Flywheel Tools

Data Curation and Manipulation on the Flywheel Platform

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Introduction

> Paragraph 1. The challenge of reproducible neuroscience. What is the state of the field / why is this needed? End paragraph by pointing out two major advances in reproducibility: imaging databases and bids

As the field of neuroimaging continues to grow, datasets being collected have seen similar growth in volume, variety, and velocity. This expansion provides researchers with novel opportunities to answer questions using much larger sample sizes, but also presents challenges to reproducibility. Researchers carrying out different tasks on different operating systems, while attempting to reproduce an analysis, can often end up with disparate and irreplicable results **CITE examples?**. Two major advances in the field help to stave off this reproducibility challenge: imaging databases, and Brain Imaging Data Structure (BIDS).

> Paragraph 2. Imaging databases. How do they help reproducibility? What platforms are out there? How does flywheel fit and why is it good?

Imaging databases have have become powerful software tools for storing, accessing, and analyzing imaging data in a reproducible manner. They reduce considerable computational and storage overhead by ensuring data is stored and structured efficiently. Without the technical experience and expertise, finding appropriate resources for storage space and computation time can be a challenging and laborious task. Fortunately, many imaging databases come equipped with such decisions already made for the user, and with a plethora of customizable tools. Importantly, these softwares provide opportunities for strict data provenance, where all changes made to a dataset can be tracked, recorded, and reproduced at any time. These imaging databases can be open- source, or commercial; notable examples include **CITE examples**. Flywheel, the focus of this paper, is a recent addition to the list of commercially available databases. Their model strongly emphasizes the use of flexible data storage, prepackaged data analysis pipelines, and transparent data provenance.

Paragraph 3. BIDS – a major response to the reproducibility challenge. Would define what BIDS seeks to achieve, how it was developed, and what does it get users (inc BIDS APPS).

In addition to the rise of database options, the neuroimaging community has also developed data storage standards — most notably the Brain Imaging Data Structure (BIDS) — to improve scientific reproducibility. BIDS is an open source standard for neuroimaging data storage that specifies how files should be named and how directories should be organized **CITE nature paper**. The benefits of adopting BIDS include:

- Minimized curation efforts, as datasets can be easily understood, operated on, and shared within and between sites;
- Reduced usage error, as important metadata are explicitly declared in each file's name and path;
- Access to software tools and pipelines (BIDS apps) that can automatically configure themselves as necessary, as metadata is machine-readable.

BIDS was initially developed at Stanford in 2015, and through open-source community participation has grown into a globally recognised neuroimaging standard **CITE ?**, publishing an official *BIDS specification* defining the currently practices and schemas. The spec publication is governed by both community input, and a democratically elected steering committee from members of the community. A wide array of BIDS apps are available in the BIDS ecosystem – notably, the BIDS validator is a common tool for validating datasets after they have been curated into BIDS **CITE ?**. Importantly, the BIDS specification is updated to match the latest imaging techniques and sequences through community participation and open governance, which allows BIDS apps to be continually developed for cutting-edge science. Hence, imaging databases like Flywheel have adopted BIDS standards and BIDS apps as core functionalities that are reliable, flexible to change, and serve to increase reproducibility.

Paragraph 4. Heudiconv. How do users usually get their data into BIDS? What is a typical heudiconv workflow? End by noting that this workflow is NOT present in flywheel at present, and that reproducible curation of data is absolutely essential for true reproducible science . This sets up the gap in the field / unmet need for your product.

To further reduce error and increase reproducibility, researchers can choose to curate their datasets into BIDS programmatically with version-controlled software. The most common BIDS curation tool is `HeuDiConv` **CITE heudiconv website?**, (shorthand for *Heuristic DICOM Converter*). `HeuDiConv` curates data using simple heuristics that map DICOM files to BIDS paths and file names. These heuristics are defined in machine-readable Python scripts, allowing them to be version controlled for reproducibility. For the typical user, BIDS curation with `HeuDiConv` follows a simple, yet highly flexible workflow using `HeuDiConv` commands and the BIDS validator tool **CITE bids validator?**:

1. Scrape DICOM metadata from the dataset

2. Examine metadata to find scan parameters that discriminate files
3. Create a heuristic script mapping DICOM metadata to BIDS-valid NIfTI file names, by applying boolean logic to scan parameters
4. Convert DICOMs to NIfTI files and apply mapping with the the HeuDiConv curator
5. Use the BIDS validator to assess results, adjust heuristic, and repeat curation as necessary

> Paragraph 5: Goals of paper. Say explicitly what you are trying to do with this tool. Orient reader to outline of paper. Close with a strong statement on the functionality of the tool.

`HeuDiConv` establishes a robust and reproducible workflow for BIDS curation that has been widely adopted throughout the neuroimaging community **CITE ?**. However, although BIDS is supported on Flywheel, the platform's functionality only offers automated BIDS curation of incoming datasets, without the option to effectively and flexibly curate data using a `HeuDiConv`-like workflow. This can lead to invalid BIDS curation on Flywheel in a handful of crucial scenarios:

- Importing legacy datasets to Flywheel that may not have originally been well suited for BIDS;
- Importing novel imaging modalities or scanning sequences not yet defined in the BIDS specification;
- Importing datasets with significant errors that can't be handles by the automated system.

In order to meet the need for a more reproducible and reliable BIDS curation workflow on Flywheel, this paper presents the `FlywheelTools` package: a software toolkit designed to implement a more flexible BIDS curation workflow on the Flywheel platform, and expand on current Flywheel functionality for addressing BIDS curation. In this paper, we describe the Flywheel platform, BIDS, and the software design approach in further detail in the Methods section. In the Results section, we demonstrate a reproducible BIDS curation workflow on Flywheel. We believe `FlywheelTools` brings an array of powerful functionality for curating data on the Flywheel database and interacting with BIDS data on the platform, whilst maintaining the simplicity and usability of the common `HeuDiConv` workflow and expanding on Flywheel's BIDS functionality.

Methods

The FlywheelTools toolkit allows users to follow a reproducible workflow for BIDS curation and audit of their data. This workflow typically includes: inspection of sequences collected during a study; design of a curation schema; implementation of curation schema; curated data inspection and export; and finally audit of data and analyses (see Figure 1).

Programming Languages & Technologies

Flywheel Tools is built primarily in Python 3.6 (Van Rossum and Drake 2009) in order to leverage its highly accessible SDK. Additionally, R 3.4.1 (R Core Team 2019) is used for HTML report generation. For reproducibility and workflow management, Flywheel Tools' modules are packaged in version-controlled software containers built and managed in Docker (Merkel 2014). Lastly, the Flywheel Tools package relies on users adopting the Brain Imaging Data Structure (BIDS) to curate their data. BIDS has rapidly evolved to become the field standard directory standard in the neuroimaging community for reproducible data organization (Gorgolewski et al. 2016). Importantly, BIDS has a large community of participants contributing to its development and adoption, and proposals for BIDS schema go through rigorous community testing and approval before being added. This leads to a trustworthy common framework for data curation shared amongst researchers. Software developers leverage this ubiquity by creating analysis and processing pipelines that can operate directly on BIDS data sets as inputs, enhancing reproducibility and interoperability on various software platforms.

Flywheel

Flywheel is a data management and analysis platform for research, which lends itself well to neuroimaging. The platform focuses heavily on collaborative and reproducible science. User-facing components of the platform itself are the web User Interface (UI), the Software Development Kits (SDK), and the Application Programming Interface (API) (Figure 2).

Flywheel Web UI

The web UI is accessible through any modern web browser and is the primary method of interacting with Flywheel data. Through this point-and-click interface, users are able to upload, view, download, and analyse data with ease and simplicity. However, accomplishing tasks with many repetitive steps or a large number of subjects/sessions to iterate over can be tiresome and error-prone. Alongside knowledge of navigating the web UI, many users also make use of the SDK to manipulate and analyse data programmatically.

Flywheel API & SDK

Flywheel's database utilises MongoDB for data storage and access, meaning that all Flywheel data is represented by hierarchical relationships between document objects. This allows users to create and store complex structures with ease, and query data rapidly (Banker 2011). In order to access this data, Flywheel uses a

RESTful Application Programming Interface (REpresentational State Transfer) (Biehl 2016), and hence each document or data object is accessible through a a specific URL that a web browser or SDK can access by requesting the data and waiting for a response from the server. The Flywheel Python SDK provides a powerful interface for inspecting and manipulating data through this API. By standardising this underlying data model into Pythonic Objects, the flywheel SDK is effectively an object relationship mapper (ORM), similar to the popular SQLAlchemy software.

Flywheel Data Model

Objects in Flywheel's data model follow a specific hierarchical structure (Figure 3) — at the top level is the Flywheel *instance*, a process running that serves the API to users (for example, a neuroimaging center). Within the Flywheel instance, there are multiple *groups*, which are typically labs or research units that collaborate on one or more *projects*. Each project object can have one or many *subjects* (i.e. participants), and each subject can have one or many *sessions* (i.e. scanning visits). Within a session, there may be one or many *acquisition* objects which represent the scanning sequence collected during a particular scan or examination (e.g. rs-fMRI, DWI, PET), and under each acquisition is *attached* the data file associated with the sequence (e.g. a NIfTI file or DICOM). Note that a file can be attached to any object type, and each object can have metadata associated with it. Hence, a subject object may have de-identified demographic metadata associated to that participant, and the subject may also have a text file attached to it (such as clinical data). A notable exception to the hierarchical structure rule is the analysis object, which behaves in much the same way as others but can be a child object of any other object, allowing researchers to create analyses of entire projects, for example, each with their own associated metadata and files (such as inputs and outputs).

Abstracting this data model in Python results in simple hierarchical objects, each with methods for handling metadata and files, and methods for accomplishing object-specific tasks like traversing the hierarchical structure or running analyses. Flywheel Tools' modules make use of this data model to accomplish a wide range of tasks.

Flywheel Gears

Flywheel encourages the use of pre-packaged computational workflows, called *gears*. Gears are run by virtual machines/containers using Docker and hence are version-controlled and software/platform agnostic. Gears can accomplish tasks such as data manipulation, pre-processing, analysis, and summarisation. In addition to the multitude of gears available on the platform, users are able to package their own software in a gear and use it for running analysis workflows on their Flywheel data, via the web UI or SDK. The complexity and frequency of the task suggests whether to accomplish a task using the web UI, programmatically using the SDK, or by wrapping it as a workflow into a gear (Figure 4). Gears can take existing Flywheel data, such as images or file attachments, as inputs to the workflow, and can be created with clickable configuration options. Once a workflow has completed running, Flywheel collects any files remaining in the container's pre-defined output directory and attaches them to a resulting analysis object. The resultant files of a gear (such as an HTML report or tabulated data) can be viewed on the Flywheel UI, downloaded to disk for further data sharing or analysis, or be used as input to a subsequent gear themselves.

Results

Flywheel Tools is implemented using the Flywheel SDK to enable easy inspection, curation, validation, and audit of Flywheel data through a handful of user-friendly gears and command-line interfaces.

The first module of the package is called `fw-heudiconv`, and is largely inspired by the popular HeuDiConv Python package.[1] `fw-heudiconv` is a multi-part toolbox for reprodicible curation of neuroimaging data into BIDS on Flywheel. The second module, `flaudit`, is a tool for accomplishing a complete audit of a Flywheel project, giving users a broad overview of the key elements of their data set.

`fw-heudiconv`

The first tool, `fw-heudiconv`, is a multi-purpose command-line interface and Flywheel gear designed for comprehensive BIDS curation on Flywheel. It is designed to be intuitive, flexible, and reproducible.

Architecture & Design

`fw-heudiconv` is inspired in large part by the Heuristic Dicom Converter (HeuDiConv) package, and shares much of its design practices. In order to curate data into BIDS, `fw-heudiconv` first considers Dicom data to be the "ground truth" data, and builds its curation approach using data in the Dicoms' headers. Ultimately, `fw-heudiconv` only has permission to manipulate metadata attached to NIfTI files, in the "Info: BIDS" field, which ensures that curation can be repeated from the stage of Dicom ingress reliably and safely.

`fw-heudiconv` can be downloaded as a Python command-line interface from the Python Package Index using `pip`, and is available as a point-and-clickable gear on the Flywheel UI. The gear is managed by Docker containerisation, meaning

[1] https://github.com/nipy/heudiconv

that versioning is reliable and reproducible. There are a number of commands available in `fw-heudiconv`, and each of them starts by querying data from Flywheel. Users can filter their queries, so as to operate on an entire Flywheel project, a subset of subjects, or a subset of sessions. Notably each command has the ability to safely test and evaluate its effects without manipulating metadata on Flywheel or writing data to disk. In particular, there are five commands users can access:

1. `fw-heudiconv-tabulate`

The tabulate tool is used to parse and extract DICOM header information in a project (or within a filtered subset of that project) and tabulate this data for the user to examine with ease. By collecting DICOM header information into tabular format, the tabulate tool gives users a comprehensive overview of the different scanning sequences that have been collected in the query, including their sequence parameters. Additionally, users have the option to limit the tabulation to a unique combination of common DICOM header fields, which significantly decreases complexity of the table. The table output by this command can be written to a local disk if run from the command line, or is saved in the output section of a Flywheel gear if run on Flywheel.

2. `fw-heudiconv-curate`

The curate tool is used to curate a dataset on Flywheel into BIDS format. Much like HeuDiConv, curation is done through the use of a heuristic, a Python file which programmatically defines the templates of a range of BIDS valid filenames, and defines the boolean logic that would assign a given scanning sequence to each template. This boolean logic is based on the sequence information users find in the tabulation of sequences, and all fields available in the Dicom header can be used to parse out which template a particular file can be assigned to. Additionally, the curate tool can be used to manipulate BIDS metadata that may need to be added to the dataset. The process of curation only manipulates BIDS metadata of NIfTI files, and hence can be repeated or updated at any time at the user's discretion.

3. `fw-heudiconv-export`

The export tool is used to export a BIDS dataset on Flywheel to disk. The tool is primarily used as a helper tool for other gears and scripts to quickly and easily extract their BIDS data into the workspace of their analysis pipeline, or by individuals who need their BIDS data exported from Flywheel.

4. `fw-heudiconv-validate`

The validate tool is a wrapper around the popular BIDS Validator package **CITE** and is use to check if the applied curation results in a BIDS-valid dataset. After exporting a data set with `fw-heudiconv-export`, the validate tool runs the BIDS validator on the dataset and returns the result and verbose description of the errors and warnings given by the BIDS Validator.

5. `fw-heudiconv-clear`

The clear tool is used to clear BIDS information cleanly and safely from the project or subjects and sessions queried. This can be useful when overwriting by re-curating current BIDS data doesn't fully erase existing data.

Heuristic File

The heuristic file is a Python file used as input to the `fw-heudiconv-curate` command. It instructs `fw-heudiconv` how to programmatically sort and parse through each acquisition object in Flywheel, and assign it to a BIDS-valid naming template. This is done by checking attributes of a list of `seqInfo` objects — generated from each DICOM's header information — against user-defined boolean rules. For example, if a T1-weighted image is present in a dataset, the user could define a string with a BIDS-valid naming template for this type of file, such as:

```
t1w = 'subject-{SubjectLabel}_session-{SessionLabel}_T1w.nii.gz'
```

Where the `SubjectLabel` and `SessionLabel` portions are expected to be automatically generated for each subject and session. After a DICOM's `SeriesDescription` field is added to the `seqInfo`'s `SeriesDescription` attribute, the user can create simple boolean rules to check if the string 'T1w' is in the `SeriesDescription`. If such a rule is met, this acquisition and its NIfTI file will be assigned to the T1-weighted image naming template. The NIfTI file will ultimately have this BIDS naming added to its metadata, and be named correctly when exported to a filesystem.

In addition to setting naming templates, the heuristic file can also be used to hardcode and assign metadata in BIDS. These data are hard-coded into the file object's metadata on Flywheel, and are assigned by using specially reserved functions and keywords in `fw-heudiconv`. For example, the heuristic file can be used to point fieldmap scans to their intended sequences using a list:

```
IntendedFor = {

  fieldmap1: ['sub-{SubjectLabel}_{SessionLabel}_task-rest_bold.nii.gz']

}`
```

By reserving select keywords for functions and metadata, heuristic files become versatile tools for defining and manipulating a wide array of metadata in Flywheel BIDS curation.

Curation Workflow

For most users, the curation workflow follows the sequence detailed above; after ingress of a batch of DICOMs from a scan, Flywheel's automated utility gears convert the DICOMs to NIfTI files. Users can then begin running `fw-heudiconv-tabulate` to gather the information stored in the DICOM headers necessary for creating a heuristic. Once the tabulation has been completed, the output file can be opened by any program that can read tabular data. Users at this stage can begin creating a heuristic file and running `fw-heudiconv-curate`, using the `--dry-run` flag to test the heuristic changes incrementally with informative logging. When satisfied, users can simply remove the `--dry-run` flag to apply the changes. The user can then use `fw-heudiconv-validate` to run the BIDS validator on the dataset, or start over by removing all BIDS metadata with `fw-heudiconv-clear`.

Additionally, if being run on the Flywheel UI, each of the commands is available as a Flywheel gear. This option can be beneficial for data provenance as all of a gear's commands and inputs, as well as outputs and log files, are stored and attached to each gear run.

`flaudit`

The second module is a Flywheel project auditor, aptly named `flaudit`. The module is intended to give Flywheel users a broad overview of their entire Flywheel project. Features of this overview include a comprehensive visualization of scanning sequences and their parameters; the corresponding BIDS curated result of each sequence; an enumeration of gear analyses and their runtimes and success rates; and a visualization of the various analysis workflows run on each session (Figures 6, **??**, 7, 7). This information is compiled in a portable HTML report that can be opened in the Flywheel UI or in any web browser.

Architecture & Design

Using similar internal machinery to `fw-heudiconv-tabulate`, `flaudit` loops over existing data in a project and tabulates information about scanning sequences, BIDS metadata, and gear jobs that have been run. These 3 tables are saved internally and then passed as input to an R markdown script that generates a dynamic HTML report. The data are also saved as output for the user to access and analyse at their own discretion.

Discussion

As the neuroimaging community embraces Big Data and the various platforms available for storage and analysis, it is becoming increasingly important for researchers to eschew the *ad hoc* analysis procedures previously run on a single machine or cluster. Instead, cloud-based platforms like Flywheel provide opportunities for more reproducible, reliable, and shareable science. Flywheel Tools provides software that maximizes these opportunities on the Flywheel platform.

Figures

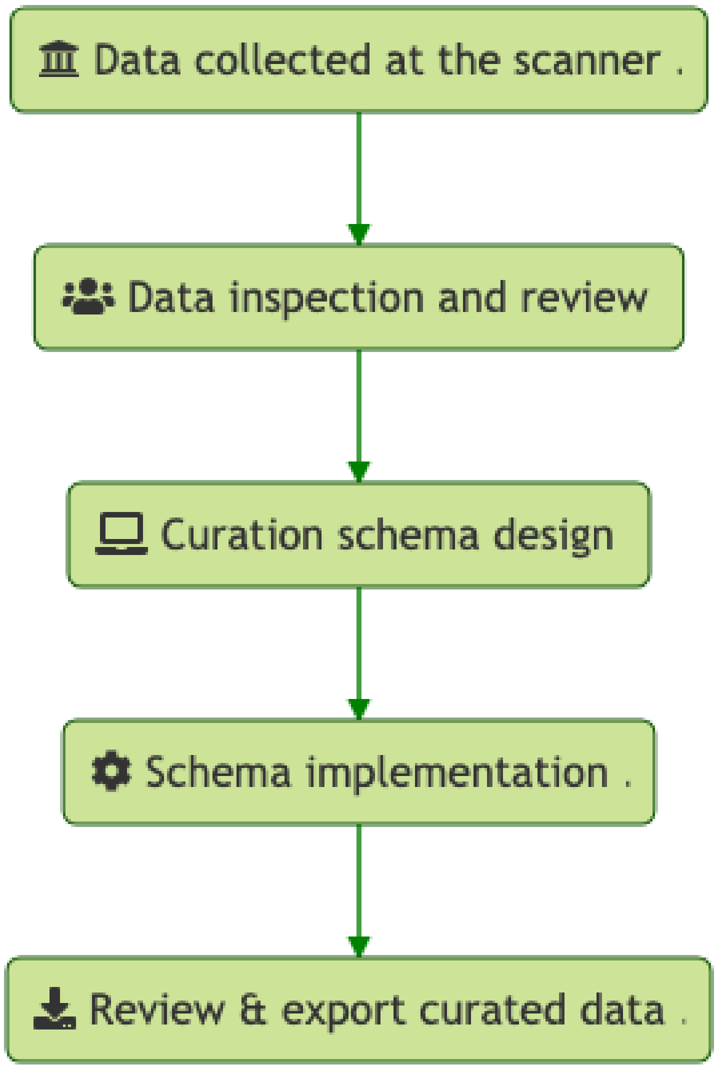

Data collected at the scanner .
Data inspection and review
Curation schema design
Schema implementation .
Review & export curated data .

Figure 1: Flywheel Tools Workflow

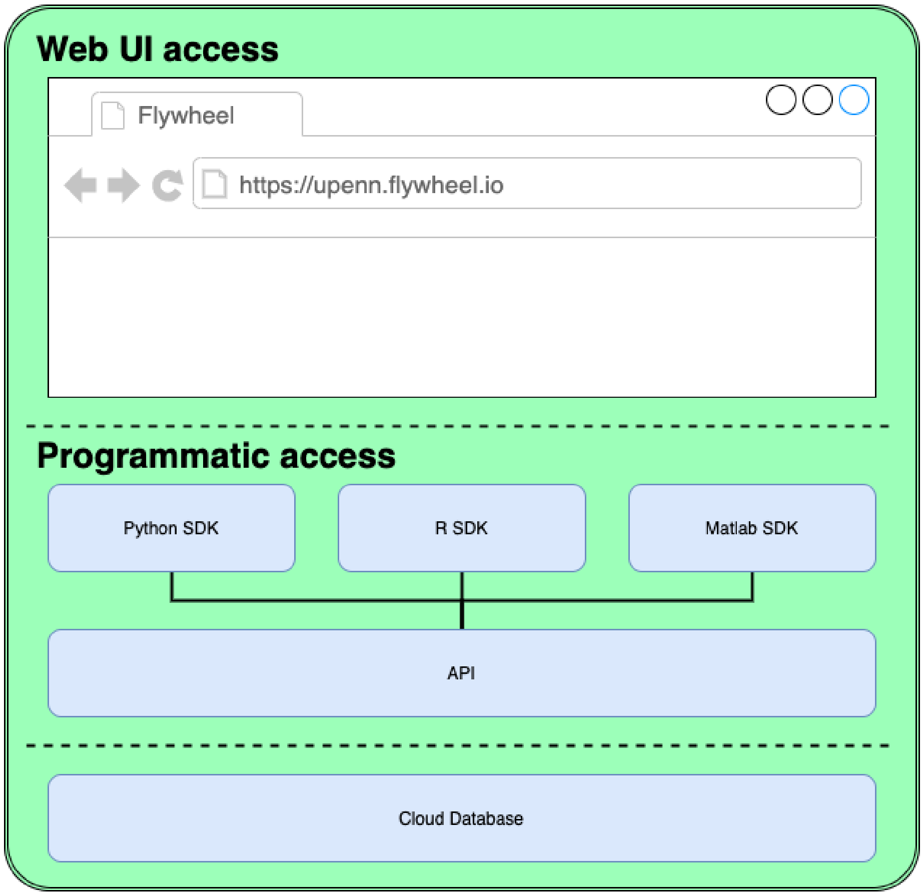


Figure 2: Flywheel General Architecture

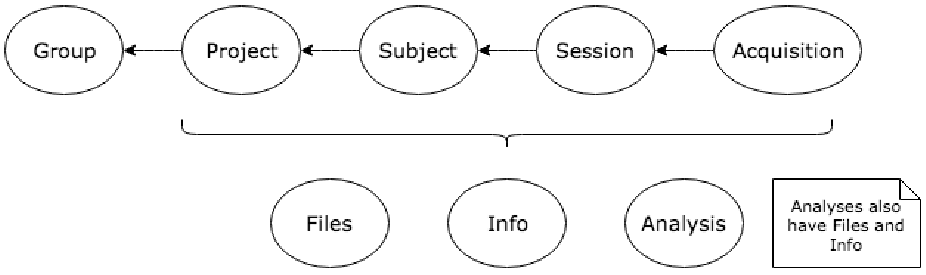


Figure 3: Flywheel Data Model

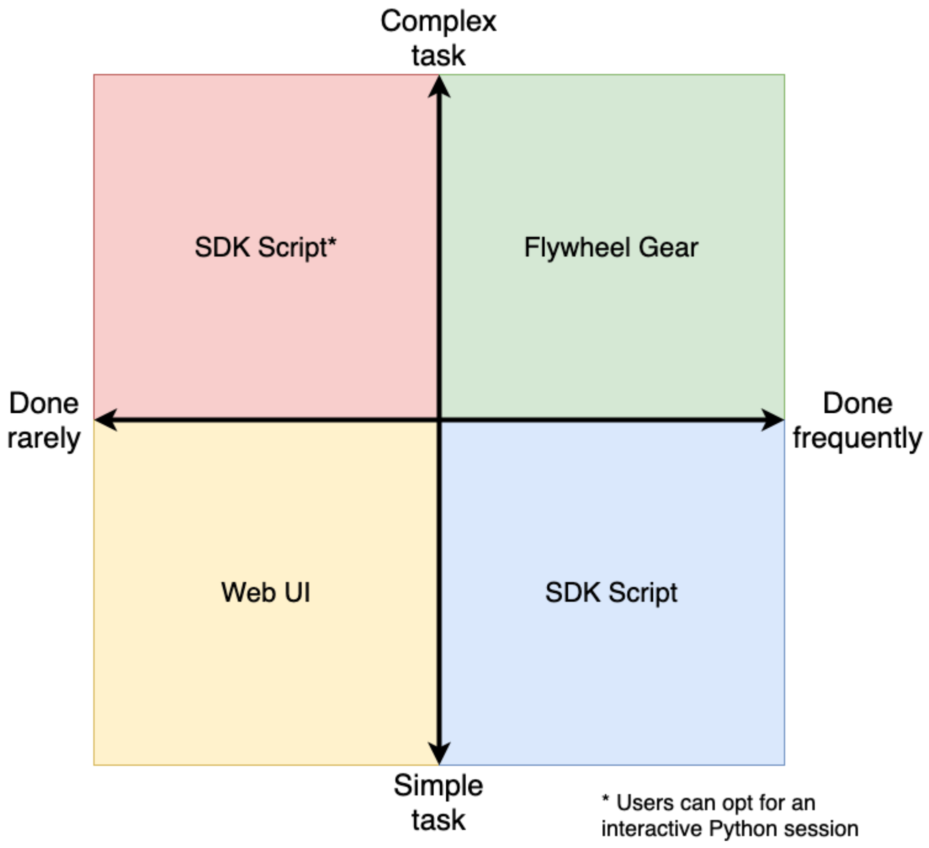


Figure 4: Decision Framework for Accomplishing Tasks on Flywheel

We visualise the above frequencies below:

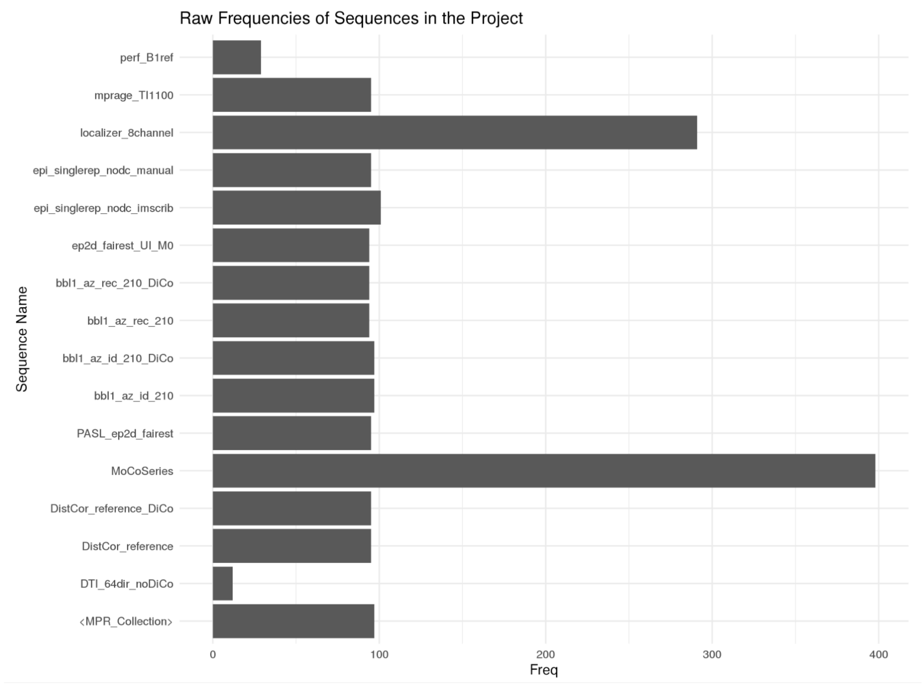
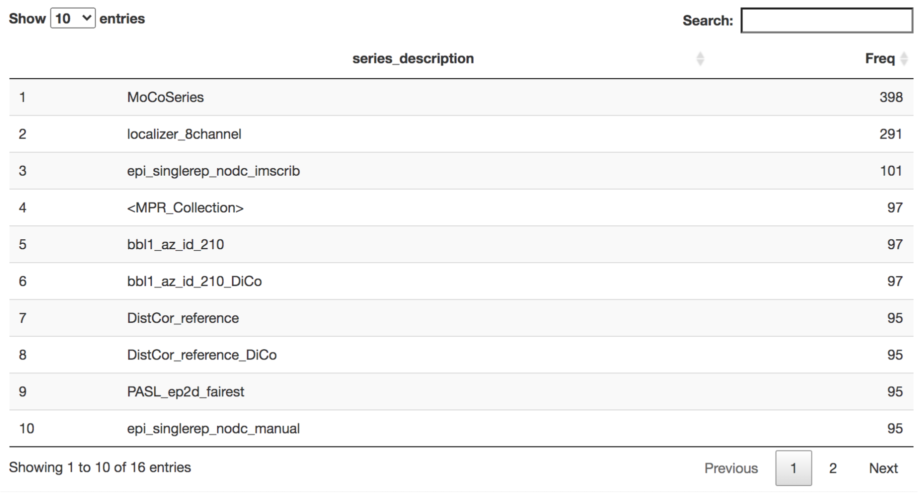


Figure 5: Plot Enumerating Available Sequences in a Flywheel Project

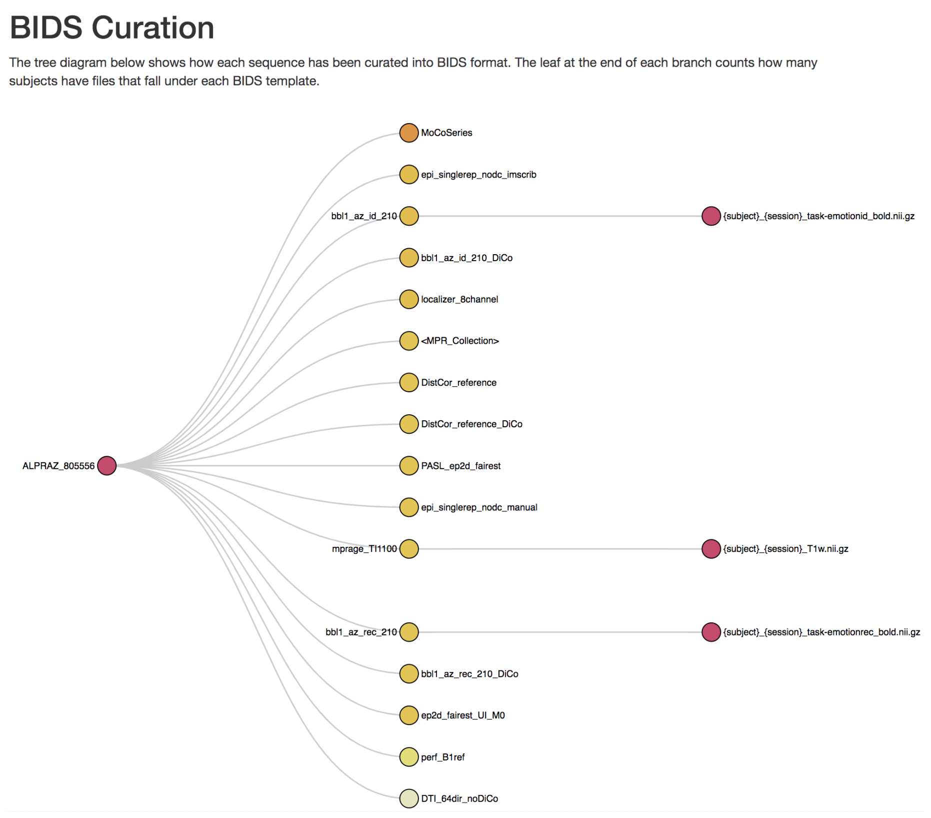

Show 10 entries

Search:

	series_description	Freq
1	MoCoSeries	398
2	localizer_8channel	291
3	epi_singlerep_nodc_imscrib	101
4	<MPR_Collection>	97
5	bbl1_az_id_210	97
6	bbl1_az_id_210_DiCo	97
7	DistCor_reference	95
8	DistCor_reference_DiCo	95
9	PASL_ep2d_fairest	95
10	epi_singlerep_nodc_manual	95

Showing 1 to 10 of 16 entries

Figure 6: Interactive Table of Available Sequences in a Flywheel Project



BIDS Curation

The tree diagram below shows how each sequence has been curated into BIDS format. The leaf at the end of each branch counts how many subjects have files that fall under each BIDS template.

Figure 7: Interactive Tree Diagram Illustrating BIDS Curation

Here are the gear completion statistics:

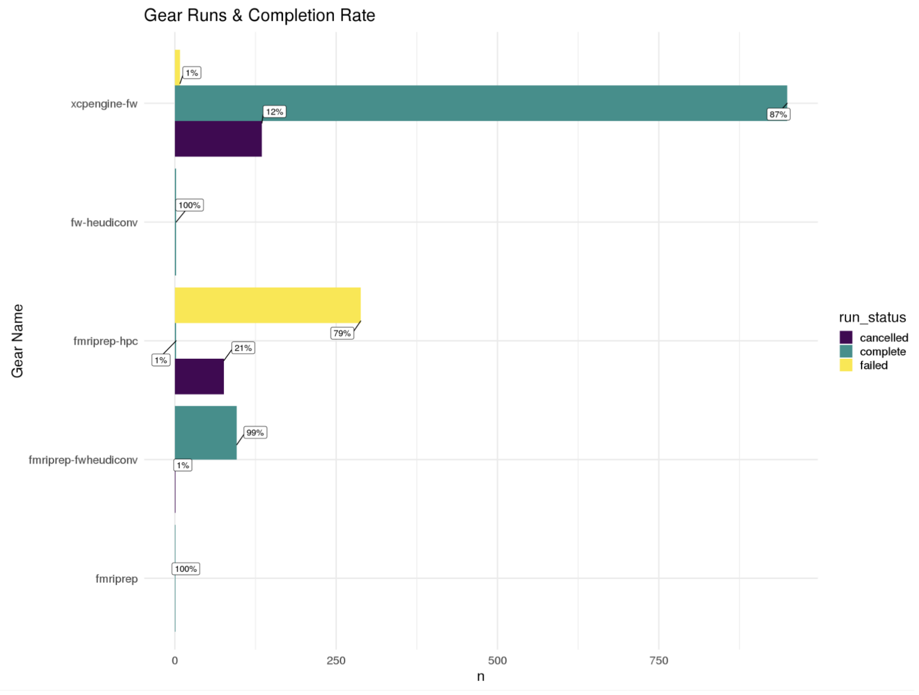


Figure 8: Plot Enumerating Gear Runs in a Flywheel Project

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