

DATASET VERSIONING THROUGH CHANGELOG ANNOTATION

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ACKNOWLEDGMENT

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ABSTRACT

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CHAPTER 1

INTRODUCTION

Software development followed a stiff production cycle prior to the early 2000s. However, as technology developed, software development required a system to adapt and change to evolving conditions leading to the Agile Manifesto. Likewise, data collected by researchers grew at an astounding rate with new technology. NASA's Atmospheric Science Data Center reported a growth from hosting around five million files to twenty million files between 2001 and 2004¹. Many datasets have required reprocessings of their data, either to improve data quality or to correct for errors [CALIPSO, ARM]. Indeed, version control systems can provide contexts for modifications when combined with error detection systems, providing a more complete picture of the system's behavior [Reference 9]. (Dynamic dataset generation?)

Dataset versioning tracks and documents the changes which occur in datasets. There exists a tendency to model dataset change using methods from software versioning. Dot-decimal style version numbers are commonly seen in relation to new releases of software such as MATLAB or R, and current version naming schemes in data often use dot-decimal notation. However, this convention results in semantically poor version names as the decimal numbers generally function solely as counts. The Ubuntu versioning scheme appears to follow a major-minor numbering pattern, but the major and minor numbers correspond to the year and month of the release, respectively. As a result, the version name holds no significance as the extent of difference between two versions. Additionally, this method breaks down since it is difficult to predict the impact changes in data will have on data consumers. Depending on how the data is processed or what subsets are used, dataset changes that the producers perceives as minor changes may have significant repercussions for the consumer. This demonstrates the structural difference between software and datasets in that a revision in data only constitutes an adjustment to the relevant

¹Agencies and research groups have collected new data at an incredible rate. The amount of data housed by NASA quadrupled from 2001 to 2004 [4] and high energy physics labs can generate on the order of 4000 new datasets every day [5].

subsets. An alteration to a software file constitutes a change to the project as a whole. As a result, datasets provide a context which does not completely translate from software project versioning.

1.1 Types of Change

Change is the fundamental characteristic in the study of versioning. Continuing the comparison with software, the measure of change in applications is primarily functional. Data, on the other hand, has not only function but also structure. While swapping the ordering of columns in a spreadsheet may not effect the usability of the data, it could cause issues with codes that use the data. It is, therefore, clear that many different forms of change exist with differing degrees of intensity. In this document, change is divided into three general categories: scientific, technical, and

1.2 Provenance and Provenance Distance

In a number of papers, authors describe models or systems that track changes in the workflow and track how modifications to the flow would then generate new versions of datasets. The information that details the activities and agents involved in generating a data entity is known as provenance. Barkstrom identifies times when new versions should be generated by locating changes in provenance (specifically calibrations, scripts, and input data) at different levels of data processing in NASA remote sensing workflows. Software revision management tools such as Git and SVN also keep track of provenance information when logging new commits to a project. Since it plays a significant role in triggering new version generations, provenance is often conflated with versioning by scientists. However, it does not sufficiently characterize a versioning event.

In the field of semantic technologies, the W3C recommendation, PROV provides a data model to encode provenance information so that the lineage of data products can be traced. However, PROV expresses relationships between versions with the `wasRevisionOf` or `alternateOf` property. The properties do not allow for more elaboration as to what changes were made to transform version one into its alternate, nor should it. The priority of provenance tracking is understanding where

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and how a data object was generated. Explicitly itemizing the changes is unnecessary in order to communicate the provenance relationship between the two versions. That there exists an association is sufficient within the scope of lineage tracking. This gap illustrates why versioning information is necessary because itemization allows data consumers to determine the significance of changing to a new version.

1.3 Changelogs

1.4 RDFa

1.5 Why Semantic Technologies?

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CHAPTER 2

PREVIOUS WORK

PROV is a W3C recommendation that deliniates a method to express data prove-nance with semantic technologies. Using the model of relating activities, agents, and entities, data managers can express the origins of their datasets. However, when an entity is revised, the PROV data model can only express the relationship as a revision or that the new dataset was derived from the original. This leaves

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CHAPTER 3

CONCEPTUAL MODEL

The conceptual model used within this thesis is built around the expression of three core versioning operations: addition, invalidation, and modification. These three activities can be represented by interacting with three types of concepts: versions, attributes, and changes. Versions represent the data entities being compared. These could be two different editions of a book or versions of software. It is important to understand that a version is an abstraction as it can be represented by multiple physical files. In the sections that follow, operations will only consider the interaction between two versions and will be explained later in the chapter. Versions then contain attributes representing a quantity being modified. Specifically for tabular data, attributes would correspond to an identifier that refers to particular rows or columns within the data. Attributes of the two versions are then connected by a change. This link functions as a very general concept which can be subclassed into more informative types such as unit changes, improving the expressiveness of the model beyond PROV's revisionOf concept.

3.1 ADDITION

When a change adds a new attribute to a version, it only needs to refer to version two and its corresponding attribute. The reasoning should be fairly obvious as the attribute never existed in version one, and therefore, there is nothing to refer to and no need to form a relationship between the change and version one. However, by linking the addition change to version one, we address a difficulty with comparing provenance graphs. When two data objects have identical structures, it is difficult to determine what time the objects were added to the dataset and which version they belong to. As a result, determining the comparability of the two objects becomes difficult. The change contributions to the dataset evolution appears naturally using this construction. The resulting model can be seen in Figure 3.1. Some relationships are specifically left out, such as that between Change A and Version 2, to not confuse

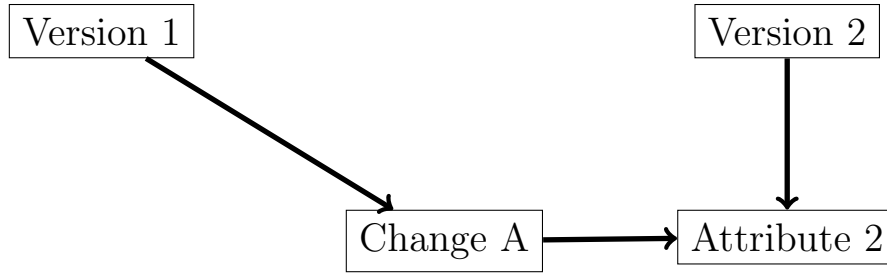


Figure 3.1: Model of the relationships between Versions 1 and 2 when adding an Attribute 2 to Version 2 as a result of Change A

identification of other types of changes. The relationship between Change A and Version 2 can still be implied from Attribute 2.

3.2 INVALIDATION

The Invalidation operation corresponds to the delete concept found in other applications. The choice of invalidation over delete results from the policy that, in versioning, data should never be deleted. In practicality, this may not be particularly feasible due to space limitations and relative validity. In either case, the change invalidates an attribute in version one, resulting in version two. Unlike the Addition operation, Invalidation forms a clear relationship between both versions, which can be seen in Figure 3.2. Notice again that since Attribute 1 no longer exists in Version 2, there is no corresponding Attribute 2 to refer to.

From Figure 3.1, we can see the confusion that could result from requiring explicit relationships between versions and changes in both the Addition and Invalidation operations. Linking Change A to Version 2 would create a duplicate connection and provides a mechanism to identify when items specifically enter or leave a version.

3.3 MODIFICATION

The final operation is Modification, and it maps a change from one attribute from version one to its corresponding attribute in version two. The particular type of change in this case is purposely left out in order to allow data producers to subclass and customize the resulting graph to properly reflect the versioning that they desire.

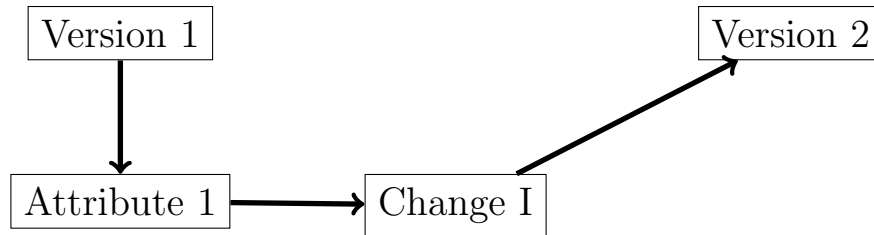


Figure 3.2: Model of the relationships between Versions 1 and 2 when invalidating Attribute 1 from Version 1 as a result of Change I

3.4 MULTIPLE LINKED VERSIONS

Using the construction outlined in the previous three sections, many changes can be compiled together into a graph in a changelog. After all additions, invalidations, and modifications have been compiled into a single graph, a complete mapping from version one to version two may be developed. The orientation of the relationships in the graph allows a flow to be created from attributes in version one to corresponding attributes in version two. Taking version two and performing the same graph construction to a version three results in not only a flow from version two to version three, but also from version one to version three. As a result, the flow can be used to construct a mapping from version one to version three or any future version.

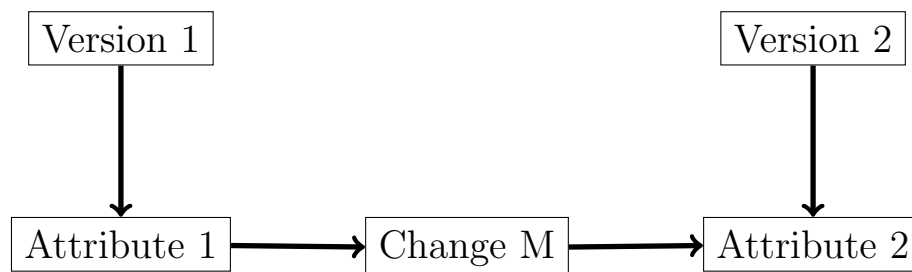


Figure 3.3: Model of the relationships between Versions 1 and 2 when modifying Attribute 1 from Version 1 as a result of Change M, resulting in Attribute 2 from Version 2

CHAPTER 4

VERSIONING SPREADSHEETS

Two datasets were initially studied. The "Noble gas isotopes in hydrocarbon gases, oils and related ground waters" database, initially published on June 11, 2013 and then republished a second version on March 8, 2015. The physical structure of the database changed from eight separate Excel spreadsheets to a single sheet. The model does not explicitly account for a change like this except that the identifiers used to refer to the versions or attributes involved may show that the items from version one originate from different files. The original dataset also had 195 columns. However, these were reduced to 54 columns in the second release. In addition, many new locations were surveyed and added to the second release. These are the most challenging

The Paragenetic Mode for Copper Minerals database produced two versions, one at a workshop on June 8, 2016 and another at a following workshop on August 21, 2016. These both take the form of Excel spreadsheets, which has the benefit of having strict row and column numbering. This allows unique identifiers to be used when referring to individual pieces of data and providing a level of abstraction. The structural changes made to the Copper Dataset resemble those found in the Noble Gas Dataset.

4.1 Provenance Analysis

The first approach to determining the provenance distance for the datasets began with the Noble Gas Dataset. The dataset provides a set of references from which the values were extracted and compiled into the dataset. As a result, a simple provenance mapping was constructed, using PROV, from each reference to its corresponding row in the spreadsheet. After this was done for each version of the dataset, we can generate graphs to compare objects from the two versions like the one found in Figure 4.1. We can tell from the labels that different Activities were used to compile the data entry, but the structure of the graph does not provide

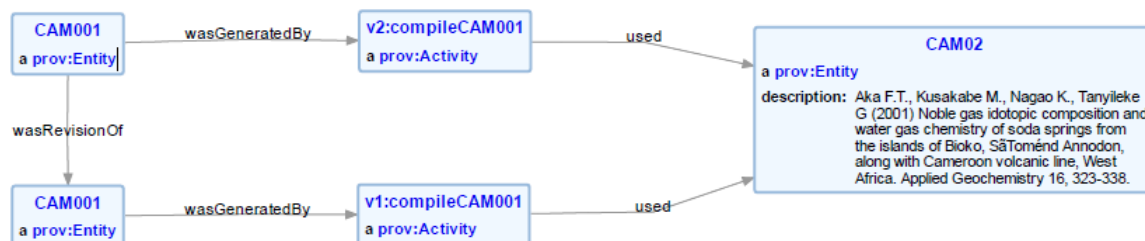


Figure 4.1: Provenance graph for the entry CAM001 entry of the Noble Gas Database. Other than the labels, the structure of each of the data objects is very much the same.

any information as to how extensive this change was for this version. Here we can see how the `wasRevisionOf` relationship would break down in determining the magnitude of change between the two versions. The relationship must, therefore, be expanded in order to provide the desired data necessary to make an evaluation.

4.2 Versioning Comparison

The initial challenge for both of these datasets is producing an appropriate mapping between their previous and latest versions. Through the second compilation process, many columns were removed from the dataset or moved around, and as a result, the identifiers associated with the Attribute in version two did not necessarily correspond to their identifier in version one. The column headings in the Noble Gas Dataset is stored in the spreadsheet as data and makes it difficult for a general system to automate mapping columns between the two versions since any number of rows may contain metadata information. Additionally, while the second release of the Noble Gas Dataset did have a document detailing the organization of the columns contained within the dataset, it did not have any information to map entries from the old dataset to the new dataset. This limits the ability to map and update changes to human actors. Immediately apparent is that any columns that have a mapping from version one to version two means that these columns (Attributes from the model) will only undergo Modification operations since there exists an associated Attribute in both the previous and current version. The conclusion then follows that all remaining Attributes (including both columns and rows)

belonging to version one were Invalidated and those belonging to version two were Added. Using this conclusion, we can pre-calculate the Added and Invalidated Attributes and separate any report into changes grouped by operator.

Once a mapping exists between the two versions, a comparison was performed to determine whether an Attribute of the data object changed. In this case, a simple equality operator was used to determine if anything was modified. In practice, more advanced or complicated methods can be used to determine equality. Since, all Additions and Invalidations have already been predetermined, we can output each Modification as we see them. As is common in versioning, the changes were outputted to a changelog document formatted using HTML. The idea here is that by providing the changelog in HTML, the changes can be made available online and therefore accessible by data consumers. Another benefit of providing a changelog in HTML is that the document can be additionally enriched by RDFa. The changelog document becomes no longer restricted to human consumption, but allows autonomous agents to more intelligently interact with dynamic data systems. The conceptual model detailed in Chapter 3 becomes encoded into the changelog and the graph resulting from the log can be extracted automatically.

The resulting graph provides a structure upon which a flow may be calculated. This becomes an alternative method to determine the provenance distance between two datasets with a much higher fidelity. As mentioned previously, the Change concept is meant to be sub-classed to provide more freedom to represent the particular change bridging the two versions. For example, the He Count entry for the Noble Gas Database changed its units from parts per million to cc STP of given gas specie per cc STP of the total gas. This would be better qualified as a unit change and would be associated with a certain weight in contribution to the total change to the dataset.

CHAPTER 5

DATABASE VERSIONING

The RRUFF Database is "an integrated database of Raman spectra, X-ray diffraction and chemistry data for minerals" (RRUFF homepage). One of the features of RRUFF which is pertinent to this document is that RRUFF provides a web accessible changelog. As rows in specific tables are changed, these changes are reported through the log. The framework for communicating change information resembles the spreadsheet context. However, the main difference is the method to refer to the Attributes as they are mapped across versions. Database tables do not have strict identifiers for rows and columns as spreadsheets do. Row identification relies on indexed keys to uniquely identify entries, but these entries can also be arranged and presented in different orderings depending on the queries used to view the database. From Reference 24, elements within the database do not have to be digitally organized in the same way that it is physically presented.

Databases are also meant to be kept online for extended periods of time. Spreadsheets must be entirely republished in order for a change to the data to be made public. Changes in a database are therefore more sparse in between each version. In order to make changelogs more comprehensive, they can describe changes by day or other increment of time or describe the latest particular subset of time.

Once the changes within the database are encoded into the versioning conceptual model, publishing the changes can follow the methods detailed in Chapter 4

CHAPTER 6

ONTOLOGY VERSIONING

The Global Change Master Directory is a repository to find Earth science data from NASA. They employ a strict set of keywords to tag and label datasets in order to make them more searchable. Version 1.0.0 of GCMD Keywords was published on April 24, 1995, and as of the time of writing, the most recent version of the keywords is 8.4. As can be seen, the naming scheme of the versions changed since the first publication of the keywords. In the initial scheme, each part of the decimal system represented a different level of the GCMD Keyword hierarchy. When a change occurred to a concept in a level of the hierarchy, the associated version number increments.

Since there exists an implementation of the GCMD Keywords in RDF, the URIs can be used as references for the Attributes in the concept model. As mentioned in Reference 8, in order for a data consumer to understand how to use a new version of an ontology, they need not only understand what concepts are new and what concepts are old, but also how to map the old ontology onto the new ontology. The mapping then informs the migration of Keyword labeling of datasets between versions.

CHAPTER 7

CONCLUSION

REFERENCES

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