NYU

Reproducible Open Benchmarks for Data Analysis

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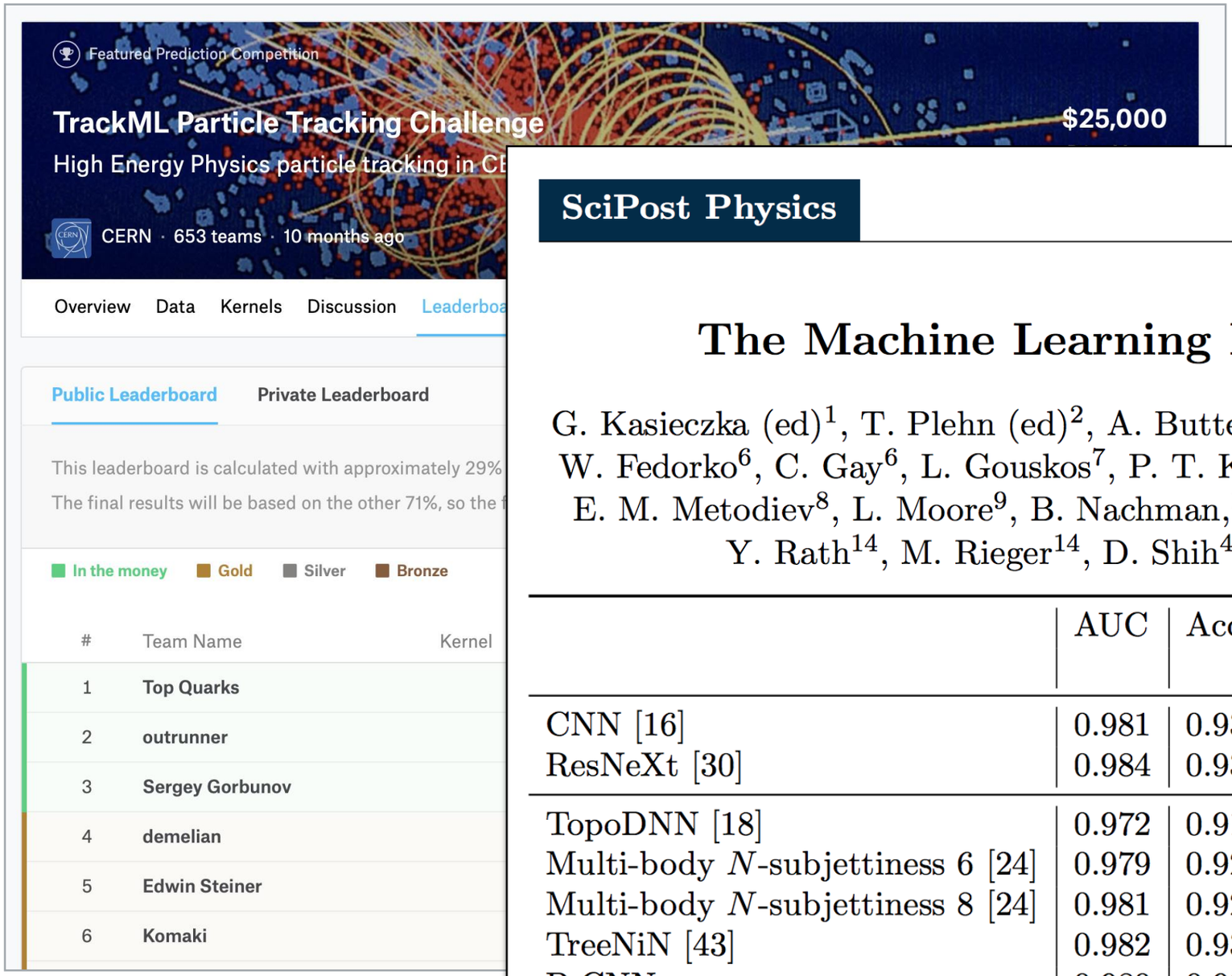


SciPost Physics Submission

The Machine Learning Landscape of Top Taggers

G. Kasieczka (ed)[1], T. Plehn (ed)[2], A. Butter[2], K. Cranmer[3], D. Debnath[4], M. Fairbairn[5], W. Fedorko[6], C. Gay[6], L. Gouskos[7], P. T. Komiske[8], S. Leiss[1], A. Lister[6], S. Macaluso[3,4], E. M. Metodiev[8], L. Moore[9], B. Nachman,[10,11], K. Nordström[12,13], J. Pearkes[6], H. Qu[7], Y. Rath[14], M. Rieger[14], D. Shih[4], J. M. Thompson[2], and S. Varma[5]

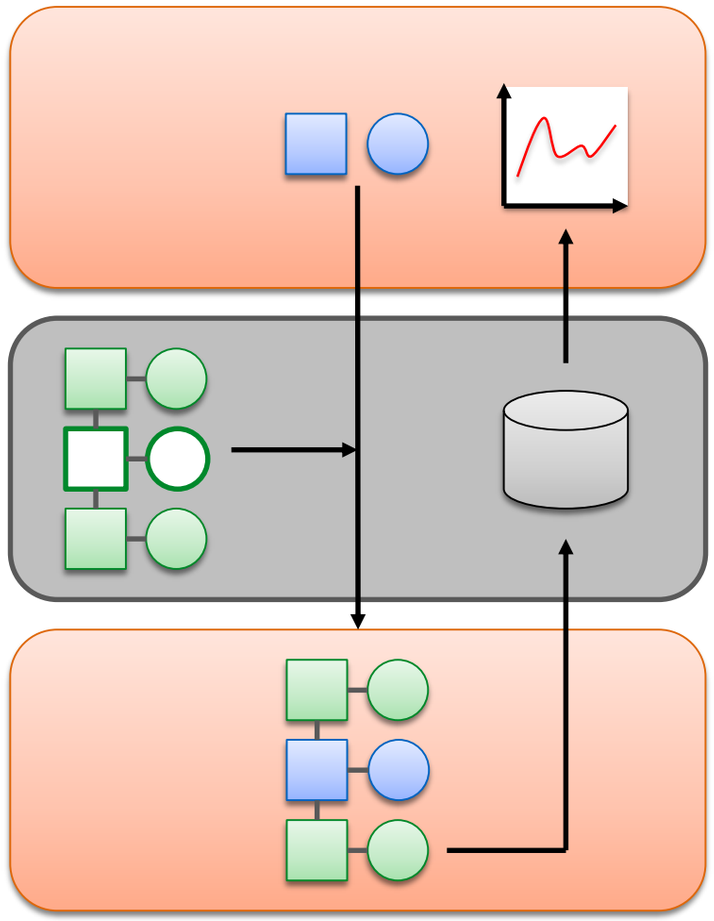
	AUC	Acc	$1/\epsilon_B$ ($\epsilon_S = 0.3$) single	mean	median	#Param
CNN [16]	0.981	0.930	914±14	995±15	975±18	610k
ResNeXt [30]	0.984	0.936	1122±47	1270±28	1286±31	1.46M
TopoDNN [18]	0.972	0.916	295±5	382± 5	378 ± 8	59k
Multi-body N-subjettiness 6 [24]	0.979	0.922	792±18	798±12	808±13	57k
Multi-body N-subjettiness 8 [24]	0.981	0.929	867±15	918±20	926±18	58k
TreeNiN [43]	0.982	0.933	1025±11	1202±23	1188±24	34k
P-CNN	0.980	0.930	732±24	845±13	834±14	348k
ParticleNet [47]	0.985	0.938	1298±46	1412±45	1393±41	498k
LBN [19]	0.981	0.931	836±17	859±67	966±20	705k
LoLa [22]	0.980	0.929	722±17	768±11	765±11	127k
Energy Flow Polynomials [21]	0.980	0.932	384			1k
Energy Flow Network [23]	0.979	0.927	633±31	729±13	726±11	82k
Particle Flow Network [23]	0.982	0.932	891±18	1063±21	1052±29	82k
GoaT	0.985	0.939	1368±140		1549±208	35k

Reproducible Open Benchmarks Platform

Exploratory work for enabling such community benchmarks.

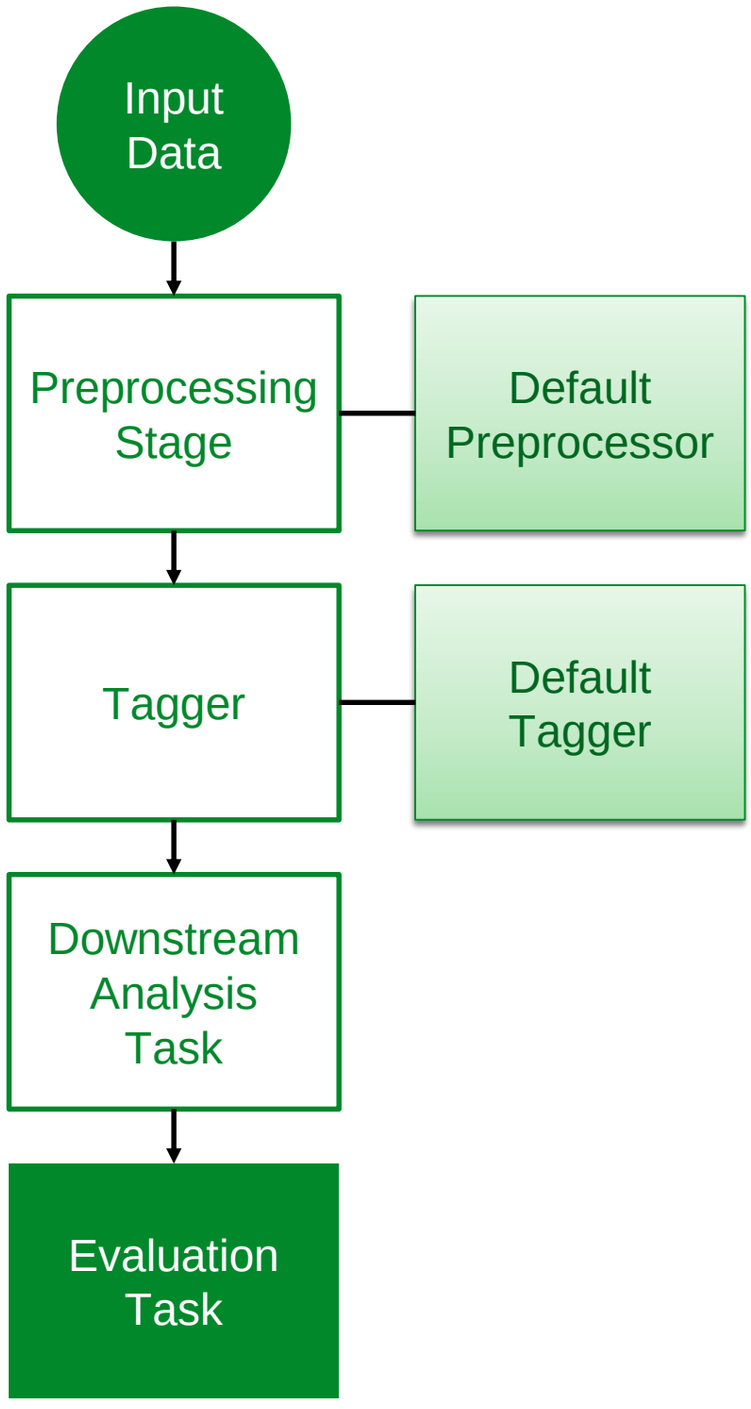
Components and Actors in ROB

1. Benchmark workflow defined by **coordinator** along with input data.
2. **Users** provide code (e.g. docker containers) that satisfy workflow stages, input parameters, and input data (file upload).
3. **Back-end** processes workflows and evaluates metrics (powered for example by REANA).
4. **Front-end** to collect input and display results.



Reproducible research data analysis platform

Benchmark Workflow Example

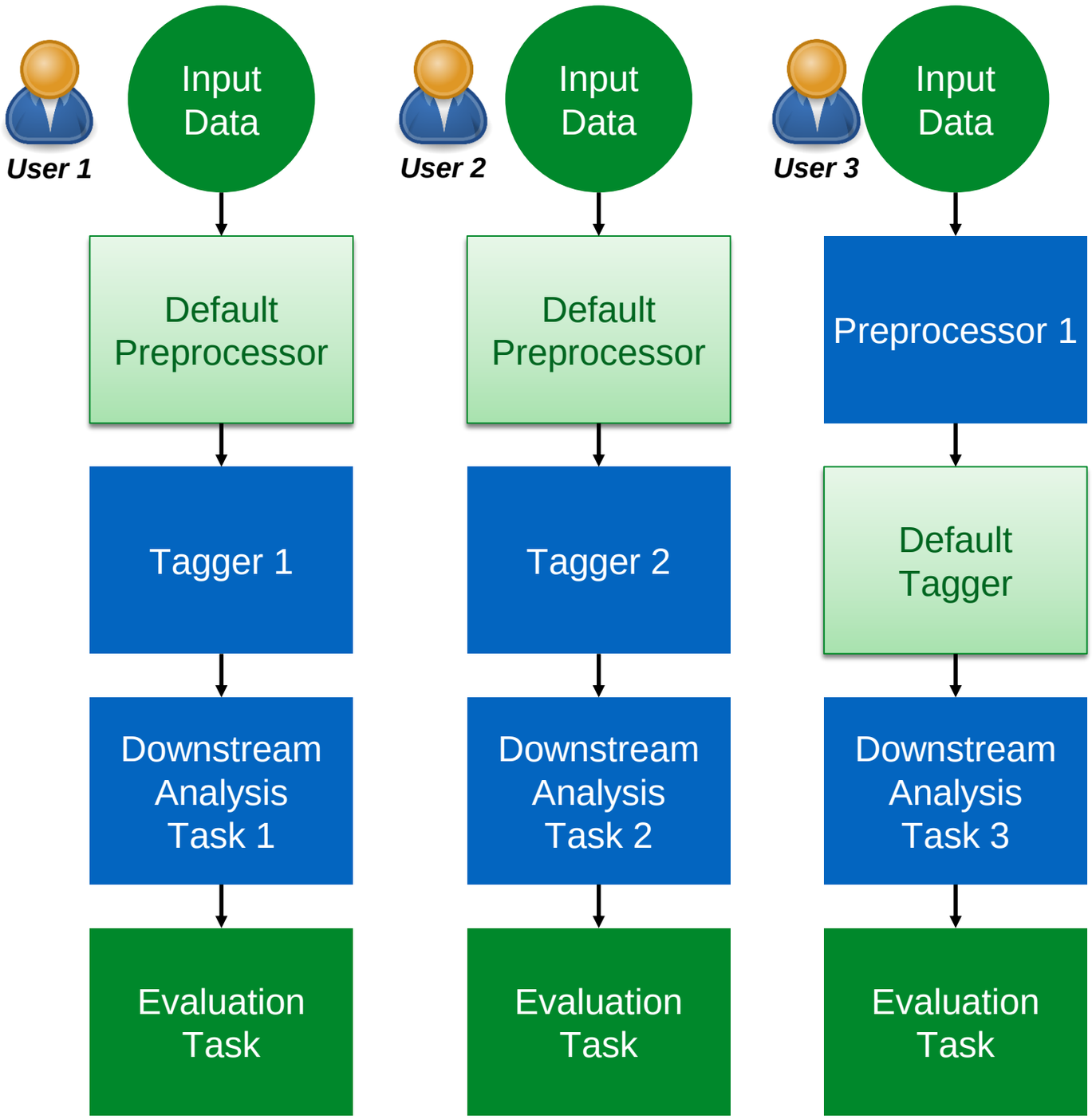


Workflow Templates

Coordinator defines structure of the workflow:

- Static input data
- Implementation for static workflow stages
- Default implementation for variable workflow stages
- Variable (user-provided) workflow stages
- User-provided input data

Benchmark Workflow Example (cont.)



Benchmark Participants

Users create different instances of the workflow by providing **implementation for variable workflow stages** (and variable input data).

Components of Workflow Templates

1. Workflow specification (e.g. REANA serial workflow) with optional references to template parameters.

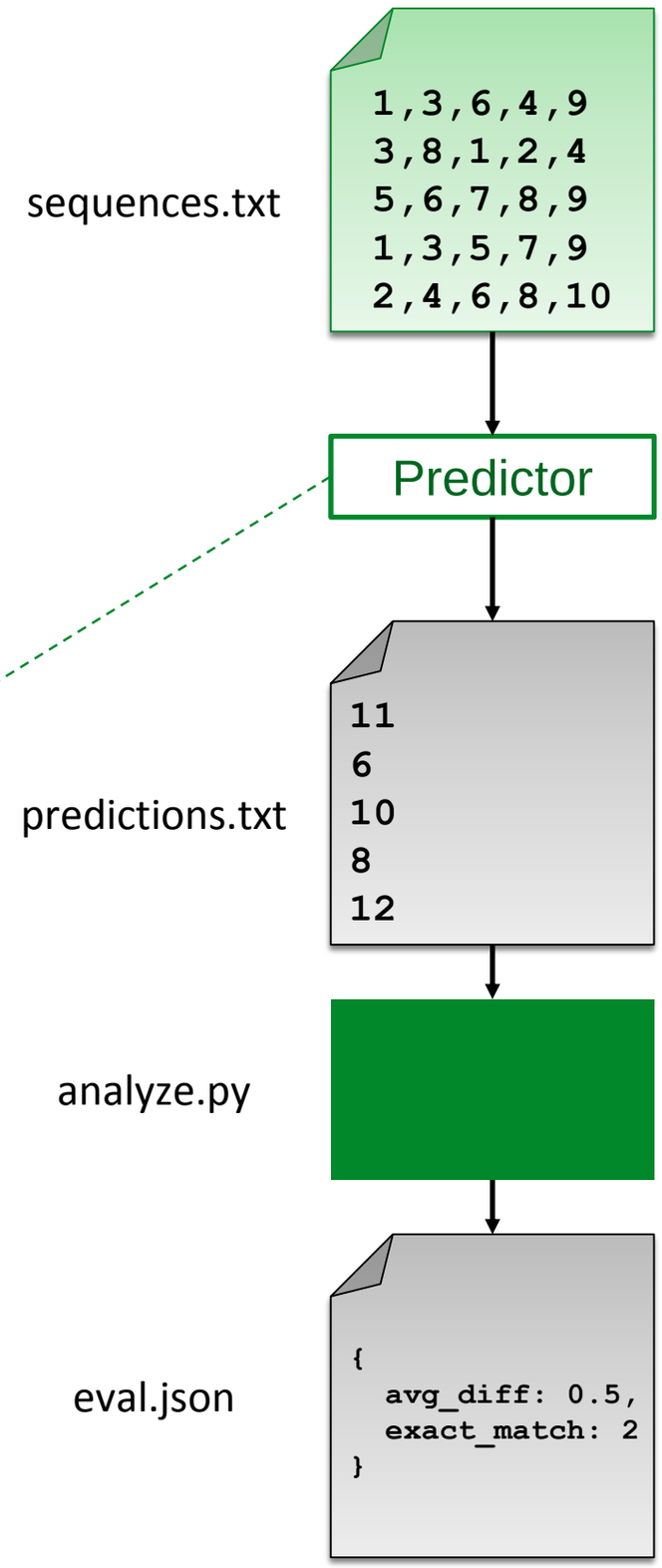
2. Declaration of template parameters (used by front-end for data input)

3. Specification of result schema to generate '*leader board*'.

```yaml
workflow:
    version: 0.3.0
    inputs:
      files:
        - $[[code]]
        - code/analyze.py
        - data/sequences.txt
      parameters:
        codefile: $[[code]]
        inputfile: data/sequences.txt
        outputfile: results/predictions.txt
    workflow:
      type: serial
      specification:
        steps:
          - environment: 'python:3.7'
            commands:
              - python "${codefile}"
                --inputfile "${inputfile}"
                --outputfile "${outputfile}"
              - python code/analyze.py
                --inputfile "${outputfile}"
                --outputfile results/eval.json
    outputs:
      files:
       - results/predict.txt
       - results/eval.json
parameters:
    - id: code
      name: 'Code file'
      datatype: file
results:
    file: results/eval.json
    schema:
        - id: avg_diff
          name: 'Deviation'
          type: decimal
        - id: exact_match
          name: 'Exact Predictions'
          type: int
    orderBy:
        - id: avg_diff
          sortDesc: false
        - id: exact_match
          sortDesc: true
```

Workflow Templates (cont.)

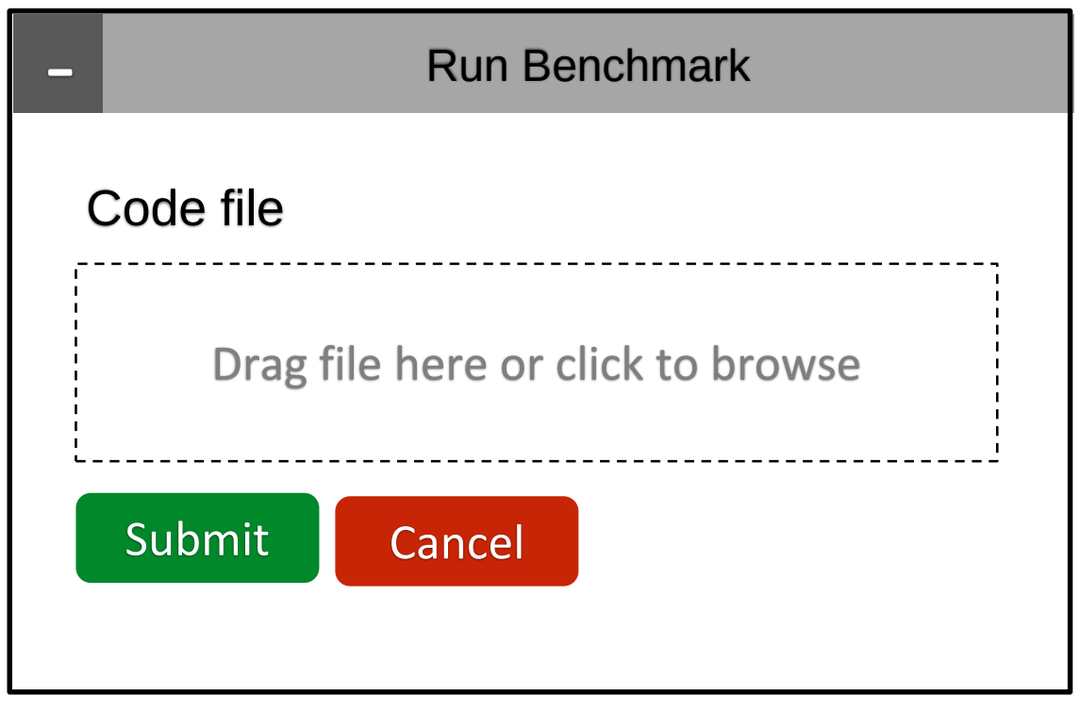
```yaml
workflow:
    version: 0.3.0
    inputs:
      files:
        - $[[code]]
        - code/analyze.py
        - data/sequences.txt
      parameters:
        codefile: $[[code]]
        inputfile: data/sequences.txt
        outputfile: results/predictions.txt
    workflow:
      type: serial
      specification:
        steps:
          - environment: 'python:3.7'
            commands:
              - python "${codefile}"
                  --inputfile "${inputfile}"
                  --outputfile "${outputfile}"
              - python code/analyze.py
                  --inputfile "${outputfile}"
                  --outputfile results/eval.json
    outputs:
      files:
       - results/predictions.txt
       - results/eval.json
```

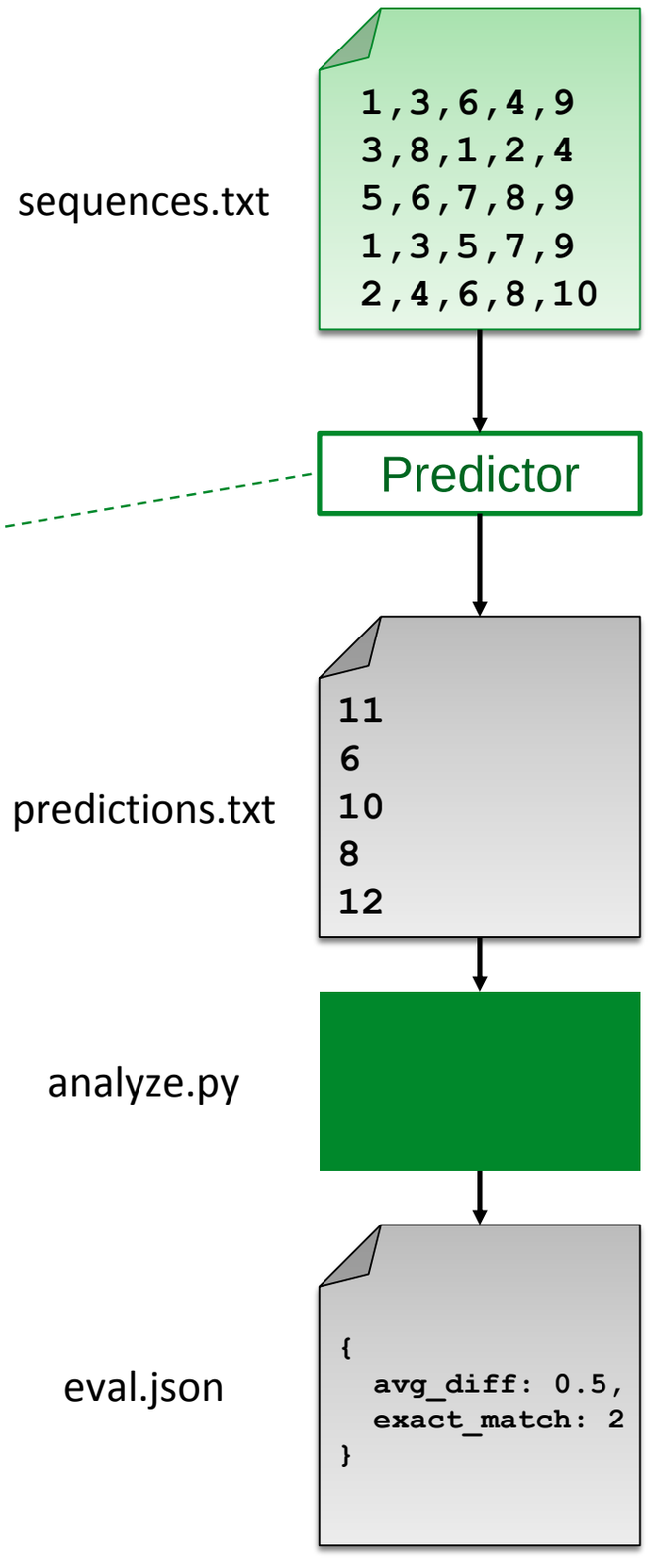


Workflow Templates (cont.)

Render input form from parameter declarations

```
28  parameters:
29      - id: code
30        name: 'Code file'
31        datatype: file
```





Workflow Templates (cont.)

Parameters for 'Hello World'

```
31  parameters:
32      - id: names
33        name: 'Input file'
34        datatype: file
35        as: data/names.txt
36      - id: sleeptime
37        datatype: int
38        defaultValue: 10
39      - id: greeting
40        datatype: string
41        defaultValue: 'Hello'
```

Workflow Templates (cont.)

Result schema to store benchmark results in database and to generate ranking

```
32  results:
33      file: results/eval.json
34      schema:
35          - id: avg_diff
36            name: 'Deviation'
37            type: decimal
38          - id: exact_match
39            name: 'Exact Predictions'
40            type: int
41      orderBy:
42          - id: avg_diff
43            sortDesc: false
44          - id: exact_match
45            sortDesc: true
```