

# Test Evaluation Report

## Metadata

**Template used:** /Users/weilinhan/FixML/fixml/src/fixml/data/templates/eval\_report.md.jinja

## Run details

- **Checklist Path:** /Users/weilinhan/FixML/fixml/src/fixml/data/checklist/checklist.csv
- **Repository Path:** /Users/weilinhan/FixML/repos/proteiML
- **HEAD Commit:** eef65f8d65240e785ca57060d2a0b05d23635aa6
- **Start Time:** 2024-09-20 09:41:50.939413
- **End Time:** 2024-09-20 09:42:40.916553
- **Time Taken:** 0:00:49.977140
- **Total Input/Output Tokens Used:** 7916/3795
- **Successful/Failed Calls:** 5/0 (100% Success Rate)
- **Files Evaluated:**
  - /Users/weilinhan/FixML/repos/proteiML/tests/test\_format\_mutation\_dataset.py
  - /Users/weilinhan/FixML/repos/proteiML/tests/test\_construct\_new\_library.py
  - /Users/weilinhan/FixML/repos/proteiML/tests/test\_model\_training.py
  - /Users/weilinhan/FixML/repos/proteiML/tests/test\_scrape\_aaindex\_matrix.py
  - /Users/weilinhan/FixML/repos/proteiML/tests/test\_ensemble\_and\_cross\_validate.py
- **LLM Model Used:** gpt-3.5-turbo

## Evaluation Summary

**Completeness Score:** 3.0/7

**Completeness Score per Checklist Item:**

ID Title	is_Satisfied
2.1 Ensure Data File Loads as Expected	1
3.2 Data in the Expected Format	1
3.5 Check for Duplicate Records in Data	1
4.2 Verify Data Split Proportion	0
5.3 Ensure Model Output Shape Aligns with Expectation	0
6.1 Verify Evaluation Metrics Implementation	0
6.2 Evaluate Model's Performance Against Thresholds	0

## Evaluation Details

### 2.1 Ensure Data File Loads as Expected

**Requirement:** Verify if data-loading functions correctly fetch datasets from predefined sources, such as a data file in repository, or online repositories, such as a url. Verify if the data-loading functions gracefully handle errors when unable to load data or correctly handle edge cases.

**Observations:**

- (test\_format\_mutation\_dataset.py) The code includes functions for reading sequence data, combining datasets, and checking for duplicates, which are related to loading and processing data.
- (test\_construct\_new\_library.py) The code snippet imports data\_processing.construct\_new\_library and data\_processing.constants modules. It defines a fixture metadata\_fixture that reads a CSV file 'Input\_Data.csv' from BACKEND\_DATA\_DIR and returns the data as a dictionary. The fixture is used in the test\_create\_and\_clean\_variant\_df\_fixture test function.
- (test\_model\_training.py) The code imports data\_processing.model\_training as mt, reads data from 'combined\_dataset.csv', and prepares encoding data for training models.
- (test\_scrape\_aaindex\_matrix.py) The code snippet imports necessary modules and defines a test function test\_aaindex\_scrape\_or\_load. It checks if SCRAPE\_AAINDEX is True, then it scrapes aaindex indices, finds accession numbers, and saves the dataset to a CSV file. If SCRAPE\_AAINDEX is False, it reads the dataset from a CSV file. Finally, it asserts the shape of the property\_dataset to be (20, 6).
- (test\_ensemble\_and\_cross\_validate.py) The code imports data\_processing.ensemble\_and\_cross\_validate module and uses data from BASE\_DIR to load datasets. The code uses pandas to read CSV files and sort values based on 'Test Set R Squared'.

## Function References:

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_format\_mutation\_dataset.py', 'Referenced Functions': ['[read\\_seq\\_data](#)', '[combine\\_seq\\_datasets](#)', '[check\\_for\\_duplicates](#)']}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_construct\_new\_library.py', 'Referenced Functions': ['[pd.read\\_csv](#)', '[to\\_dict](#)', '[create\\_variant\\_dataframe](#)', '[clean\\_variant\\_dataframe](#)']}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_model\_training.py', 'Referenced Functions': ['[prepare\\_encoding\\_data](#)']}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_scrape\_aaindex\_matrix.py', 'Referenced Functions': ['[scrape\\_aaindex\\_indices](#)', '[find\\_accession\\_numbers](#)']}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_ensemble\_and\_cross\_validate.py', 'Referenced Functions': ['[pd.read\\_csv](#)', '[sort\\_values](#)']}

## 3.2 Data in the Expected Format

**Requirement:** Verify if the data matches the expected format that specified by the function. This step must involves checking the shape of data, data types, values, and any other properties that specified by the function.

### Observations:

- (test\_format\_mutation\_dataset.py) The code does not explicitly verify the format of the data loaded.
- (test\_construct\_new\_library.py) The test\_create\_and\_clean\_variant\_df\_fixture test function checks the length of variant\_df columns, the length of variant\_df, and the presence of duplicate records in cleaned\_variants.
- (test\_model\_training.py) The code prepares encoding data for training models, which involves checking the shape of data, data types, and values.
- (test\_scrape\_aaindex\_matrix.py) Not applicable
- (test\_ensemble\_and\_cross\_validate.py)

## Function References:

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_format\_mutation\_dataset.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_construct\_new\_library.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_model\_training.py', 'Referenced Functions': ['[prepare\\_encoding\\_data](#)']}

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_scrape\_aaindex\_matrix.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_ensemble\_and\_cross\_validate.py', 'Referenced Functions': []}

### 3.5 Check for Duplicate Records in Data

**Requirement:** Verify if there is no duplicate record in the loaded data.

#### Observations:

- (test\_format\_mutation\_dataset.py) The code includes a function 'check\_for\_duplicates' to verify and remove duplicate records.
- (test\_construct\_new\_library.py) The test\_create\_and\_clean\_variant\_df\_fixture test function checks for duplicate records in cleaned\_variants.
- (test\_model\_training.py) The code does not explicitly check for duplicate records in the loaded data.
- (test\_scrape\_aaindex\_matrix.py) Not applicable
- (test\_ensemble\_and\_cross\_validate.py)

#### Function References:

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_format\_mutation\_dataset.py', 'Referenced Functions': ['[check\\_for\\_duplicates](#)']}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_construct\_new\_library.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_model\_training.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_scrape\_aaindex\_matrix.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_ensemble\_and\_cross\_validate.py', 'Referenced Functions': []}

### 4.2 Verify Data Split Proportion

**Requirement:** Verify if the data is split into training and testing sets by the proportion specified by the function. Verify the split by checking the actual fraction of data points in the training and test sets.

#### Observations:

- (test\_format\_mutation\_dataset.py) The code does not include functionality to verify data split proportion.
- (test\_construct\_new\_library.py) Not applicable
- (test\_model\_training.py) The code trains models using training and testing data, but does not explicitly verify the data split proportion.
- (test\_scrape\_aaindex\_matrix.py) Not applicable
- (test\_ensemble\_and\_cross\_validate.py)

#### Function References:

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_format\_mutation\_dataset.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_construct\_new\_library.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_model\_training.py', 'Referenced Functions': []}

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_scrape\_aaindex\_matrix.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_ensemble\_and\_cross\_validate.py', 'Referenced Functions': []}

## 5.3 Ensure Model Output Shape Aligns with Expectation

**Requirement:** Verify if the structure of the model's output matches the expected format specified by the function, such as checking the dimensions of the output versus the number of labels in classification task.

### Observations:

- (test\_format\_mutation\_dataset.py) The code does not relate to model output shape alignment.
- (test\_construct\_new\_library.py) Not applicable
- (test\_model\_training.py) The code trains models but does not explicitly verify the model's output shape alignment with expectations.
- (test\_scrape\_aaindex\_matrix.py) Not applicable
- (test\_ensemble\_and\_cross\_validate.py)

### Function References:

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_format\_mutation\_dataset.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_construct\_new\_library.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_model\_training.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_scrape\_aaindex\_matrix.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_ensemble\_and\_cross\_validate.py', 'Referenced Functions': []}

## 6.1 Verify Evaluation Metrics Implementation

**Requirement:** Verify if the evaluation metrics are correctly implemented and appropriate for the model's task. Verify if the metric computations with expected values to validate correctness.

### Observations:

- (test\_format\_mutation\_dataset.py) The code does not include functionality to verify evaluation metrics implementation.
- (test\_construct\_new\_library.py) Not applicable
- (test\_model\_training.py) The code trains models but does not explicitly verify the evaluation metrics implementation.
- (test\_scrape\_aaindex\_matrix.py) Not applicable
- (test\_ensemble\_and\_cross\_validate.py)

### Function References:

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_format\_mutation\_dataset.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_construct\_new\_library.py', 'Referenced Functions': []}

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_model\_training.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_scrape\_aaindex\_matrix.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_ensemble\_and\_cross\_validate.py', 'Referenced Functions': []}

## 6.2 Evaluate Model's Performance Against Thresholds

**Requirement:** First compute evaluation metrics for both the training and testing datasets, then verify if these metrics exceed threshold values, indicating acceptable model performance.

### Observations:

- (test\_format\_mutation\_dataset.py) The code does not include functionality to evaluate model performance against thresholds.
- (test\_construct\_new\_library.py) Not applicable
- (test\_model\_training.py) The code trains models but does not explicitly evaluate the model's performance against thresholds.
- (test\_scrape\_aaindex\_matrix.py) Not applicable
- (test\_ensemble\_and\_cross\_validate.py)

### Function References:

- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_format\_mutation\_dataset.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_construct\_new\_library.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_model\_training.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_scrape\_aaindex\_matrix.py', 'Referenced Functions': []}
- {'File Path': '/Users/weilinhan/FixML/repos/proteiML/tests/test\_ensemble\_and\_cross\_validate.py', 'Referenced Functions': []}