SOFTWARE TOOL ARTICLE

**REvised** The Neuroimaging Data Model Linear Regression Tool (nidm_linreg): PyNIDM Project [version 2; peer review: 1 approved with reservations, 1 not approved]

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Abstract

The Neuroimaging Data Model (NIDM) is a series of specifications for describing all aspects of the neuroimaging data lifecycle from raw data to analyses and provenance. NIDM uses community-driven terminologies along with unambiguous data dictionaries within a Resource Description Framework (RDF) document to describe data and metadata for integration and query. Data from different studies, using locally defined variable names, can be retrieved by linking them to higher-order concepts from established ontologies and terminologies. Through these capabilities, NIDM documents are expected to improve reproducibility and facilitate data discovery and reuse. PyNIDM is a Python toolbox supporting the creation, manipulation, and querying of NIDM documents. Using the query tools available in PyNIDM, users are able to interrogate datasets to find studies that have collected variables measuring similar phenotypic properties. This, in turn, facilitates the transformation and combination of data across multiple studies.

The focus of this manuscript is the linear regression tool which is a part of the PyNIDM toolbox and works directly on NIDM documents. It provides a high-level statistical analysis that aids researchers in

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gaining more insight into the data that they are considering combining across studies. This saves researchers valuable time and effort while showing potential relationships between variables. The linear regression tool operates through a command-line interface integrated with the other tools (pynidm linear-regression) and provides the user with the opportunity to specify variables of interest using the rich query techniques available for NIDM documents and then conduct a linear regression with optional contrast and regularization.

**Keywords**
Linear Regression, Neuroimaging, PyNIDM, Neuroimaging Data Model, Machine Learning

This article is included in the Artificial Intelligence and Machine Learning gateway.

This article is included in the INCF gateway.
Introduction

Background

The Neuroimaging Data Model (NIDM) (Keator et al. 2013; NIDM Working Group; Maumet et al. 2016) (Neuroimaging Data Model, RRID:SCR_013667) was started by an international team of volunteers to create specifications for describing all aspects of the neuroimaging data lifecycle. NIDM is built upon the PROV Standard (Moreau et al. 2008; ‘PROV-Overview’), which means it provides information about the people, tools, and other metadata involved in creating a piece of data, which can be used to determine how reliable and thorough it is. The PROV Standard consists of three specifications: Experiment, Results, and Workflow, and it depends on semantic web. Unlike the internet, which supports a “Web of documents”, the semantic web supports a “Web of data” that can be viewed as a global database. The goal of semantic web is to link data, organize it, and allow it to be queried as is done in a database (“Semantic Web - W3C”). Using semantic web, the PROV Standard’s three specifications were envisioned to capture information on all aspects of the neuroimaging data lifecycle, producing graphs linking each result’s artifact with the workflow that produced it and the data used in the computation. These graphs can be serialized into a variety of text-based formats (NIDM documents), and with the capabilities of the semantic web, can be used to link datasets together through annotations with terms from formal terminologies, complete data dictionaries of study variables, and linkage of study variables to broader concepts. These annotations provide a critical capability to aid in reproducibility and replication of studies, as well as data discovery in shared resources. The NIDM-Experiment model consists of a simple project-session-acquisition hierarchy which can be used to describe both the content and metadata about experimental studies and derived (e.g., regional brain volume, mass-univariate functional brain analysis) neuroimaging data. It has been used to describe many large publicly-available human neuroimaging datasets (e.g. ABIDE (Di Martino et al. 2014), ADHD200 (Milham et al. 2011), CoRR (Zuo et al. 2014) (Consortium for Reliability and Reproducibility, RRID:SCR_003774), OpenNeuro (“OpenNeuro”) (OpenNeuro, RRID:SCR_005031) datasets) along with providing unambiguous descriptions of the clinical, neuropsychological, and imaging data collected as part of those studies.

PyNIDM (PyNIDM) (PyNIDM, RRID:SCR_021022) v3.9.7 (PyNIDM v3.9.7) is a Python toolbox under active development that supports the creation, manipulation, and query of NIDM documents. It is open-source and hosted on GitHub, distributed under the Apache License, Version 2.0 (“Apache License, Version 2.0”). PyNIDM consists of tools to work with NIDM documents such as conversion from BIDS (Gorgolewski et al. 2016), graph visualization, serialization format conversion, merging and query. Querying of NIDM documents is supported using a command-line RESTful (Ravan et al. 2020) interface (i.e. pynidm query) which executes SPARQL (“SPARQL Query Language for RDF”) queries. Using the query functionality and the NIDM document semantics, users can quickly identify datasets that measured similar properties and may be combined for further investigation.

Beyond the existing tools that have been written to support NIDM documents, some high-level statistical analysis tools are needed to provide investigators with an opportunity to gain more insight into data they may be interested in combining for a complete scientific investigation. Combining datasets collected across different studies is not a trivial task. It requires both a complete, unambiguous description of the data and how it was collected, along with a varying number of transformations to align, where possible, disparate data. The process of transforming data is often quite time-consuming and therefore understanding whether the identified datasets, at a high level, might have some interesting relationships prior to committing to a full scientific study is prudent. Here we report on a tool that provides such capabilities; namely, a simple linear modeling tool supporting NIDM documents and integrated into the existing PyNIDM suite of tools.

Statement of need

While tools and libraries for statistics and machine learning algorithms are numerous, there are none that can be directly applied to NIDM documents. The linear regression algorithm presented here allows scientists studying the human brain to easily find relationships between variables across datasets while retaining the provenance present in NIDM documents. The algorithm has the ability to query for specific variables or across similar variables from different studies using concept annotations on the variables. It then provides the user with the ability to construct arbitrary linear models on those data, supporting interactions between variables, contrasts of learned parameter sets, and L1 and L2
regularization (Nagpal 2017). L1 and L2 Regularization are two different techniques used to reduce the error of a linear fit while avoiding overfitting, creating a less complex model. They will be explained later in the paper.

There is no comparable tool for this use case.

Methods
Implementation
The linear regression tool, `nidm_linreg`, uses the PyNIDM query functionality to aggregate data in NIDM documents serialized using the standard Terse Resource Description Framework (RDF) Triple Language (TURTLE) (“RDF 1.1 Turtle”), a common semantic-web serialization format that is both structured for ease of use with computers and relatively easy for humans to read. Researchers have the ability to construct custom models based on their scientific goals. The source code is available on Zenodo and full details can be found in the Software Availability statement (Keator et al. 2021).

Thus, nidm_linreg is a machine learning algorithm that can work on complex datasets described using the NIDM linked-data format, while being reasonably easy to use. Researchers have the ability to conduct a preliminary analysis to understand if it is worth the effort to pursue combining datasets and doing the transformations necessary to integrate those datasets. One can quickly determine if there are high-level relationships in the datasets and look at the different weights to decide what variables may warrant further study.

The tool provides a simple command-line user interface (Figure 1) based on the “Click” Python library (“Welcome to Click — Click Documentation (8.0.X)”) which integrates the linear regression module with existing PyNIDM tools (e.g. pynidm linear-regression, pynidm query, pynidm convert, etc.).

To use the tool, the user runs the command `pynidm linear-regression` with a variety of required and optional parameters. The first parameter, “-nl”, is a comma-separated list of NIDM serialized TURTLE files, each representing a single dataset or a collection site within a multi-site research project or multiple datasets (Figure 2). A useful set of NIDM documents describing publicly-available neuroimaging data from the ABIDE, ADHD200, and CoRR studies along with datasets in the OpenNeuro database can be found on GitHub (A. Kumar, D. Keator) The next parameter, “-model” provides the user with the ability to construct a linear model using notation found in popular statistics packages (e.g., R statistical software (Ripley 2001)( R Project for Statistical Computing, RRID:SCR_001905)). The syntax follows the scheme “dependent variable (DV) = independent variable 1 (IV1) + independent variable 2 (IV2) + … + IVX”. To encode interactions between IV1 and IV2 in the above example, one can use the common “*” syntax: “DV = IV1 + IV2 + IV1*IV2”.

![Figure 1. pynidm linear-regression parameters; demonstrating options for a researcher using the tool.](image-url)
To determine what variables or data elements are available from a set of NIDM documents, the first step is to use “pynidm query” to do a data element search of the NIDM documents. From this search, the user can see what data elements are available in the selected NIDM documents and understand some details of those data elements (e.g., ranges, categories, data type, etc.). After performing the data elements query of the NIDM documents and selecting independent and dependent variables of interest, one proceeds with constructing the linear model with the pynidm linear-regression tool.

One can select data elements from the NIDM documents for linear regression using three specific forms: (1) using the UUID of the objects in the NIDM graph documents; (2) using the distinct variable name from the original dataset, also stored as metadata in the NIDM graph documents; (3) using a high-level concept that has been associated with specific variables described by the concept across datasets, used to make querying across datasets with different variable names but measuring the same phenomenon easier. We support these three distinct forms of selecting data elements to enable distinct usage patterns. Some investigators will use NIDM documents of their internal studies and want to be able to reference data elements using their study-specific variable names. Other investigators may want to use variables from different studies and thus the variable names are unlikely to be the same; thus, we support the use of selecting variables based on high-level concepts. In practice, users will not often mix forms of referring to data elements within the same model, but we show it in our use cases to make evident the flexibility of the tool.

After the model and data elements are selected by the user, the NIDM files are queried with a command-line interface which uses SPARQL to gather data from the files. It is done in this way because the NIDM file depends on the PROV Standard, and thus uses semantic web techniques, as mentioned in the introduction. For that reason, the NIDM file acts like a database, and a query is needed to collect the data.

However, since no modules for machine learning operate based on the same semantic web standard as the NIDM files, the data returned from the query is not easily usable. Thus, the data is placed in an array, then reorganized and manipulated with the pandas module and array functions to return a readable array that is returned to the user. That array is used as the dataset in the linear regression, executed with methods made available by the Scikit-Learn library.

The optional “-contrast” parameter allows one to select one or more IVs to contrast the parameter estimates for those IVs. Our tool supports multiple methods of coding treatment variables (e.g., treatment coding (Figure 3), simple coding, sum coding, backward difference coding, and Helmert coding) as made available by the Patsy Python library (Brooke 1923). The user can select multiple independent variables to contrast and/or contrasts on interactions.

The optional “-r” parameter allows the user to select L1 (Lasso) or L2 (Ridge) regularization implemented in scikit-learn (Varoquaux et al. 2015) (scikit-learn, RRID:SCR_002577). In either case, regularizing prevents the data from being overfit, potentially improving model generalizability and demonstrating which variables have the strongest relationships with the dependent variable. The regularization weight is iteratively determined across a wide range of regularization weightings using 10-fold cross-validation, selecting the regularization weight yielding the maximum likelihood.

There are error checks within the code to make sure the researcher has feedback on why a model cannot run, whether it is because there are not enough data points or because one or more variables could not be found in one or more of the NIDM documents. This makes the experience as simple as possible for the user, which is important, as our intended audience for these tools are investigators who may have no prior experience with the semantic web and/or NIDM documents. The first error check is apparent when the user inputs a command. All inputs are stripped of extra spaces, and the command is presented back to the user so if there is a syntax error, the user can easily trace it. Furthermore, regardless of whether the user puts spaces between the specified parameters or not, the code breaks it into its constituent parts, reducing burden on the user to type it in a particular way. It also handles different signage used by the user, for example treating an equal sign or tilde the same way. Finally, if the same variable is a dependent variable and independent variable according to the user’s model, the user is told that this is impossible, and the code is halted before an error occurs.
Another built-in error check ensures the variables in the model are found in the NIDM files specified. If the variable is not found in a file, those variables are listed out for the user, allowing them to understand what is wrong and exiting before errors are caused. Furthermore, if there are fewer than 20 datapoints, the result will not be as accurate, so the user is warned if too few data points are provided and given the option to proceed or not.

**Use cases**

We present two use cases in this paper. In the example shown in Figure 2, we have first run a pynidm query operation on the NIDM documents and identified four variables of interest: supratentorial brain volume (fs_000008), diagnostic group (DX_GROUP), performance IQ (PIQ_tca9ck), and age. The model specified establishes the relationship between the DV, brain volume, and the IVs, diagnostic group, performance IQ, and age. In this example, fs_000008 is the fixed unique identifier (UUID) of the supratentorial brain volume computed with the FreeSurfer software (Fischl 2012) (FreeSurfer, RRID:SCR_001847) using the original Magnetic Resonance Imaging (MRI) structural scans of the brain. This particular UUID is fixed because it identifies a specific brain region and measurement computed with the FreeSurfer software and will not change across datasets that derive brain volume measurements with FreeSurfer. DX_GROUP is the name of the study-specific variable describing the diagnostic group assigned to participants. PIQ_tca9ck is the performance IQ measure collected on study participants and is the UUID created for this data element when the NIDM documents were created for this dataset. Note, this particular UUID is not guaranteed to be the same across NIDM documents from different studies.

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The contrast variable in this example is “DX_GROUP” which describes the diagnostic group of each participant. The results of the treatment coding contrast applied in Figure 2 can be seen in Figure 3. Finally, we conducted L1 regularization on the data, determining the optimal weight.

Another example is shown in Figure 4. We have first run a pynidm query operation on the NIDM documents and identified 4 variables of interest: fs_003343, age, sex, and group. Here, fs_003343 is the fixed unique identifier (UUID) of the left hippocampus volume while age, sex, and group are names of the study-specific variables concerning the age of the participant at the time of the study, the gender, and the group the participant was in. The model specified establishes the relationship between the DV, left hippocampus volume, and the IVs, group, age, and sex. However, in this case, we also encode interactions between age and sex and age and group, as denoted by the asterisks. Also, in this model, we have used multiple IVs to contrast the parameter estimates for those IVs. The contrast variables are age and group. Finally, L2 regularization is selected for regularization.

The results of the Helmert coding contrast can be seen in Figure 5.
**Operation**

The data must be in a NIDM document(s) to be used with this tool. Data can be transformed into a NIDM document directly from BIDS or tabular data files using the PyNIDM tools “bidsmri2nidm” and “csv2nidm”. Once data is transformed into NIDM, the user only needs to have a functional installation of PyNIDM and access to a terminal window or similar command-line processing tool with a functional version of Python 3. Once the user specifies the parameters, data is aggregated from the NIDM files, re-structured for the linear regression algorithm, and parameter estimates learned using ordinary least squares and returning either a printout or output file of the various coefficients and summary statistics.

**Conclusions**

In this work, we have designed a linear regression tool that works on linked-data NIDM documents in support of understanding relationships between variables collected across studies. This tool helps scientists evaluate relationships between data prior to fully integrating datasets for hypothesis testing which may require considerable time and resources. In our initial evaluations, this tool has shown utility for these use cases. In future work, we are creating additional machine learning tools allowing users to cluster data in a similar fashion to the linear regression tool presented here. Further, the NIDM community is working on additional functionality for the PyNIDM toolkit that transforms the value representations of the variables selected for modeling to be consistent across all NIDM documents used in the model. These transformations are made using the detailed data dictionaries included in the NIDM documents. This functionality will be included in the PyNIDM query application programmers’ interface (API) and will be immediately available to the linear regression tool presented here.
Software availability
Source code available from: https://github.com/incf-nidash/PyNIDM/blob/master/nidm/experiment/tools/nidm_linreg.py


License: Apache License, Version 2.0

References

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OpenNeuro: Copyright 2022, Stanford Center for Reproducible Neuroscience. Reference Source

PROV-Overview: Copyright 2013, W3C. Reference Source


RDF 1.1 Turtle: Copyright 2008-2014, W3C. Reference Source


Semantic Web - W3C: Copyright 2015, W3C. Reference Source

SPARQL Query Language for RDF: Copyright 2006-2007, W3C. Reference Source


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Version 1

Reviewer Report 11 April 2022

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Karsten Specht
Department of Biological and Medical Psychology, University of Bergen, Bergen, Norway

In this software tool article, the authors describe a tool that allows high-level statistical analysis for combining studies that follow the Neuroimaging Data Model (NIDM) framework. The tool is/will be part of the PyNDIM toolbox.

In general, this appears as a very useful tool that a larger community might want to use. However, the article is phrased and organized in a way that this might not happen. The audience of the current manuscripts is almost exclusively the NDIM community that is involved in developing the tools, but it is not directed to potential users. The main problem is, in my view, that the level of explanation and description of the tool is very minimalistic. Of course, all important aspects and relevant tools are mentioned, but only as keywords with the appropriate references. My main concern is that readers not entirely familiar with all aspects and methods incorporated into this tool will not get its importance and relevance.

I would like to see just a few more sentences describing the key elements in a revised version. For example, readers unfamiliar with the PROV standard or the semantic web technique are already lost after the third sentence. And the introduction continues like that. For example, the “L1 and L2 regularization” is just thrown in on the first page, assuming that every reader immediately gets its relevance, but a more relevant discussion follows much later.

Similarly, I would have expected a more detailed description of the implementations in the section that is called “implementation and use cases”, but this section is mainly on “use cases” and very little on implementation.

So, in summary, I think a revised version of this article would benefit from just a few more describing lines so that this very relevant tool generates interest in a broader audience.

Is the rationale for developing the new software tool clearly explained?

Yes
Is the description of the software tool technically sound?
Yes

Are sufficient details of the code, methods and analysis (if applicable) provided to allow replication of the software development and its use by others?
Partly

Is sufficient information provided to allow interpretation of the expected output datasets and any results generated using the tool?
Yes

Are the conclusions about the tool and its performance adequately supported by the findings presented in the article?
Yes

**Competing Interests:** No competing interests were disclosed.

**Reviewer Expertise:** Neuroimaging, methods development, reliability measures

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

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Author Response 30 Apr 2022

**Ashmita Kumar,** Troy High School, Fullerton, USA

Thank you for the time you have taken to review this paper. We will add more specifics to make it more accessible to potential users, defining our implementation, data structures, and technique in more detail. We apologize for the time it has taken to respond, but rest assured we are working to address it in our next version.

**Competing Interests:** No competing interests were disclosed.

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Reviewer Report 08 April 2022

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The authors have written about the nidm_linreg tool which is a linear regression tool that is now a part of the PyNIDM software. nidm_linreg was added because PyNIDM did not have a tool like this in its suite yet. The tool's design and the paper's focus on usage are both very thorough. This software tool article is likely of interest to PyNIDM and other members of the neuroimaging community. We have the following comments and concerns about the software and the paper:

1. Echoing the concern expressed in Dec 2021 in the PyNIDM GitHub issue 309 (https://github.com/incf-nidash/PyNIDM/issues/309), it is bad practice to install Python packages outside of dependency management functionality. The nidm_linreg.py tool currently tries to quietly install 4 packages using pip if they are not present in the Python environment. This will likely cause problems and/or confusion for the user. A safe and reproducible way to provide the end-user with the dependencies they need is to provide a requirements.txt file with the repository which lets users use a specific version of the expected package dependencies. https://pip.pypa.io/en/stable/reference/requirements-file-format/

2. We ran the commands on the GitHub README.md (with some necessary modifications) to install and test PyNIDM (see below), pytest returned several errors and warnings (on two different platforms) that should be corrected:

   conda create -n pynidm_py3 python=3
git clone https://github.com/incf-nidash/PyNIDM.git
cd PyNIDM
pip install -e .
pytest
[snip]
= 4 failed, 24 passed, 14 skipped, 3 warnings, 36 errors in 35.41s ==

3. Running the commands as-written in Figures 2 and 4 did not work. We cloned the simple2_NIDM_examples repository (https://github.com/dbkeator/simple2_NIDM_examples) and tried to use the data within, but we were only able to run one of the example commands successfully.

   This felt insufficient to evaluate the reproducibility of the tool. The authors should provide commands, script, or a container such that users can reproduce the same outputs presented in the paper.

4. The Methods section “Implementation and use cases” covers a blend of those two things where we think it would read better to see a focused section on Implementation and a focused section on Use cases. The Implementation section could discuss the design decisions and software architecture as well as planned support. Most of the current content could move over to a Use cases section covering a use case or two (as it does now).

5. The paper mentioned there are “error checks” built into the tool, but no examples are
shown. Including a sentence about the kinds of errors being checked for would be another useful addition.

6. The reference for the Patsy Python Library (Brooke 1923), on page 5 of the PDF (Methods section, 8th paragraph) is incorrect.

Is the rationale for developing the new software tool clearly explained?
Yes

Is the description of the software tool technically sound?
Yes

Are sufficient details of the code, methods and analysis (if applicable) provided to allow replication of the software development and its use by others?
No

Is sufficient information provided to allow interpretation of the expected output datasets and any results generated using the tool?
Yes

Are the conclusions about the tool and its performance adequately supported by the findings presented in the article?
Partly

**Competing Interests:** No competing interests were disclosed.

**Reviewer Expertise:** Neuroimaging, Neuroscience, Computer Science, Data Science

We confirm that we have read this submission and believe that we have an appropriate level of expertise to state that we do not consider it to be of an acceptable scientific standard, for reasons outlined above.

Author Response 30 Apr 2022

**Ashmita Kumar,** Troy High School, Fullerton, USA

Thank you for your feedback on our tool. We appreciate your thoroughness and will ensure to make the required changes. To your first point, we will make sure that our package requirements are presented to the user before installation instead of using a quiet install. To your second point, while we are unsure why the error appeared, we are looking into it and attempting to reproduce it. We will be sure to address it in our next version. To your third point, we will make sure to provide a way for users to replicate the outputs in the paper by providing more specifics on how we obtained them. To your fourth point, we will separate the two sections and add to our Implementation section in our next version. To your fifth point, the error checks built in include data validation for type and quantity of that data, which we will explain in more detail. To your final point, we will try to find the correct citation.
Thank you for taking the time to make this review, and we are sorry for the length of time it has taken to respond. We really appreciate it.

**Competing Interests:** No competing interests were disclosed.

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