`pandera`: Statistical Data Validation of Pandas Dataframes

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What's a `DataFrame`?

```
dataframe.head()
```

	hours_worked	wage_per_hour
person_id		
aafee0b	38.5	15.1
0a917a3	41.25	15.0
2d1786b	35.0	21.3
263cf89	27.75	17.5
89a09dc	22.25	19.5

What's Data Validation?

Data validation is the act of *falsifying* data against explicit assumptions for some downstream purpose, like analysis, modeling, and visualization.

> *"All swans are white"*

(https://commons.wikimedia.org/wiki/File:Black_Swans.jpg#/media/File:Black_Swans.jpg)

Why Do I Need it?

- It can be difficult to reason about and debug data processing pipelines.
- It's critical to ensuring data quality in many contexts especially when the end product informs business decisions, supports scientific findings, or generates predictions in a production setting.

Everyone has a personal relationship with their dataframes

One day, you encounter an error log trail and decide to follow it...

```
/usr/local/miniconda3/envs/pandera-presentations/lib/python3.7/site-packages/pandas/core/ops/__init__.py in masked_
arith_op(x, y, op)
    445         if mask.any():
    446             with np.errstate(all="ignore"):
--> 447                 result[mask] = op(xrav[mask], com.values_from_object(yrav[mask]))
    448 
    449     else:

TypeError: can't multiply sequence by non-int of type 'float'
```

And you find yourself at the top of a function...

```python
def process_data(df):
    ...
```

You look around, and see some hints of what had happened...

```python
def process_data(df):
    return (
        df.assign(
            weekly_income=lambda x: x.hours_worked * x.wage_per_hour
        )
    )
```

You sort of know what's going on, but you want to take a closer look!

```python
def process_data(df):
    import pdb; pdb.set_trace()  # <- insert breakpoint
    return (
        df.assign(
            weekly_income=lambda x: x.hours_worked * x.wage_per_hour
        )
    )
```

And you find some funny business going on...

```
>>> print(df)
```

```
           hours_worked  wage_per_hour
person_id
aafee0b            38.5           15.1
0a917a3           41.25           15.0
2d1786b            35.0           21.3
263cf89           27.75           17.5
89a09dc           22.25           19.5
e256747           -20.5           25.5
```

```
>>> df.dtypes
```

```
hours_worked      object
wage_per_hour    float64
dtype: object
```

```
>>> df.hours_worked.map(type)
```

```
person_id
aafee0b    <class 'float'>
0a917a3    <class 'float'>
2d1786b      <class 'str'>
263cf89    <class 'float'>
89a09dc    <class 'float'>
e256747    <class 'float'>
Name: hours_worked, dtype: object
```

You squash the bug and add documentation for the next weary traveler who happens upon this code.

```python
def process_data(df):
    return (
        df
        .astype({"hours_worked": float, "wage_per_hour": float})  # <- make sure columns are floats
        .assign(
            hours_worked=lambda x: x.hours_worked.where(  # <- replace negative values with nans
                x.hours_worked >= 0, np.nan
            )
        )
        .assign(
            weekly_income=lambda x: x.hours_worked * x.wage_per_hour
        )
    )
```

```
>>> process_data(df)
```

	hours_worked	wage_per_hour	weekly_income
person_id			
aafee0b	38.50	15.1	581.350
0a917a3	41.25	15.0	618.750
2d1786b	35.00	21.3	745.500
263cf89	27.75	17.5	485.625
89a09dc	22.25	19.5	433.875
e256747	NaN	25.5	NaN

A few months later...

You find yourself at a familiar function, but it looks a little different from when you left it...

```
@pa.check_input(in_schema)
@pa.check_output(out_schema)
def process_data(df):
    return (
        df.assign(
            hours_worked=lambda x: x.hours_worked.where(  # <- replace negative values with nans
                x.hours_worked >= 0, np.nan
            )
        )
        .assign(
            weekly_income=lambda x: x.hours_worked * x.wage_per_hour
        )
    )
```

You look above and see what `in_schema` and `out_schema` are, finding a `NOTE` that a fellow traveler has left for you.

```python
import pandera as pa
from pandera import DataFrameSchema, Column, Check

# NOTE: this is what's supposed to be in `df` going into `process_data`
in_schema = DataFrameSchema({
    "hours_worked": Column(pa.Float, coerce=True, nullable=True),
    "wage_per_hour": Column(pa.Float, coerce=True, nullable=True),
})

# ... and this is what `process_data` is supposed to return.
out_schema = (
    in_schema
    .update_column("hours_worked", checks=Check.greater_than_or_equal_to(0))
    .add_columns({"weekly_income": Column(pa.Float, nullable=True)})
)

@pa.check_input(in_schema)
@pa.check_output(out_schema)
def process_data(df):
    ...
```

Moral of the Story

The better you can reason about the contents of a dataframe, the faster you can debug.

The faster you can debug, the sooner you can focus on downstream tasks that you care about.

Outline

- Data validation in theory and practice.
- Brief introduction to `pandera`
- Case Study: **Fatal Encounters** dataset
- Roadmap

Data Validation in Theory and Practice

According to the European Statistical System:

> *Data validation is an activity in which it is verified whether or not a combination of values is a member of a set of acceptable value combinations. [Di Zio et al. 2015 (https://ec.europa.eu/eurostat/cros/system/files/methodology_for_data_validation_v1.0_rev-2016-06_final.pdf)]*

Data Validation in Theory and Practice

More formally, we can relate this definition to one of the core principles of the scientific method: **falsifiability**

$$v(x) \twoheadrightarrow \{True, False\}$$

Where x is a set of data values and v is a surjective validation function, meaning that there exists at least one x that maps onto each of the elements in the set $\{True, False\}$ [van der Loo et al. 2019 (https://arxiv.org/pdf/1912.09759.pdf)].

Case 1: Unfalsifiable

$v(x) \rightarrow True$

> ***Example:*** *"my dataframe can have any number of columns of any type"*
>
> ```
> lambda df: True
> ```

Case 2: Unverifiable

$v(x) \rightarrow False$

> ***Example:*** *"my dataframe has an infinite number of rows and columns"*
>
> ```
> lambda df: False
> ```

Types of Validation Rules

[van der Loo et al. 2019 (https://arxiv.org/pdf/1912.09759.pdf)]

Technical Checks

Have to do with the properties of the data structure:

- `income` is a numeric variable, `occupation` is a categorical variable.
- `email_address` should be unique.
- null (missing) values are permitted in the `occupation` field.

Domain-specific Checks

Have to do with properties specific to the topic under study:

- the `age` variable should be between the range 0 and 120
- the `income` for records where `age` is below the legal working age should be `nan`
- certain categories of `occupation` tend to have higher `income` than others

Types of Validation Rules

Deterministic Checks

Checks that express hard-coded logical rules

> *the mean `age` should be between `30` and `40` years old.*
>
> ```
> lambda age: 30 <= age.mean() <= 40
> ```

Probabilistic Checks

Checks that explicitly incorporate randomness and distributional variability

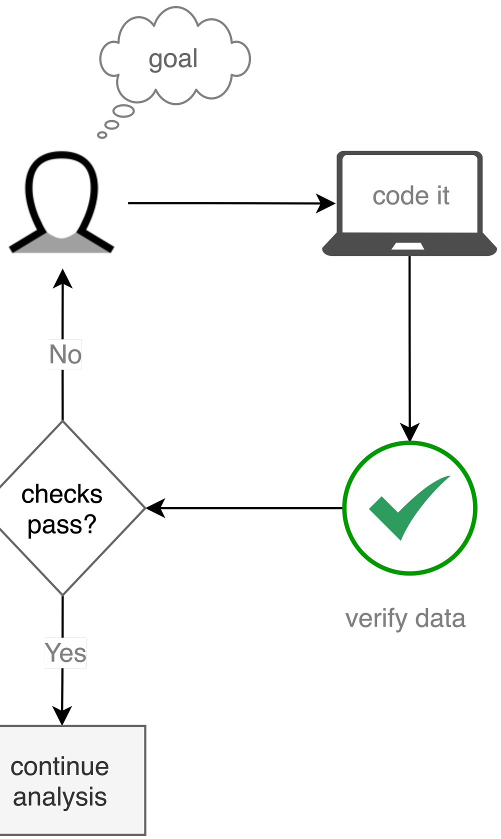
> *the 95% confidence interval or mean `age` should be between `30` and `40` years old.*
>
> ```
> def prob_check_age(age):
>     mu = age.mean()
>     ci = 1.96 * (age.std() / np.sqrt(len(age))
>     return 30 <= mu - ci and mu + ci <= 40
> ```

Statistical Type Safety

Verifying the assumptions about the distributional properties of a dataset to ensure that statistical operations on those data are valid.

- "the training samples are independently and identically distributed"
- "features `x1`, `x2`, and `x3` are not correlated"
- "the variance of feature `x` is greater than some threshold `t`"
- "the label distribution is consistent across the training and test set"

Data Validation Workflow in Practice



User Story

> *As a machine learning engineer who uses `pandas` every day, I want a data validation tool that's intuitive, flexible, customizable, and easy to integrate into my ETL pipelines so that I can spend less time worrying about the correctness of a dataframe's contents and more time training models.*

Introducing `pandera`

A design-by-contract data validation library that exposes an intuitive API for expressing dataframe schemas.

Refactoring the Validation Function

$$v(x) \twoheadrightarrow \{True, False\}$$

$$s(v, x) \rightarrow \begin{cases} \text{x}, & \text{if } v(x) = true \\ \text{error}, & \text{otherwise} \end{cases}$$

Where s is a *schema* function that takes two arguments: the validation function v and some data x.

Why?

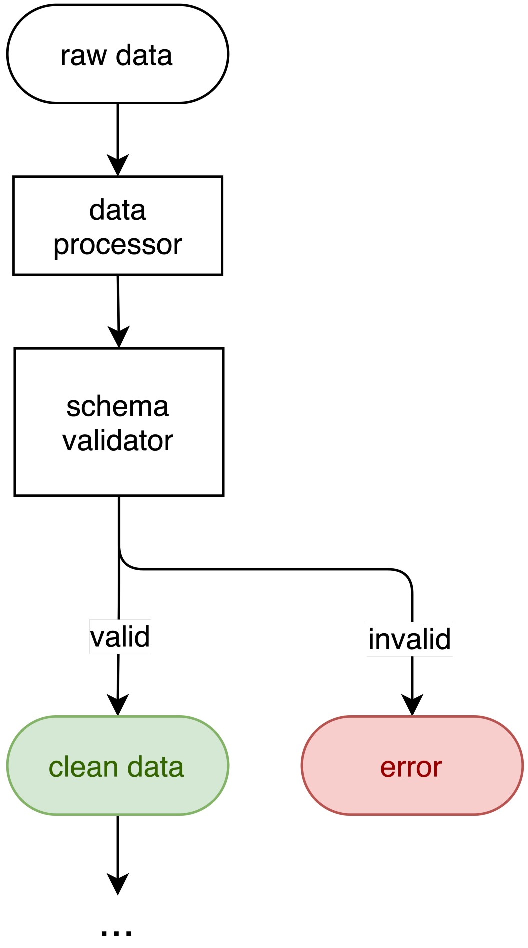
Compositionality

Consider a data processing function $f(x) \rightarrow x'$ that cleans the raw dataset x.

We can use the schema to define any number of composite functions:

- $f(s(x))$ first validates the raw data to catch invalid data before it's preprocessed.
- $s(f(x))$ validates the output of f to check that the processing function is fulfilling the contract defined in s
- $s(f(s'(x)))$: the data validation 🥪

Architecture



Case Study: Fatal Encounters Dataset

"A step toward creating an impartial, comprehensive, and searchable national database of people killed during interactions with law enforcement."

https://fatalencounters.org (https://fatalencounters.org)

Bird's Eye View

- 26,000+ records of law enforcement encounters leading to death
- Records date back to the year 2000
- Each record contains:
    - demographics of the decedent
    - cause and location of the death
    - agency responsible for death
    - court disposition of the case (e.g. "Justified", "Accidental", "Suicide", "Criminal")

What factors are most predictive of the court ruling a case as "Accidental"?

Example 1:

> *Undocumented immigrant Roberto Chavez-Recendiz, of Hidalgo, Mexico, was fatally shot while Rivera was arresting him along with his brother and brother-in-law for allegedly being in the United States without proper documentation. The shooting was "possibly the result of what is called a 'sympathetic grip,' where one hand reacts to the force being used by the other," Chief Criminal Deputy County Attorney Rick Unklesbay wrote in a letter outlining his review of the shooting. The Border Patrol officer had his pistol in his hand as he took the suspects into custody. He claimed the gun fired accidentally.*

Example 2:

> *Andrew Lamar Washington died after officers tasered him 17 times within three minutes.*

Example 3:

> *Biddle and his brother, Drake Biddle, were fleeing from a Nashville Police Department officer at a high rate of speed when a second Nashville Police Department officer, James L. Steely, crashed into him head-on.*

Caveats

- As mentioned on the [website (https://fatalencounters.org)](https://fatalencounters.org), the records in this dataset are the most comprehensive to date, but by no means is it a finished project. Biases may be lurking everywhere!
- I don't have any domain expertise in criminal justice!
- The main purpose here is to showcase the capabilities of `pandera`.

VALIDATE ALL THE THINGS !!!

Notebook is Available Here:

Jupyter notebook classic:

(https://mybinder.org/v2/gh/pandera-dev/pandera-presentations/master?filepath=notebooks%2F20200505_scipy_conference.ipynb)

https://bit.ly/scipy-2020-pandera (https://bit.ly/scipy-2020-pandera)

Jupyter lab:

(https://mybinder.org/v2/gh/pandera-dev/pandera-presentations/master?urlpath=lab%2Ftree%2Fnotebooks%2F20200505_scipy_conference.ipynb)

https://bit.ly/scipy-2020-pandera-jlab (https://bit.ly/scipy-2020-pandera-jlab)

Read the Data

```
import janitor
import requests
from pandas_profiling import ProfileReport

dataset_url = (
    "https://docs.google.com/spreadsheets/d/"
    "1dKmaV_JiWcG8XBoRgP8b4e9Eopkpgt7FL7nyspvzAsE/export?format=csv"
)
fatal_encounters = pd.read_csv(dataset_url, skipfooter=1, engine="python")
```

	Unique ID	Subject's name	Subject's age	Subject's gender	Subject's race	Subject's race with imputations	Imputation probability	URL of image of deceased	Date of injury resulting in death (month/day/year)	Location of injury (address)	Loca of de (c
0	25746	Samuel H. Knapp	17	Male	European-American/White	European-American/White	not imputed	NaN	01/01/2000	27898-27804 US-101	Willits
1	25747	Mark A. Horton	21	Male	African-American/Black	African-American/Black	not imputed	NaN	01/01/2000	Davison Freeway	Detroi
2	25748	Phillip A. Blurbridge	19	Male	African-American/Black	African-American/Black	not imputed	NaN	01/01/2000	Davison Freeway	Detroi

Clean up column names

To make the analysis more readable

```
def clean_columns(df):
    return (
        df.clean_names()
        .rename(
            columns=lambda x: (
                x.strip("_")
                .replace("&", "_and_")
                .replace("subjects_", "")
                .replace("location_of_death_", "")
                .replace("_resulting_in_death_month_day_year", "")
                .replace("_internal_use_not_for_analysis", "")
            )
        )
    )

fatal_encounters_clean_columns = clean_columns(fatal_encounters)
```

Minimal Schema Definition

Just define columns that we need for creating the training set, and specify which are `nullable`.

```
clean_column_schema = pa.DataFrameSchema(
    {
        "age": Column(nullable=True),
        "gender": Column(nullable=True),
        "race": Column(nullable=True),
        "cause_of_death": Column(nullable=True),
        "symptoms_of_mental_illness": Column(nullable=True),
        "dispositions_exclusions": Column(nullable=True),
    }
)
```

Validate the output of `clean_columns` using `pipe` at the end of the method chain

```
def clean_columns(df):
    return (
        df.clean_names()
        .rename(
            columns=lambda x: (
                x.strip("_")
                .replace("&", "_and_")
                .replace("subjects_", "")
                .replace("location_of_death_", "")
                .replace("_resulting_in_death_month_day_year", "")
                .replace("_internal_use_not_for_analysis", "")
            )
        )
        .pipe(clean_column_schema)  # <- validate output with schema
    )
```

Sidebar

If a column is not present as specified by the schema, a `SchemaError` is raised.

```python
corrupted_data = fatal_encounters.drop("Subject's age", axis="columns")
try:
    clean_columns(corrupted_data)
except pa.errors.SchemaError as exc:
    print(exc)
```

```
column 'age' not in dataframe
  unique_id                   name gender                     race  \
0     25746        Samuel H. Knapp   Male  European-American/White
1     25747         Mark A. Horton   Male   African-American/Black
2     25748  Phillip A. Blurbridge   Male   African-American/Black
3     25749             Mark Ortiz   Male          Hispanic/Latino
4         2           Lester Miller   Male         Race unspecified

     race_with_imputations imputation_probability url_of_image_of_deceased  \
0  European-American/White            not imputed                      NaN
1   African-American/Black            not imputed                      NaN
2   African-American/Black            not imputed                      NaN
3          Hispanic/Latino            not imputed                      NaN
4   African-American/Black            0.947676492                      NaN

  date_of_injury location_of_injury_address       city  ...  \
0     01/01/2000          27898-27804 US-101    Willits  ...
1     01/01/2000             Davison Freeway    Detroit  ...
2     01/01/2000             Davison Freeway    Detroit  ...
3     01/01/2000             600 W Cherry Ln   Carlsbad  ...
4     01/02/2000       4850 Flakes Mill Road  Ellenwood  ...

  a_brief_description_of_the_circumstances_surrounding_the_death  \
0  Samuel Knapp was allegedly driving a stolen ve...
1  Two Detroit men killed when their car crashed ...
2  Two Detroit men killed when their car crashed ...
3  A motorcycle was allegedly being driven errati...
4  Darren Mayfield, a DeKalb County sheriff's dep...

   dispositions_exclusions intentional_use_of_force_developing  \
0               Unreported                     Vehicle/Pursuit
1               Unreported                     Vehicle/Pursuit
2               Unreported                     Vehicle/Pursuit
3               Unreported                     Vehicle/Pursuit
4                 Criminal    Intentional Use of Force, Deadly

  link_to_news_article_or_photo_of_official_document  \
0  https://drive.google.com/file/d/10DisrV8K5ReP1...
1  https://drive.google.com/file/d/1-nK-RohgiM-tZ...
2  https://drive.google.com/file/d/1-nK-RohgiM-tZ...
3  https://drive.google.com/file/d/1qAEefRjX_aTtC...
4  https://docs.google.com/document/d/1-YuShSarW_...
```

Explore the Data with `pandas-profiling` (https://github.com/pandas-profiling/pandas-profiling)

Overview

Dataset statistics

Number of variables	29
Number of observations	28367
Missing cells	75102
Missing cells (%)	9.1%
Duplicate rows	0
Duplicate rows (%)	0.0%
Total size in memory	6.3 MiB
Average record size in memory	232.0 B

Variable types

CAT	22
NUM	5
URL	2

Declare the Training Data Schema

```python
training_data_schema = pa.DataFrameSchema(
    {
        # feature columns
        "age": Column(pa.Float, Check.in_range(0, 120), nullable=True),
        "gender": Column(pa.String, Check.isin(genders), nullable=True),
        "race": Column(pa.String, Check.isin(races), nullable=True),
        "cause_of_death": Column(pa.String, Check.isin(causes_of_death), nullable=True),
        "symptoms_of_mental_illness": Column(pa.Bool, nullable=True),
        # target column
        "disposition_accidental": Column(pa.Bool, nullable=False),
    },
    coerce=True  # <- coerce columns to the specified type
)
```

Serialize schema to yaml format:

```python
print(training_data_schema.to_yaml())
```


```yaml
schema_type: dataframe
version: 0.4.2
columns:
  age:
    pandas_dtype: float
    nullable: true
    checks:
      in_range:
        min_value: 0
        max_value: 120
  gender:
    pandas_dtype: string
    nullable: true
    checks:
      isin:
      - female
      - male
      - transgender
      - transexual
  race:
    pandas_dtype: string
    nullable: true
    checks:
      isin:
      - african_american_black
      - asian_pacific_islander
      - european_american_white
      - hispanic_latino
      - middle_eastern
      - native_american_alaskan
      - race_unspecified
  cause_of_death:
    pandas_dtype: string
    nullable: true
    checks:
      isin:
      - asphyxiated_restrained
      - beaten_bludgeoned_with_instrument
      - burned_smoke_inhalation
      - chemical_agent_pepper_spray
      - drowned
      - drug_overdose
      - fell_from_a_height
      - gunshot
      - medical_emergency
      - other
      - stabbed
```

Clean the Data

The cleaning function should normalize string values as specified by `training_data_schema` .

```
def clean_data(df):
    return (
        df.dropna(subset=["dispositions_exclusions"])
        .transform_columns(
            [
                "gender", "race", "cause_of_death",
                "symptoms_of_mental_illness", "dispositions_exclusions"
            ],
            lambda x: x.str.lower().str.replace('-|/| ', '_'),  # clean string values
            elementwise=False
        )
        .transform_column(
            "symptoms_of_mental_illness",
            lambda x: x.mask(x.dropna().str.contains("unknown")) != "no",  # binarize mental illness
            elementwise=False
        )
        .transform_column(
            "dispositions_exclusions",
            lambda x: x.str.contains("accident", case=False),  # derive target column
            "disposition_accidental",
            elementwise=False
        )
        .query("gender != 'white'")  # probably a data entry error
        .filter_string(
            "dispositions_exclusions",
            "unreported|unknown|pending|suicide",  # filter out unknown, unreported, or suicide cases
            complement=True
        )
    )
```

Add the data validation 🥪

```python
@pa.check_input(clean_column_schema)
@pa.check_output(training_data_schema)
def clean_data(df):
    return (
        df.dropna(subset=["dispositions_exclusions"])
        .transform_columns(
            [
                "gender", "race", "cause_of_death",
                "symptoms_of_mental_illness", "dispositions_exclusions"
            ],
            lambda x: x.str.lower().str.replace('-|/| ', '_'),  # clean string values
            elementwise=False
        )
        .transform_column(
            "symptoms_of_mental_illness",
            lambda x: x.mask(x.dropna().str.contains("unknown")) != "no",  # binarize mental illness
            elementwise=False
        )
        .transform_column(
            "dispositions_exclusions",
            lambda x: x.str.contains("accident", case=False),  # derive target column
            "disposition_accidental",
            elementwise=False
        )
        .query("gender != 'white'")  # probably a data entry error
        .filter_string(
            "dispositions_exclusions",
            "unreported|unknown|pending|suicide",  # filter out unknown, unreported, or suicide cases
            complement=True
        )
    )
```

`ValueError`: Unable to `coerce` column to schema data type

```python
try:
    clean_data(fatal_encounters_clean_columns)
except ValueError as exc:
    print(exc)
```

```
could not convert string to float: '18 months'
```

Normalize the age column

So that string values can be converted into `float`

```
def normalize_age(age):
    return (
        age.str.replace("s|`", "")
        .pipe(normalize_age_range)
        .pipe(normalize_age_to_year, "month|mon", 12)
        .pipe(normalize_age_to_year, "day", 365)
    )
```

Apply `normalize_age` inside the `clean_data` function.

```python
# data validation 🥪
@pa.check_input(clean_column_schema)
@pa.check_output(training_data_schema)
def clean_data(df):
    return (
        df.dropna(subset=["dispositions_exclusions"])
        .transform_columns(
            [
                "gender", "race", "cause_of_death",
                "symptoms_of_mental_illness", "dispositions_exclusions"
            ],
            lambda x: x.str.lower().str.replace('-|/| ', '_'),  # clean string values
            elementwise=False
        )
        .transform_column(
            "symptoms_of_mental_illness",
            lambda x: x.mask(x.dropna().str.contains("unknown")) != "no",  # binarize mental illness
            elementwise=False
        )
        .transform_column("age", normalize_age, elementwise=False)  # <- clean up age column
        .transform_column(
            "dispositions_exclusions",
            lambda x: x.str.contains("accident", case=False),  # derive target column
            "disposition_accidental",
            elementwise=False
        )
        .query("gender != 'white'")  # probably a data entry error
        .filter_string(
            "dispositions_exclusions",
            "unreported|unknown|pending|suicide",  # filter out unknown, unreported, or suicide cases
            complement=True
        )
    )
```

Create Training Set

```
fatal_encounters_clean = clean_data(fatal_encounters_clean_columns)
with pd.option_context("display.max_rows", 5):
    display(fatal_encounters_clean.filter(list(training_data_schema.columns)))
```

	age	gender	race	cause_of_death	symptoms_of_mental_illness	disposition_accidental
4	53.0	male	race_unspecified	gunshot	False	False
8	42.0	female	race_unspecified	vehicle	False	False
...	...	...	...	...	...	...
28236	35.0	male	european_american_white	drowned	False	False
28276	26.0	male	hispanic_latino	gunshot	False	False

8068 rows × 6 columns

Sidebar

Informative Error Messages

If, for some reason, the data gets corrupted, `Check` failure cases are reported as a dataframe indexed by failure case `value`.

```python
corrupt_data = fatal_encounters_clean.copy()
corrupt_data["gender"].iloc[:50] = "foo"
corrupt_data["gender"].iloc[50:100] = "bar"
try:
    training_data_schema(corrupt_data)
except pa.errors.SchemaError as exc:
    print(exc)
```

```
<Schema Column: 'gender' type=string> failed element-wise validator 0:
<Check _isin: isin({'transgender', 'female', 'male', 'transexual'})>
failure cases:
                                                           index  count
failure_case
bar           [146, 147, 148, 151, 153, 162, 165, 168, 171, ...     50
foo           [4, 8, 9, 11, 12, 13, 17, 22, 31, 32, 40, 41, ...     50
```

Fine-grained debugging

The `SchemaError` exception object contains the invalid dataframe and the failure cases, which is also a dataframe.

```python
with pd.option_context("display.max_rows", 5):
    try:
        training_data_schema(corrupt_data)
    except pa.errors.SchemaError as exc:
        print("Invalid Data:\n-------------")
        print(exc.data.iloc[:, :5])
        print("\nFailure Cases:\n--------------")
        print(exc.failure_cases)
```

```
Invalid Data:
-------------
      unique_id                      name   age gender  \
4             2             Lester Miller  53.0    foo
8         25752              Doris Murphy  42.0    foo
...         ...                       ...   ...    ...
28236     28209      Joe Deewayne Cothrum  35.0   male
28276     28358  Jose Santos Parra Juarez  26.0   male

                         race
4           race_unspecified
8           race_unspecified
...                       ...
28236  european_american_white
28276          hispanic_latino

[8068 rows x 5 columns]

Failure Cases:
--------------
    index failure_case
0       4          foo
1       8          foo
..    ...          ...
98    280          bar
99    284          bar

[100 rows x 2 columns]
```

Summarize the Data

What percent of cases in the training data are "accidental"?

```
percent_accidental = fatal_encounters_clean.disposition_accidental.mean()
display(Markdown(f"{percent_accidental * 100:0.02f}%"))
```

2.74%

Hypothesis: "the `disposition_accidental` target has a class balance of ~2.75%"

```python
from pandera import Hypothesis

# use the Column object as a stand-alone schema object
target_schema = Column(
    pa.Bool,
    name="disposition_accidental",
    checks=Hypothesis.one_sample_ttest(
        popmean=0.0275, relationship="equal", alpha=0.01
    )
)

target_schema(fatal_encounters_clean);
```

Prepare Training and Test Sets

For functions that have tuple/list-like output, specify an integer index `pa.check_output(schema, <int>)` to apply the schema to a specific element in the output.

```python
from sklearn.model_selection import train_test_split

target_schema = pa.SeriesSchema(
    pa.Bool,
    name="disposition_accidental",
    checks=Hypothesis.one_sample_ttest(
        popmean=0.0275, relationship="equal", alpha=0.01
    )
)
feature_schema = training_data_schema.remove_columns([target_schema.name])


@pa.check_input(training_data_schema)
@pa.check_output(feature_schema, 0)
@pa.check_output(feature_schema, 1)
@pa.check_output(target_schema, 2)
@pa.check_output(target_schema, 3)
def split_training_data(fatal_encounters_clean):
    return train_test_split(
        fatal_encounters_clean[list(feature_schema.columns)],
        fatal_encounters_clean[target_schema.name],
        test_size=0.2,
        random_state=45,
    )

X_train, X_test, y_train, y_test = split_training_data(fatal_encounters_clean)
```

Model the Data

Import the tools

```
from sklearn.calibration import CalibratedClassifierCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.impute import SimpleImputer
from sklearn.pipeline import Pipeline, make_pipeline
from sklearn.preprocessing import OneHotEncoder, StandardScaler
from sklearn.compose import ColumnTransformer
```

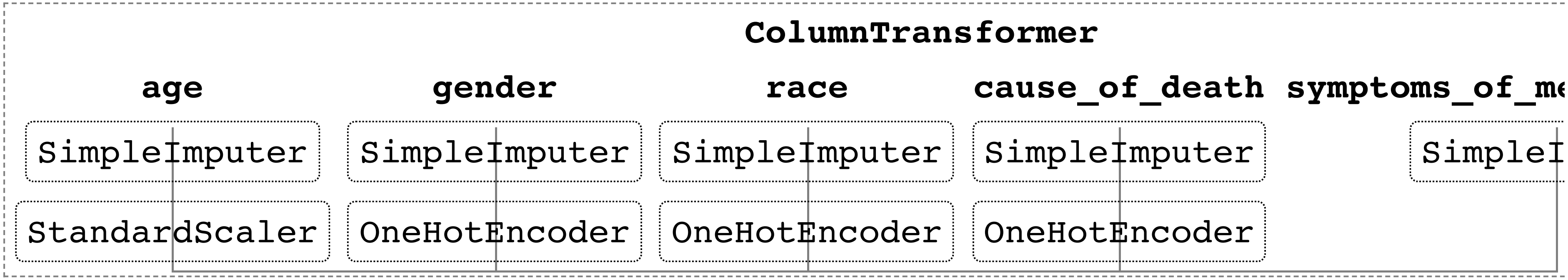
`DataFrameSchema -> ColumnTransformer` 🤯

Create a transformer to numericalize the features using a `schema` object. `Check` s have a `statistics` attribute that enables access to the properties defined in the `schema` .

```python
def column_transformer_from_schema(feature_schema):

    def transformer_from_column(column):
        column_schema = feature_schema.columns[column]
        if column_schema.pandas_dtype is pa.String:
            return make_pipeline(
                SimpleImputer(strategy="most_frequent"),
                OneHotEncoder(categories=[get_categories(column_schema)])
            )
        if column_schema.pandas_dtype is pa.Bool:
            return SimpleImputer(strategy="median")

        # otherwise assume numeric variable
        return make_pipeline(
            SimpleImputer(strategy="median"),
            StandardScaler()
        )

    return ColumnTransformer([
        (column, transformer_from_column(column), [column])
        for column in feature_schema.columns
    ])

def get_categories(column_schema):
    for check in column_schema.checks:
        if check.name == "isin":
            return check.statistics["allowed_values"]
    raise ValueError("could not find Check.isin")
```

Define the transformer

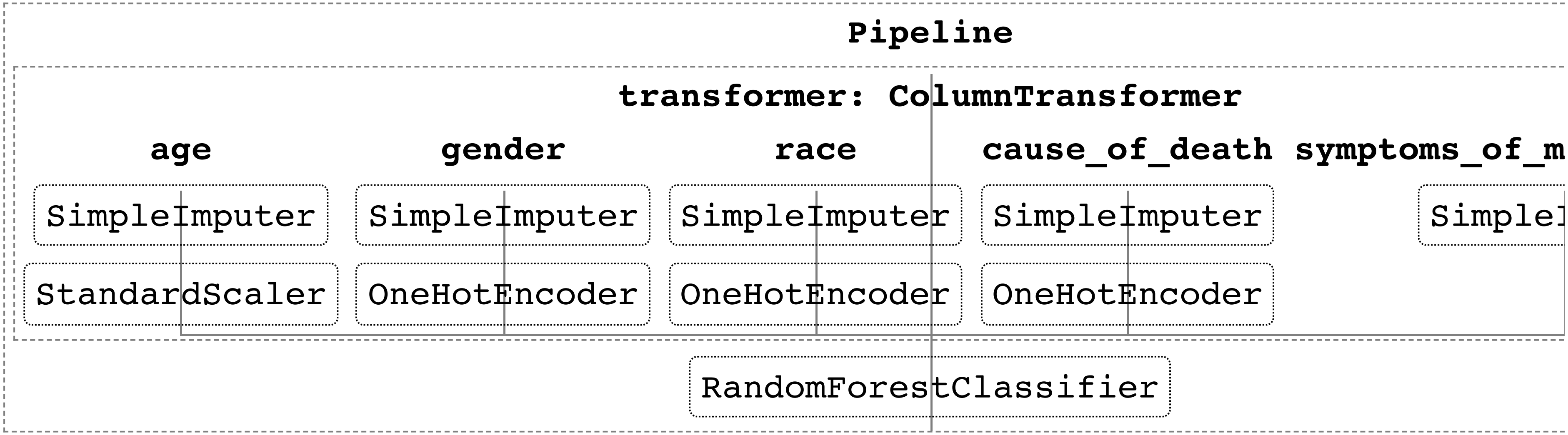
```
transformer = column_transformer_from_schema(feature_schema)
```



Define and fit the modeling pipeline

You can even decorate object methods, specifying the argument name that you want to apply a schema to.

```
pipeline = Pipeline([
    ("transformer", transformer),
    (
        "estimator",
        RandomForestClassifier(
            class_weight="balanced_subsample",
            n_estimators=500,
            min_samples_leaf=20,
            min_samples_split=10,
            max_depth=10,
            random_state=100,
        )
    )
])

fit_fn = pa.check_input(feature_schema, "X")(pipeline.fit)
fit_fn = pa.check_input(target_schema, "y")(fit_fn)
fit_fn(X_train, y_train)
```



Evaluate the Model

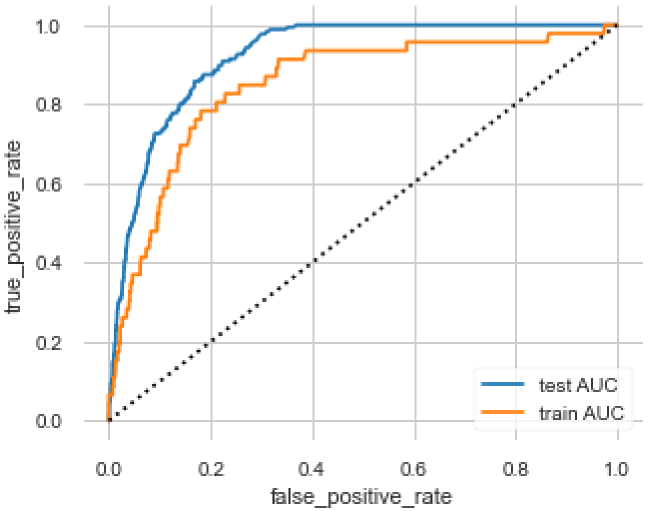
Use the `check_input` and `check_output` decorators to validate the `estimator.predict_proba` method.

```python
from sklearn.metrics import roc_auc_score, roc_curve

pred_schema = pa.SeriesSchema(pa.Float, Check.in_range(0, 1))

# check that the feature array input to predict_proba method adheres to the feature_schema
predict_fn = pa.check_input(feature_schema)(pipeline.predict_proba)

# check that the prediction array output is a probability.
predict_fn = pa.check_output(pred_schema, lambda x: pd.Series(x))(predict_fn)

yhat_train = pipeline.predict_proba(X_train)[:, 1]
print(f"train ROC AUC: {roc_auc_score(y_train, yhat_train):0.04f}")

yhat_test = pipeline.predict_proba(X_test)[:, 1]
print(f"test ROC AUC: {roc_auc_score(y_test, yhat_test):0.04f}")
```

```
train ROC AUC: 0.9207
test ROC AUC: 0.8479
```

Plot the ROC curves using an in-line `schema` .

```python
def plot_roc_auc(y_true, y_pred, label, ax=None):
    fpr, tpr, _ = roc_curve(y_true, y_pred)
    roc_curve_df = pd.DataFrame({"fpr": fpr, "tpr": tpr}).pipe(
        pa.DataFrameSchema({
            "fpr": Column(pa.Float, Check.in_range(0, 1)),
            "tpr": Column(pa.Float, Check.in_range(0, 1)),
        })
    )
    return roc_curve_df.plot.line(x="fpr", y="tpr", label=label, ax=ax)

with sns.axes_style("whitegrid"):
    _, ax = plt.subplots(figsize=(5, 4))
    plot_roc_auc(y_train, yhat_train, "test AUC", ax)
    plot_roc_auc(y_test, yhat_test, "train AUC", ax)
    ax.set_ylabel("true_positive_rate")
    ax.set_xlabel("false_positive_rate")
    ax.plot([0, 1], [0, 1], color="k", linestyle=":")
```



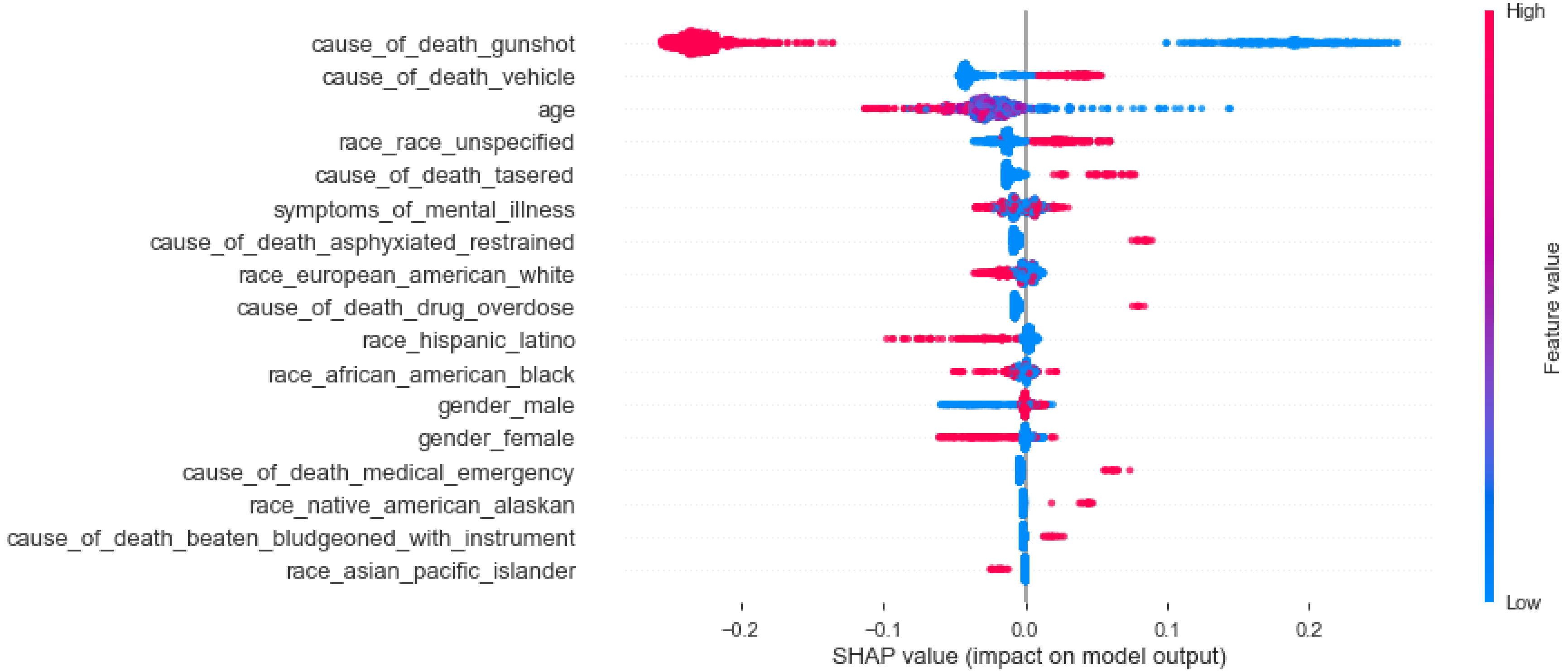
Audit the Model

`shap` package: [https://github.com/slundberg/shap (https://github.com/slundberg/shap)](https://github.com/slundberg/shap)

Create an `explainer` object. Here we want to check the inputs to the `transformer.transform` method.

```
import shap

explainer = shap.TreeExplainer(
    pipeline.named_steps["estimator"],
    feature_perturbation="tree_path_dependent",
)

transform_fn = pa.check_input(feature_schema)(
    pipeline.named_steps["transformer"].transform
)

X_test_array = transform_fn(X_test).toarray()

shap_values = explainer.shap_values(X_test_array, check_additivity=False)
```

What factors are most predictive of the court ruling a case as "Accidental"?



The probability of the case being ruled as `accidental` ⬆️ if the `cause_of_death` is `vehicle`, `tasered`, `asphyxiated_restrained`, `medical_emergency`, or `drug_overdose`, or `race` is `race_unspecified` or `native_american_alaskan`.

The probability of the case being ruled as `accidental` ⬇️ if the `cause_of_death` is `gunshot` or `race` is `european_american_white`, or `asian_pacific_islander`.

Write the Model Audit Schema

Create a dataframe with `{variable}` and `{variable}_shap` as columns

```
audit_dataframe = (
    pd.concat(
        [
            pd.DataFrame(X_test_array, columns=feature_names),
            pd.DataFrame(shap_values[1], columns=[f"{x}_shap" for x in feature_names])
        ],
        axis="columns"
    ).sort_index(axis="columns")
)

audit_dataframe.head(3)
```

	age	age_shap	cause_of_death_asphyxiated_restrained	cause_of_death_asphyxiated_restrained_shap	cause_of_death_beaten_bludgeoned_with_ir
0	-0.534156	-0.039886	0.0	-0.007479	0.0
1	-0.820163	-0.012115	0.0	-0.008413	0.0
2	-0.319651	-0.037459	0.0	-0.008016	0.0

3 rows × 56 columns

Define two sample t-test that tests the relative impact of a variable on the output probability of the model

```python
def hypothesis_accident_probability(feature, increases=True):
    relationship = "greater_than" if increases else "less_than"
    return {
        feature: Column(checks=Check.isin([1, 0])),
        f"{feature}_shap": Column(
            pa.Float,
            checks=Hypothesis.two_sample_ttest(
                sample1=1,
                sample2=0,
                groupby=feature,
                relationship=relationship,
                alpha=0.01,
            )
        ),
    }
```

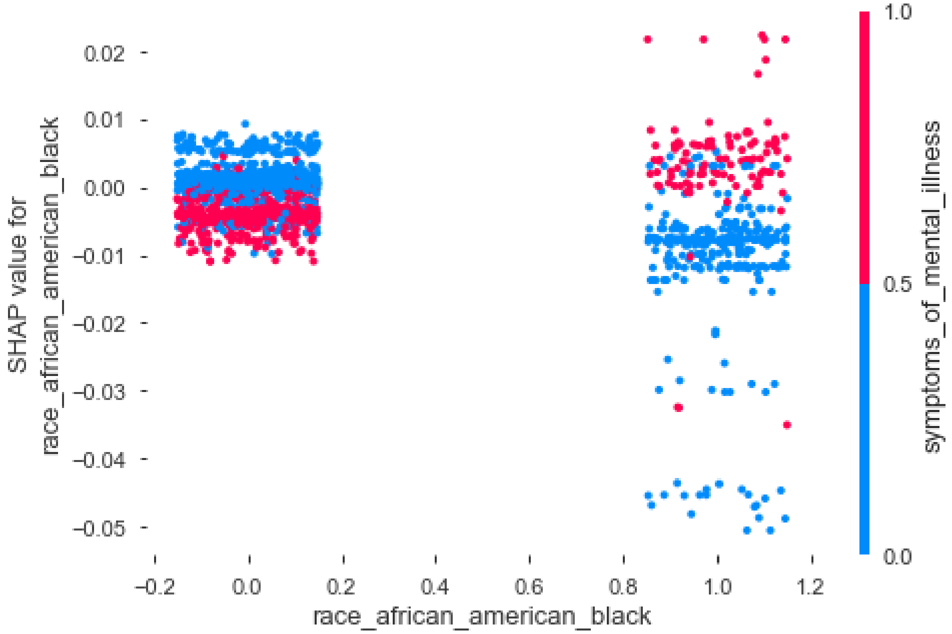
Programmatically construct the schema and validate `feature_shap_df` .

```
columns = {}
# increases probability of disposition "accidental"
for column in [
    "cause_of_death_vehicle",
    "cause_of_death_tasered",
    "cause_of_death_asphyxiated_restrained",
    "cause_of_death_medical_emergency",
    "cause_of_death_drug_overdose",
    "race_race_unspecified",
    "race_native_american_alaskan",
]:
    columns.update(hypothesis_accident_probability(column, increases=True))

# decreases probability of disposition "accidental"
for column in [
    "cause_of_death_gunshot",
    "race_european_american_white",
    "race_asian_pacific_islander",
]:
    columns.update(hypothesis_accident_probability(column, increases=False))

model_audit_schema = pa.DataFrameSchema(columns)

try:
    model_audit_schema(audit_dataframe)
    print("Model audit results pass! ✅ ")
except pa.errors.SchemaError as exc:
    print("Model audit results fail ❌ ")
    print(exc)
```

```
Model audit results pass! ✅
```

More Questions 🤔

- Why would `race_unspecified` be associated with a higher probability of `accidental` rulings?
- Can we predict/impute the `disposition` of unreported, unknown, or pending cases? What would that get us?
- What's the generative process by which these data are being created and collected?
- Are the interaction effects between different demographic variables, e.g. `race_african_american_black` and other variables?



Takeaways

- Data validation is a means to multiple ends: *reproducibility*, *readability*, *maintainability*, and *statistical type safety*
- It's an iterative process between exploring the data, acquiring domain knowledge, and writing validation code.
- `pandera` schemas are executable contracts that enforce the statistical properties of a dataframe at runtime and can be flexibly interleaved with data processing and analysis logic.
- `pandera` doesn't automate data exploration or the data validation process. The user is responsible for identifying which parts of the pipeline are critical to test and defining the contracts under which data are considered valid.

Experimental Features

Schema Inference

```python
schema = pa.infer_schema(dataframe)
```

Schema Serialization

```python
pa.io.to_yaml(schema, "schema.yml")
pa.io.to_script(schema, "schema.py")
```

Roadmap: Feature Proposals

Define domain-specific schemas, types, and checks, e.g. for machine learning

```python
# validate a regression model dataset
schema = pa.machine_learning.supervised.TabularSchema(
    targets={"regression": pa.TargetColumn(type=pa.ml_dtypes.Continuous)},
    features={
        "continuous": pa.FeatureColumn(type=pa.ml_dtypes.Continuous),
        "categorical": pa.FeatureColumn(type=pa.ml_dtypes.Categorical),
        "ordinal": pa.FeatureColumn(type=pa.ml_dtypes.Ordinal),
    }
)
```

Generate synthetic data based on schema definition as constraints

```python
dataset = schema.generate_samples(100)
X, y = dataset[schema.features], dataset[schema.targets]
estimator.fit(X, y)
```

Contributions are Welcome!

Repo: [https://github.com/pandera-dev/pandera (https://github.com/pandera-dev/pandera)](https://github.com/pandera-dev/pandera)

1. Improving documentation
2. Submit feature requests (e.g. additional built-in `Check` and `Hypothesis` methods)
3. Submit bugs/issues or pull requests on Github

Thank you!

@cosmicBboy (https://twitter.com/cosmicBboy)