Rapid Time Serires Datasets Library

Efficient AI with Rust Lab

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1 Introduction

2 Binding and Design

Since our goal is to create a time series data library that is usable in Python, but implemented in Rust, we used PyO3 to create a Python binding for our Rust library. PyO3 is a Rust crate that allows you to write native Python modules in Rust. It provides a way to make Rust methods, types and classes available in Python by annotating Rust code with special macros, and building a library that can be imported in Python.

2.1 Passing data to Rust

Since our library is used in Python, users will have loaded a time series dataset into their Python environment, and then use our library on this data to prepare it for usage e.g. in machine learning tasks. As our library is implemented in Rust, we need to pass the data from Python to Rust somehow, to be able to operate on it.

PyO3 natively supports data-APIs from Python to Rust, where e.g. a Python list of floating point numbers can be passed to a Rust Vector. This native API operates py passing the data by value, and therefore creates a copy of the data on which the Rust implementation then works. Time series datasets can become quite large. Therefore, passing the data using the native API is slow, it takes around 9 seconds on a medium size dataset (the "ElectricityLoadDiagrams20112014" dataset, which has a size of 678.1 MB) on one of our modern machines. We use Rust for its superior performance, therefore having such a high overhead simply for passing the data to Rust, without performing any operations, is unacceptable.

We solved this problem by passing the data by reference. Natively, this would not be possible, but the Rust crate `numpy` offers a Rust API to `numpy` arrays, which makes passing data by reference from Python to Rust possible. Since in that case, we only need to pass a reference to where the data is stored, the passing is instantaneous and does not slow down the library in any way.

It has to be mentioned that this approach limits the library to only work with `numpy` arrays. By design, `numpy` arrays only consist of elements of the same type, and therefore only arrays of 64-bit floating point numbers are supported. But this is not a serious limitation, as time series data is typically represented as floating point numbers, and the PyTorch `DataLoader`, which is a standard way to load data in PyTorch for machine learning tasks, also only supports floating point data.

2.2 Interface design

The implementation supports two kinds of time series datasets: Forecasting datasets and classification datasets. Since the requirements for the two types of datasets are sufficiently different, we decided to implement them as separate classes. Nevertheless, our goal was to implement the offered preprocessing operations only once, and make them usable for both kinds of datasets.

For consistency of the data layout between the different kinds of datasets, data is expected to be passed as a 3D `numpy` array. The first dimension represents the number of instances. For forecasting datasets this is typically one, for classification datasets this is higher. The second dimension represents the number of timesteps, and the third dimension represents the number of features. This is a common way to represent time series data, and it allows for efficient processing in Rust.

The overall idea is that the class is to be used as a kind of pipeline, storing and manipulating the data internally. The user only passes a reference to the data in the constructor, and retrieves the ready results in the end, and does not have to worry about its storage in the process. For both kinds of datasets, that is, both classes, the interface and expected call order is almost the same, with only two differences in the method parameters. These will be explained in the following sections.

The overall structure of the pipeline looks as shown in Figure 1 (exemplary for a `ForecastingDataSet`, but it is almost equivalent for the `ClassificationDataSet` class):

```
# Create a ForecastingDataSet instance (pass data)
forecasting_data_set = ForecastingDataSet(data, 0.7, 0.2, 0.1)

# call the pipeline methods
forecasting_data_set.impute(ImputeStrategy.LeaveNaN)
forecasting_data_set.downsample(2)
forecasting_data_set.split()
forecasting_data_set.normalize()
forecasting_data_set.standardize()

# collect the results (returns the ready data)
forecasting_data_set_res = forecasting_data_set.collect(3, 1, 1)
```

Figure 1: Example usage of the `ForecastingDataSet` class

The overall pipeline workflow goes as follows:

1. The data is passed to Rust in the constructor, which instantiates the provided class. Additionally, the user specifies the proportions of the data that are to be used for training, validation, and testing.
2. If the user wants to impute the missing data, the `impute(strategy)` method can be called. Here, the user can specify the imputation strategy to be used.
3. If the user wants to downsample the data by some factor, the `downsample()` method is called.
4. Calling the `split()` method on `ForecastingDataSet`, no arguments have to be passed, since the split proportions are passed in the constructor. For classification strategies, the `split_strategy` that should be used can also be indicated.
5. If the user wants to normalize the data, the `normalize()` method is called.
6. If the user wants to standardize the data, the `standardize()` method is called.
7. To collect the results, the `collect()` method is called. For forecasting datasets, this method takes three arguments (`past_window`, `future_horizon`, `stride`), for classification datasets, this does not take arguments.

The `split()` and `collect()` operations are mandatory, since they're essential parts of the pipelines data-flow. The preprocessing operations `impute()`, `downsample()`, `normalize()`, and `standardize()` are optional. Note that, in a realistic use case, the user would choose to call either the `normalize()` or the `standardize()` method, but not both. The call order is expected to be as shown in the example. In case an incorrect call order is used that would lead to a loss of data integrity, an error is raised preventing the user from proceeding with the pipeline.

The difference between the interface of the `split()` method is due to the fact that for forecasting datasets, the temporal splitting strategy is the only valid one, while for classification datasets, the user can choose between in-order and random splitting - requiring a parameter. Similarly, the `collect()` method for forecasting datasets takes three additional parameters (`past_window`, `future_horizon`, `stride`) that are used to construct sliding windows from the data, while for classification datasets, no such parameters are needed, since the data is not converted into sliding windows.

2.3 Internal data handling

In the constructor, a reference to the data that is to be operated on is passed as a reference to a `numpy` array. This reference is then stored to the class. Since the data that is referenced is stored in the Python memory, this reference needs to be stored using a `Py<...>` smart pointer, which is a "GIL-independent reference to an object allocated on the Python heap" [Dev]. In subsequent method calls, where access to the data is needed, this reference is used to "bind" the data in Rust, which aquires the GIL (Global Interpreter Lock) to ensure that the data is not modified while it is being accessed.

As a general principle, we designed the library to copy data only when it is absolutely necessary. Apart from the `downsample()` operation, on which we'll elaborate in a later section, this is exactly once in the librarys data-flow. It is not possible to implement our functionality without copying the data at least once, since we offer splitting capabilities, which split the data into multiple independent arrays. Where the split and therefore the actual copying is performed is different for the two types of datasets.

Forecasting datasets For forecasting datasets, the `collect(past_window, future_horizon, stride)` method returns the data split into the three aforementioned parts (train, validation, test) and additionally converts them into sliding windows, using the specified parameters. This will be elaborated on in a later section. For now, it is only important to understand that in addition to splitting the data, it is also converted to a different format. This conversion must happen at the final step, just before returning the data. Otherwise, e.g. normalizing the data would cause a huge overhead, since in the process of constructing the sliding windows, data is possibly duplicated - and therefore all copies would have to be changed instead of just the original data.

But if we now actually split the data during the `split()` method, which requires a full copy of the data, and then construct the sliding windows during the `collect()` method which also requires copying the data, we would have to copy the data twice. To avoid this, for forecasting datasets, the `split()` method only computes the indices of the original full data array, where the split would be performed. No actual splitting - and therefore no copying of the data - is done yet. Since for forecasting data, a temporal split is the only valid splitting strategy, this index suffices to store an unambiguous division of the original array into the three parts. The actual split is performed in the `collect()` method, together with the construction of the sliding windows. Therefore, the data is only copied once in the implementation for forecasting datasets.

Classification datasets For classification datasets, the requirements look slightly different.

On the one hand, there are two valid splitting strategies: in-order and random splitting. While for in-order splitting, the instances are kept in the original order, which is the order in which they were passed, in random splitting they are randomly shuffled before being divided into three parts. As a consequence, for classification data using the random splitting strategy, simply storing the indices on which to split the data into three parts does not suffice anymore, since the re-ordering of the datapoints due to the shuffle would then be lost.

On the other hand, the data does not have to be converted into sliding windows, the format of returned values looks like the original data. In sum, this allows for an implementation of the data-flow that is different from the one of the forecasting data, but also only requires to copy the data once: The data can be split and copied into three separate arrays in the `split()` method. The `normalize()` and `standardize()` method then work on the copies of the data, and not on the original array. In the `collect()` method, the previously copied arrays are then simply returned directly, without having to be copied again. Hence, the data is only copied once in the implementation for classification datasets, too.

Generic interfaces for normalize and standardize At first glance, this now poses a problem to our goal to implement preprocessing operations only once, and use them for both kinds of datasets, since we have to call the `normalize()` and `standardize()` methods in very different scenarios: For forecasting datasets, the data remains in the original array, and only the split indices were computed. For classification data, the data is already split into three separate arrays.

But we found a way to use one single generic implementation for both cases: In the Rust `numpy` implementation, there are two kinds of arrays. The struct `Array<...>` represents an actual owned array. The struct `ArrayView<...>` on the other hands represents a view on an array, or possibly also on a part of it. Both of them are inheritants of the `ArrayBase<...>` class, which is one of the fundamental classes of the Rust `numpy` implementation. It offers an interface that allows to read and manipulate the underlying array, be it an actual owned array, or a view on another array.

Creating a view on a part of an array is highly efficient, since no data has to be copied. Hence, given the split indices of the original array, it is possible to create views on the three parts of

the array (train, validate and test) very easily for forecasting datasets. Using the generic parent class `ArrayBase<...>` as a parameter type, it is possible to make the `normalize()` and `standardize()` methods callable using both actual owned arrays and array views - mitigating the overhead of having to implement the functionality twice.

The method signature then looks as shown in Figure 2 (exemplary for `normalize()`, but it is the same for `standardize()`):

```
pub fn normalize<S>(
    train_view: &mut ArrayBase<S, Dim<[usize; 3]>>,
    val_view: &mut ArrayBase<S, Dim<[usize; 3]>>,
    test_view: &mut ArrayBase<S, Dim<[usize; 3]>>
) -> PyResult<()>
    where S: DataMut<Elem = f64>
{ ... }
```

Figure 2: Signature of the `normalize()` method

As mentioned before, it can be called using both owned arrays and array views, as shown in Figure 3 and Figure 4.

```
fn normalize(&mut self, _py: Python) -> PyResult<()> {
    check_arrays_set(&self.train_data, &self.val_data, &self.test_data)?;

    normalize(
        &mut self.train_data.as_mut().unwrap(),
        &mut self.val_data.as_mut().unwrap(),
        &mut self.test_data.as_mut().unwrap()
    )?;
    Ok(())
}
```

Figure 3: Calling the `normalize()` method with owned arrays in the `ClassificationDataSet` class

```
fn normalize(&mut self, _py: Python) -> PyResult<()> {
    let (mut train_view, mut val_view, mut test_view) = get_split_views_mut(
        _py,
        &self.data,
        self.train_split_index,
        self.val_split_index
    )?;

    normalize(&mut train_view, &mut val_view, &mut test_view)?;
    Ok(())
}
```

Figure 4: Calling the `normalize()` method with array views in the `ForecastingDataSet` class

2.4 Data-flow Visualization

The different data handling strategies for forecasting and classification datasets result in distinct data-flows, as visualized in Figure 5. The key difference lies in when the actual data copying occurs: forecasting datasets defer copying until the final `collect()` step to avoid double-copying (once for splitting, once for sliding windows), while classification datasets perform the split immediately to accommodate random shuffling strategies.

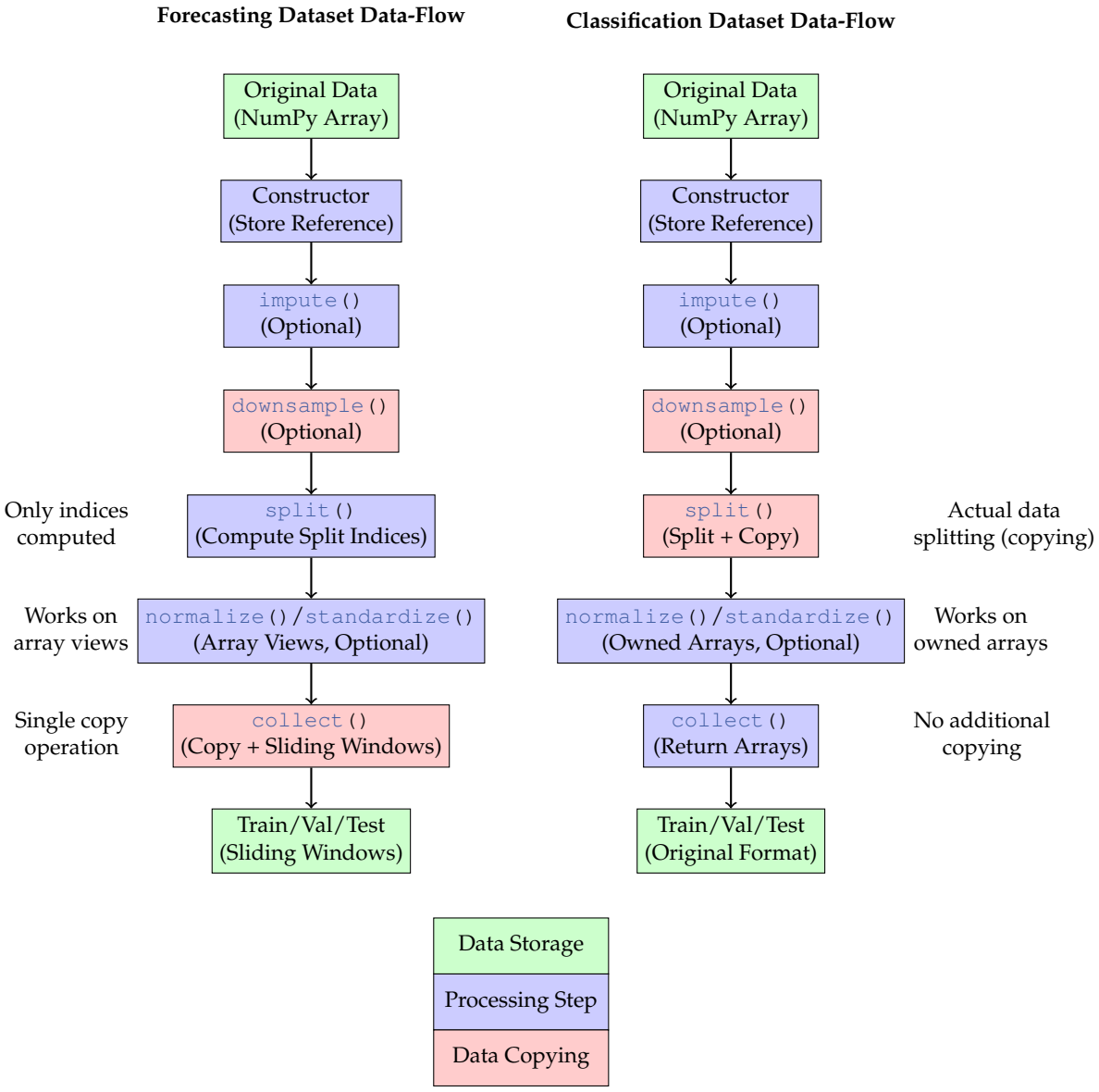

Figure 5: Data-flow comparison between forecasting and classification datasets. Red boxes indicate where data copying occurs, blue boxes indicate where data is processed without copying. Green boxes represent Python-side data storage.

Why it is necessary to copy data in the `downsample()` step is explained in section 5.

2.5 Integration with LightningDataModule

To make the library usable in a machine learning context, we integrated it with the PyTorch Lightning framework. This allows users to easily use our library in their machine learning pipelines, with the user not even having to understand our libraries interface. The integration is done by implementing a class that inherits from the `LightningDataModule` class, which is the base class for all Lightning data modules. Such a `LightningDataModule` can then be used in the `LightningModule` as a data source. The `LightningModule` offers a unified interface for simplifying machine learning workflows. Our class is called `RustDataModule`, and it provides a simple interface to use our library in a Lightning context.

The user only ever needs to interact with the `RustDataModule` class by passing the data as a `numpy` array to the constructor, along with all parameters that let him choose which optional preprocessing features should be used, how the data should be split, and so on. No knowledge about the internal workings of the Rust implmentation is required. The user can then use the `RustDataModule` class in the `LightningModule` as a data source, and the data will be automatically prepared for usage in the machine learning pipeline. The signature of the `RustDataModule` constructor looks as follows:

```
def __init__(
    self,
    dataset: np.ndarray,
    dataset_type: DatasetType,
    past_window: int = 1,
    future_horizon: int = 1,
    stride: int = 1,
    labels: np.ndarray | None = None,
    batch_size: int = 32,
    num_workers: int = 0,
    downsampling_rate: int = 0,
    normalize: bool = False,
    standardize: bool = False,
    impute_strategy: ImputeStrategy = ImputeStrategy.LeaveNaN,
    splitting_strategy: SplittingStrategy = SplittingStrategy.InOrder,
    splitting_ratios: tuple = (0.7, 0.2, 0.1),  # Train, validation, test ratios
):
...
```

Figure 6: Signature of the `RustDataModule` constructor

The reference to the `numpy` array, along with all options, are saved to the class. At the appropriate time, when the data modules `setup()` method is called, an instance of the appropriate class (`ForecastingDataSet` or `ClassificationDataSet`) is created, and the data is passed to it. All preprocessing methods are called according to the chosen options. The resulting split data is then again stored to the `RustDataModule` class. It can be retrieved in the form of a PyTorch `DataLoader`, which is a standard way to load data in PyTorch. The `DataLoader` is used automatically by the `LightningModule` to load the different parts of the data.

3 Random and In-Order Splitting

With this library, we provide a simple and efficient way to split time series datasets into the three training, validation, and test sets. We support both random and In-Order splitting.

Random splitting is useful for datasets where the order of the data points does not matter like in classification data, while In-Order splitting is essential for time series data where the order is crucial like in the forecasting data.

List of supported splitting methods:

- classification data : random splitting AND In-Order splitting
- forecasting data : In-Order splitting

When calling the function `split()` we would need to pass four parameters:

- `split_strategy`: the splitting strategy to use.
- `train_prop`: the proportion of the training set, which is a float between 0 and 1.
- `val_prop`: the proportion of the validation set, which is a float between 0 and 1.
- `test_prop`: the proportion of the test set, which is a float between 0 and 1.

As we can see the pipeline of **random splitting** in Figure 7, the steps are as follows:

1. Validate the proportions of the training, validation, and test sets.
2. Compute the number of instances in the dataset.
3. Compute the split offsets for the training, validation, and test sets.
4. Shuffle the dataset.
5. Split the dataset into the three sets.
6. Return the training, validation, and test sets.

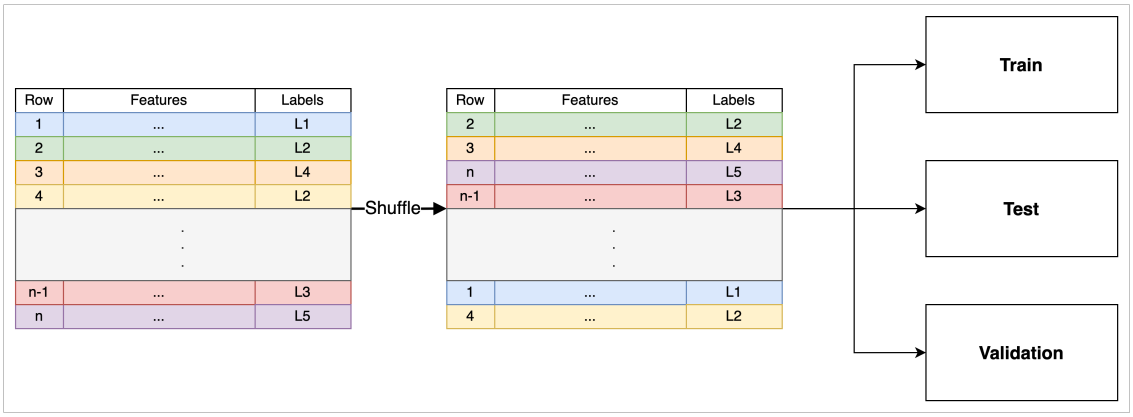

Figure 7: Random Splitting

In case of **In-Order splitting**, as shown in Figure 8, we follow a similar approach, but we do not shuffle the dataset. The steps are as follows:

1. Validate the proportions of the training, validation, and test sets.
2. Compute the number of timesteps in the dataset.
3. Compute the split offsets for the training, validation, and test sets.
4. Split the dataset into the three sets.
5. Return the training, validation, and test sets.

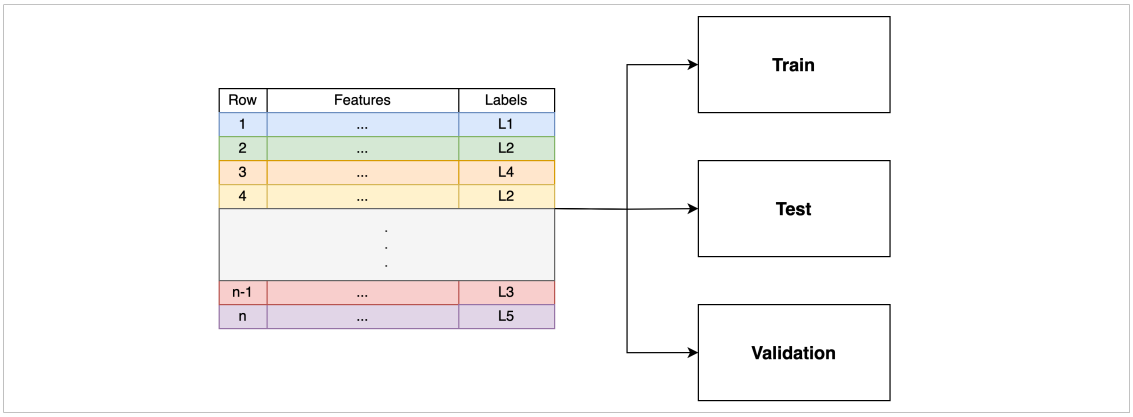

Figure 8: In-Order Splitting

A code snippet of how one may use the splitting method is shown in Figure 9.

```
classification_data_set.split(SplittingStrategy.InOrder, 0.7, 0.2, 0.1)
```

Figure 9: Usage of the `split()` method for `ClassificationDataSet`

4 Standardization and Normalization

Another important step in preprocessing time series data is standardization and normalization.

Standardization is the process of scaling the data to have a mean of 0 and a standard deviation of 1, while min-max normalization scales the data to a range between 0 and 1.

We perform these two operations distinctly on each column of the dataset, which is essential for time series data where each column represents a different feature.

It is also worth mentionaning that key features such as mean, standard deviation, min, and max are computed only once for the training set and then applied to the validation and test sets. This is crucial to avoid data leakage, which can lead to overfitting and unrealistic performance metrics.

4.1 Standardization

Standardization is performed by subtracting the mean and dividing by the standard deviation for each feature. This ensures that the data has a mean of 0 and a standard deviation of 1.

Here are the main steps of the standardization process:

1. Compute the mean and standard deviation for each feature in the training set.
2. Through a for loop iterate over each feature and apply the standardization formula:

$$x' = \frac{x - \text{mean}}{\text{std}} \tag{1}$$

3. Apply the same mean and standard deviation to the validation and test sets.

4.2 Min-Max Normalization

Min-max normalization scales the data to a range between 0 and 1. This is particularly useful for algorithms that are sensitive to the scale of the data, such as neural networks.

Here are the main steps of the min-max normalization process:

1. Compute the minimum and maximum values for each feature in the training set.
2. Through a for loop iterate over each feature and apply the min-max normalization formula:

$$x' = \frac{x - \min}{\max - \min} \tag{2}$$

3. Apply the same min and max values to the validation and test sets.

In the bottle neck scenario, where the difference between the minimum and maximum values is zero, we set their values to 1, which avoids division by zero errors.

A code snippet of how one may use the standardization and normalization methods is shown in Figure 10.

```
classification_data_set.normalize()
classification_data_set.standardize()
```

Figure 10: Usage of the standardization and normalization methods

5 Downsampling

Downsampling is the process of reducing the number of data points in a time series dataset. This is useful for reducing the size of the dataset and speeding up the training process, especially when dealing with large datasets.

When calling the function `downsample()`, we need to pass one parameter:

- `factor`: the factor by which to downsample the dataset, which is an integer greater than 1.

The downsampling process works by taking every `factor`-th data point in the dataset. For example, if the factor is 2, we take every second data point, effectively halving the size of the dataset.

An illustration of how downsampling with `factor` 2 works is shown in Figure 11.

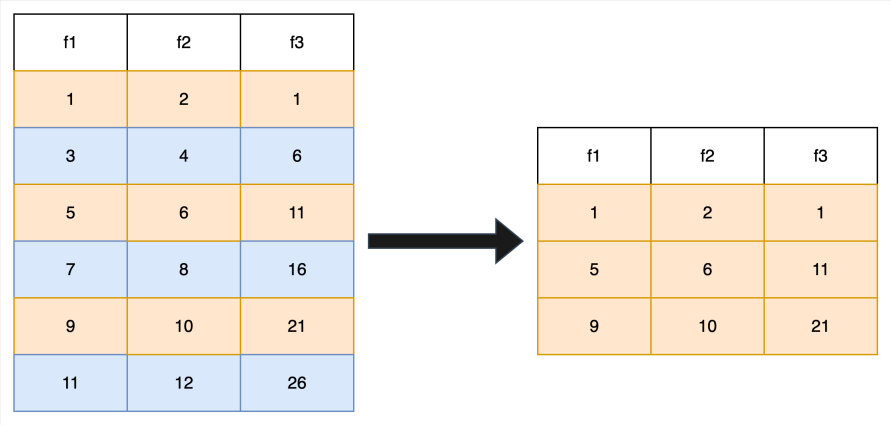

Figure 11: Downsampling

In the Rust side, we loop through the dataset and create a new dataset with only the data points that are at indices that are multiples of the downsampling factor. This is done efficiently using the `ndarray` library.

A code snippet of how one may use the downsampling method is shown in Figure 12.

```
classification_data_set.downsample(2)
```

Figure 12: Usage of the downsampling method

As elaborated on before, the Rust `numpy` crate allows to use views on arrays, which are highly efficient and do not require copying the data. Therefore, our first idea was to use a view on the downsampled part the original array, instead of creating a downsampled copy. But this is not possible, since it is only possible to create views on contiguous parts of the original array, and downsampling does not yield a contiguous part of the original array. Therefore, we have to copy the data in the downsampling step.

6 Imputing

7 Testing

We have implemented unit tests for nearly all the methods in the library. These tests cover various scenarios and edge cases to ensure the correctness of the implementation.

Since our rust code is deeply integrated with bindings and the the Pyo3 library, we were not able to write pure Rust tests. Instead, we have mimicked python environment in the Rust tests, which allows us to test the methods as if they were called from Python. We did this by using the `pyo3` library, which allows us to write Python code in Rust and test it as if it were called from Python.

One might wonder why we did not use the `pytest` library to test the Python code directly. The reason is that we wanted to ensure that the Rust code is working correctly and that the bindings are working as expected. This way, we can catch any issues in the Rust code before they propagate to the Python side. Also, there were some functions that were not directly callable from Python, as they were private functions in the Rust code. We wanted to test these functions as well, so we had to write tests in Rust and compile them differently from how we compiled for the Python bindings.

7.1 Running the Tests

To run the tests, we would need to follow these steps:

1. One may want to clean up all the build artifacts from previous builds. This can be done by running the following command:

   ```
   cargo clean
   ```

2. Ensure that the `maturin` library is installed. This can be done by running the following command:

   ```
   pip install maturin
   ```

3. Now build the Rust code with the `test_expose` feature enabled. This can be done by running the following command:

   ```
   maturin develop --features test_expose
   ```

4. (Only on Mac) Find the location of the `libpython3.12.dylib` file. This can be done by running the following command:

   ```
   find $(python3 -c "import sys; print(sys.prefix)") -name "libpython3.12.dylib"
   ```

5. (Only on Mac) Set the `DYLD_LIBRARY_PATH` environment variable to the path of the `libpython3.12.dylib` file. This can be done by running the following command:

   ```
   export DYLD_LIBRARY_PATH=given_path_from_above
   ```

6. Finally, run the tests with the following command:

   ```
   cargo test --features test_expose
   ```

7.2 Test Coverage

As also mentioned above, we have implemented the unit tests through mimicking the Python environment in Rust. This came with some down sides, which doesn't allow us to use the `cargo-tarpaulin` library to measure the test coverage. However, we have manually checked the coverage of the tests and ensured that all the methods are covered by the tests. We have also ensured that the tests cover various scenarios and edge cases to ensure the correctness of the implementation.

In order to have a rough estimate of the test coverage, we have counted the number of all the functions in the library and the number of functions that are covered by the tests.

The results are as follows:

- Total number of functions(excluding bindings): 47
- Number of test cases: 40
- Test coverage: **85%**

Please note that this is a rough estimate and the actual test coverage may vary. We have also ensured that the tests cover various scenarios and edge cases to ensure the correctness of the implementation.

8 Benchmarking

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Wer vor einer zur Abnahme einer Versicherung an Eides Statt zuständigen Behörde eine solche Versicherung falsch abgibt oder unter Berufung auf eine solche Versicherung falsch aussagt, wird mit Freiheitsstrafe bis zu drei Jahren oder mit Geldstrafe bestraft.
Para. 156 StGB (German Criminal Code): False Statutory Declarations
Whoever before a public authority competent to administer statutory declarations falsely makes such a declaration or falsely testifies while referring to such a declaration shall be liable to imprisonment not exceeding three years or a fine.
§ 161 StGB: Fahrlässiger Falscheid; fahrlässige falsche Versicherung an Eides Statt
(1) Wenn eine der in den §§ 154 bis 156 bezeichneten Handlungen aus Fahrlässigkeit begangen worden ist, so tritt Freiheitsstrafe bis zu einem Jahr oder Geldstrafe ein.
(2) Straflosigkeit tritt ein, wenn der Täter die falsche Angabe rechtzeitig berichtigt. Die Vorschriften des § 158 Abs. 2 und 3 gelten entsprechend.
Para. 161 StGB (German Criminal Code): False Statutory Declarations Due to Negligence
(1) If a person commits one of the offences listed in sections 154 through 156 negligently the penalty shall be imprisonment not exceeding one year or a fine.
(2) The offender shall be exempt from liability if he or she corrects their false testimony in time. The provisions of section 158 (2) and (3) shall apply accordingly.

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Matriculation No. (optional)

Ich versichere hiermit an Eides Statt, dass ich die vorliegende Arbeit/Bachelorarbeit/ Masterarbeit* mit dem Titel
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