pyradigm Documentation

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Contents:

Pyradigm is a PYthon based data structure to ease and improve Dataset's InteGrity in Machine learning workflows.

CHAPTER 1

About

Background

A common problem for machine learning developers is keeping track of the source of the features extracted, and to ensure integrity of the dataset (e.g. not getting data mixed up from different subjects and/or classes). This is incredibly hard as the number of projects grow, or personnel changes are frequent. These aspects can break the chain of hyper-local info about various datasets, such as where did the original data come from, how was it processed or quality controlled, how was it put together, by who and what does some columns in the table mean etc. This package provides a Python data structure to encapsulate a machine learning dataset with key info greatly suited for neuroimaging applications (or any other domain), where each sample needs to be uniquely identified with a subject ID (or something similar). Key-level correspondence across data, labels (e.g. 1 or 2), classnames (e.g. 'healthy', 'disease') and the related helps maintain data integrity, in addition to offering a way to easily trace back to the sources from where the features have been originally derived.

Context

For users of Panadas, some of the elements in *pyradigm*'s API/interface may look familiar. However, the aim of this data structure is not to offer an alternative to pandas, but to ease the machine learning workflow for neuroscientists by 1) offering several well-knit methods and useful attributes specifically geared towards neuroscience research, 2) aiming to offer utilities that combines multiple or advanced patterns of routine dataset handling and 3) using a more accessible language (compared to hard to read pandas docs aimed at econometric audience) to better cater to neuroscience developers (esp. the novice).

Check the *Usage* and *API Reference* pages, and let me know your comments.

Thanks for checking out. Your feedback will be appreciated.

CHAPTER 2

Installation

Pyradigm can easily be installed with a single command:

```
pip install pyradigm
```

If you lack `sudo` access, try

```
pip install pyradigm --user
```

Requirements

- Packages: `numpy`
- Supported versions: 2.7, 3.5 and 3.6

CHAPTER 3

API Reference

A tutorial-like presentation is available at *Usage*, using the following API.

class pyradigm.**MLDataset**(*filepath=None*, *in_dataset=None*, *data=None*, *labels=None*, *classes=None*, *description=''*, *feature_names=None*)

Bases: object

An ML dataset to ease workflow and maintain integrity.

add_classes(*classes*)

Helper to rename the classes, if provided by a dict keyed in by the orignal keys

classes [dict] Dict of class named keyed in by sample IDs.

TypeError If classes is not a dict.

ValueError If all samples in dataset are not present in input dict, or one of they samples in input is not recognized.

add_sample(*sample_id*, *features*, *label*, *class_id=None*, *feature_names=None*)

Adds a new sample to the dataset with its features, label and class ID.

This is the preferred way to construct the dataset.

sample_id [str, int] The identifier that uniquely identifies this sample.

features [list, ndarray] The features for this sample

label [int, str] The label for this sample

class_id [int, str] The class for this sample. If not provided, label converted to a string becomes its ID.

feature_names [list] The names for each feature. Assumed to be in the same order as *features*

ValueError If *sample_id* is already in the MLDataset, or If dimensionality of the current sample does not match the current, or If *feature_names* do not match existing names

TypeError If sample to be added is of different data type compared to existing samples.

class_set
Set of unique classes in the dataset.

class_sizes
Returns the sizes of different objects in a Counter object.

classes
Identifiers (sample IDs, or sample names etc) forming the basis of dict-type MLDataset.

data
data in its original dict form.

data_and_labels()
Dataset features and labels in a matrix form for learning.

Also returns sample_ids in the same order.

data_matrix [ndarray] 2D array of shape [num_samples, num_features] with features corresponding row-wise to sample_ids

labels [ndarray] Array of numeric labels for each sample corresponding row-wise to sample_ids

sample_ids [list] List of sample ids

del_sample(*sample_id*)
Method to remove a sample from the dataset.

sample_id [str] sample id to be removed.

UserWarning If sample id to delete was not found in the dataset.

description
Text description (header) that can be set by user.

dtype
number of features in each sample.

extend(*other*)
Method to extend the dataset vertically (add samples from anotehr dataset).

other [MLDataset] second dataset to be combined with the current (different samples, but same dimensionality)

TypeError if input is not an MLDataset.

feature_names
Returns the feature names as an numpy array of strings.

get_class(*class_id*)
Returns a smaller dataset belonging to the requested classes.

class_id [str] identifier of the class to be returned.

MLDataset With subset of samples belonging to the given class.

ValueError If one or more of the requested classes do not exist in this dataset. If the specified id is empty or None

get_feature_subset(*subset_idx*)
Returns the subset of features indexed numerically.

subset_idx [list, ndarray] List of indices to features to be returned

MLDataset [MLDataset] with subset of features requested.

UnboundLocalError If input indices are out of bounds for the dataset.

get_subset(*subset_ids*)
Returns a smaller dataset identified by their keys/sample IDs.

subset_ids [list] List od sample IDs to extracted from the dataset.

sub-dataset [MLDataset] sub-dataset containing only requested sample IDs.

glance(*nitems=5*)
Quick and partial glance of the data matrix.

nitems [int] Number of items to glance from the dataset. Default : 5

dict

keys
Sample identifiers (strings) forming the basis of MLDataset (same as sample_ids)

static **keys_with_value**(*dictionary*, *value*)
Returns a subset of keys from the dict with the value supplied.

label_set
Set of labels in the dataset corresponding to class_set.

labels
Returns the array of labels for all the samples.

num_classes
Total number of classes in the dataset.

num_features
number of features in each sample.

num_samples
number of samples in the entire dataset.

random_subset(*perc_in_class=0.5*)
Returns a random sub-dataset (of specified size by percentage) within each class.

perc_in_class [float] Fraction of samples to be taken from each class.

subdataset [MLDataset] random sub-dataset of specified size.

random_subset_ids(*perc_per_class=0.5*)
Returns a random subset of sample ids (of specified size by percentage) within each class.

perc_per_class [float] Fraction of samples per class

subset [list] Combined list of sample ids from all classes.

ValueError If no subjects from one or more classes were selected.

UserWarning If an empty or full dataset is requested.

random_subset_ids_by_count(*count_per_class=1*)

Returns a random subset of sample ids of specified size by count, within each class.

count_per_class [int] Exact number of samples per each class.

subset [list] Combined list of sample ids from all classes.

sample_ids
Sample identifiers (strings) forming the basis of MLDataset (same as keys).

sample_ids_in_class(*class_id*)
Returns a list of sample ids belonging to a given class.

class_id [str] class id to query.

subset_ids [list] List of sample ids belonging to a given class.

save(*file_path*)
Method to save the dataset to disk.

file_path [str] File path to save the current dataset to

IOError If saving to disk is not successful.

summarize_classes()
Summary of classes: names, numeric labels and sizes

tuple : class_set, label_set, class_sizes

class_set [list] List of names of all the classes

label_set [list] Label for each class in class_set

class_sizes [list] Size of each class (number of samples)

train_test_split_ids(*train_perc=None*, *count_per_class=None*)
Returns two disjoint sets of sample ids for use in cross-validation.

Offers two ways to specify the sizes: fraction or count. Only one access method can be used at a time.

train_perc [float] fraction of samples from each class to build the training subset.

count_per_class [int] exact count of samples from each class to build the training subset.

train_set [list] List of ids in the training set.

test_set [list] List of ids in the test set.

ValueError If the fraction is outside open interval (0, 1), or If counts are outside larger than the smallest class, or If unrecongized format is provided for input args, or If the selection results in empty subsets for either train or test sets.

CHAPTER 4

Usage

A tutorial-like example is given in the following Jupyter notebook:

Pyradigm Example,

which is reproduced here for your convenience.

Table of Contents

Illustration of Pyradigm's utility via examples and their use-cases

This class is greatly suited for neuroimaging applications (or any other domain), where each sample needs to be uniquely identified with a subject ID (or something similar).

Key-level correspondence across data, labels (1 or 2), classnames ('healthy', 'disease') and the related helps maintain data integrity and improve the provenance, in addition to enabling traceback to original sources from where the features have been originally derived.

Just to given you a concrete examples, let's look at how an ML dataset is handled traditionally.

You have a matrix X of size n x p, with n samples and p features, and a vector y containing the target values (or class labels or class identifiers). This X and y serves as training (and test set) for a classifier like SVM to fit the data X to match y as accurately as possible.

Let's get a little more concrete:

```
import sys, os
import numpy as np
import matplotlib
%matplotlib
%matplotlib inline
import matplotlib.pyplot as plt

n = 10 # number of samples
p = 3  # number of features

X = np.random.random([n, p]) # random data for illustration
y = [1]*5 + [2]*5            # random labels ...

np.set_printoptions(precision=2) # save some screen space
print 'X : \n', X
print 'y : \n', y
```

```
Using matplotlib backend: TkAgg
X :
[[ 0.64  0.48  0.88]
 [ 0.19  0.05  0.12]
 [ 0.13  0.1   0.68]
 [ 0.99  0.19  0.39]
 [ 0.86  0.36  0.91]
 [ 0.83  0.98  0.32]
 [ 0.86  0.35  0.3 ]
 [ 0.32  0.65  0.83]
 [ 0.6   0.75  0.53]
 [ 0.12  0.52  0.41]]
y :
[1, 1, 1, 1, 1, 2, 2, 2, 2, 2]
```

Almost all the machine learning toolboxes take their input in this form: X and y, regardless of the original source that produced these features in the first place.

This is all fine if all you ever wanted to do is to extract some features, do some machine learning and dispose these features away!

** But this is almost never the case!**

Because it doesn't simply end there.

At a minimum, I often need to know * which samples are misclassified - meaning you need to know what the identifiers are and not simply their row indices in X? * what are the charecteristics of those samples? * what classes do they belong to?

And all this info needs to be obtained * without having to write lots of code connecting few non-obvious links to disparate sources of data (numerical features X, and sample identifiers in a CSV file) to find the relevant info * without having to track down who or which method originally produced these features * how the previous personnel or grad student organized the whole dataset, if you haven't generated the features yourself from scratch

And if you are like me, you would be thinking about how would you organize your workflow such that the aforementioned tasks can be accomplished with ease.

This data structure attempts to accomplish that with ease. By always organizing the extracted features keyed-in into a dictionary with their *sample id*, and other important info such as *target values* and other identified info. This, by definition, preserves the integrity of the data (inability to incorrectly label samples etc).

No, this data structure doesn't offer the full provenance tracking, which is quite a challenging problem. But it tries make your life a little easier in your ML workflows.

An example application is shown below, touching upon the following topics:

- Motivation
- Constructing a dataset
- Attributes
- Iteration over samples
- Subset selection
- Saving/reloading a dataset (Serialization)
- Combining multiple datasets and arithmetic on useful subsets within datasets
- Exporting to numpy and portability (e.g. with sklearn)

Improting the necessary modules and our fancy class definition:

```
from pyradigm import MLDataset
```

We can now instantiate it and give it a description:

```
dataset = MLDataset()
dataset.description = 'ADNI1 baseline: cortical thickness features from Freesurfer v4.
↪3, QCed.'
```

```
dataset
```

```
ADNI1 baseline: cortical thickness features from Freesurfer v4.3, QCed.
Empty dataset.
```

You can see the dataset some description attached to it, however we know it is empty. This can be verified in a boolean context as shown below:

```
bool(dataset)
```

```
False
```

Let's add samples to this dataset which is when this dataset implementation becomes really handy. Before we do that, we will define some convenience routines defined to just illustrate a simple yet common use of this dataset.

So now we have IO routines to read the data for us. Let's define where the data will come from:

```
work_dir = '/project/ADNI/FreesurferThickness_v4p3'
class_set = ['Cntrl', 'Alzmr', 'MCI']
class_sizes = [15, 12, 18]
```

This would obviously change for your applications, but this has sufficient properties to illustrate the point.

Let's look at what methods this dataset offers us:

```
dir(dataset)
```

```
['add_classes',
 'add_sample',
 'class_set',
 'class_sizes',
 'classes',
 'data',
 'data_and_labels',
 'del_sample',
 'description',
 'extend',
 'get_class',
 'get_feature_subset',
 'get_subset',
 'glance',
 'keys',
 'num_classes',
 'num_features',
 'num_samples',
 'random_subset',
 'random_subset_ids',
 'random_subset_ids_by_count',
 'sample_ids',
 'sample_ids_in_class',
 'save',
 'summarize_classes',
 'train_test_split_ids']
```

Constructor

You can see there few methods such as add_sample, get_subset etc: important method being add_sample, which is key to constructing this dataset. Let's go ahead and some samples:

```
import random
from datetime import datetime
random.seed(datetime.now())

def read_target_list(class_name, class_size):
    "Generates a random target list. In reality, you would do something like the␣
↪commented code below."
    target_list = list()
    for idx in range(class_size):
        target_list.append('{}{:04d}'.format(class_name[0],np.random.randint(1000)))

    return target_list

#     target_list_path = os.path.join(work_dir,'scripts','test_sample.{}'.
↪format(class_name))
#     with open(target_list_path,'r') as tf:
#         target_list = tf.readlines()
#         target_list = [sub.strip() for sub in target_list]
```

```
for class_index, class_id in enumerate(class_set):
    print('Working on class {:>5}'.format(class_id))

    target_list = read_target_list(class_id,class_sizes[class_index])
    for subj_id in target_list:
        print('\t reading subject {:>15}'.format(subj_id))
        thickness_wb = get_features(work_dir, subj_id)

        # adding the sample to the dataset
        dataset.add_sample(subj_id, thickness_wb, class_index, class_id)
```

```
Working on class Cntrl
     reading subject           C0102
     reading subject           C0589
     reading subject           C0246
     reading subject           C0776
     reading subject           C0483
     reading subject           C0622
     reading subject           C0547
     reading subject           C0296
     reading subject           C0981
     reading subject           C0782
     reading subject           C0767
     reading subject           C0451
     reading subject           C0065
     reading subject           C0592
     reading subject           C0665
Working on class Alzmr
     reading subject           A0502
     reading subject           A0851
     reading subject           A0402
     reading subject           A0460
     reading subject           A0166
     reading subject           A0264
     reading subject           A0866
     reading subject           A0375
     reading subject           A0971
     reading subject           A0624
     reading subject           A0153
     reading subject           A0735
Working on class   MCI
     reading subject           M0450
     reading subject           M0207
     reading subject           M0647
     reading subject           M0752
     reading subject           M0037
     reading subject           M0171
     reading subject           M0173
     reading subject           M0733
     reading subject           M0551
     reading subject           M0698
     reading subject           M0256
     reading subject           M0642
     reading subject           M0924
     reading subject           M0543
     reading subject           M0751
     reading subject           M0950
     reading subject           M0143
```

```
    reading subject           M0670
```

Nice. Isn't it?

So what's nice about this, you say? *The simple fact that you are constructing a dataset as you read the data* in its most elemental form (in the units of the dataset such as the subject ID in our neuroimaging application). You're done as soon as you're done reading the features from disk.

What's more - you can inspect the dataset in an intuitive manner, as shown below:

```
dataset
```

```
ADNI1 baseline: cortical thickness features from Freesurfer v4.3, QCed.
45 samples and 4 features.
Class Cntrl : 15 samples.
Class   MCI : 18 samples.
Class Alzmr : 12 samples.
```

Even better, right? No more too much typing of several commands to get the complete and concise sense of the dataset.

Convenient attributes

If you would like, you can always get more specific information, such as:

```
dataset.num_samples
```

```
45
```

```
dataset.num_features
```

```
4
```

```
dataset.class_set
```

```
['Cntrl', 'MCI', 'Alzmr']
```

```
dataset.class_sizes
```

```
Counter({'Alzmr': 12, 'Cntrl': 15, 'MCI': 18})
```

```
dataset.class_sizes['Cntrl']
```

```
15
```

If you'd like to take a look data inside for few subjects - shall we call it a glance?

```
dataset.glance()
```

```
{'C0102': array([ 0.06,  0.16,  0.8 ,  0.9 ]),
 'C0246': array([ 0.93,  0.91,  0.09,  0.62]),
 'C0483': array([ 0.27,  0.97,  0.84,  0.63]),
```

```
 'C0589': array([ 0.34,  0.06,  0.33,  0.24]),
 'C0776': array([ 0.67,  0.06,  0.08,  0.03])}
```

We can control the number of items to glance, by passing a number to dataset.glance() method:

```
dataset.glance(2)
```

```
{'C0102': array([ 0.06,  0.16,  0.8 ,  0.9 ]),
 'C0589': array([ 0.34,  0.06,  0.33,  0.24])}
```

Or you may be wondering what are the subject IDs in the dataset.. here they are:

```
dataset.sample_ids
```

```
['C0102',
 'C0589',
 'C0246',
 'C0776',
 'C0483',
 'C0622',
 'C0547',
 'C0296',
 'C0981',
 'C0782',
 'C0767',
 'C0451',
 'C0065',
 'C0592',
 'C0665',
 'A0502',
 'A0851',
 'A0402',
 'A0460',
 'A0166',
 'A0264',
 'A0866',
 'A0375',
 'A0971',
 'A0624',
 'A0153',
 'A0735',
 'M0450',
 'M0207',
 'M0647',
 'M0752',
 'M0037',
 'M0171',
 'M0173',
 'M0733',
 'M0551',
 'M0698',
 'M0256',
 'M0642',
 'M0924',
 'M0543',
 'M0751',
 'M0950',
```

```
 'M0143',
 'M0670']
```

Iteration over samples

Thanks to its dictionary based implementation, data for a given sample '007_S_1248' can simply be obtained by:

```
sample_id = dataset.sample_ids[20]
print sample_id, dataset.data[sample_id]
```

```
A0264 [ 0.63  0.14  0.23  0.15]
```

we can easily iterate over all the samples to obtain their data as well as class labels. Let's see it in action:

```
for sample, features in dataset.data.items():
    print "{} : {:>10} : {}".format(sample, dataset.classes[sample], features)
```

```
C0102 :      Cntrl : [ 0.06  0.16  0.8   0.9 ]
C0589 :      Cntrl : [ 0.34  0.06  0.33  0.24]
C0246 :      Cntrl : [ 0.93  0.91  0.09  0.62]
C0776 :      Cntrl : [ 0.67  0.06  0.08  0.03]
C0483 :      Cntrl : [ 0.27  0.97  0.84  0.63]
C0622 :      Cntrl : [ 0.4   0.53  0.08  0.53]
C0547 :      Cntrl : [ 0.66  0.49  0.45  0.68]
C0296 :      Cntrl : [ 0.32  0.33  0.21  0.52]
C0981 :      Cntrl : [ 0.51  0.09  0.93  0.91]
C0782 :      Cntrl : [ 0.12  0.42  0.2   0.65]
C0767 :      Cntrl : [ 0.59  0.18  0.26  0.77]
C0451 :      Cntrl : [ 0.2   0.08  0.25  0.18]
C0065 :      Cntrl : [ 1.    0.56  0.71  0.6 ]
C0592 :      Cntrl : [ 0.05  0.48  0.28  0.57]
C0665 :      Cntrl : [ 0.87  0.07  0.62  0.68]
A0502 :      Alzmr : [ 0.57  0.69  0.23  0.17]
A0851 :      Alzmr : [ 0.06  0.71  0.86  0.66]
A0402 :      Alzmr : [ 0.9   0.54  0.6   0.2 ]
A0460 :      Alzmr : [ 0.75  0.71  0.19  0.46]
A0166 :      Alzmr : [ 0.14  0.54  0.01  0.09]
A0264 :      Alzmr : [ 0.63  0.14  0.23  0.15]
A0866 :      Alzmr : [ 0.55  0.5   0.97  0.13]
A0375 :      Alzmr : [ 0.89  0.66  0.53  0.44]
A0971 :      Alzmr : [ 0.41  0.86  0.86  0.58]
A0624 :      Alzmr : [ 0.74  0.01  0.13  0.41]
A0153 :      Alzmr : [ 0.82  0.37  0.81  0.52]
A0735 :      Alzmr : [ 0.79  0.02  0.59  0.57]
M0450 :        MCI : [ 0.04  0.51  0.44  0.44]
M0207 :        MCI : [ 0.76  0.65  0.53  0.43]
M0647 :        MCI : [ 0.63  0.07  0.41  0.62]
M0752 :        MCI : [ 0.3   0.92  0.64  0.64]
M0037 :        MCI : [ 0.07  0.82  0.57  0.39]
M0171 :        MCI : [ 0.38  0.43  0.22  0.22]
M0173 :        MCI : [ 0.74  0.81  0.63  0.33]
M0733 :        MCI : [ 0.64  0.93  0.13  0.13]
M0551 :        MCI : [ 0.79  0.03  0.28  0.29]
M0698 :        MCI : [ 1.    0.54  0.71  0.72]
M0256 :        MCI : [ 0.26  0.58  0.24  0.44]
```

```
M0642 :         MCI : [ 0.16  0.93  0.74  0.44]
M0924 :         MCI : [ 0.39  0.41  0.25  0.19]
M0543 :         MCI : [ 0.83  0.51  0.06  0.86]
M0751 :         MCI : [ 0.11  0.38  0.55  0.57]
M0950 :         MCI : [ 0.77  1.    0.03  0.54]
M0143 :         MCI : [ 0.84  0.12  0.94  0.9 ]
M0670 :         MCI : [ 0.57  0.72  0.97  0.33]
```

Thanks to the choice of the OrderedDict() for each of the data, classes and labels, the order of sample addition is retained. Hence the correspondence across samples in the dataset not only key-wise (by the sample id), but also index-wise.

Another example to illustrate how one can access the subset of features e.g. cortical thickness for a particular region of interest (say posterior cingulate gyrus) is below:

```
# let's make a function to return the indices for the ROI
def get_ROI_indices(ctx_label=None):
    if ctx_label == 'post_cingulate_gyrus':
        return xrange(2) # dummy for now
    else:
        return xrange(dataset.num_features) # all the features
```

Now the following code iterates over each sample and prints the average cortical thickness in the specific ROI:

```
avg_thickness = dict()
for sample, features in dataset.data.items():
    avg_thickness[sample] = np.mean(features[get_ROI_indices('post_cingulate_gyrus')])
    print "{} {:>10}  {:.2f}".format(sample, dataset.classes[sample], avg_
↪thickness[sample] )
```

```
C0102       Cntrl  0.11
C0589       Cntrl  0.20
C0246       Cntrl  0.92
C0776       Cntrl  0.36
C0483       Cntrl  0.62
C0622       Cntrl  0.46
C0547       Cntrl  0.58
C0296       Cntrl  0.32
C0981       Cntrl  0.30
C0782       Cntrl  0.27
C0767       Cntrl  0.39
C0451       Cntrl  0.14
C0065       Cntrl  0.78
C0592       Cntrl  0.27
C0665       Cntrl  0.47
A0502       Alzmr  0.63
A0851       Alzmr  0.39
A0402       Alzmr  0.72
A0460       Alzmr  0.73
A0166       Alzmr  0.34
A0264       Alzmr  0.38
A0866       Alzmr  0.52
A0375       Alzmr  0.77
A0971       Alzmr  0.63
A0624       Alzmr  0.37
A0153       Alzmr  0.60
A0735       Alzmr  0.41
M0450         MCI  0.27
```

```
M0207        MCI  0.71
M0647        MCI  0.35
M0752        MCI  0.61
M0037        MCI  0.44
M0171        MCI  0.40
M0173        MCI  0.77
M0733        MCI  0.78
M0551        MCI  0.41
M0698        MCI  0.77
M0256        MCI  0.42
M0642        MCI  0.54
M0924        MCI  0.40
M0543        MCI  0.67
M0751        MCI  0.25
M0950        MCI  0.88
M0143        MCI  0.48
M0670        MCI  0.64
```

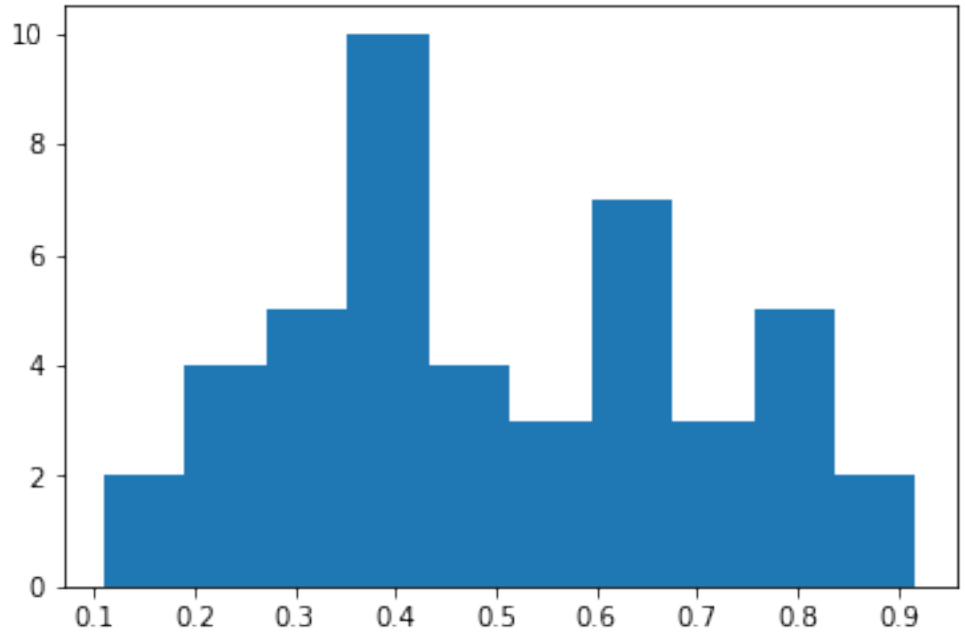
Let's make a bar plot with the just computed numbers:

```
avg_thickness.values()
```

```
[0.77419317627756634,
 0.274568477535865,
 0.52456600133438958,
 0.10988851639242048,
 0.9173077195848538,
 0.67215738787506218,
 0.78073124498823832,
 0.34319836534987225,
 0.36466613282060334,
 0.40681014189609904,
 0.77075603570250351,
 0.2672873843477836,
 0.3979586538904154,
 0.41057586141404956,
 0.24687851327074922,
 0.54467083900315094,
 0.63490203247374355,
 0.26986173065211588,
 0.35136691981491958,
 0.38601865045543871,
 0.57797853866707183,
 0.60791732543673671,
 0.41977590274138665,
 0.77760363600740945,
 0.13930958880564798,
 0.37157580525743594,
 0.47605248855507931,
 0.70524233745725029,
 0.59765881251299779,
 0.71813681129356643,
 0.47074880969405297,
 0.38743449904671035,
 0.46419007761963849,
 0.6215589295056978,
 0.1986440118547006,
 0.29957866524180221,
```

```
 0.32234483765792193,
 0.7273392116680899,
 0.63002920038567556,
 0.88383304529760121,
 0.40282387477340864,
 0.44243699049296453,
 0.77499920202425088,
 0.38313913682247508,
 0.64471408195318269]
```

```
n, bins, patches = plt.hist(avg_thickness.values())
```



Remember as the original source of data was random, this has no units, property or meaning!

Subset selection

In addition to the structured way of obtaining the various properties of this dataset, this implementation really will come in handy when you have to slice and dice the dataset (with large number of classes and features) into smaller subsets (e.g. for binary classification). Let's see how we can retrieve the data for a single class:

```
ctrl = dataset.get_class('Cntrl')
```

That's it, obtaining the data for a given class is a simple call away.

Now let's see what it looks like:

```
ctrl
```

```
 Subset derived from: ADNI1 baseline: cortical thickness features from Freesurfer v4.
↪3, QCed.
15 samples and 4 features.
Class Cntrl : 15 samples.
```

Even with updated description automatically, to indicate its history. Let's see some data from controls:

```
ctrl.glance(2)
```

```
{'C0102': array([ 0.06,  0.16,  0.8 ,  0.9 ]),
 'C0589': array([ 0.34,  0.06,  0.33,  0.24])}
```

We can also query a random subset of samples for manual inspection or cross-validation purposes. For example:

```
random_subset = dataset.random_subset(perc_in_class=0.3)
random_subset
```

```
 Subset derived from: ADNI1 baseline: cortical thickness features from Freesurfer v4.
↪3, QCed.
12 samples and 4 features.
Class Cntrl : 4 samples.
Class   MCI : 5 samples.
Class Alzmr : 3 samples.
```

You can see which samples were selected:

```
random_subset.sample_ids
```

```
['C0296',
 'C0981',
 'C0592',
 'C0665',
 'A0402',
 'A0460',
 'A0866',
 'M0207',
 'M0752',
 'M0924',
 'M0543',
 'M0143']
```

You can verify that it is indeed random by issuing another call:

```
# supplying a new seed everytime to ensure randomization
from datetime import datetime
dataset.random_subset(perc_in_class=0.3).sample_ids
```

```
['C0102',
 'C0589',
 'C0547',
 'C0767',
 'A0851',
 'A0166',
 'A0375',
 'M0450',
 'M0207',
 'M0551',
 'M0698',
 'M0751']
```

Let's see how we can retrieve specific samples by their IDs (for which there are many use cases):

```
data = dataset.get_subset(dataset.sample_ids[1:20])
data
```

```
 Subset derived from: ADNI1 baseline: cortical thickness features from Freesurfer v4.
↪3, QCed.
19 samples and 4 features.
Class Cntrl : 14 samples.
Class Alzmr : 5 samples.
```

So as simple as that.

Cross-validation

If you would like to develop a variant of cross-validation, and need to obtain a random split of the dataset to obtain training and test sets, it is as simple as:

```
train_set, test_set = dataset.train_test_split_ids( train_perc = 0.5)
```

This method returns two sets of sample ids corresponding to training set (which 50% of samples from all classes in the dataset) and the rest in test_set. Let's see what they have:

```
train_set, test_set
```

```
(['C0592',
  'C0622',
  'C0782',
  'C0776',
  'C0451',
  'C0483',
  'C0981',
  'M0752',
  'M0173',
  'M0543',
  'M0642',
  'M0751',
  'M0256',
  'M0207',
  'M0143',
  'M0924',
  'A0851',
  'A0402',
  'A0502',
  'A0971',
  'A0264',
  'A0624'],
 ['M0450',
  'A0866',
  'C0102',
  'C0246',
  'M0733',
  'A0166',
  'M0551',
  'M0698',
```

```
  'A0735',
  'M0647',
  'C0547',
  'C0065',
  'A0153',
  'C0665',
  'C0767',
  'C0589',
  'C0296',
  'A0460',
  'A0375',
  'M0171',
  'M0950',
  'M0037',
  'M0670'])
```

We can also get a train/test split by specifying an exact number of subjects we would like from each class (e.g. when you would like to avoid class imbalance in the training set):

```
train_set, test_set = dataset.train_test_split_ids( count_per_class = 3)
```

Let's see what the training set contains - we expect 3*3 =9 subjects :

```
train_set
```

```
['C0776',
 'C0065',
 'C0483',
 'M0173',
 'M0752',
 'M0698',
 'A0166',
 'A0624',
 'A0460']
```

We can indeed verify that is the case, by creating a new smaller dataset from that list of ids and getting a summary:

```
training_dataset = dataset.get_subset(train_set)
training_dataset
```

```
 Subset derived from: ADNI1 baseline: cortical thickness features from Freesurfer v4.
↪3, QCed.
9 samples and 4 features.
Class Cntrl : 3 samples.
Class   MCI : 3 samples.
Class Alzmr : 3 samples.
```

Another programmatic way to look into different classes is this:

```
class_set, label_set, class_sizes = training_dataset.summarize_classes()
class_set, label_set, class_sizes
```

```
(['Cntrl', 'MCI', 'Alzmr'], [0, 2, 1], array([ 3.,  3.,  3.]))
```

which returns all the classes that you could iterative over.

Using these two lists, we can easily obtain subset datasets, as illustrated below.

```
dataset
```

```
ADNI1 baseline: cortical thickness features from Freesurfer v4.3, QCed.
45 samples and 4 features.
Class Cntrl : 15 samples.
Class   MCI : 18 samples.
Class Alzmr : 12 samples.
```

```
binary_dataset = dataset.get_class(['Cntrl','Alzmr'])
binary_dataset
```

```
 Subset derived from: ADNI1 baseline: cortical thickness features from Freesurfer v4.
↪3, QCed.
27 samples and 4 features.
Class Cntrl : 15 samples.
Class Alzmr : 12 samples.
```

How about selecting a subset of features from all samples?

```
binary_dataset.get_feature_subset(xrange(2))
```

```
Subset features derived from:

 Subset derived from: ADNI1 baseline: cortical thickness features from Freesurfer v4.
↪3, QCed.
27 samples and 2 features.
Class Cntrl : 15 samples.
Class Alzmr : 12 samples.
```

Great. Isn't it? You can also see the two-time-point history (initial subset in classes, followed by a subset in features).

Serialization

Once you have this dataset, you can save and load these trivially using your favourite serialization module. Let's do some pickling:

```
out_file = os.path.join(work_dir,'binary_dataset_Ctrl_Alzr_Freesurfer_thickness_v4p3.
↪pkl')
binary_dataset.save(out_file)
```

That's it - it is saved.

Let's reload it from disk and make sure we can indeed retrieve it:

```
reloaded = MLDataset(filepath=out_file) # another form of the constructor!
```

```
Loading the dataset from: /project/ADNI/FreesurferThickness_v4p3/binary_dataset_Ctrl_
↪Alzr_Freesurfer_thickness_v4p3.pkl
```

```
reloaded
```

```
 Subset derived from: ADNI1 baseline: cortical thickness features from Freesurfer v4.
↪3, QCed.
27 samples and 4 features.
Class Cntrl : 15 samples.
Class Alzmr : 12 samples.
```

Dataset Arithmetic

You might wonder how can you combine two different types of features (thickness and shape) from the dataset. Piece of cake, see below ...

To concatenat two datasets, first we make a second dataset:

```
dataset_two = MLDataset(in_dataset=dataset) # yet another constructor: in its copy␣
↪form!
```

How can you check if they are "functionally identical"? As in same keys, same data and classes for each key... Easy:

```
dataset_two == dataset
```

```
True
```

Now let's try the arithmentic:

```
combined = dataset + dataset_two
```

```
Identical keys found. Trying to horizontally concatenate features for each sample.
```

Great. The add method recognized the identical set of keys and performed a horiz cat, as can be noticed by the twice the number of features in the combined dataset:

```
combined
```

```
45 samples and 8 features.
Class Cntrl : 15 samples.
Class   MCI : 18 samples.
Class Alzmr : 12 samples.
```

We can also do some removal in similar fashion:

```
smaller = combined - dataset
```

```
C0102 removed.
C0589 removed.
C0246 removed.
C0776 removed.
C0483 removed.
C0622 removed.
C0547 removed.
C0296 removed.
C0981 removed.
C0782 removed.
C0767 removed.
C0451 removed.
```

```
C0065 removed.
C0592 removed.
C0665 removed.
A0502 removed.
A0851 removed.
A0402 removed.
A0460 removed.
A0166 removed.
A0264 removed.
A0866 removed.
A0375 removed.
A0971 removed.
A0624 removed.
A0153 removed.
A0735 removed.
M0450 removed.
M0207 removed.
M0647 removed.
M0752 removed.
M0037 removed.
M0171 removed.
M0173 removed.
M0733 removed.
M0551 removed.
M0698 removed.
M0256 removed.
M0642 removed.
M0924 removed.
M0543 removed.
M0751 removed.
M0950 removed.
M0143 removed.
M0670 removed.
```

Data structure is even producing a warning to let you know the resulting output would be empty! We can verify that:

```
bool(smaller)
```

```
False
```

Portability

This is all well and good. How does it interact with other packages out there, you might ask? It is as simple as you can imagine:

```
from sklearn import svm
clf = svm.SVC(gamma=0.001, C=100.)
data_matrix, target, sample_ids = binary_dataset.data_and_labels()
```

```
clf.fit(data_matrix, target)
```

```
SVC(C=100.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma=0.001, kernel='rbf',
```

```
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

There you have it, a simple example to show you the utility and convenience of this dataset.

CHAPTER 5

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