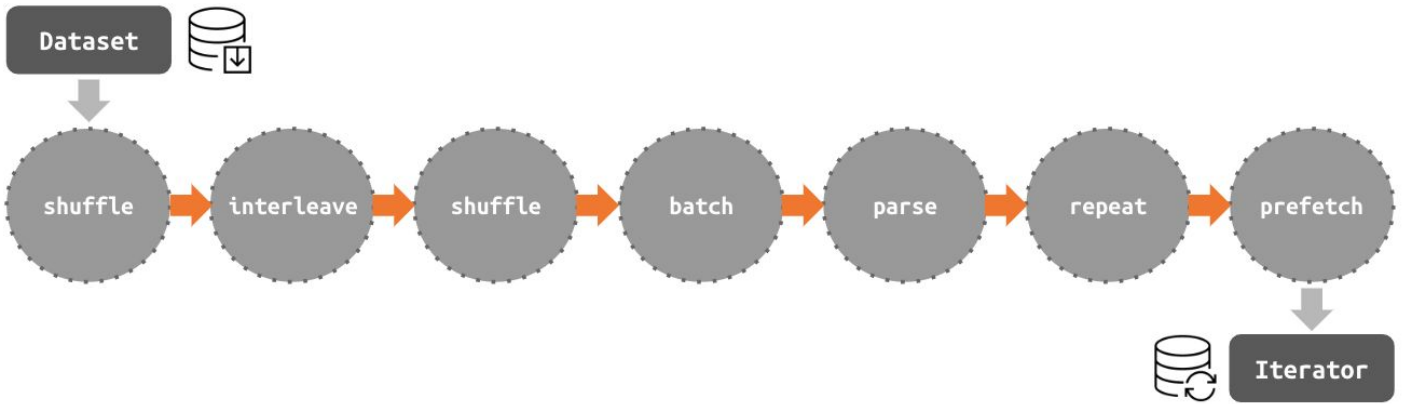
A+B ≠ B+A

The order of transformations matter.

Why? 🤷

`tf.data` API provides flexibility to users but the ordering of certain transformations have performance implications.

- **`repeat`** → **`shuffle`** - performant but no guarantee that samples processed in an epoch
- **`shuffle`** → **`repeat`** - guaranteed that samples processed in an epoch but less performant



Putting it all together

Key stages in the modelling pipeline:

Define input function for passing data to the model for training and evaluation.

Define feature columns which are specifications for how the model should interpret the input data.

Instantiate estimator with necessary parameters and feeding in the feature columns.

Train and evaluate model. Train loop saves model parameters as checkpoint. Eval loop restores model and uses it to evaluate model.

Export trained model as `SavedModel`.

Evaluate model - compute evaluation metrics over test data.

Generate predictions with trained model.

```
def input_fn():
    ...
    return features, labels

def build_feature_columns():
    f1 = tf.feature_column.numeric_column('a')
    f2 = tf.feature_column.categorical_column_with_hash_bucket('b', 5)
    return [f1, f2]

estimator = tf.estimator.LinearRegressor(build_feature_columns(),
    optimizer,
    model_dir,
    tf.estimator.RunConfig(...))

if mode == tf.estimator.ModeKeys.TRAIN:
    tf.estimator.train_and_evaluate(estimator,
        tf.estimator.TrainSpec(train_input_fn),
        tf.estimator.EvalSpec(eval_input_fn))

    estimator.export_savedmodel(export_dir_base=serving_dir,
        serving_input_receiver_fn)

elif mode == tf.estimator.ModeKeys.EVAL:
    results = estimator.evaluate(eval_input_fn)

elif mode == tf.estimator.ModeKeys.PREDICT:
    predictions = estimator.predict(eval_input_fn)
```

What about TensorFlow 2.0?

Notably among the myriad of updates with the final release of TensorFlow 2.0 is the reliance on **`tf.keras`** as its central high-level API.

Simplified and integrated workflow for Machine Learning:

- Use **`tf.data`** for data loading at scale (or `NumPy`)
- Use **`tf.keras`** or existing canned estimators in **`tf.estimator`** for model construction

One part of the tight integration with the ecosystem is the ability for Keras models to be converted into an `Estimator` and used just like any other TensorFlow estimator.

Simple examples

Existing sampling functionality

TensorFlow already provides built-in functionality for sampling.

In-memory

tf.contrib.training

+ `.resample_at_rate(inputs, rates)`
+ `.rejection_sample(tensors, accept_prob_fn, batch_size)`
+ `.stratified_sample(tensors, labels, target_probs, batch_size)`
+ `.weighted_resample(inputs, weights, overall_rate)`

tf.data API

tf.data.Dataset

+ `.take(count)`

tf.data.experimental

+ `.rejection_resample(class_func, target_dist)`
+ `.sample_from_datasets(datasets, weights)`

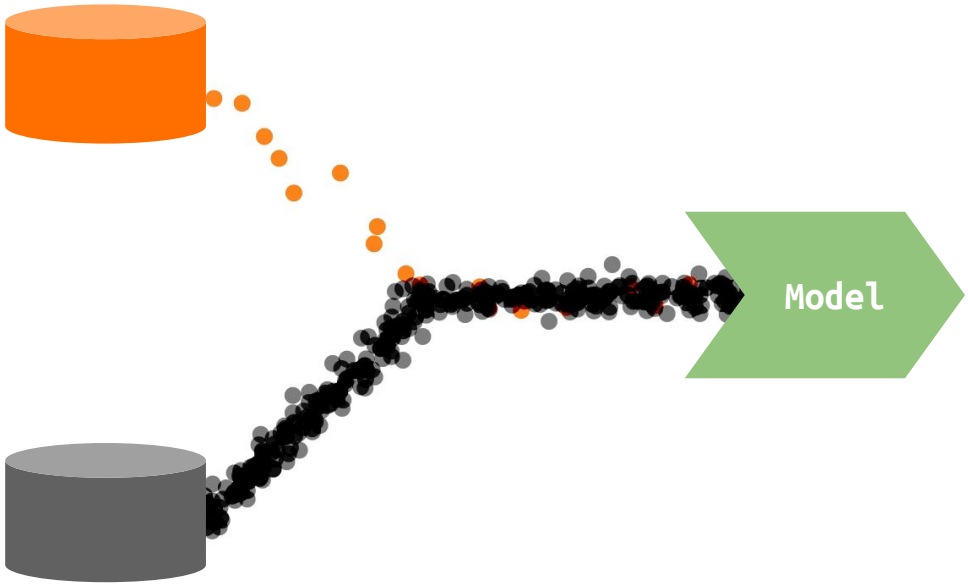
(loss sampling)

tf.random

+ `.uniform_candidate_sampler(true_classes, num_true, num_sampled, unique, range_max)`
+ `.log_uniform_candidate_sampler(true_classes, num_true, num_sampled, unique, range_max)`

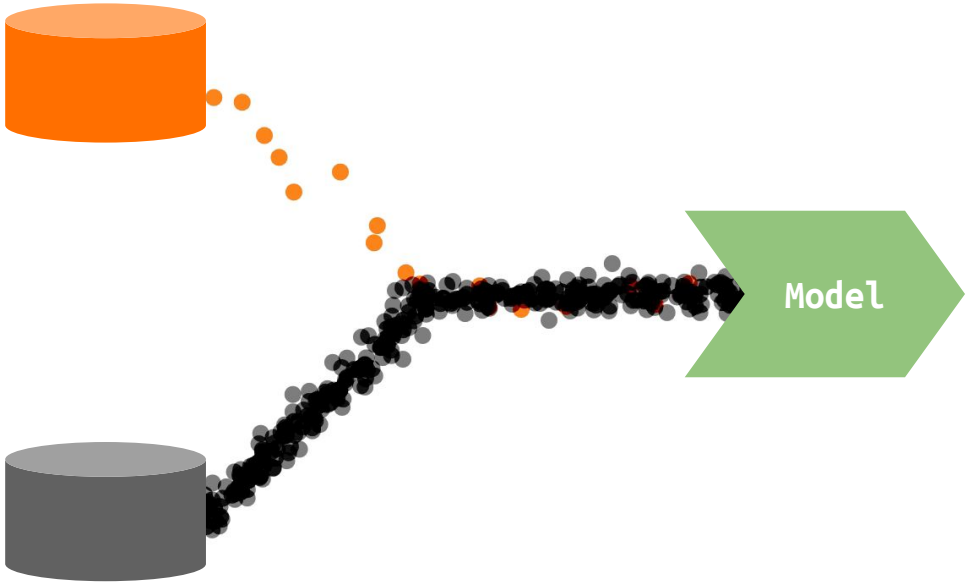
...

Without balancing




```
pos = make_examples(pos_filenames)
neg = make_examples(neg_filenames)
```

Without balancing

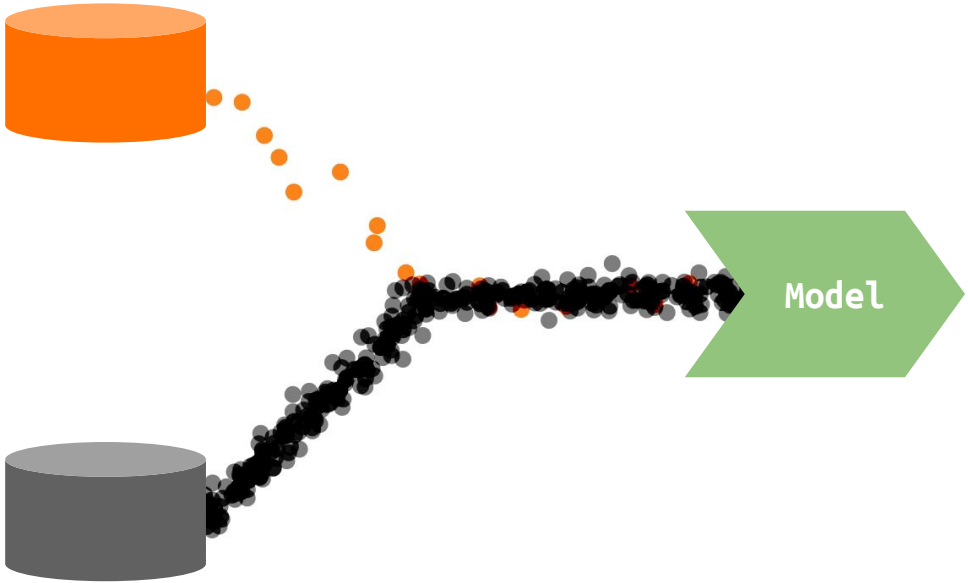



```
pos = make_examples(pos_filenames)
neg = make_examples(neg_filenames)
```

→→→ **combine the (shuffled) datasets randomly**

`tf.data.experimental.sample_from_datasets`

Without balancing




```
pos = make_examples(pos_filenames)
neg = make_examples(neg_filenames)
```

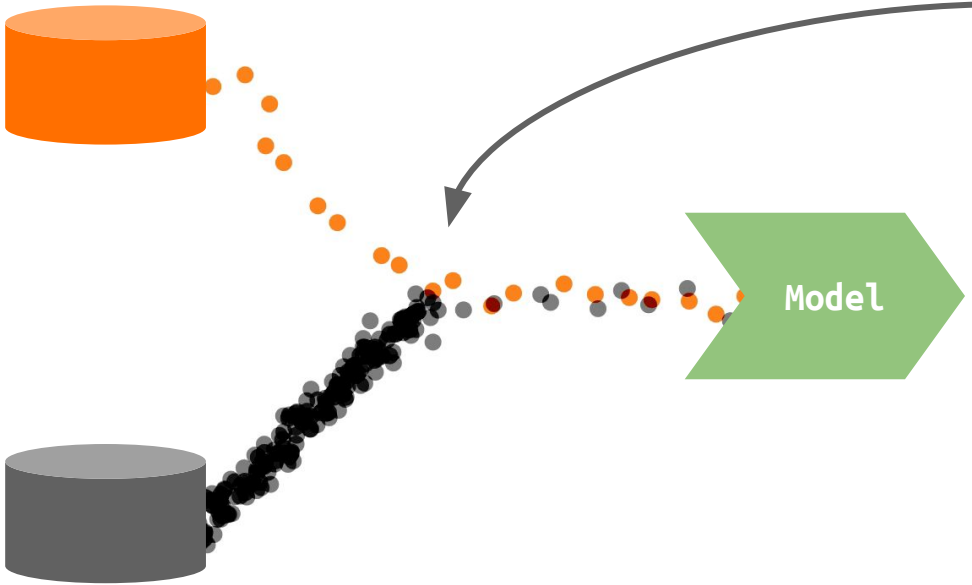
→→→ combine the (shuffled) datasets randomly
`tf.data.experimental.sample_from_datasets`

...or

→→→ combine the datasets deterministically
`tf.data.Dataset.concatenate`
`tf.data.experimental.choose_from_datasets`

→→→ then shuffle

With downsampling




```
pos = make_examples(pos_filenames)
neg = make_examples(neg_filenames)
neg = neg.take(POS_SIZE)
```

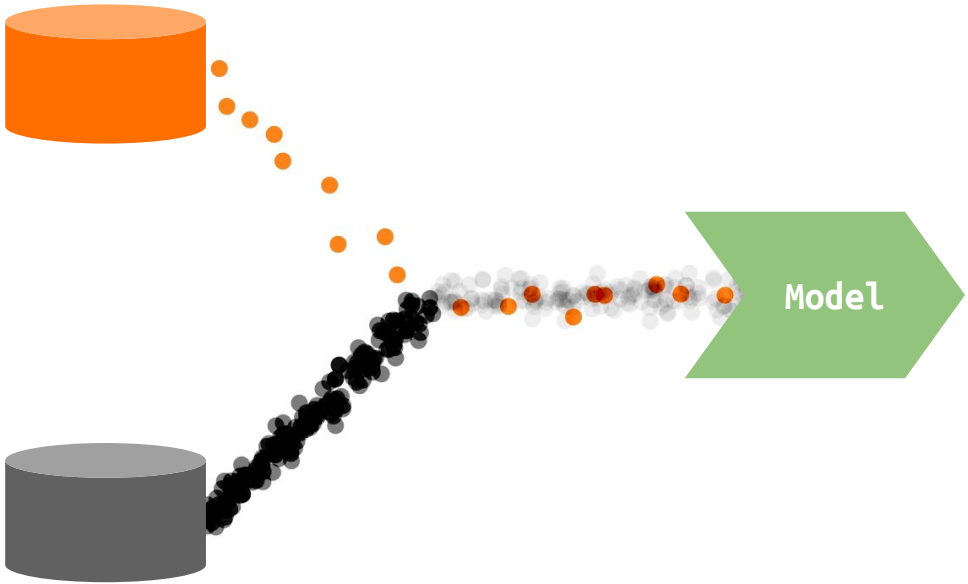
→→→ combine the (shuffled) datasets randomly
`tf.data.experimental.sample_from_datasets`

...or

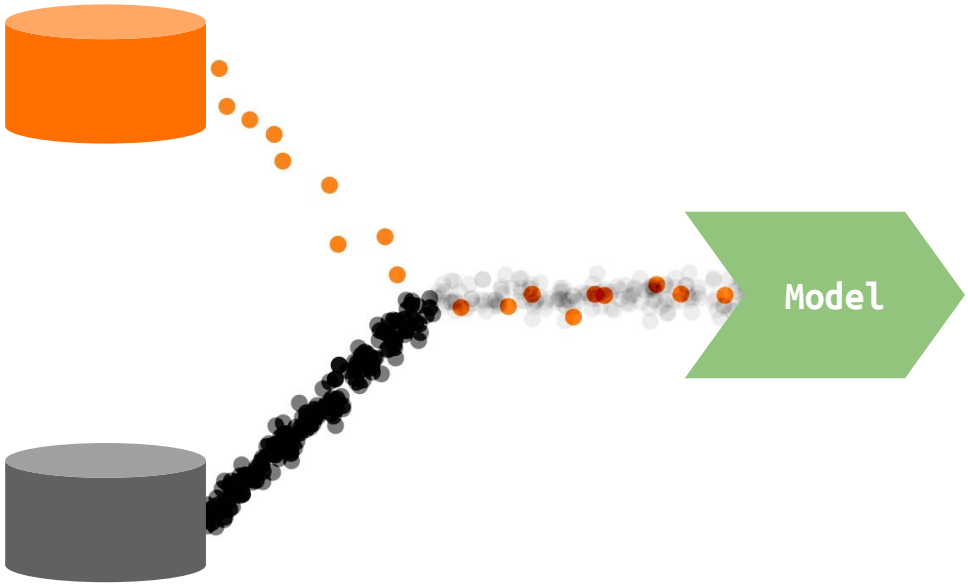
→→→ combine the datasets deterministically
`tf.data.Dataset.concatenate`
`tf.data.experimental.choose_from_datasets`

→→→ then shuffle

With example weighting



With example weighting

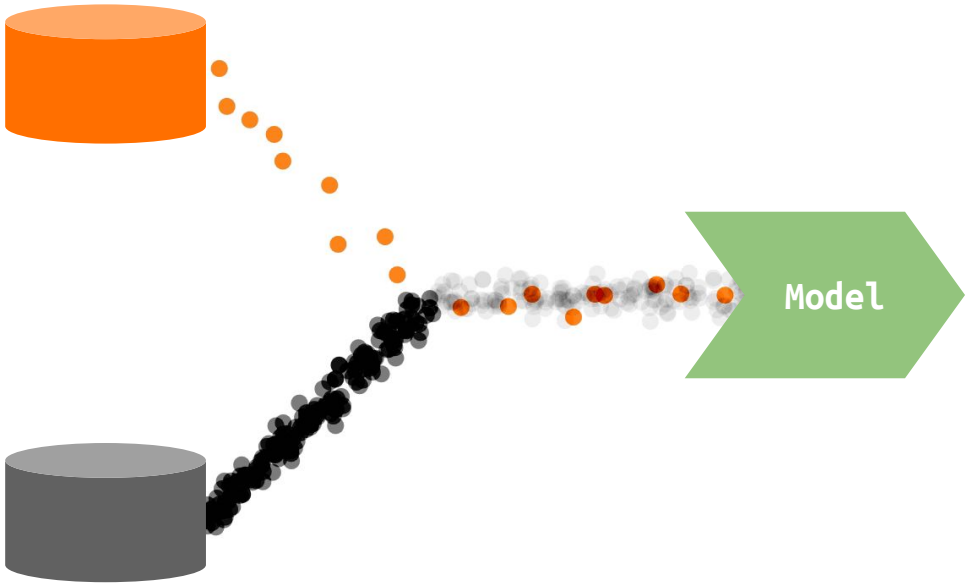



```
def pos_weighting(features, labels): ...
def neg_weighting(features, labels): ...

pos = pos.map(pos_weighting)
neg = neg.map(neg_weighting)
```

→→→ combine

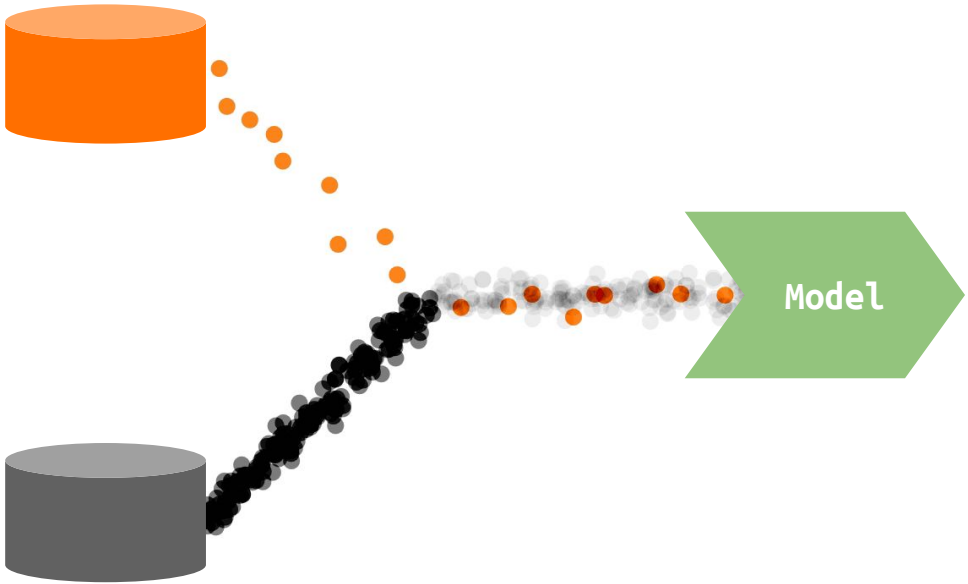
With example weighting




```
def pos_weighting(features, labels):
  weights = tf.fill(tf.shape(labels), POS_WT)
  return features, labels, weights
```

for tf.keras

With example weighting

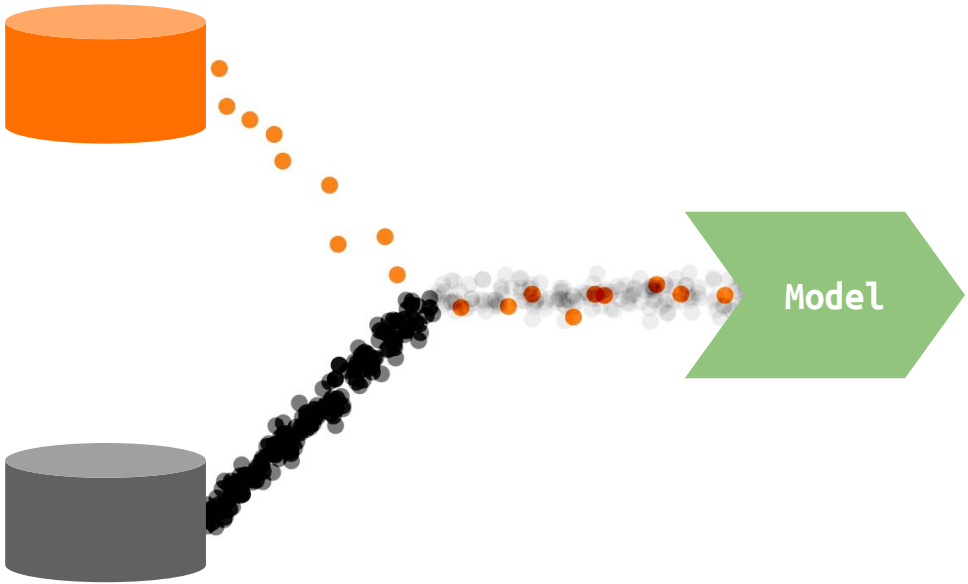



```
def pos_weighting(features, labels):
  weights = tf.fill(tf.shape(labels), POS_WT)
  features['weight'] = weights
  return features, labels
```

for tf.estimator

```
estimator = DNNClassifier(
  ...
  weight_column='weight'
  ...
)
```

With example weighting

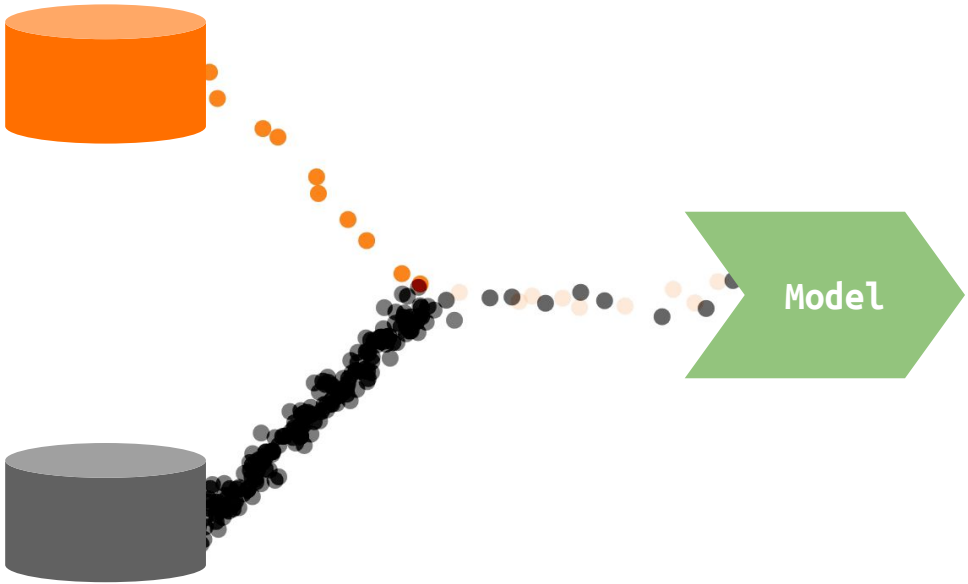



```
def pos_weighting(features, labels):
  weights = tf.fill(tf.shape(labels), POS_WT)
  ...
def neg_weighting(features, labels): ...

pos = pos.map(pos_weighting)
neg = neg.map(neg_weighting)
```

→→→ combine

Downsampling and re-weighting




```
def pos_weighting(features, labels):
  weights = tf.fill(tf.shape(labels), POS_WT)
  ...
def neg_weighting(features, labels): ...

pos = pos.map(pos_weighting)
neg = neg.map(neg_weighting)
neg = neg.take(POS_SIZE)
```

→→→ combine

Data input pipelines in TensorFlow

Summary

Data input pipelines in TensorFlow

Summary

1. **`tf.data`** defines ETL pipelines between data sources and model inputs 

Data input pipelines in TensorFlow

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Data input pipelines in TensorFlow

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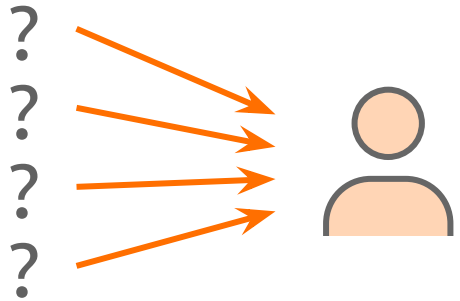
5. Simple sampling can be done with **`take`**, **`concatenate`**, and **`shuffle`** 
6. More options are **`sample_from_datasets`** and **`rejection_resample`** 

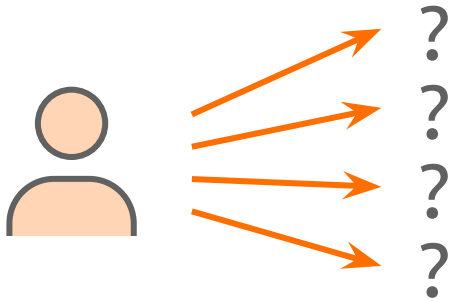
Where we use sampling...

Behavioural modelling

Recommender systems

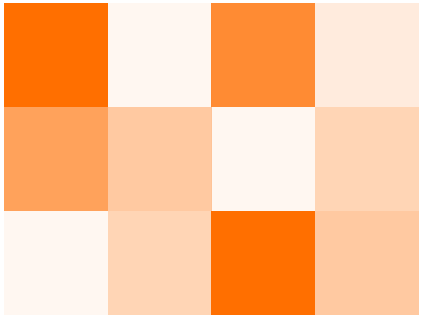


Propensity to act



Behavioural modelling

- Examples are **`(user, item)`** pairs
- Many more **unobserved** than **observed** pairs
- Unobserved pairs can be **generated**



Behavioural modelling

Two approaches for sampling:

1. **Generate all unobserved pairs on disk, and sample**

   Modification: **pre-sample** when reading

2. **Generate unobserved pairs dynamically in memory**

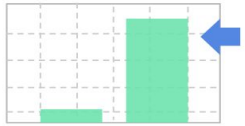
   Modification: **cache** features, **look up** keyed by `user` / `item`

Take less, prioritise more

An effective way to handle imbalanced data is to **downsample and upweight the majority class.**

1. **Downsample** - *extract random samples from the majority class known as "random majority undersampling"*

2. **Upweight** - *add a weighting to the downsampled examples*



Weight should typically be equal to the factor used to downsample:

{weight} = {original example weight} x {downsampling factor}

What are the benefits? 🕵️

Faster convergence

Minority class seen more often during training, helping model to converge quicker.

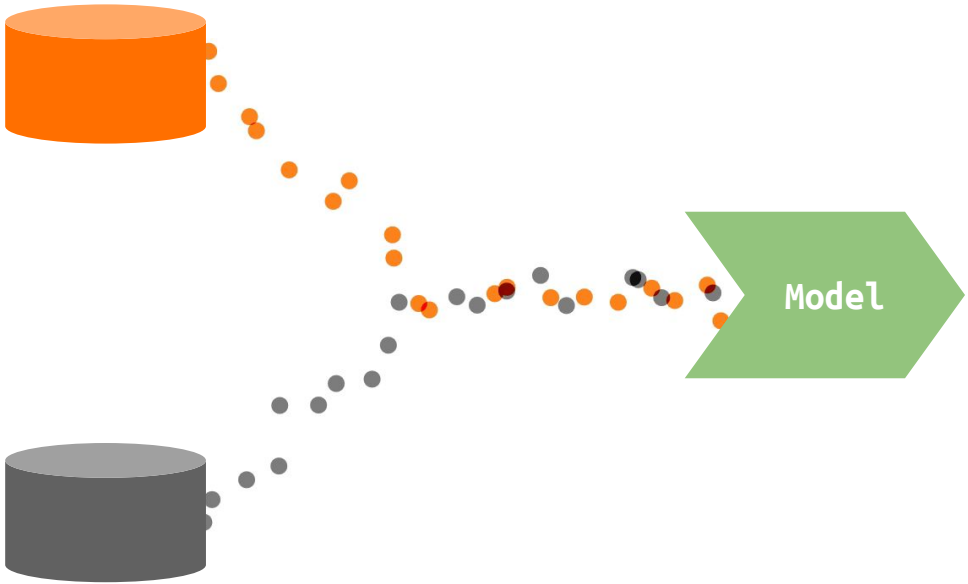
Less I/O

Consolidating majority class into fewer examples requires less processing of data.

Calibration

Upweighting ensures outputs can still be interpreted as probabilities.

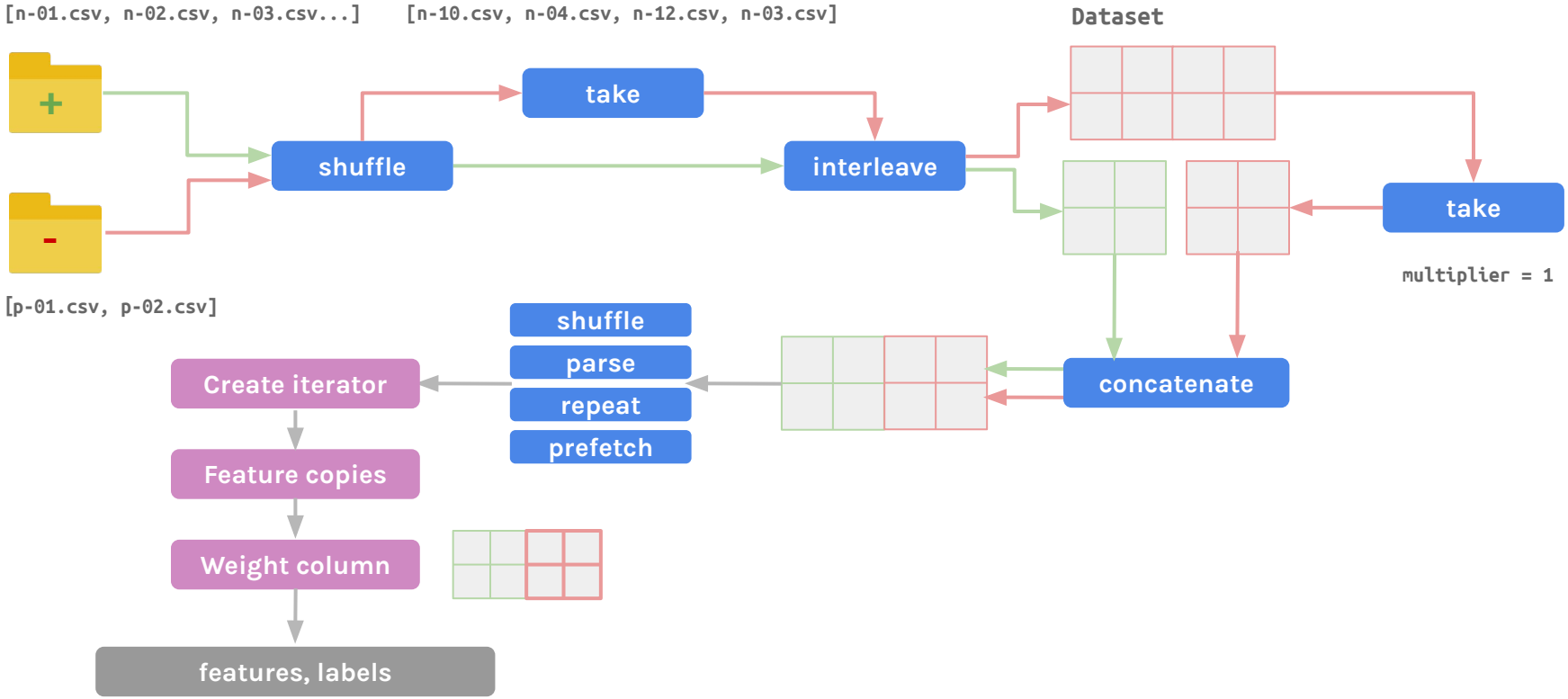
Downsampling with fewer reads



No point reading the whole dataset

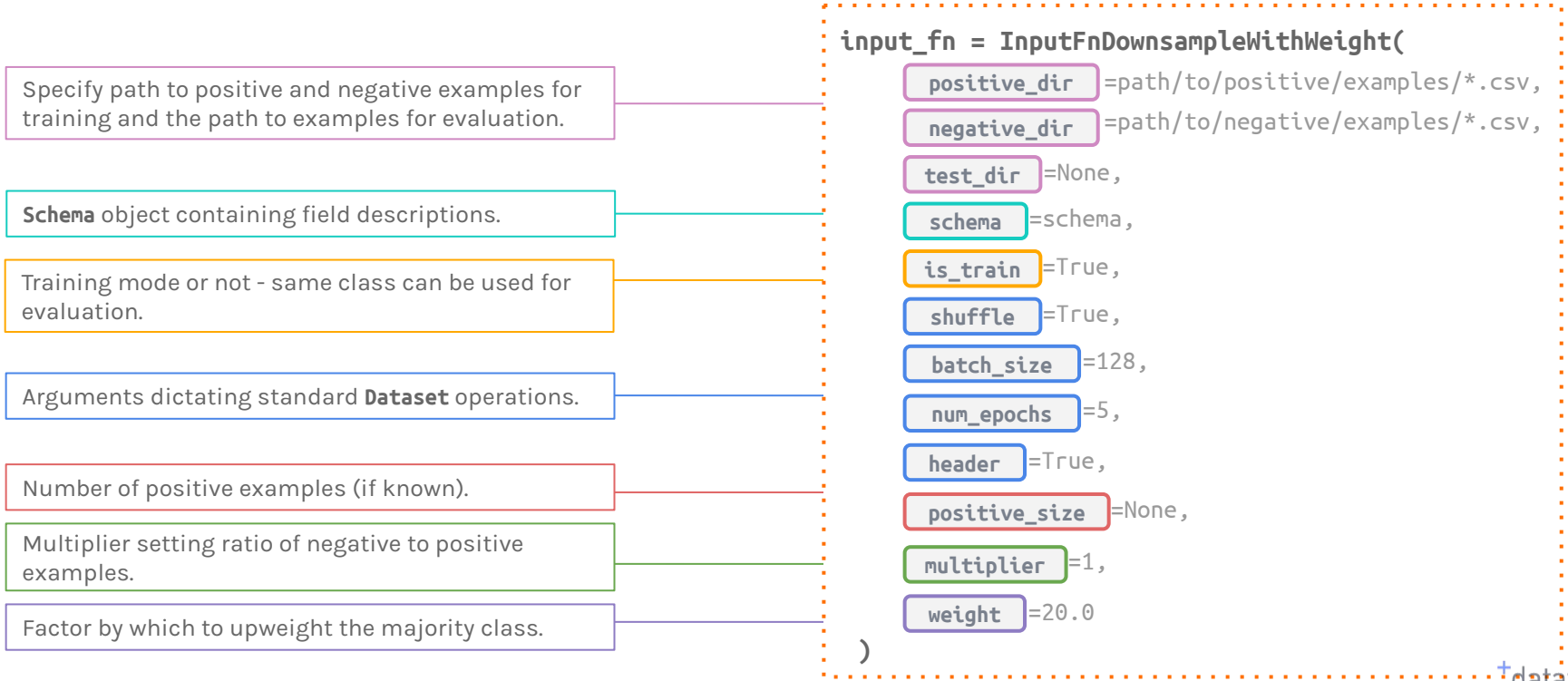
if the model won't read it all

Inner workings



Focussing on args

InputFnDownsampleWithWeight is our callable class, with arguments to instantiate an **input_fn**, including the magnitude of downsampling / upweighting required.

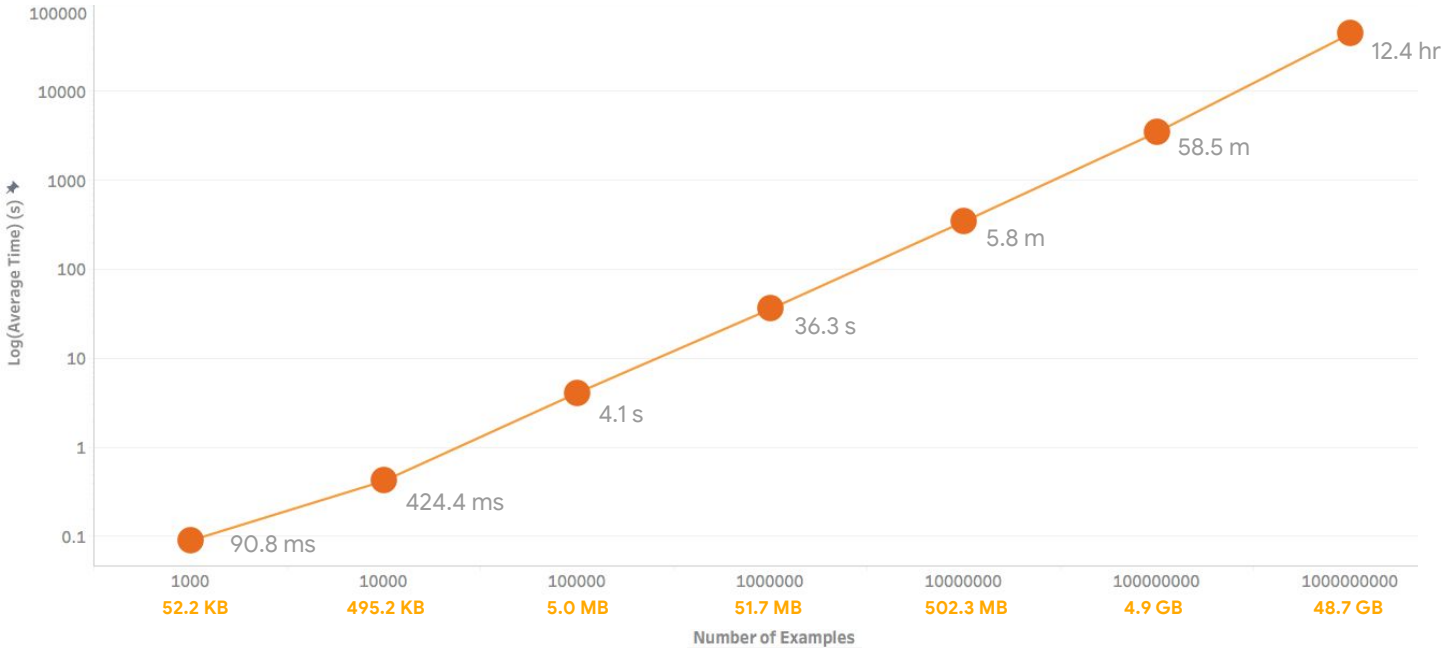


Counting the # of examples takes O(n) time

The number of positive examples in the dataset is calculated automatically if the value is not provided when instantiating the training input function.

This is where there is a **computational bottleneck**...

```
def _compute_dataset_rows(dataset):
    reducer = tf.contrib.data.Reducer(init_func=lambda _: 0,
                                      reduce_func=lambda x, _: x + 1,
                                      finalize_func=lambda x: x)
    dataset = tf.contrib.data.reduce_dataset(dataset, reducer)
    return int(tf.Session().run(dataset))
```



VM specification:

Debian GNU/Linux 9 (stretch)

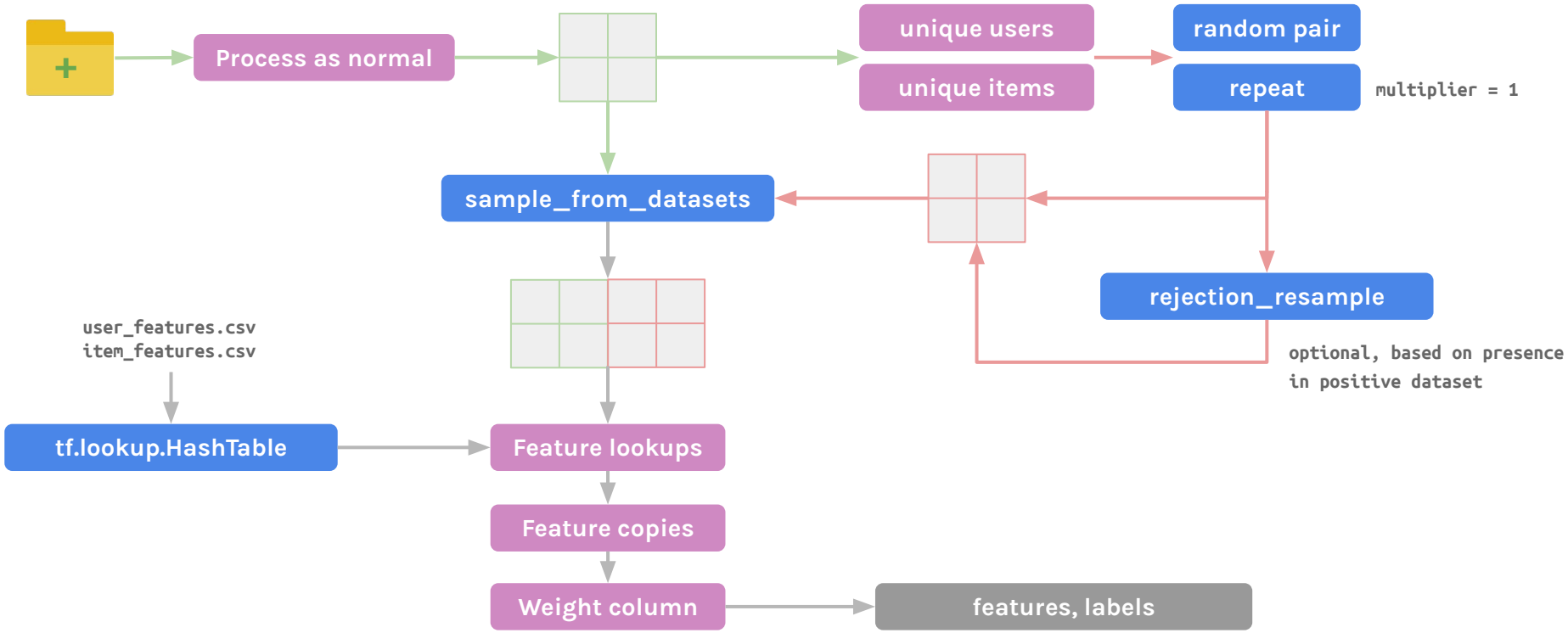
n1-standard-8
8 vCPUs, 30GB memory

100GB standard persistent disk

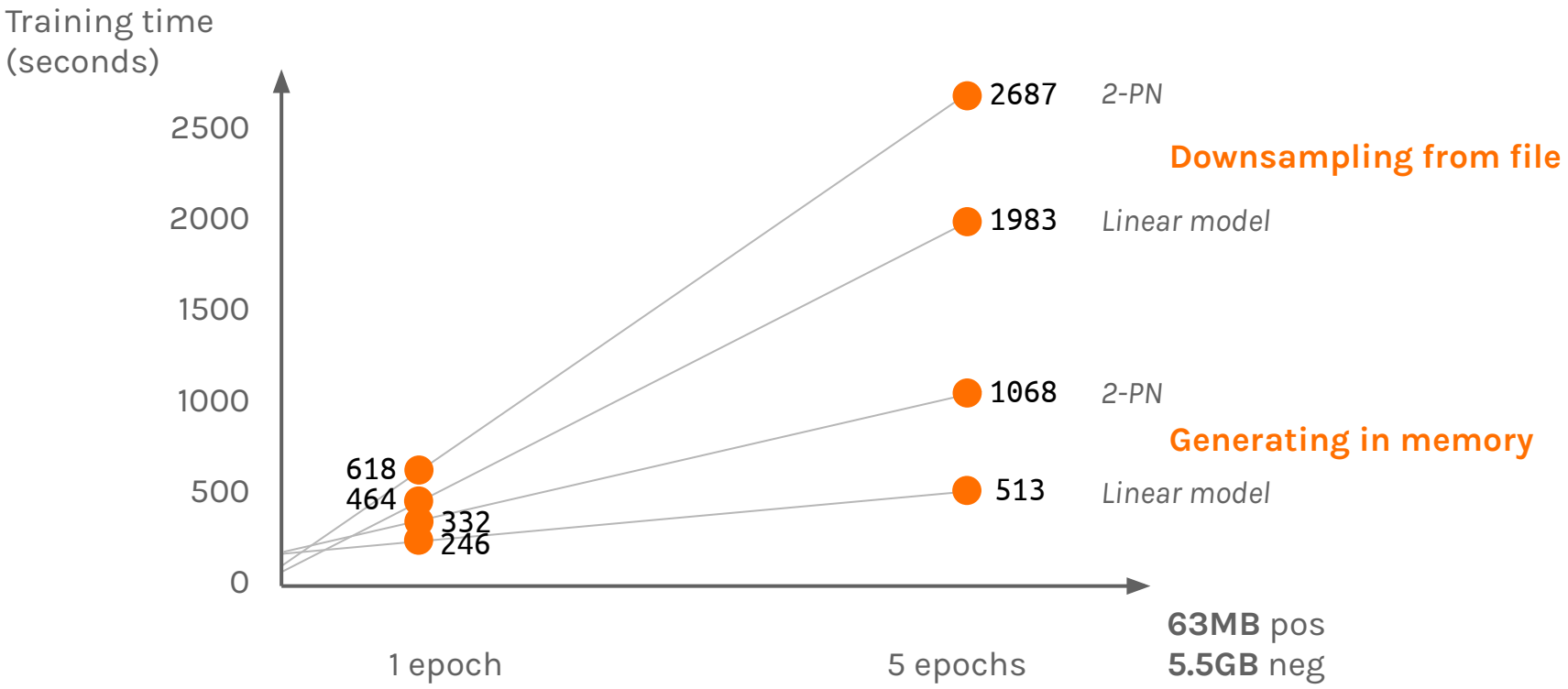
Fake example generation

No point making the fake examples on disk

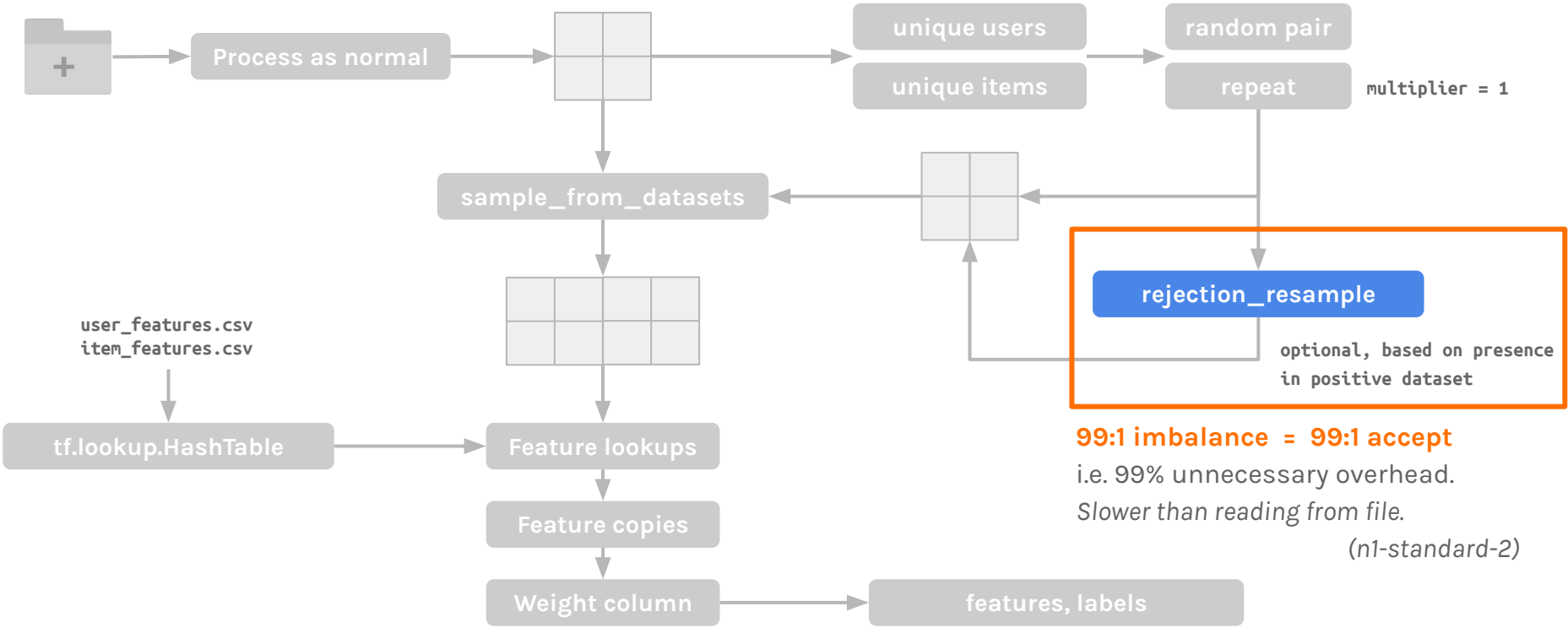
Inner workings



Speedup measurements



Inner workings



99:1 imbalance = 99:1 accept

i.e. 99% unnecessary overhead.

Slower than reading from file.

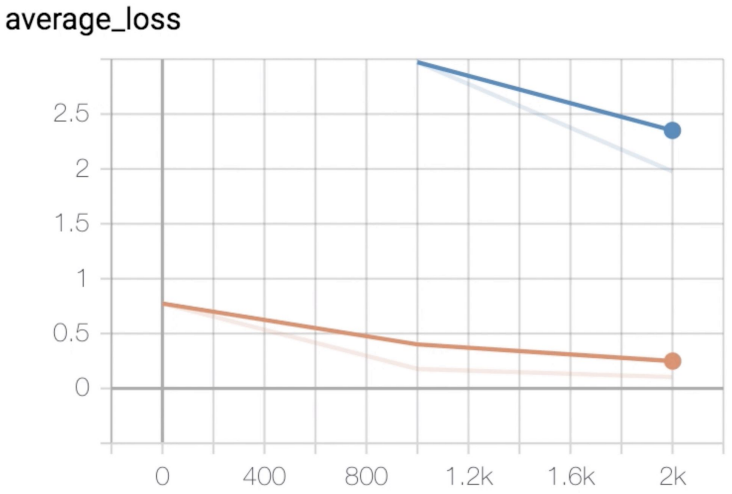
(n1-standard-2)

Working examples

1. **Propensity Modelling** - Acquire Valued Shoppers Dataset

2. **Recommender Systems** - Million Songs Dataset

```
.
├── ai-platform
│   ├── __init__.py
│   ├── setup.py
│   └── trainer
│       ├── __init__.py
│       └── task.py
├── ai-platform-deploy.sh
├── ai-platform-predict.sh
├── ai-platform-train.sh
├── local-ai-platform-train.sh
├── local-predict-evaluate.sh
├── local-train.sh
└── vocab
    ├── songs.csv
    └── users.csv
```



Wrapping up

Final thoughts 💡

Other sampling methods – random replication, SMOTE etc.

Dataset pipeline optimizations – see yesterday's talk by Taylor Robie + Priya Gupta

Sampling is meaningful – see "inverse probability weighting" in causal inference

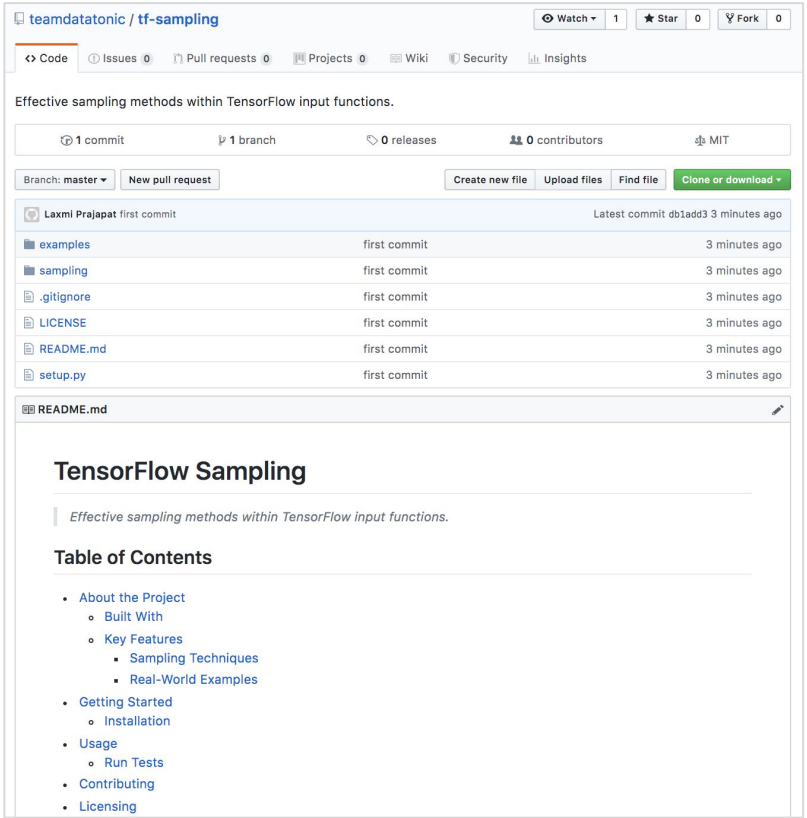
TL;DL 🙉

github.com/teamdatatonic/tf-sampling

datatonic.com

@teamdatatonic

laxmi-prajapat
wjkf



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Effective sampling methods within TensorFlow input functions

Add to Your Schedule
Add Comment or Question

Laxmi Prajapat (Datatonic), William Fletcher (Datatonic)
11:50am–12:30pm Thursday, October 31, 2019
Location: Grand Ballroom H
Applications

Who is this presentation for?

- Machine learning practitioners, data scientists, and ML engineers

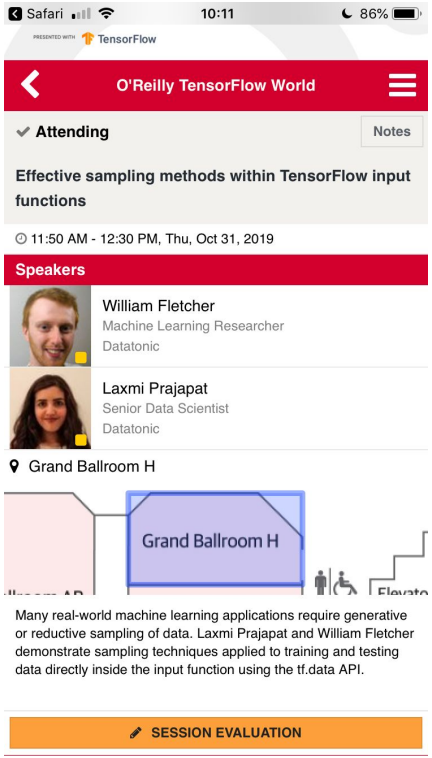
Level

Intermediate

Description

Many real-world machine learning applications require generative or reductive sampling of data. At training time this may be to deal with class imbalance (e.g., rarity of positives in a binary classification problem or a sparse user-item interaction matrix) or to augment the data stored on file; it may also simply be a matter of efficiency. Laxmi Prajapat and William Fletcher explore some sampling techniques in the context of recommender systems, using tools available in the tf.data API, and detail which methods are beneficial with given data and hardware demands. They present quantitative results, along with a closer examination of potential pros and cons.

O'Reilly Events App



+datatonic

Thank you for listening! 👋