mlinspect: Lightweight Inspection of Native Machine Learning Pipelines

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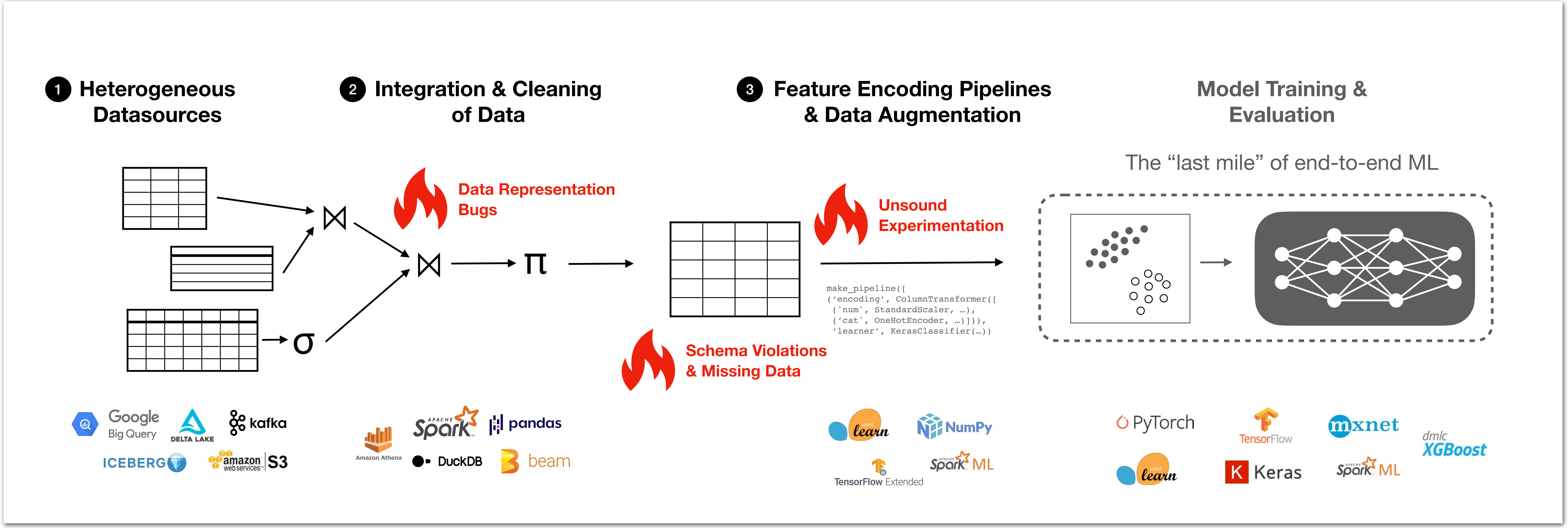
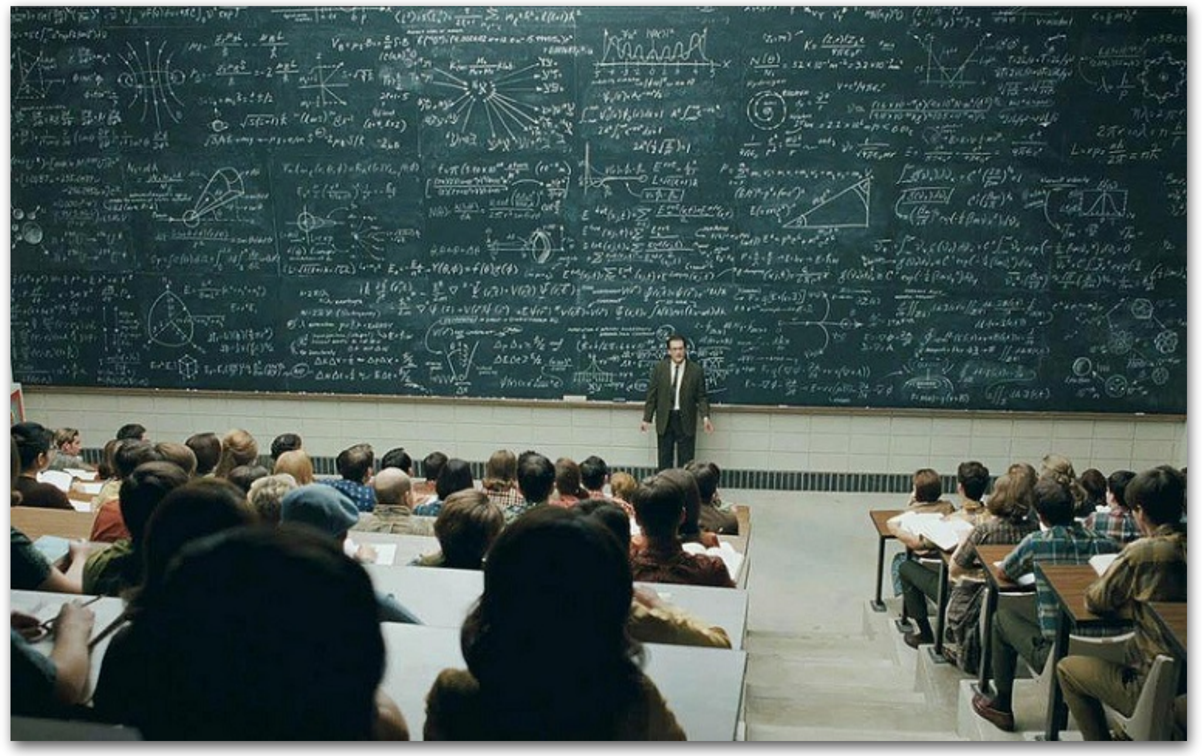
ML Pipelines in the Real World



ML in Research vs ML in Production

- **Lab conditions**
  - Mental model of working in a jupyter notebook
  - Dataset static, clean, well understood, often fits into memory
  - User has PhD in ML
- **Production conditions**
  - Data continuously produced, never clean
  - Data originates from many sources, not under control
  - Model training is only one piece of large, complex pipelines
  - Non-ML experts as end users / operators
- **Even experts make mistakes!**



https://chrisguillebeau.com/files/2016/11/Mathboard.jpg

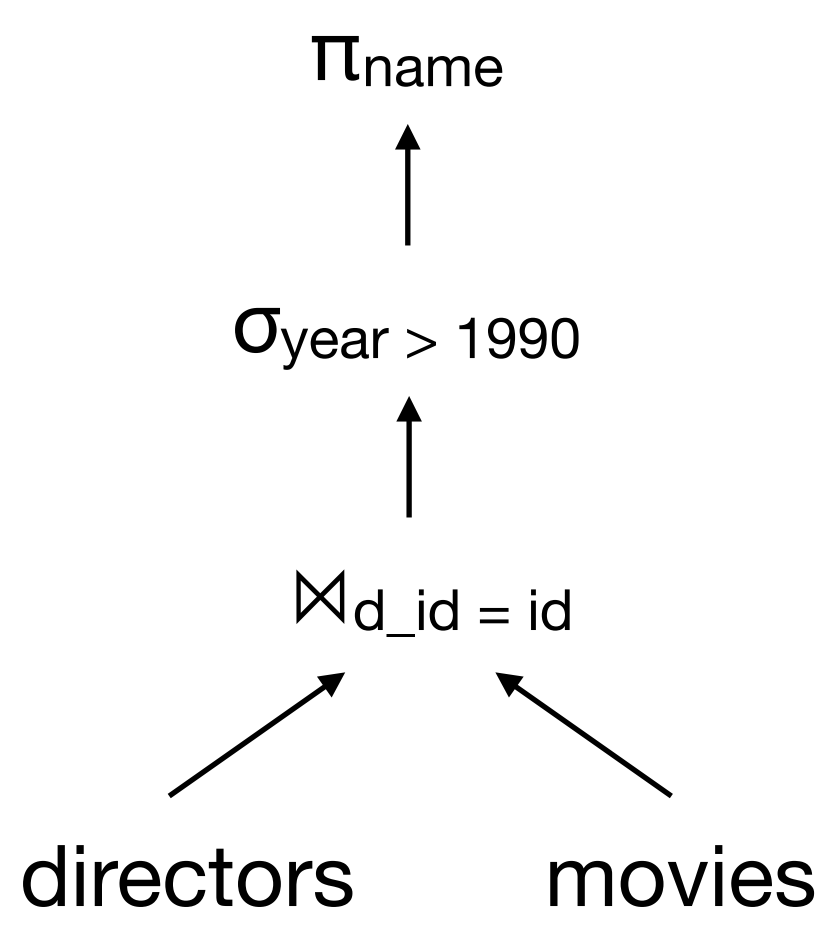
On Challenges in Machine Learning Model Management, IEEE Data Engineering Bulletin'19
FairPrep: Promoting Data to a First-Class Citizen in Studies on Fairness-Enhancing Interventions, EDBT'20

What Makes Inspection Difficult?

- **Relational DBMS:** Explicit data model (relations), computations (queries) expressed declaratively in relational algebra
- **Algebraic properties enable automatic inspection**: e.g. identifying all input records that contributed to a query result (why-provenance)
- **ML Pipelines: lack of unifying algebraic foundation** for data preprocessing, different technologies "glued together"

```
SELECT name
FROM directors
JOIN movies ON d_id = id
WHERE year > 1990
```

$\pi_{name}\ \sigma_{year\,>\,1990}\ (\text{directors} \bowtie_{d\_id\,=\,id} \text{movies})$



On Challenges in Machine Learning Model Management, Data Engineering Bulletin'19

The Way Forward

- First approach: **invent new holistic systems to regain control** -> **would require rewriting all existing code**
- Second approach: **manually annotating existing code** -> **does not happen in practice**
- **Our approach: retrofit inspection techniques into the existing DS landscape**
- Observation: **declarative specification of operations for preprocessing present in some popular ML libraries**:
    - Pandas mostly applies relational operations
    - Estimator / Transformer pipelines (scikit-learn / SparkML / Tensorflow Transform) offer nestable and composable way to declaratively specify feature transformations

Example

Potential issues in preprocessing pipeline:

1. Join might change proportions of groups in data
2. Column 'age_group' projected out, but required for fairness
3. Selection might change proportions of groups in data
4. Imputation might change proportions of groups in data
5. 'race' as a feature might be illegal!
6. Embedding vectors may not be available for rare names!

```
# load input data sources, join to single table
patients = pandas.read_csv(…)
histories = pandas.read_csv(…)
data = pandas.merge([patients, histories], on=['ssn'])

# compute mean complications per age group, append as column
complications = data.groupby('age_group')
 .agg(mean_complications=('complications','mean'))
data = data.merge(complications, on=['age_group'])

# Target variable: people with frequent complications
data['label'] = data['complications'] >
  1.2 * data['mean_complications']

# Project data to subset of attributes, filter by counties
data = data[['smoker', 'last_name', 'county',
             'num_children', 'race', 'income', 'label']]
data = data[data['county'].isin(counties_of_interest)]

# Define a nested feature encoding pipeline for the data
impute_and_encode = sklearn.Pipeline([
  (sklearn.SimpleImputer(strategy='most_frequent')),
  (sklearn.OneHotEncoder())])
featurisation = sklearn.ColumnTransformer(transformers=[
  (impute_and_encode, ['smoker', 'county', 'race']),
  (Word2VecTransformer(), 'last_name')
  (sklearn.StandardScaler(), ['num_children', 'income']])

# Define the training pipeline for the model
neural_net = sklearn.KerasClassifier(build_fn=create_model())
pipeline = sklearn.Pipeline([
  ('features', featurisation),
  ('learning_algorithm', neural_net)])

# Train-test split, model training and evaluation
train_data, test_data = train_test_split(data)
model = pipeline.fit(train_data, train_data.label)
print(model.score(test_data, test_data.label))
```

Can we find ways to **automatically hint data scientists at potentially problematic operations** in the preprocessing code of their ML pipelines?

Inspiration from software engineering, e.g. **code inspection in modern IDE's**

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Python script for preprocessing, written exclusively with native pandas and sklearn constructs

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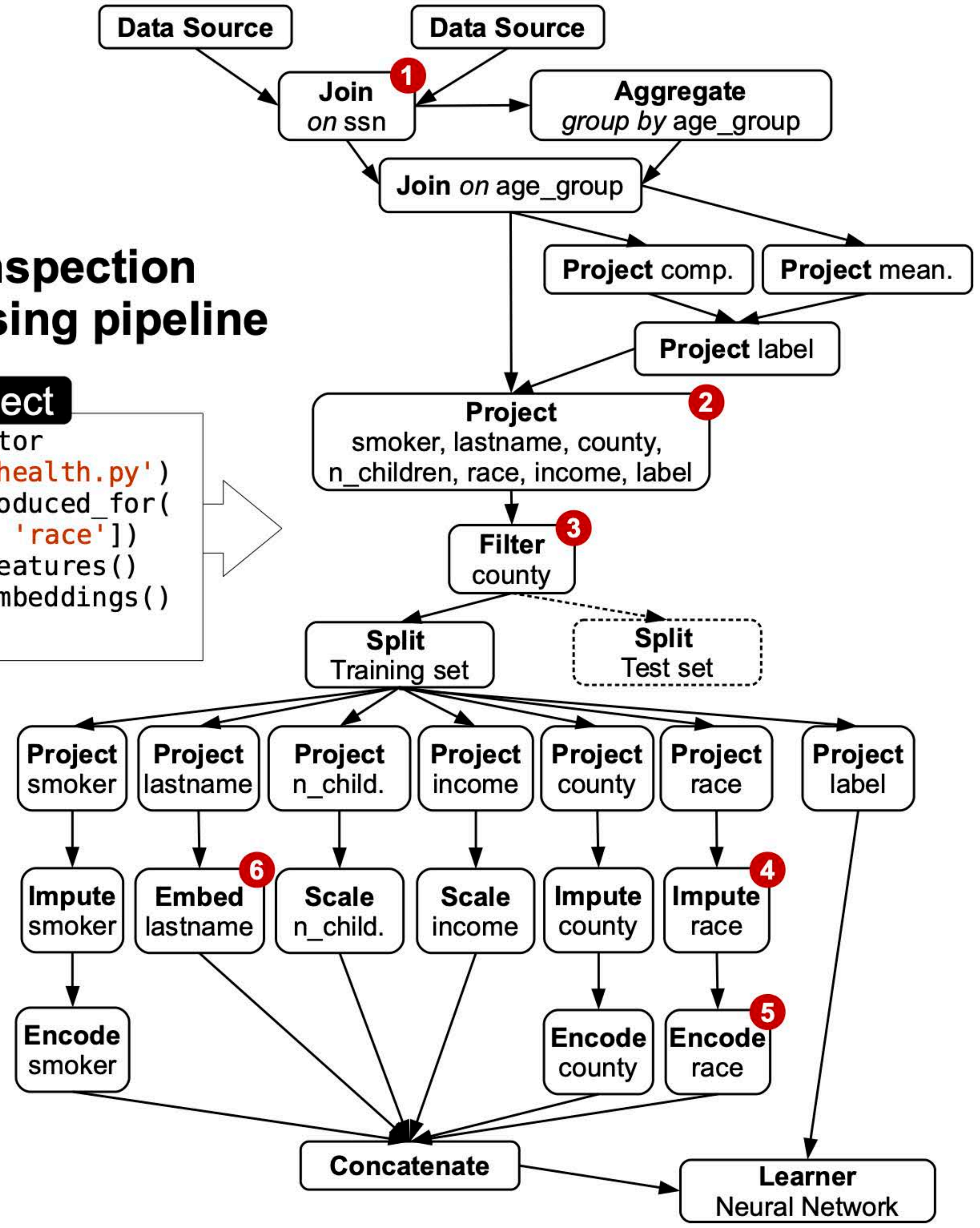
```

Declarative inspection of preprocessing pipeline

mlinspect

```
PipelineInspector
.on_pipeline('health.py')
 .no_bias_introduced_for(
 ['age_group', 'race'])
 .no_illegal_features()
 .no_missing_embeddings()
.verify()
```

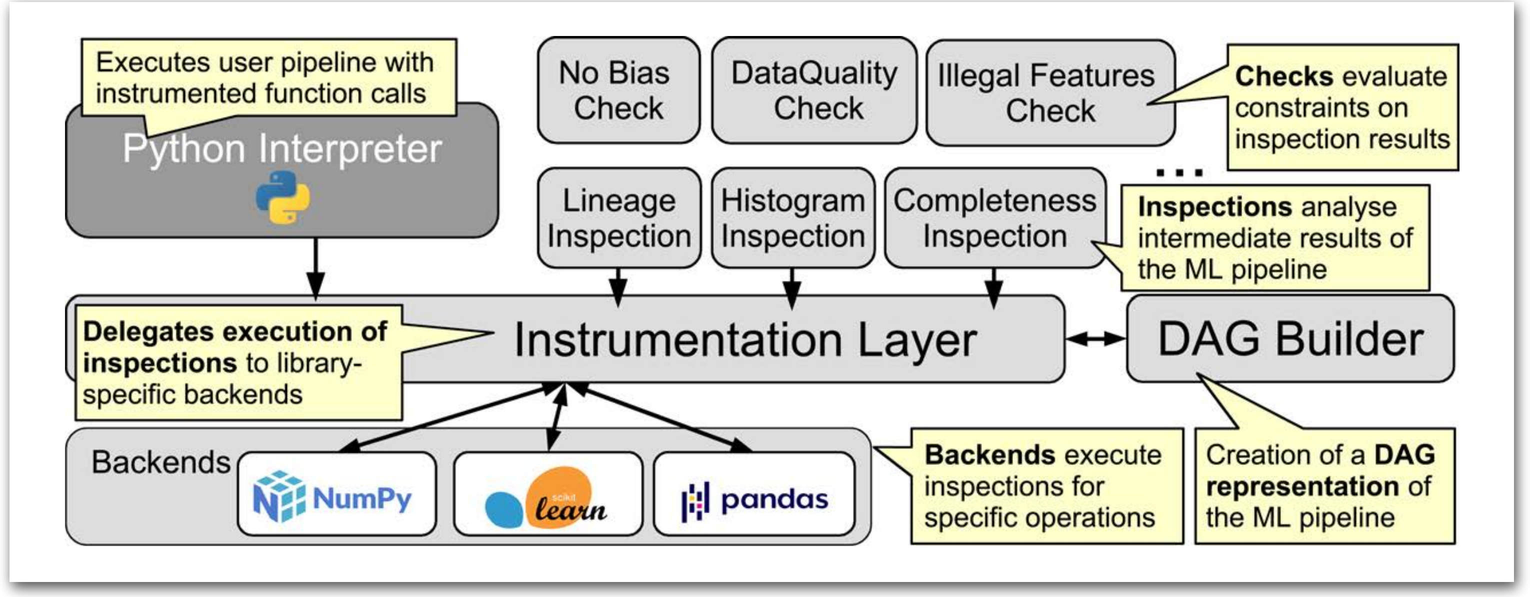
Corresponding dataflow DAG for instrumentation, extracted by *mlinspect*



mlinspect

- Library to instrument ML preprocessing code with custom inspections to **analyse a single pipeline execution and detect potential issues**
- Works with **“native” preprocessing pipelines** (no annotation / manual instrumentation required) in pandas / sklearn / keras
- **Representation of preprocessing operations based on dataflow graph**
- Allows users to **implement inspections as user-defined functions** which are **automatically applied to the inputs and outputs of certain operations**

```
PipelineInspector
 .on_pipeline_from_py_file('healthcare.py')
  .expect_no_bias_introduced_for(['age_group', 'race'])
  .expect_no_use_of_illegal_features()
  .expect_no_missing_embeddings()
 .verify()
```



Data Distribution Debugging in Machine Learning Pipelines, VLDBJ’22

Inspections & Checks

- The central entry point of mlinspect is the **PipelineInspector**
  - There, you can add **inspections** and **checks**
- **Inspections:**
  - Visit each operator in the extracted DAG to analyse the data flowing through it
  - Can also annotate individual tuples, to track how they flow through the pipeline
  - These annotations are only visible for mlinspect
- **Checks:**
  - Check constraints on the extracted DAG and, when needed, the results of inspections

```
from mlinspect import PipelineInspector
from mlinspect.inspections import MaterializeFirstOutputRows
from mlinspect.checks import NoBiasIntroducedFor

IPYNB_PATH = ...

inspector_result = PipelineInspector\
        .on_pipeline_from_ipynb_file(IPYNB_PATH)\
        .add_required_inspection(MaterializeFirstOutputRows(5))\
        .add_check(NoBiasIntroducedFor(['race']))\
        .execute()

extracted_dag = inspector_result.dag
dag_node_to_inspection_results = inspector_result.dag_node_to_inspection_results
check_to_check_results = inspector_result.check_to_check_results
```

Inspection: MaterializeFirstOutputRows

- The most simple **inspection** in mlinspect
- **Analyzes the data** flowing through each operator in your ML pipeline, and **materializes** the first *n* rows of each
- This is similar to how data scientists might try to debug their code with *print* statements, just to see what data looks like at different pipeline stages
- For pipelines using lots of data, inspections **should not materialize all intermediate data**!

```
data = pd.merge([patient, cost],
                on="ssn")
data = data[["smoke", "cost"]]
```

ssn	smoke
123	Y
456	N
789	Y
…	…

ssn	cost
123	100
789	200
…	…

ssn	smoke	cost
123	Y	100
789	Y	200
…	…	…

smoke	cost
Y	100
Y	200
…	…

Inspection: RowLineage

- This inspection uses **annotation propagation** to track individual tuples through the ML pipeline

- Operators like filters, joins, and sorting can make tracking tuples manually difficult

- Example: you encounter an unexpected *null*-value somewhere in your pipeline. Where does the *null*-value come from? What are the corresponding rows in the initial input tables?

```
data = pd.merge([patient, cost],
                 on=“ssn”)
data = data[[“smoke”, “cost”]]
```

ssn	smoke	
123	null	{(1,1)}
456	N	{(1,2)}
789	Y	{(1,3)}
…	…	

ssn	cost	
123	100	{(2,1)}
789	200	{(2,2)}
…	…	

ssn	smoke	cost	
123	null	100	{(1,1),(2,1)}
789	Y	200	{(1,3),(2,2)}
…	…	…	

smoke	cost	
null	100	{(1,1),(2,1)}
Y	200	{(1,3),(2,2)}
…	…	

HistogramForColumns & NoBiasIntroducedFor

- The *HistogramForColumns* inspection uses **annotation propagation** to track group memberships through the ML pipeline and materializes histograms of the groups
- The check *NoBiasIntroducedFor* checks for sudden distribution shifts by looking at the histograms before and after each operator
- Next to *HistogramForColumns,* there is also *IntersectionalHistogramForColumns*
- **Problem**: when should a distribution shift trigger a warning?

```
data = data[data.county = “CountyA”]
data = data[[“county”]]
```

age_group	county
< 60	CountyA
< 60	CountyA
< 20	CountyA
< 60	CountyB
< 20	CountyB
< 20	CountyB

age_group: 50% vs 50%

age_group	county
< 60	CountyA
< 60	CountyA
< 20	CountyA

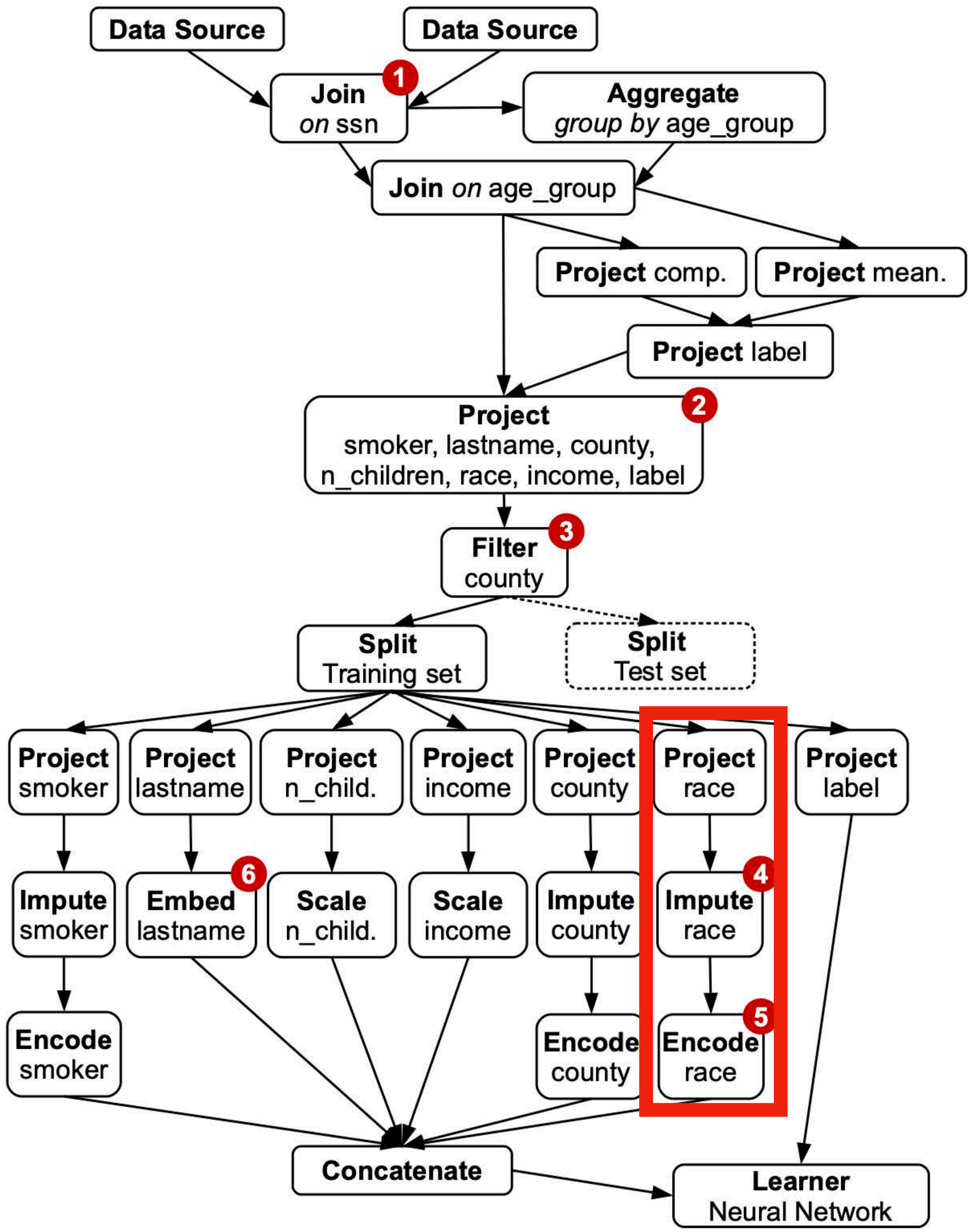
age_group: 66% vs 33%

county	
CountyA	< 60
CountyA	< 60
CountyA	< 20

age_group: 66% vs 33%

Check: NoIllegalFeatures

- This check only looks at the extracted DAG to see if columns with certain names are used as input for an ML model
- As with *NoBiasIntroducedFor*: this detection based only on comparing column names with pre-defined and user-defined lists is **no guarantee** that all features are okay to be used!
- However, this can help with spotting potential issues easier



Data Quality Inspections

- mlinspect also offers exemplary inspections for data quality checking: *CompletenessOfColumns* and *CountDistinctOfColumns*

- The completeness of a column is the fraction of non-null values in it

- On top of these inspections, it is again possible to build checks

```
data = pd.merge([patient, cost],
                on="ssn", how="right")
```

ssn	cost
123	100
456	200
789	150

smoke completeness: N/A

ssn	smoke
123	Y
789	N

smoke completeness: 100%

ssn	cost	smoke
123	100	Y
456	200	null
789	150	N

smoke completeness: 66%

Demo

https://surfdrive.surf.nl/files/index.php/s/ybriyzsdc6vcd2w 1:06-4:00

Inspection Implementation

- Experienced users can also implement their own inspections and checks
- **Implementation of inspections via for-comprehensions** on iterators
- **Efficient execution with loop fusion** (“banana-split law”)
- **Runtime overhead linear in the number of input and output records** as long as the row annotations have a fixed size limit

```
# Abstract base class for all inspections
class Inspection(metaclass=abc.ABCMeta):
  # Inspect intermediate data at a DAG operator, based on operator
  #  information (op_context), and an iterator over annotated
  #  input rows with the corresponding output rows (row_iterator);
  # Return computed annotations for output rows
  def visit_op(self, op_context, row_iterator) -> Iterable
  # Persist inspection result for the current DAG node
  def op_annotation_after_visit(self)
```

```
def visit_op(self, op_context,  row_iterator) -> Iterable
  for row in row_iterator:
    annotation = annotate_and_update_state(self, row)
    yield annotation
```

Inspection Execution

1. **Preparation**: Determination of a minimal required set of inspections based on the inspections and checks specified by the user.

2. **Instrumentation**: Instrumentation of function calls of the AST of the user program, monkey patching.

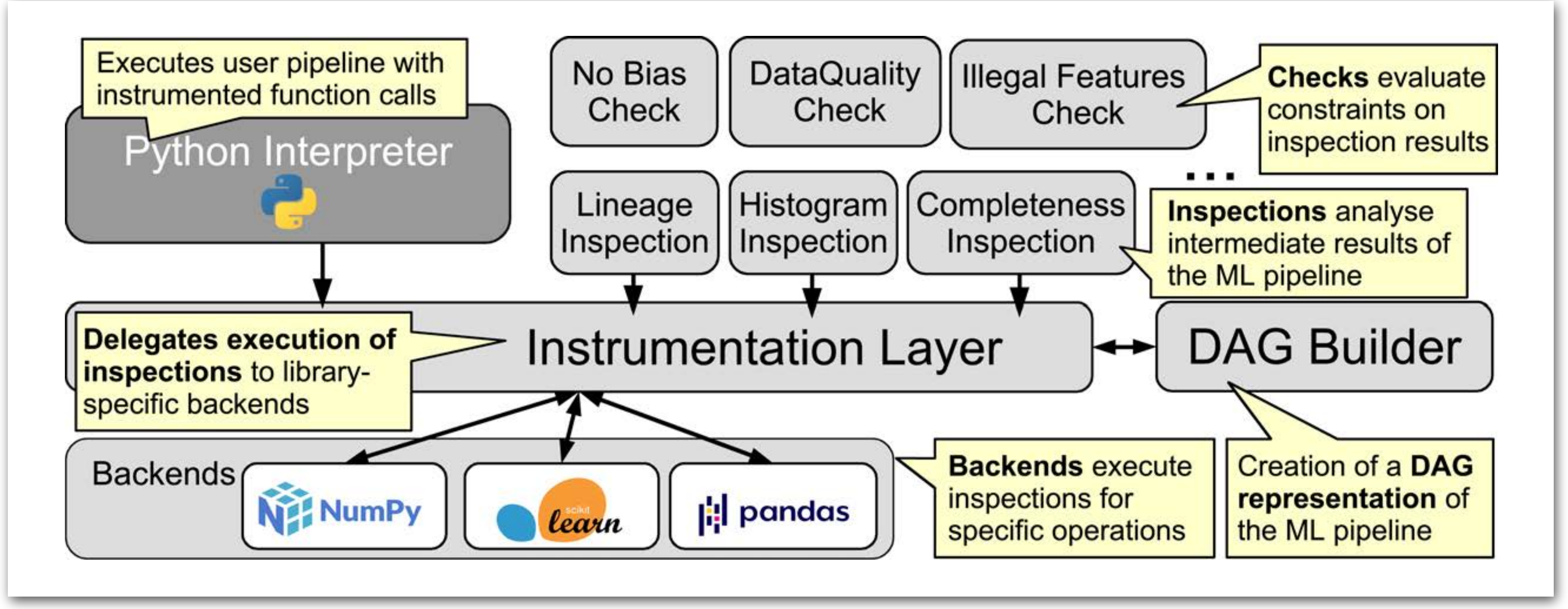
3. **Execution of the instrumented program**: Delegation of the execution of inspections to library-specific backends; joint execution with pipeline operations; creation of the dataflow DAG.

4. **Results**: Evaluation of checks using the DAG and the inspection results.

```
from mlinspect.instrumentation
 import monkey_patch, undo_monkey_patch
monkey_patch()
# ...original user code...
undo_monkey_patch()
```

```
obj.a_func("arg0", "arg1", my_arg="arg2")
```

```
obj.a_func("arg0", "arg1", my_arg="arg2",
            **set_code_reference(0,0,0,42))
```

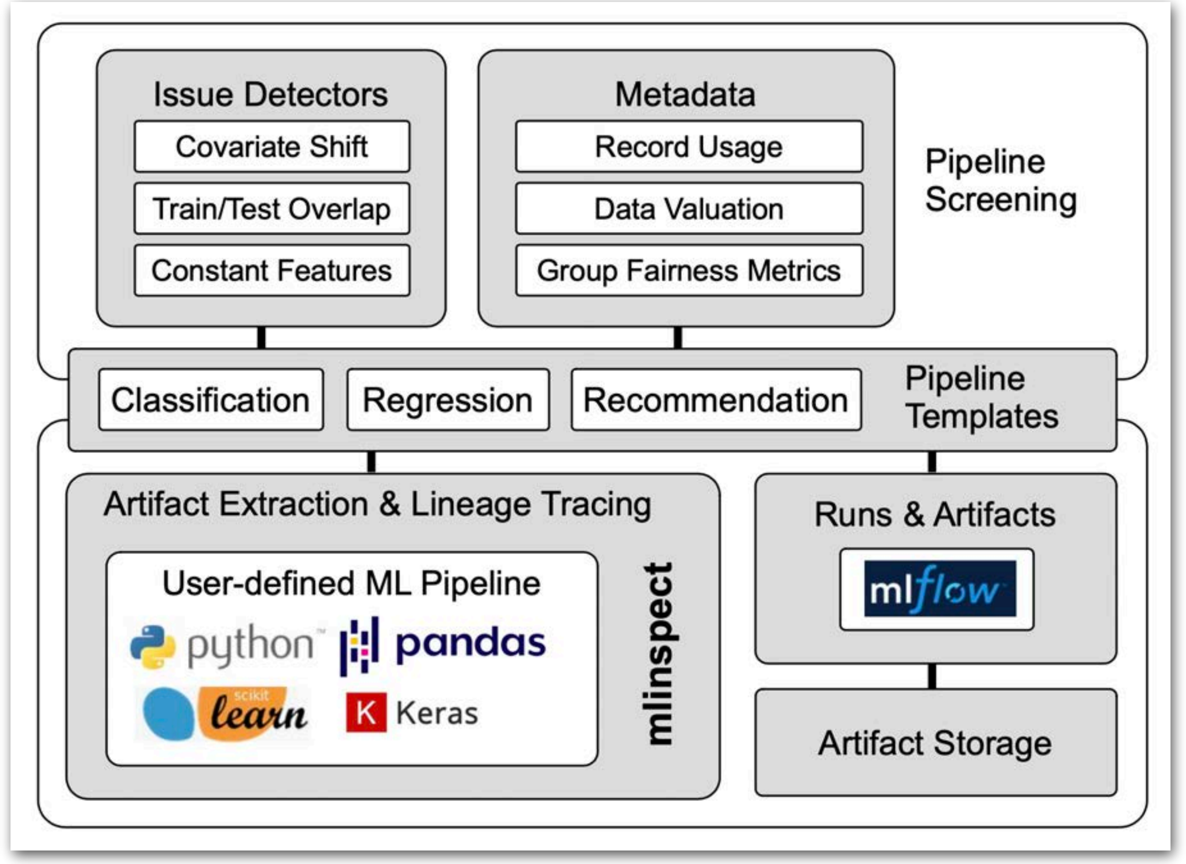


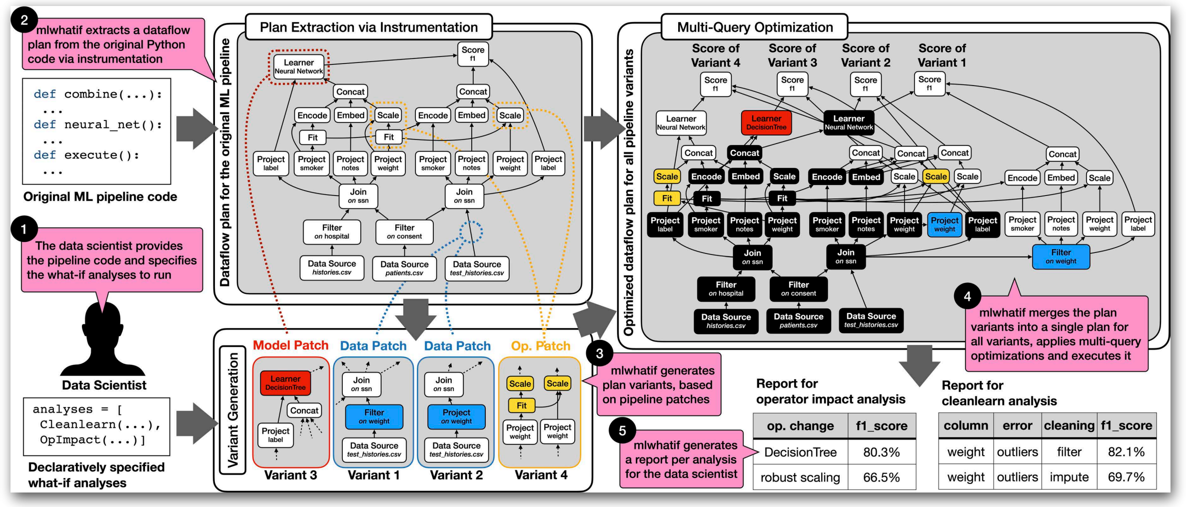
Monkey Patching

```
@gorilla.patches(sklearn.preprocessing)
class SklearnPreprocessingPatching:
  @gorilla.name('label_binarize')
  @gorilla.settings(allow_hit=True)
  def execute_label_binarize(*args, **kwargs):
    original = gorilla.get_original_attribute(sklearn.preprocessing, 'label_binarize')
    # Patched function
    def patched(...):
      function_info = FunctionInfo('sklearn.preprocessing._label', 'label_binarize')
      # Operator mapping for DAG
      op_ctx = OperatorContext(OperatorType.PROJECTION_MODIFY, function_info)
      parent_info = get_parent_node_info(args[0], ...)
      # Initiate inspection execution via backend
      input_df = SklearnBackend.before_call(op_ctx, [parent_info])
      # Execute original function
      result = original(input_df, *args[1:], **kwargs)
      # Finalize inspection execution via backend
      backend_result = SklearnBackend.after_call(op_ctx, input_df, result)
      # Append DAG node with inspection result
      add_new_operator_node_to_dag(DagNode(...), [parent_info], backend_result)
      # Return original result
      return backend_result.updated_result_df
    return execute(original, patched, *args, **kwargs)
```

Ongoing and Future Work

- **Moving the execution** of inspections **into more efficient runtime systems** like DuckDB
- Use mlinspect as runtime system to **enable different use cases**, e.g., automated screening of ML pipelines during CI pipelines (**ArgusEyes**)
- Assisting with **more advanced ML pipeline analysis that requires pipeline rewriting** and cannot be done by just observing a single execution of a given ML pipeline (**mlwhatif**)





Proactively Screening Machine Learning Pipelines with ArgusEyes, SIGMOD'23 (demo)

Automating and Optimizing Data-Centric What-If Analyses on Native Machine Learning Pipelines, SIGMOD'23

Data-Centric What-If Analysis for ML Pipelines

- ML pipelines are **often brittle with respect to input data**

- Data scientists are interested in different **what-if analyses** for their pipelines, e.g.,

  - **What-if** there are data quality problems?

  - **What-if** I used different preprocessing?

- Currently, data scientists have to implement this **manually**, which is tedious and error-prone

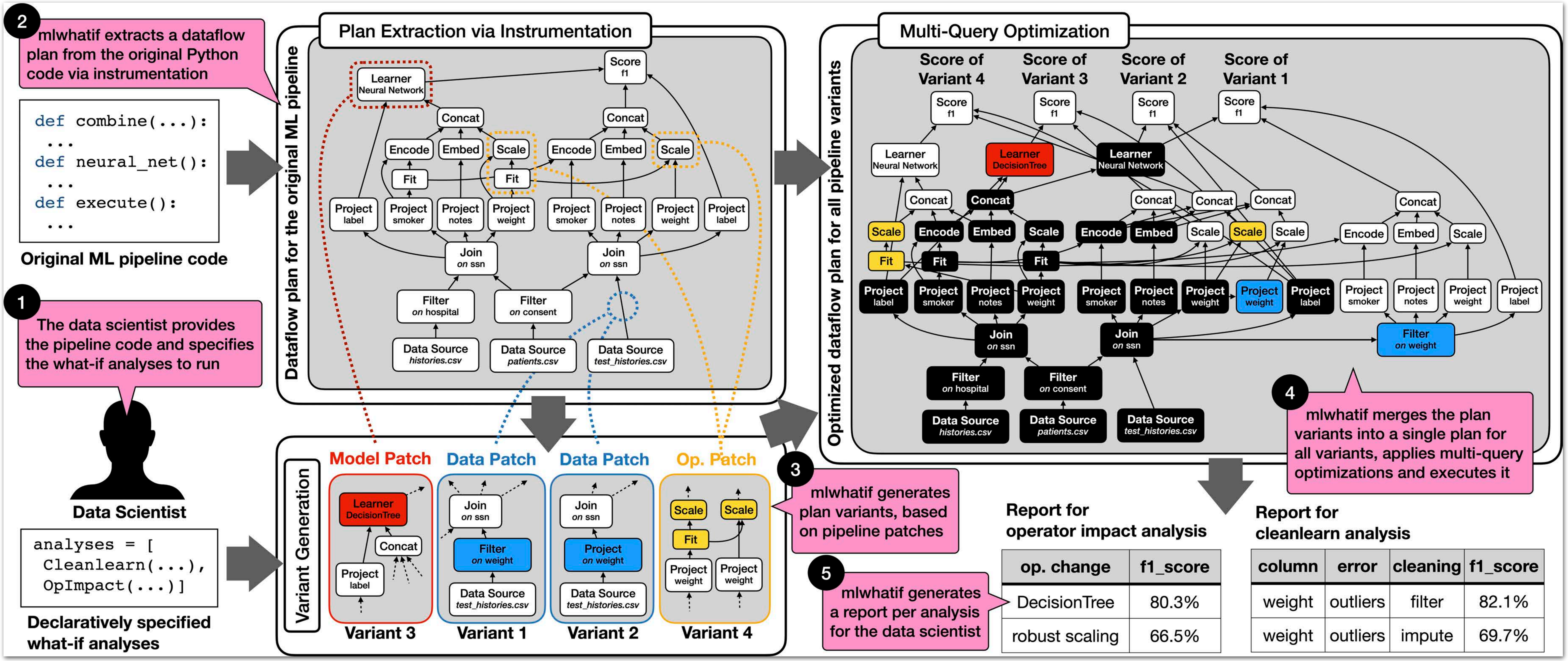
- **Goal: Allow declarative what-if analysis** by automatically rewriting extracted pipeline DAGs

```
from mlwhatif.analysis import Cleanlearn, OperatorImpact
analyses = [ # Declarative definition of what-if analyses to run
  Cleanlearn(column='weight', error=Error.OUTLIER,
             cleanings=[Clean.FILTER, Clean.IMPUTE]),
  OperatorImpact(robust_scaling=True, alternative_model=...)]
# Execution of what-if analyses on a given pipeline
report_with_scores = mlwhatif.execute_whatif('healthcare.py', analyses)
print(report_with_scores)
```

analysis	column	error_detector	cleaning	f1_score
cleanlearn	weight	outliers	filter	0.821
cleanlearn	weight	outliers	impute_const	0.697

Automating and Optimizing Data-Centric What-If Analyses on Native Machine Learning Pipelines, SIGMOD'23

mlwhatif: Data-Centric What-If Analysis




```
def combine(...):
  ...
def neural_net():
  ...
def execute():
  ...
```

```
analyses = [
 Cleanlearn(...),
 OpImpact(...)]
```

Report for operator impact analysis

op. change	f1_score
DecisionTree	80.3%
robust scaling	66.5%

Report for cleanlearn analysis

column	error	cleaning	f1_score
weight	outliers	filter	82.1%
weight	outliers	impute	69.7%

Thanks!

- **Summary**
  - **mlinspect** allows inspecting a single execution of a given input ML pipeline: **https://github.com/stefan-grafberger/mlinspect**
  - **mlwhatif** allows declarative what-if analysis **https://github.com/stefan-grafberger/mlwhatif**
  - **Limitation:** Our approach relies on“declaratively” written ML pipelines, where we can identify the semantics of the operations
- For more about my research, visit **https://stefan-grafberger.com/**

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```

Banana split law

- Operations like calculating the sum and the length of numerical data can be done using folds. All folds can be combined into a single fold.
- sumlength :: [Int] → (Int,Int)
  sumlength xs = (sum xs, length xs)
- sumlength = fold (λn (x, y) → (n + x, 1 + y)) (0, 0)
- "The strange name of this property derives from the fact that the *fold* operator is sometimes written using brackets (| |) that resemble bananas, and the pairing operator is sometimes called split."

A tutorial on the universality and expressiveness of fold, Graham Hutton, 1999