

1 DSWorkFlow: A Framework for Capturing Data Scientists' 2 Workflows 3

4 MOSHE MASH, Carnegie Mellon University
5 STEPHANIE ROSENTHAL, Carnegie Mellon University
6 REID SIMMONS, Carnegie Mellon University
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8 While machine learning algorithms continue to improve, their success often relies upon the data scientists'
9 ability to detect patterns, determine useful features and visualizations, select good models, and evaluate and
10 iterate upon results. Data scientists often spend a long time making very little progress as they struggle to
11 determine how to proceed. In this respect, the understanding of data scientists' workflows and challenges has
12 recently attracted a great deal of scholarly interest. However, the literature is mostly based on interviews and
13 qualitative research methodologies. With this in mind, we developed *DSWorkFlow*, a data collection framework
14 that provides researchers with the ability to observe and analyze data scientists' cognitive workflows as they
15 develop predictive models. Using *DSWorkFlow*, researchers can collect data from a Jupyter Notebook, to
16 reconstruct the code execution order and extract relevant information about data scientist workflow alongside
17 the concomitant collection of qualitative data. We tested the framework experimentally with seven data
18 scientists as they each created three machine learning models to inform our extraction algorithms.

19 CCS Concepts: • **Human-centered computing** → **HCI design and evaluation methods**.

20 Additional Key Words and Phrases: data science process, workflow analysis, workflow extraction
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22 1 INTRODUCTION 23

24 The increasing proliferation of vast data repositories and powerful computing resources and
25 platforms has given rise to the concomitant development of data science and machine learning (ML)
26 as disciplines concerned with the establishment and development of generalizable processes for
27 extracting knowledge and insights from data [8]. Data science in particular is a rapidly developing
28 field that has attracted a great deal of interest from organizations that seek to analyze their massive
29 troves of data in order to gain new insights and drive their decision making [7]. Companies are
30 hiring data scientists to scale their capabilities [36] in such domains as healthcare [12, 24], business
31 intelligence [25, 38], finance [5, 34] and in scientific computing for physics [32], bioinformatics
32 [4, 10] and meteorology [22, 33], among others.

33 Despite extensive research and advances in the design and development of ML algorithms, their
34 success often relies on the proficiency of data scientists in performing such actions as determining
35 useful features, selecting good models, and evaluating and iterating upon results [2, 15, 27]. A
36 considerable body of recent qualitative studies (mostly interview-based) have sought to understand
37 data scientist workflows and challenges [1, 6, 16, 20, 21, 28, 40].

38 As a whole, these studies have found that because every dataset and every data science task is
39 different, the data science workflow is not monolithic, uniform, or sequential. Rather, it is contingent
40 on the content and nature of the dataset and task and involves an iterative and exploratory process
41 of trial and error, which many data scientists find challenging. Due to the open-endedness of the task
42 of building accurate ML models, even expert data scientists often struggle during the development
43 process in determining which actions to perform and what code to write [16]. As a result of their
44 uncertainty, data scientists may collect additional data in spite of a solidified distribution [17], stop
45 the process too early if they cannot make progress [16], or repeat the same actions, such as feature
46 selection, over and over again as they focus on one aspect of the task at the expense of others [29].

47 In contrast to prior studies that have mostly relied on qualitative methodologies in the form
48 of interviews and think-aloud sessions for data scientists to self-reflect on their processes, we
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50 propose a novel framework, *DSWorkflow*, for capturing a more complete picture of data scientist
51 workflows as they create machine learning models, including code, code output, and their
52 thought processes.¹ The primary goal of *DSWorkflow* is to bridge the gap between qualitative
53 and quantitative methodologies, allowing researchers the opportunity to study data scientists as
54 they are working through realistic problems in a familiar development environment - Jupyter
55 Notebooks. Beyond its familiarity, Jupyter Notebooks also contain valuable data embedded within
56 them, including output and execution data. By logging Notebooks regularly, *DSWorkflow* can then
57 parse the collected data and extract relevant information to reconstruct code and output sequences.

58 We tested our framework with seven data scientists as they worked on three machine learning
59 tasks. Our study procedure includes a tutorial, think aloud protocol, and the three datasets and tasks.
60 We then developed tools that used the Jupyter Notebook logs and audio and screen recordings for
61 extracting action sequences that participants performed throughout their workflows. Our ongoing
62 work uses the extracted output from *DSWorkflow* to predict when data scientists may be stuck.

63 This paper describes the three distinct components of *DSWorkflow*: Workflow Collection,
64 Reconstruction, and Extraction. As a whole, we believe that using the *DSWorkflow* framework
65 will enable researchers like us to capture a richer understanding of the data science workflow and
66 challenges that data scientists face as they work, and to develop better tools to support them.

67 2 WORKFLOW COLLECTION

68 The first component of *DSWorkflow* is Workflow Collection. *DSWorkflow* supports the complete
69 collection of realistic workflow data in a lab setting with a focus on two major goals: 1) the ability
70 to extract the entire cognitive workflow, including both digital artifacts and thought processes; and
71 2) the capacity to collect a broad set of workflows in a variety of domains and tasks.

72 2.1 Digital Artifact Collection

73 In order to reduce the variability in programming languages and coding environments, we chose
74 to limit our collection to Python code as it is currently the most popular language for data science
75 [3, 19] and Jupyter Notebooks on account of their popularity for data science applications [13].

76 **Jupyter Notebooks:** A Jupyter Notebook is an interactive Python development environment
77 that is used by the overwhelming majority of the data science community and which allows the
78 development of Python code that can be sensibly replicated by others [31]. The notebook consists
79 of a sequence of cells of various types. A code cell allows a developer to write and edit code, which
80 is executed using the Python interpreter and output in real time in the space under that code
81 cell. Markdown cells allow the developer to use rich text in order to document the computational
82 process. Developers can add, remove, combine, and execute cells in any order at any time during
83 the development process. Jupyter Notebooks are particularly well-suited to the initial development
84 of machine learning models in which data scientists work iteratively to produce a proof of concept
85 since the code in the notebook is executed immediately and the output is presented in-line.

86 **Notebook Snapshots** In addition to their popularity among data scientists, Jupyter Notebooks
87 can be parsed to extract the data science process. The underlying structure of a Jupyter Notebook
88 is a JSON document containing structured descriptions of all the cells in the notebook. The JSON
89 document encodes the content of each cell, the output of those cells when run, and the execution
90 order of the cells within its code. We make use of this format and structure to reconstruct the data
91 scientists' workflow from a sequence of Jupyter Notebooks.

92 The content of the Jupyter Notebook files changes as data scientists write and execute cells.
93 Cells that occur sequentially within the interface may never actually be run sequentially, but

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97 ¹The complete framework can be obtained from our open-source data repository.

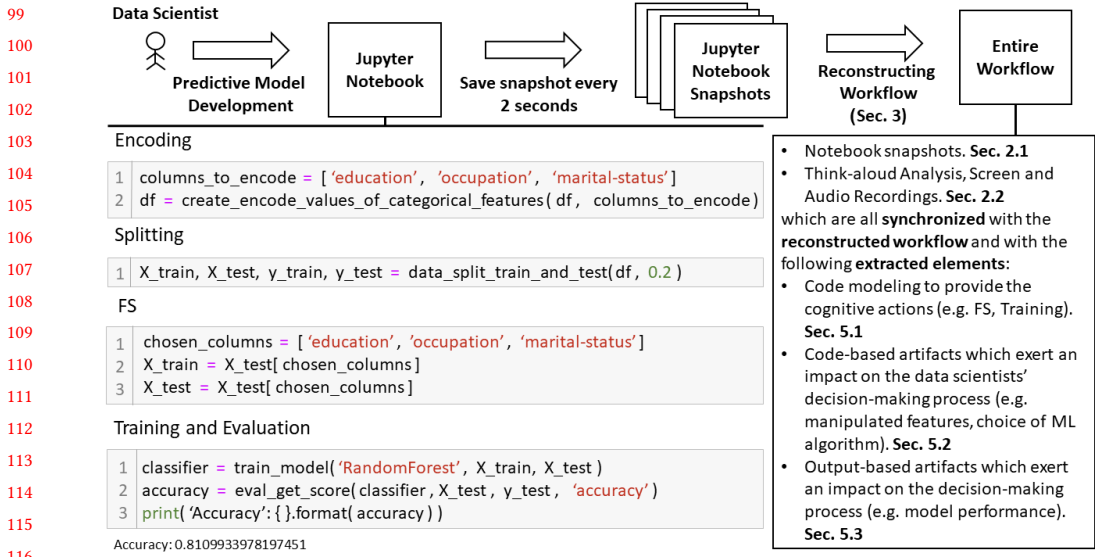


Fig. 1. DSWorkflow process for reconstructing the entire cognitive workflow

120 a record of their execution order is embedded in the Notebook. Since we wish to preserve a
 121 complete chronological record of the data scientists' workflow including their code writing and
 122 code execution, DSWorkflow automatically saves a copy of the Notebook, including the embedded
 123 data, in IPYNB files at regular intervals (2 seconds in our case). The procedure used to parse and
 124 sequence these Notebooks in order to recreate the development process is described in Section 3.

125
126 **2.2 Cognitive Workflow Collection**

127 In addition to capturing the code, output, and execution history, we also record the data scientist's
 128 screen and audio in order to track their visible and audible (i.e. think-aloud) interactions with the
 129 Jupyter Notebook interface (or with other applications such as a web browser).

130 **Think-Aloud Protocol:** The goal of our think-aloud protocol is to encourage the data scientists
 131 to express their thought processes as they are writing and executing code, interpreting the results,
 132 and testing their assumptions [11] (see Van Someren et al. [35] for an in-depth review of one
 133 such protocol). There are many possible reasons that this introspection could be important and
 134 complementary to other qualitative data collection techniques. For example, one could use the think
 135 aloud to determine what triggers data scientists to perform the actions they choose or alternatively
 136 the actions she or he perform while they struggle.

137 **Screen and Audio Recording:** We recorded the screen and the think-aloud audio using Screen-
 138 Rec [23], in order to allow the broadest possible range of analyses. The records includes comple-
 139 mentary information that is not saved in the data logs. A record of the screen enables researchers
 140 to observe what the data scientist was looking at and for how long (e.g., if they are viewing output,
 141 scrolling through their code, or even if they leave the notebook to search the web for a specific API
 142 function call of a specific library). These audio and screen recordings could be synchronized with
 143 data logs to provide an additional dimension for analysis. While we did not use such devices in our
 144 test, additional devices such as eye trackers according to research needs as well.

145 **Simplified Machine Learning API:** The Python libraries most commonly used for non-specialized
 146 machine learning applications contain a variety of functionality, only some of which may be familiar
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148 to any particular data scientist [13]. To prevent any impact a lack of API expertise may exert on
149 our own workflow collection (e.g., slowing down development, frequent online searches for API
150 calls, etc.), we developed a set of functions on top of these libraries for participants in our study to
151 use. These functions still allow for variation in different data scientists' development style in each
152 part of the data science process (e.g., visualization, model training, evaluations) without requiring
153 data scientists to navigate extensive APIs. More specifically, our machine learning API incorporates
154 elements from the following Python libraries: SciKit-Learn [30] machine learning library; Pandas
155 [26, 39] data analysis library, and Matplotlib [18] and Seaborn [37] visualization libraries. The
156 current version of our API was designed for general classification tasks. Nonetheless, it is broad
157 enough to support a variety of functions necessary for generating ML models and could be extended
158 to specific tasks (e.g., Natural Language Processing or Computer Vision) and to regression problems
159 by expanding it accordingly. The full API can be obtained from our open-source data repository at
160 <https://github.com/MoshikMash/DSWorkflow>.

161 The main advantage of our API is that it aggregates several methods from different objects into a
162 single function. For example, when a data scientist would like to train and evaluate a ML algorithm
163 model using SciKit-learn, they would need to create an algorithm-specific object, fit the training
164 data to it, transform it to the test set and finally use a suitable function for the metric she or he
165 would like to use for evaluation. On the other hand, our API allows the data scientist to attain the
166 same objectives with only two functions – *train_model* with a parameter specifying the name of
167 the ML algorithm and *eval_get_score* with a parameter specifying the evaluation metric to be used).
168 An actual example of how the API was used by one of our participants is presented in Figure 1.

169 The use of our API is an optional part of DSWorkflow depending on what aspects of the data
170 science process that researchers could desire to focus on. Not using the API does not affect the
171 functionality of DSWorkflow.

172 3 WORKFLOW RECONSTRUCTION

174 The second component of DSWorkflow is Workflow Reconstruction, which sequences the executed
175 code cells from the Notebook Snapshots logged by the Workflow Collection component. An
176 important piece of information embedded in the Jupyter Notebook is an execution counter that
177 increments each time a cell is run. For example, if two cells *A* and *B* are executed in the following
178 order *A, B, A, B*, DSWorkflow can observe the execution counts increasing over the 4 executions as
179 well as any code changes that are made to the cells between executions: (*A* : 1, *B* : -), (*A* : 1, *B* :
180 2), (*A* : 3, *B* : 2), (*A* : 3, *B* : 4).

181 Concatenating cell code in increasing execution order in a new IPYNB file reconstructs the entire
182 code execution from start to finish with execution timestamps that can be matched against the
183 think-aloud recordings. No execution counts are lost since the notebook is saved at regular intervals
184 even if the data scientist deletes or modifies the cells. The execution timestamps could also be
185 useful for other analyses (e.g., determining the rate at which a data scientist is executing code or the
186 best classifier they have trained in the last 15 minutes). This new reconstructed Jupyter Notebook
187 associates each line of executed code with the corresponding snapshot that it was extracted from.
188 This allows the researcher to refer back to the original Notebook file alongside the screen and audio
189 recordings in order to examine the data scientist's decision making process qualitatively.

190 To illustrate the workflow reconstruction process, imagine that a data scientist ran the code
191 described in Figure 1 (according to the figure's cell order). Then, they wanted to examine whether
192 Random Forest would attain better performance by dropping the feature "age" by modifying the first
193 line of code in the third (FS) cell to `columns = [['education', 'occupation']]`, and running
194 this cell followed by the next code cell (Training and Evaluation). DSWorkflow will capture and
195 save the Jupyter Notebook including the cells' code, their output (e.g., accuracy for the Training and
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197 Evaluation code cell), and their execution number after each time cells are run. The reconstructed
198 workflow will be made up of the code rows described in the figure, followed by the modified FS cell
199 and the Training and Evaluation code cell.

200 201 4 TESTING THE FRAMEWORK

202 Before proceeding to a discussion of DSWorkflow's Workflow Extraction component, we present
203 an application of DSWorkflow in which we employed the aforementioned testing procedure and
204 which will appear in a future publication. More specifically, we tested our data collection and
205 reconstruction components on seven M.Sc. data science students (5 females and 2 males aged 23-28),
206 and used their data to help inform our third DSWorkflow component - Workflow Extraction.

207 The application relates to a common scenario that occurs when data scientists develop predictive
208 models – they repeat the same actions, such as feature selection, over and over again as they
209 focus on one aspect of the task at the expense of others, even if it does not help them improve the
210 ML model [29]. This state of affairs wastes a lot of expensive time that could be more gainfully
211 employed to other ends.

212 With this in mind, we labeled these moments using the records and think-aloud analysis and, in
213 turn, used the data logs to develop a predictive model that could predict this "stuckness". Preliminary
214 results show that this prediction task can be accomplished with a relatively high degree of recall
215 (i.e., detecting when they are stuck) and low precision (i.e., predicting stuckness when they are not).

216 217 4.1 Experimental Procedure

218 We chose a within-subject in-lab study where each participant was asked to develop a machine
219 learning model for each of three different datasets. Studying a data scientist performing on mul-
220 tiple datasets will eventually enable us to analyze the effects that a given dataset can exert on a
221 participant's workflow and understand the similarities and differences across data scientists.

222 Based on pilot data, we determined that 90 minutes would be enough time for a data scientist to
223 both explore a new dataset and iterate on ML modeling several times. Because 4.5 hours is compar-
224 atively long for a single session, we split the study into two parts; participants got instructions and
225 performed one modeling task on the first day and then came back on a different day to complete
226 two more tasks. In the first meeting, participants signed a consent form and completed a tutorial to
227 build a sample machine learning model using our API and Jupyter Notebooks.

228 After the participants completed each task, they filled out a questionnaire that was meant to
229 validate their understanding of the task, to capture their final thoughts about their models and their
230 performance, and to assess the impact of DSWorkflow on their workflow. The participants were
231 also paid \$45 (USD) per meeting for their time at the end of each of the two experimental sessions.
232 The study was also approved by Carnegie Mellon University's Institutional Review Board (IRB).

233 234 4.2 Tasks

235 We selected three publicly available datasets which relate to general knowledge domains (i.e.,
236 which require no specific expertise to understand) and which contain mixed data types (categorical,
237 numerical, binary, dates, etc.) and the participants were asked to develop models to predict the
238 target variables given the features provided.

239 **Census Income Task (Census):** The dataset [9] contains demographic information about a
240 sample of the US population (e.g., age, marital status, degrees conferred, occupation). The target is
241 to predict whether a person earns more than \$50,000 (USD) per year.

242 **Telecom Customer Churn Task (Telecom)** The dataset [14] contains information about a
243 telecommunication company's customers (e.g., demographic information, tenure, monthly payment,
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246 enrolment in services). The target is to predict whether the customer was retained or if they closed
 247 their account.

248 **Australian Rain Task (Rain)** The dataset [41] contains daily weather observations from Aus-
 249 tralian weather stations (e.g., wind speed, wind direction, temperature). The target is to predict
 250 whether it would rain the following day.

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5 WORKFLOW EXTRACTION

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5.1 Action Modeling

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There are several possible levels of abstraction that DSWorkflow could employ to model the workflows from a code function level up to such tasks as wrangling, profiling and modeling as defined in [20]. We chose an intermediate *action* level representing functionality categories in SciKit-Learn as [1] and is reflected in the statements used by participants in our study. For example, participants performed feature selection (FS) several different ways since the code does not use any API code or any library function but rather uses Pandas syntax to filter columns from a dataframe. Sometimes, they used double brackets:

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```
X_train[['education', 'occupation', 'marital-status', 'age']]
```

while other times they declared a list and then used single brackets for the feature selection:

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columns = ['education', 'occupation', 'marital-status', 'age']
X_train[columns]
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These different methods represent the same functionality. The advantage of using a list variable is that the data scientist does not need to write feature names twice when choosing from the train set and the test set though both are possible and appeared in our small dataset.

Representing code at a higher level, which we call *actions* could allow analysis to focus on the meaning of the lines and not the actual code writing itself. In particular, we chose the following actions: 1) Visualization; 2) Feature Engineering (FE); 3) Encoding i.e., transforming the values of a feature from categorical to numerical; 4) Splitting data into train and test sets; 5) Scaling features or the normalization of the feature values; 6) Feature Selection (FS); 7) Training of models; 8) Hyperparameter tuning (HPT); and 9) Evaluation by computing or visualizing performance metrics. Our action extraction method is a semi-automated parsing approach to assign each line or several lines of code into one of these nine action categories.

Many of the action assignments are straightforward, particularly when the code contains the names of one of our API functions or is included among a data science library's functionality categories. Some cases, however, require more sophisticated reasoning for correct labelling, such as the FS code shown in Figure 1. In order to label these lines of code properly, our parsing algorithm detects when a list is first created and then searches for the list's variable name in subsequent lines in order to label those lines according to the latter action. In a small number of cases, such as visualizations that are not supported by the API or selecting features to be printed rather than used for training models, the parser cannot assign labels and we must label them manually. After

295 automated and manual labeling, 8571 actions were collected across our 7 data scientist participants
296 in each of their three tasks (99% were labeled automatically).

298 5.2 Extracting Code-Based Artifacts

299 In addition to actions, DSWorkflow extracts code-based artifacts that our study showed to be rele-
300 vant to the data scientists' decision making process. For instance, an important piece of information
301 that is extracted by the framework is the features that the data scientist selected or engineered
302 when performing FS or FE. For example, as described in the FS part in Figure 1, the framework
303 searches the lines of code labeled action FS, and extracts the set of features that the participant
304 chose for the model (e.g., education, occupation, marital-status) using the same code that searches
305 for lists described above. Because DSWorkflow extracts these lists over the whole workflow, it also
306 indicates which features were added or removed from the set since the last time the data scientist
307 performed Feature Selection.

308 Similarly, the framework extracts the chosen model (e.g., Random Forest (RF) in the training
309 part in Figure 1), the parameters chosen when training models with non-default parameters (e.g.,
310 maximum tree length for Random Forest) and the specific metric used when evaluating the model
311 (e.g., accuracy). All participants in our study used our API, and thus this extraction is performed by
312 analyzing the *train_model* and *eval_get_score* function calls. Performing this extraction on general
313 SciKit-Learn functions is feasible, but would require modifying this component.

314 In addition, DSWorkflow extracts an indicator of whether code has changed since the last time
315 the cell was executed. This indicator is important because data scientists often execute cells without
316 modifying them just because they formed part of their model development pipeline's "flow." This
317 is accomplished in practice by carrying out comparisons between the current code snapshot and
318 previous code snapshots.

320 5.3 Extracting Output Artifacts

321 During our studies, our participants commented on several of the output artifacts that were
322 relevant to their decision making. The most common observation was the evaluation metric score.
323 Participants used the score values to determine what models to use next (e.g., "...LR's accuracy
324 is greater than KNN's so I prefer using LR [logistic regression]..."), and which features to use (e.g.,
325 "...The performance is better for some of the classifiers (e.g. LR and Random Forest) once I remove the
326 'education' feature..." and "...I am trying to see whether there are features with strong correlations with
327 the target that are not correlated with other features that I did not include in the model. So, I will add
328 Temp3pm (strong correlation and not correlated with any other feature)..."). We also observed them
329 comparing several different metrics to compare classifiers (e.g., "...The AUC is better for LR. However,
330 the recall for KNN is higher...").

331 We implemented an algorithm to extract the results for all the metrics that the data scientists
332 printed, because the metrics that different data scientists care about varied given the task and the
333 person. Moreover, we found that data scientists often use several metrics to evaluate their model.

334 We detect the type of metric by searching for the metric's name as an API function parameter
335 (for example, see the last cell in Figure 1) and extract the score from the output. This can also be
336 done in a very similar manner with other APIs too. For example, if we were to search for accuracy
337 in SciKit-Learn, then we would be looking for the "accuracy_score" function within the Jupyter
338 Notebook (since SciKit-Learn contains a dedicated function for each metric). Alternately, the data
339 scientist could evaluate a model and assign the result into a variable and print it later. In this case,
340 the framework detects when the variable was saved in order to associate it with its metric type.
341 Another possible scenario we need to take into account is one where a confusion matrix includes
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344 several metrics (e.g. TP, FP, TN, and FN for binary classifications). In this case, the framework
345 extracts all metric scores.

346 An additional and interesting scenario relates to the iterative cycle of analysis associated with
347 writing code for analyzing and manipulating data, training ML algorithms and evaluating and
348 inspecting the output to maximize the predictive model's performance [2, 15, 27]. In this case, the
349 framework saves a counter variable that counts the number of training and evaluation iterations to
350 allow the researcher to distinguish between different iterations. For example, a researcher might
351 check whether the performance improved between iterations. In addition, DSWorkflow saves an
352 indicator of whether a line of code generates an error from the Python interpreter along with the
353 error output displayed, as this can be indicative of fixing code and rerunning cells.

354 The Workflow Extraction tools that we contribute are general purpose and can be useful for a
355 variety of applications. The action modeling allows researchers to investigate patterns at a higher
356 level than the lines of code, and our code and output extraction algorithms detect a variety of useful
357 information, including the models, metrics, and features used. Our framework is also extensible and
358 researchers can write Python code to extract new features for their own applications. For example,
359 we developed features that describe the number of times the data scientist succeeded in improving
360 their model's performance over time, which we use in predicting when a data scientist is stuck.

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362 6 CONCLUSION

363 Data science and machine learning are new, rapidly growing, and highly influential fields. Thus,
364 scholars have expressed a great deal of interest in attempting to understand data scientists' cognitive
365 workflows. With this in mind, this paper introduces DSWorkflow, a novel framework for the
366 collection of data scientists' workflows, containing Workflow Collection, Reconstruction, and
367 Extraction components.

368 A primary goal in developing DSWorkflow was capturing as much of the data science workflow
369 as possible. With this in mind, our framework allows the collection of data from several sources
370 (both quantitative and qualitative) such as think-aloud analyses, screen and audio recordings,
371 reconstructed code and output workflow from Jupyter notebooks, and the extraction of relevant
372 information. This, in turn, enables researchers to conduct extensive analyses of data scientist
373 workflow and "connect the dots" by synchronizing information from different sources.

374 We posit that DSWorkflow will facilitate a broad range of quantitative research on data scientists'
375 cognitive workflow, and help establish a bridge between theoretical and applied research, as well as
376 between quantitative and qualitative methodologies in the field. Using our DSWorkflow framework,
377 researchers will be able to study data scientists as they are exploring data and developing models
378 and open the door to the development of a number of applications to support data scientists, such
379 as predicting when data scientists are struggling and providing them feedback about how they can
380 make progress, comparing data scientists from varying levels of expertise or fields and facilitating
381 data science training and instruction in both academic and corporate settings.

382

383 ACKNOWLEDGMENTS

384 This paper is based in part upon work funded and supported by the Department of Defense under
385 contract FA8702-15-D-0002. This research was also funded in part by JPMorgan Chase & Co. Any
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