

Making Machine Learning Datasets and Models FAIR for HPC: A Methodology and Case Study

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Abstract—The FAIR Guiding Principles aim to improve the findability, accessibility, interoperability, and reusability of digital content by making them both human and machine actionable. However, these principles have not yet been broadly adopted in the domain of machine learning-based program analyses and optimizations for High-Performance Computing (HPC). In this paper, we design a methodology to make HPC datasets and machine learning models FAIR after investigating existing FAIRness assessment and improvement techniques. Our methodology includes a comprehensive, quantitative assessment for elected data, followed by concrete, actionable suggestions to improve FAIRness with respect to common issues related to persistent identifiers, rich metadata descriptions, license and provenance information. Moreover, we select a representative training dataset to evaluate our methodology. The experiment shows the methodology can effectively improve the dataset and model’s FAIRness from an initial score of 19.1% to the final score of 83.0%.

Index Terms—FAIR, machine learning, HPC, ontology

I. INTRODUCTION

Research activities in high-performance computing (HPC) community have applied machine learning (ML) for various research needs such as performance modeling and prediction [9], memory optimization [13, 14], and so on. A typical ML-enabled HPC study generates a large amount of valuable datasets from the HPC experiment outputs. The datasets serve as training inputs for the ML models applied in research. There is an increasing awareness of the need for data reuse in the HPC community. However, the community still lacks guidelines and experiences to effectively access and share the data that was collected in various research experiments.

The FAIR Guiding Principles [12] were published to advocate the reuse of data and other digital contents, including algorithms, software tools, source codes, and workflows that led to the generation of data. These principles serve as a guideline, but not the specification, to make digital data and contents findable, accessible, interoperable, and reusable by both humans and machines. The FAIR principles have been

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broadly adopted in certain research communities, such as biomedical and health science, with a range of studies and implementations to address the challenges in achieving data FAIRness. There are various initiatives and active community activities started to promote the importance of data FAIRness and assist to FAIRify the existing datasets. However, these principles and practices haven’t yet been tailored to benefit the HPC community.

In this paper, we present a methodology and a case study to make HPC machine learning training datasets and models FAIR, in the domain of machine learning-based program analyses and optimizations for HPC. We investigate the needs and challenges to FAIRify a HPC dataset following the established data FAIRification workflows used in other research communities. Seeing limitations of existing FAIRness evaluation approaches, we propose a hybrid assessment step with both manual and automated assessments. Concrete actions are then suggested to improve FAIRness. The methodology is evaluated using a representative dataset and ML model, demonstrating significant FAIRness improvement from 19.1% to 83.0%.

This paper has the following contributions: 1) We survey the best practices and approaches for data FAIRification. 2) A comprehensive, quantitative methodology is proposed to evaluate and improve FAIRness of HPC datasets and ML models. 3) The methodology leverages a hybrid assessment to generate a single FAIRness score. An ontology is developed to help address common issues for FAIRness improvement. 4) Using a concrete dataset and ML model, we evaluate the proposed methodology for its effectiveness.

II. BACKGROUND OF THE FAIR GUIDING PRINCIPLES

FAIR Guiding Principles: With a massive amount of data generated and collected in research activities, the scientific communities are pursuing good data management and data stewardship that can simplify data discovery, evaluation, and reuse in downstream studies. The FAIR Guiding Principles, standing for findable, accessible, interoperable and reusable, were jointly prepared by representatives and interested stakeholder groups as guidelines for data management and stewardship [12]. These independent but related principles together define the data characteristics to improve the data discoverability and reusability. Instead of serving as specifications to enforce

the implementations, they are meant to guide data generators, researchers, and stewards to create a FAIR data environment.

FAIRness Evaluation: FAIRness evaluation is critical in the FAIRification process by providing assessments and feedbacks to data creators and stewards. The FAIR data maturity model released by the Research Data Alliance (RDA) [4] defines three essential elements for an evaluation framework: 1) FAIRness indicators derived from the FAIR principles to formulate measurable aspects of each principle; 2) priorities reflecting the relative importance of the indicators; and 3) the evaluation method defining a quantitative approach to report the evaluation results. There are three commonly seen FAIRness evaluation approaches used in research communities: 1) *Discrete-answer questionnaire-based evaluation*: This approach, accompanied by a scoring system, provides a checklist of single-selection questions to reflect the FAIR principles and related concepts. It requires little knowledge about the FAIR principles and is relatively straightforward to exploit the evaluation with discrete-answer questionnaire. 2) *Open-answer questionnaire-based evaluation*: This approach also exploits a list of metrics reflecting the FAIR principles. Different from the discrete-answer approach, the open-answer approach requires concrete answers and statements to the metric as evidences to the implementation of FAIRness. 3) *Automated evaluation*: This approach automatically retrieves and evaluates a given digital resource, simplifies the evaluation process and eliminates the human subjectiveness. Automated evaluation service could also provide evaluation feedback and recommendation to improvement. However, the evaluation capability of this approach is limited by the metrics chosen, the software support, target granularity of data objects, and the resource availability of the metadata providers.

FAIRification Processes: As the FAIR Guiding Principles get higher attention in various research communities, many initiatives started to advocate the application of FAIR data principles. GO FAIR[3], a global, stakeholder-driven and self-governed initiative, has been working towards implementations of the FAIR Guiding Principles and proposes FAIRification process aiming at addressing the conversion of raw datasets into FAIR datasets. This FAIRification process emphasizes on FAIRification for both data and metadata, including seven steps: (1) retrieve non-FAIR data, (2) analyze the retrieved data, (3) define the semantic model, (4) make data linkable, (5) assign license, (6) define metadata for the dataset, and (7) deploy/publish FAIR data resource. The process is proposed for general purpose without considering specific requirements and needs from individual community. Challenges may arise when applying the process for data coming from a specific domain. For instance, without standardized data format in HPC community, the analyses used for the retrieved data vary based on the selected custom data formats. The development of a HPC semantic model needs iterative reviews and revisions to ensure consistency in providing accurate and unambiguous meaning of entities and relations in the HPC domain.

III. A METHODOLOGY TO MAKE DATASETS FAIR

We propose a 3-step methodology to improve the FAIRness of HPC datasets and ML models: 1) initial FAIRness assessment, 2) improving FAIRness based on assessment results, and 3) final assessment. We elaborate the first two steps since the last step is a repetition of the first one.

A. Initial FAIRness Assessment

After surveying the existing FAIRness evaluation methods, we have found that while the questionnaire-based manual evaluations have advantages to cover more details, the manual input process and the tendency to cause biased result due to subjectiveness are not ideal. On the other hand, automated evaluation avoids manual intervention and biased result. But they are less flexible and limited by the implementation for supported data granularity and metadata. As a result, we propose a hybrid approach involving both manual and automated assessments to have a more productive, flexible and informative evaluation.

We choose the FAIRness assessment service by F-UJI [2] as the automated evaluation service due to many desirable features it has. The F-UJI service designs automatic testings for evaluation based on 17 FAIRness metrics derived from the 41 RDA FAIRness maturity indicators. It uses a scoring system to provide quantitative evaluation result, in percentage, reflecting the ratio of the achieved score number to the full score number. Moreover, F-UJI provides detailed output to each metric evaluation as a guidance to assist users to improve the FAIRness maturity. Finally, F-UJI is an open-source project that can be expanded to include new features and support. However, F-UJI has insufficient support for many FAIR Guiding Principles related to metadata.

The chosen manual evaluation is the self-assessment tool by RDA FAIR data maturity model. It is a discrete-answer questionnaire-based evaluation and uses the same 41 RDA FAIRness maturity indicators referenced by F-UJI. Users provide an answer, with an associated level number, to each indicator from one of the following options to determine the maturity: (0) not applicable; (1) not been considered; (2) under consideration or in planning; (3) in implementation; and (4) fully implemented. Visualized report is available from the tool to present the maturity of the FAIRness.

In the proposed hybrid assessment, we consolidate 41 RDA indicators and 17 F-UJI metrics to form a new list of 47 indicators as shown in Table I. There are 11 indicators, marked * in Table I, originated from both RDA indicators and F-UJI metrics. The hybrid evaluation for these 11 indicators will take the result from the F-UJI metric due to the need to avoid biased result from manual evaluation.

To generate quantitative assessment results, we design a scoring system as follows: each indicator is given one point if its result is determined by the RDA maturity indicator as fully implemented, or by the F-UJI metric as a fully passed test. A total of 47 points for the whole hybrid evaluation (8 for 'F', 13 for 'A', 14 for 'I', and 12 for 'R') where the points correspond to the number of FAIRness indicators for each FAIR principle.

The final score is represented as the percentage of the earned points divided by the total point count.

B. Improving FAIRness

Improving the FAIRness can be achieved by systematically addressing issues reported by the manual and automated assessments. Users can iterate through all the metrics that are not marked as fully implemented or passed. The evaluation reports often give reasons for the failed tests associated with the metrics. Due to page limit, we present example actions users can take to address some commonly seen inadequacies in FAIRness revealed by our hybrid assessment process.

- *Getting persistent identifier:* The web address (URL) is commonly used by data collector as the identifier for a dataset. However, URLs tend to change over time which leads to broken links to the data. A persistent and unique identifier, such as digital object identifier (DOI), is the preferred identifier for a FAIR dataset. It is recommended to register the dataset at general or domain-specific registry systems to make the data more discoverable. We select Zenodo[15], a general-purpose open access repository, as our default platform to generate DOIs.
- *Providing coarse-grain metadata information:* Inadequate metadata is a common issue for datasets to fulfill the FAIR principles. Again, we use public data hosting services such as `zenodo.org` to leverage their built-in metadata. The metadata information are provided by filling in the required information during the data registering/uploading process. This type of metadata tends to describe general information of the associated dataset. Data collectors can also prepare metadata by following guidance for general data, e.g. Dublin Core metadata initiative, or domain-specific data, e.g. Data Documentation Initiative (DDI) for social, behavioral, economic and health sciences. Manual assessment has greater flexibility to assess various styles of metadata, whereas the automated evaluation assesses if metadata is complying specific metadata format and requirements. The F-UJI automated evaluation supports multidisciplinary metadata standards, e.g. Dublin Core and DataCite Metadata Schema, and metadata standards from several scientific domains, e.g. biology, botany, and paleontology. General metadata information supported by `zenodo.org` are recognized by the F-UJI evaluation.
- *Generating rich attributes for different granularity of data:* It is relatively easy to make a whole dataset and ML model FAIR. However, significant work is needed to make fine-grain contents inside a dataset or model FAIR. There is a lack of community standards to provide rich attributes for the data elements of various science domains. In HPC, datasets can be generated from performance profiling tools, compilers, runtime systems with very different attributes. For ML models, standardized set of attributes is not yet available to describe various types of ML models and the associated meta information. To address this problem, we are developing the HPC Ontology [8] to provide standard attributes which can be used to annotate fine-grain data

elements in different subdomains of HPC, including GPU profiling results, program analysis (e.g. call graph analysis), and machine learning models (e.g. decision trees). The design of HPC Ontology is modular so it can be extended to include more subdomains in the future.

- *Automatic annotating data elements:* Even with existing standard attributes, it is impractical to manually annotate data elements one by one. For many HPC datasets are published in CSV files, we leverage Tarql[11], a command-line tool for converting data stored in CSV files into the Resource Description Framework (RDF) format using standard metadata and attributes provided by the HPC Ontology.
- *Provenance information:* Provenance information is required to fulfill ‘R’ FAIR principle. Similar to the metadata, `zenodo.org` provides basic support for provenance information such as publication date and publisher. Formal provenance metadata, such as PROV, is recommended for advanced provenance information support.
- *License information:* Data collectors should choose and apply license information to the collected dataset to fulfill ‘R1.1’ FAIR principle. A recommended choice for data is one of the Creative Commons license.

IV. XPLACER DATASETS

In this paper, we pick a dataset and ML model generated by the XPlacer [13] to study how to FAIRify HPC datasets and ML models. The reason to choose XPlacer is that the authors released raw data with detailed documents explaining how data was generated and processed. They also describe the meanings of each row and column for the corresponding CSV files. The rich human-readable documentation provides a good foundation for FAIRness evaluation and improvement.

XPlacer is a memory optimization tool developed to use machine learning to guide the optimal use of memory APIs available on Nvidia GPUs. It has both offline training and online adaptation steps, including collecting training datasets, generating machine learning models, and applying the generated model to predict the best memory usage advise.

The offline data collection uses seven benchmarks from the Rodinia benchmark [1] with seven available memory advises applied to different arrays in the benchmarks. In each experiment with a selected benchmark, profiling tools were used to collect kernel level and data object level metrics. After data normalization and feature dimensionality reduction, the collected XPlacer dataset has a total of 2688 samples prepared for the machine learning models. The raw data collected from XPlacer experiments is hosted at a public Github repository¹. Figure 1 shows how the raw profiling data generated from different GPU machines are first parsed and stored into CSV files, which are merged and labeled to generate training datasets to build various machine learning models.

Multiple machine learning classification models were generated by XPlacer from the training datasets. These models include Random Forest, Random Tree, and Decision Tree.

¹https://github.com/AndrewXu22/optimal_unified_memory

TABLE I: FAIR Guiding Principles: maturity indicators and assessment metrics

P ¹	Indicator	Description	S ²
F1	RDA-F1-01M	Metadata is identified by a persistent identifier	4
	RDA-F1-01D *	Data is identified by a persistent identifier	
	FsF-F1-02D	Metadata is identified by a globally unique identifier	
	RDA-F1-02M *	Data is identified by a globally unique identifier	
F2	RDA-F2-01M	Rich metadata is provided to allow discovery	2
	FsF-F2-01M	Metadata includes descriptive core elements to support data findability	
F3	RDA-F3-01M *	Metadata includes the identifier for the data	1
	FsF-F3-01M		
F4	RDA-F4-01M *	Metadata is offered in such a way that it can be harvested and indexed	1
	FsF-F4-01M		
A1	RDA-A1-01M	Metadata contains information to enable the user to get access to the data	9
	RDA-A1-02M	Metadata can be accessed manually	
	RDA-A1-02D	Data can be accessed manually	
	RDA-A1-03M	Metadata identifier resolves to a metadata record or digital object	
	RDA-A1-03D	Data identifier resolves to a metadata record or digital object	
	RDA-A1-04M *	Metadata is accessed through standardised protocol	
	RDA-A1-04D *	Data is accessed through standardized protocol	
	FsF-A1-03D		
A1.1	RDA-A1.1-01M	Metadata is accessible through a free access protocol	2
	RDA-A1.1-01D	Data is accessible through a free access protocol	
A1.2	RDA-A1.2-01D	Data is accessible through an access protocol that supports authentication and authorization	1
A2	RDA-A2-01M *	Metadata is guaranteed to remain available after data is no longer available	1
	FsF-A2-01M		
I1	RDA-I1-01M	Metadata uses knowledge representation expressed in standardized format	6
	RDA-I1-01D	(Data uses knowledge representation expressed in standardized format	
	RDA-I1-02M	Metadata uses machine-understandable knowledge representation	
	RDA-I1-02D	Data uses machine-understandable knowledge representation	
	FsF-I1-01M	Metadata is represented using a formal knowledge representation language	
	FsF-I1-02M	Metadata uses semantic resources	
I2	RDA-I2-01M	Metadata uses FAIR-compliant vocabularies	2
	RDA-I2-01D	Data uses FAIR-compliant vocabularies	
I3	RDA-I3-01M *	Metadata includes references to other (meta)data	6
	FsF-I3-01M		
	RDA-I3-01D	Data includes references to other (meta)data	
	RDA-I3-02M	Metadata includes references to other data	
	RDA-I3-02D	Data includes references to other data	
	RDA-I3-03M	Metadata includes qualified references to other metadata	
RDA-I3-04M	Metadata include qualified references to other data		
R1	RDA-R1-01M	Plurality of accurate and relevant attributes are provided to allow reuse	2
	FsF-R1-01MD	Metadata specifies the content of the data	
R1.1	RDA-R1.1-01M	Metadata includes information about the license under which the data can be reused	3
	RDA-R1.1-02M	Metadata refers to a standard reuse license	
	RDA-R1.1-03M *	Metadata refers to a machine-understandable reuse license	
R1.2	RDA-R1.2-01M	Metadata includes provenance information according to community-specific standards	3
	RDA-R1.2-02M	Metadata includes provenance information according to a cross-community language	
	FsF-R1.2-01M	Metadata includes provenance information about data creation or generation	
R1.3	RDA-R1.3-01M *	Metadata complies with a community standard	4
	FsF-R1.3-01M		
	RDA-R1.3-01D	Data complies with a community standard	
	RDA-R1.3-02M	Metadata is expressed in compliance with a machine-understandable community standard	
	RDA-R1.3-02D *	Data is in compliance with a machine-understandable community standard	

¹ FAIR Guiding Principle ID

² Max score allocated to each sub-principle

* Both RDA FAIRness indicator and F-UJI metric represent the same evaluation

The decision tree model is selected in this FAIRification study. Each non-leaf tree node in the decision tree represents a decision determined by a feature with a threshold value whereas a leaf node contains a label value representing the final decision.

V. EXPERIMENT

This section presents the FAIRification process of applying our methodology, presented in section III, to the XPlacer

datasets and the decision tree model.

Initial Assessment: The initial hybrid assessment results reveal that a selected XPlacer dataset (generated on an IBM machine) has a 19.1% FAIRness score. The detailed reports from both RDA manual evaluation and the F-UJI evaluation reveal that persistent identifier is missing to fulfill the ‘F’ FAIR principle. Missing license and provenance information are the major factors for its low fulfillment in the ‘R’ FAIR principle. For the rest covered in ‘A’ and ‘I’ FAIR principles, missing

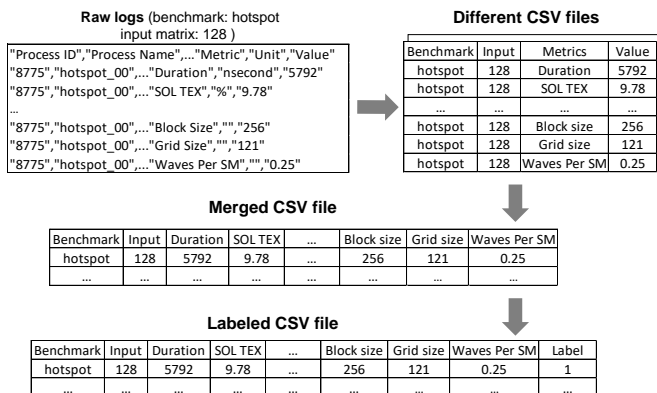


Fig. 1: XPlacer data processing pipeline

metadata information is the root cause for its low fulfillment in FAIRness.

Improving FAIRness: With the assessment feedback and recommendations, we apply the methods mentioned in Section III-B to achieve a higher assessment result.

- We uploaded the XPlacer dataset to Zenodo.org to obtain an DOI for persistent identifier and fulfill metric FsF-F1-02D.
- As part of the uploading process, we carefully filled in required metadata information in zenodo.org. The enhancement is able to fulfill eleven more metrics.
- Basic provenance information is also provided by zenodo.org but does not comply formal provenance metadata such as PROV. Therefore, only partial fulfillment is achieved for metric FsF-R1.2-01M.
- We chose the Creative Commons 4.0 license (CC-BY 4.0) for the XPlacer dataset to fulfill the R1.1 principle.
- We extended the HPC ontology [8] to provide required attributes to describe fine-grain data elements. A unit ontology (QUDT) is also used to annotate the units for numerical values to enable maximum data interoperability and fulfill the RDA-I3-01M FAIRness indicator.
- We used Tarql to automatically convert the corresponding CSV file into linked data using the JSON-LD format, with attributes provided by the HPC Ontology. Listing 1 shows an example output of the conversion. A set of key-value pairs are generated to describe data cells of a CSV file. Each key is a standard metadata tag or an attribute provided by an ontology. For example, *hpc:hostToDeviceTransferSize* at line 9 is used to indicate CPU to GPU data transfer size. The corresponding value at line 10 is pointing to an object defined between line 13 and 23, which include two other nested objects for precisely encoding unit (KiloByte) and value (7872.0), respectively. This level of fine-grain details is required to enable maximal interoperability among datasets.
- For the decision tree model, High-level metadata describing the model is provided in the FAIRification process. In addition, we leverage and extend HPC ontology to provide standard attributes to annotate fine-grain information in the

decision tree. The decision tree model can then be presented as linked data using JSON-LD format tree by annotating the tree nodes with the feature and threshold value for the non-leaf nodes and the label property for the leaf nodes.

Listing 1: Example JSON-LD output

```

{
  "@id": "http://example.org/test.csv#L1",
  "@type": "hpc:TableRow",
  "hpc:codeVariant": "111100",
  "hpc:allocatedDataSize": 8000000,
  "hpc:arrayID": "0",
  "hpc:commandLineOption": "graph1MW.6",
  "hpc:gpuPageFault": 5,
  "hpc:hostToDeviceTransferSize": {
    "@id": "Nbdd222a0d12a483d8f1a4cef274f18fc"
  }
},
{
  "@id": "Nbdd222a0d12a483d8f1a4cef274f18fc",
  "@type": "http://qudt.org/schema/qudt/QuantityValue",
  "http://qudt.org/schema/qudt/unit": {
    "@id": "http://qudt.org/vocab/unit/KiloBYTE"
  },
  "http://qudt.org/schema/qudt/value": {
    "@type": "http://www.w3.org/2001/XMLSchema#decimal",
    "@value": "7872.0"
  }
}

```

Final FAIRness Assessment: The final FAIRness evaluation by the hybrid evaluation reveals a 83.0% score, improved from 19.1%, after the improvements (Figure 2).

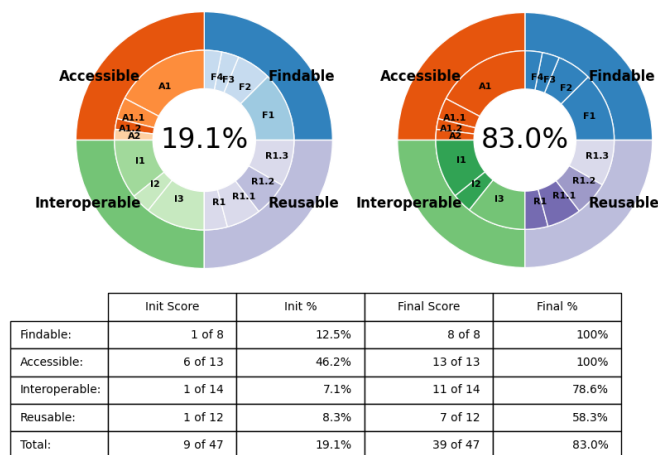


Fig. 2: Final hybrid assessment

The results show that the dataset and ML model do not fulfill FsF-I1-02M that requires namespaces of known semantic resources to be present in the metadata of an object. This is due to the limited support by the data hosting service by zenodo.org to provide namespaces for specific semantic resources. A partial fulfillment is reported by F-UJI for FsF-R1-01MD that requires metadata for technical properties of the data file. We find that this is due to the implementation limitations on both F-UJI and zenodo.org after investigation. The metric is considered fulfilled in our final manual assessment. Another partial fulfillment report is for FsF-R1.2-01M that requires provenance metadata provided in a machine-readable version of PROV-O or PAV. We encoded the provenance information for XPlacer dataset at the fine-level granularity through HPC ontology and link to PROV-O ontology. However, these provenance metadata cannot be annotated into registry in zenodo.org due to its limited

support. This metric is also considered passed in our manual assessment.

The final assessment shows that the use of the HPC ontology significantly improves the metadata support for the XPlacer dataset, resulting in full fulfillment for all FAIRness indicators for 'F and A' FAIR principles. However, providing full and qualified references to other data standards is still ongoing development for the HPC ontology. This leads to a lower fulfillment, in implementation phase, for RDA-I3-01D (Data includes references to other data), RDA-I3-02D (Data includes qualified references to other data), and RDA-I3-04M (Metadata include qualified references to other data). In the 'R' FAIR principle, RDA-R1.2-02M (Metadata includes provenance information according to a cross-community languages) that checks if metadata includes provenance information according to a cross-community languages is also considered in implementation phase to support PROV-O ontology as the cross-community languages for provenance information. There is no community standard specified for data and metadata in HPC community. We propose to use the HPC ontology as one metadata standard for HPC. As HPC ontology is still under development, we consider RDA-R1.3-01M, RDA-R1.3-01D, RDA-R1.3-02M and RDA-R1.3-02D still in the implementation phase.

VI. DISCUSSION & FUTURE WORK

Summary: This paper presents a concrete methodology and a case study to make HPC datasets and ML models FAIR, after surveying existing techniques used to assess and improve FAIRness of scientific data. Our methodology can enjoy the benefits of both automatic and manual assessments while avoiding their limitations. It also includes a set of actionable suggestions to address reported FAIRness issues, including using ontologies to provide rich and standard data attributes. The experiment has shown that our methodology can effectively improve the FAIRness maturity for a selected dataset and ML model.

Discussion: To make general datasets and ML models FAIR, it can be discussed from three different aspects:

- FAIRness assessment: In this study, we have observed that existing FAIRness assessment tools have several major weaknesses: insufficient coverage for details in FAIR principles, tendency to report biased assessment result, with emphasis to limited group of users (data curators, data stewards, and data users), and with support for only specific domains (with attributes and vocabularies in specific scientific communities). Improving the FAIRness assessment support addressing the above weaknesses can provide a trustworthy gauge of data FAIRness. Data generators, curators, stewards and users can jointly improve the data FAIRness based on a standardized and creditable metric of data FAIRness.
- FAIR-aware data store and management: Data hosting and management service have great impact to the FAIRness for the hosted/managed data. In this paper, zenodo.org is recommended for its support in DOI generation, general metadata, provenance and license information support. It

provides relatively smooth transition for users, who heavily rely on git repositories to store data and digital contents, to FAIRify the data. Several leading services for hosting/managing ML datasets and models [6, 7, 5, 10] are commonly used by ML developers and users. We survey and evaluate their support for FAIRness and observe several commonly seen issues: missing persistent identifier representing the datasets or models, insufficient coarse and fine-level metadata, and accessing (meta)data and model is constrained by hosting service APIs. Providing FAIR-aware data store and management systems is also a critical factor to make general datasets and ML models FAIR.

- FAIRification for ML models: As FAIR principles are applicable to any digital object, FAIRness for ML models should also be considered. We apply data annotation with support from HPC Ontology as an example to achieve FAIRness fulfilment for the selected decision tree model. However, the same approach might not be practical to many large scale ML models that contain millions or billions of parameters. Supporting rich metadata describing the ML models would be the alternative approach for the FAIRification. There is not yet a dedicated list of attributes and metadata information to represent all ML models (reflecting 'R1' sub-principle). We also observe there are many information associated with the Interoperability and Reusability of a ML model cannot easily be found. For example, the NLP model BERT comes in many flavors: varying its size, preprocessing applied to the dataset (case and special characters), and additional fine-tuning objectives. Such information might not be shown by existing model hosting services and cannot be checked by any FAIRness assessment tool. And last, ML models closely related to the datasets used for training. The reusability of a ML model is likely to be limited to a specific type of dataset, or learning goal. Attributes describing the dataset requirements and learning goal need to be properly defined. Therefore, identifying the FAIR-centric metadata and attributes for the ML models (e.g. model architecture, training configuration, and training objectives), together with automated evaluation to assess the metadata, can greatly promote the FAIR for ML models.

Future work: We will continue to improve the HPC ontology to have required references to other data standards. We hope that the HPC ontology can be adopted as one standard to FAIRify data within the HPC community. We will also incorporate some manual correction and assessment steps into the automated assessment step to further improve the FAIRness assessment. Last but not the least, we will extend our work to support FAIRification for ML models and workflows. Ultimately, we aim to pursue trustable machine learning by achieving better FAIRness in machine learning models and datasets.

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