Toward Reliable Biodi sity Dataset References Michael Elliott¹, Jorrit H. Poelen², José A.B. Fortes¹

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Toward Reliable Biodiversity Dataset References

Abstract

No systematic approach has yet adopted to reliably reference	2
and provide access to our digital biodiversity datasets. Based on	3
accumulated evidence, we argue that location-based identifiers such	4
as URLs are not sufficient to ensure long-term data access. We	!
introduce a method that uses dedicated data observatories to	(
evaluate long-term URL reliability.	7
After taking periodic inventories from March through October	8
2019 of the data served by major biodiversity aggregators, including	9
GBIF, iDigBio, DataONE, and BHL, we found that, for each	10
network, 5% to 43% of registere Ls were intermittently or	11
consistently unresponsive, 0% to 63% produced unstable content,	12
and 13% to 76% became either unresponsive or unstable over the	13
period of observation.	14
We propose the use of crypt grahpic hashing to generate	15
content-based identifiers that can reliably reference datasets. We	10
show that content-based identifiers facilitate decentralized archival	17
and reliable distribution of biodiversity sets. Among other	18
potential benefits, our proposed identifiers enable reliable dataset	19
citations and long-term reproducibility of biodiversity studies.	20
Keywords — Biodiversity, Ecological Informatics, Information	21
Systems, Information Retrieval	22

Introduction 23

Over the course of hundreds of years, naturalists and biologists have systematically collected physical evidence from an ever-changing natural 25 world. Through well-established protocols and institutional support, many of these natural history collections have withstood the ravages of time (Davis and Schmidt 1996, Hortal et al. 2015). Records that describe these carefully collected specimens are now made available digitally through online search indices, registries, and data archives (Page et al. 2015). The 30 increased availability of digital natural history records helps work toward Charles Elton's realization that ecosystems can only be fully understood when we "provide conceptions which can link up into some complete 33 scheme the colossal store of facts about natural history which has 34 accumulated up to date in this rather haphazard manner" (Elton 1927). So far, various initiatives have succeeded to vide comprehensive aggregate views from previously scattered natural history record siloes ((alias?), GBIF 2019, Matsunaga et al. 2013, Michener et al. 2011, 38 Rinaldo and Norton 2009). However, we show that these aggregate views 39 are subject to change as their underlying digital source data changes or 40 becomes inaccessible. Although efforts have been made to keep track of 41 changes in dataset networks, such as using version numbers and last 42 modified dates (Robertson et al. 2014, Wieczorek et al. 2012) and periodic archival (Costello et al. 2013), we not aware of the adoption of any systematic approach to preserve the accessibility as well as longevity of our digital natural history record and derived datasets. We have collected 46 evidence that, despite hundreds of years of experience in preserving our physical natural history records, we are currently faced with a growing 48 body of digital data that changes daily and can disappear with the push of a button.

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Our scholarly record is stitched there by an intricate web of 51 associations between scientific studies and the datasets on which they are 52 based. These associations are made explicit through citations that can be 53 used to reconstruct a study's context and provide the chain of evidence Eprt its claims (Garfield et al. 1964). In the pre-internet era, the lookup of cited references required access to one or more of the many academic libraries in the world. With the rise of internet cessible 57 scientific publications, authors and readers access these references by using a networked device to download content from publication websites. This means that researchers are increasingly citing online works to support their claims. Because the citation format of online works typically documents only when (e.g., 2019-10-01) and where (e.g., https://doi.org/10.123/456) the referenced work was accessed by the author (DataONE 2012, GBIF 63 2019, iDigBio 2016), the reader expects the web-accessed resource to 64 remain accessible and unaltered via this single web location. Readers may 65 attempt to find a version of the works referenced by searching online data networks for the matching author and title, but there is no guarantee that information found this way will be exactly the same as what was originally referenced. Any reference that does not allow readers to find the referenced work fails to satisfy the FAIR principle of findability: "F1. (meta)data are assigned a globally unique and eternally persistent identifi (Wilkinson 71 et al. 2016). Our study is not alone in imiding evidence that suggests 72 that networked, location-based access to digital objects is an unreliable 73 mechanism for providing continued access to the unaltered original work 74

(Klein et al. 2014, Vision 2010). Unless we change the way we preserve and cite our digital scholarly works, our physical records stored in libraries and museums around the world are likely to outlast our digital ones.

Problem Characterization

We show that the current practice of using Uniform Resource Locators (URLs) (Berners-Lee et al. 1994) to reference online biodiversity datasets provides no guarantee of long-term data accessibility. Readers who encounter references that use URLs as dataset identifiers cannot be certain that the referenced dataset will continue to be accessible and in its original form. This uncertainty might be cause for a for researchers because, over time, the integrity of the scholarly record itself is damaged when existing references become unreliable to the loss of access to the data they reference. When data access is lost, documented research results may become impossible to reproduce and the justification for conclusions or hypotheses that

The current practice of relest on URLs to locate and identify referenced data is hazardous due their demonstrated risk of link rot and content drift (Klein et al. 2014). Link rot occurs when a URL, or link, that previously responded to queries can no longer be reached. This can happen, for example, due to temporary outages, URL retirement, or URL migration. A link exhibits content drift when a query to the link provides content that is different from the content it provided in the past. The extent of content drift can vary; content may have received only minor edits with no changes in semantics, or it may reference a different entity altogether. When a single URL is used to locate data that may change

over time, access to any particular version of the data is likely to be 100 ved. We show that, in the event of link rot or content drift, any 101 ng references that on the affected URL may become unreliable. In one study on the $G \sqsubseteq$ ics journal, it was reported that 40% of links (URLs) to supplemental materials became unavailable due to link rot 104 within one year of publication (Vision 2010). Another study (Klein et al. 105 2014) confirmed that as many as one in five articles burnal of Sc 106 Technology, and Medicine p <mark>=de</mark> references that exhibit either link rot 107 and content drift and refer to the existen either as "reference rot". As 108 discussed in the results section of this paper, we have found that the use of URLs to reference biodiversity datasets according to existing biodiversity 110 network citation guidelines (DataONE 2012, GBIF 2019, iDigBio 2016) 111 can lead to unreliable dataset reference result of reference rot. The information systems used by major biodiversity data networks, such as 113 DataONE, GBIF, and iDigBio, rely on data curators and institutional 114 repositories to maintain active dataset URLs, and aggregate the data 115 found at those URLs for distribution in response to user queries. If a data 116 curator modifies, relocates, or stops serving a particular dataset, it may 117 become impossible to retrieve the original dataset and the integrity of the 118 data network will suffer as a result. 119

In this paper, we propose a methodology for measuring the existence of link rot and content drift in online data networks, then provide experimental results that confirm the existence of both link rot and content drift across all of the biodiversity data networks we considered, including BHL, DataONE, iDigBio, and GBIF. Finally, we propose a method for referencing and serving biodiversity data in a way that works

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toward satisfying the Findable, Accessible, Interoperable, and Reusable (FAIR) principles (Wilkinson et al. 2016).

Methodology

Although it has been demonstrated that reference rot does occur when URLs are used for referencing scientific works (Klein et al. 2014, Vision 2010), we are not aware of any prior studies that provide quantitative evidence that reference rot occurs specifically in biodiversity data networks. We set out to quantify the extent of reference rot in biodiversity data networks. Because reference rot occurs in the scope of individual data references, and references to digital datasets rely on URLs to locate the data, we begin by introducing terminology for characterizing the reliability of a URL according to how often it exhibits link rot and content drift.

URL Reliability

We assume that the URLs used to reference biodiversity datasets are expected to resolve to an Internet Protocol (IP) (Postel 1981) address via the Domain Name System (Mockapetris 1987). If a web server is accessible at the resolved IP address, a query (i.e., HTTP get request) to that address over the Hypertext Transfer Protocol (HTTP) will return a response code and, in some cases, associated content (Berners-Lee et al. 2005). We classify the reliability of a URL according to the content, or lack of that it provides over successive queries. If a query to a URL is unsuccessful, we say that link rot has occurred. However, if a successful response is received but the retrieved content is different from the content

retrieved by previous query, we say that content drift has occurred.

Monitoring URLs in this way allows us not only to determine whether link rot and content drift occur, but also to capture their long-term behaviors. For example, one URL that has exhibited link rot might have failed to respond only once, whereas another might have become repetally unresponsive. Likewise, one URL might exhibit content drift less frequently than another whose contents change rapidly. Furthermore, various

combinations of link rot and content drift behavior may indicate that one

URL is more reliable than another, even though both exhibit reference rot. 157

We label URLs with sets of reliability indicators according to their link rot and content drift behaviors. The defined reliability indicators are differentiated by the degree of link rot and content drift observed over a series of queries to the URL at different points in time. We characterize the responsiveness of a URL according to how often it exhibits link rot:

- Unresponsive: the link has failed to respond to one or more queries
- Responsive: the link has responded to all recorded queries

We characterize the stability of a URL according to how often it produces different content from one query to the next:

- Unstable: the content that the link points to sometimes changes
- Stable: the content that the link points to never changes

We characterize the overall reliability of a URL according to both its responsiveness and stability:

• Unreliable: the link does not always provide the expected content; it is either unresponsive, unstable, or both

• Reliable: the link always provides the expected content; it is both responsive and stable

Before we can determine the reliability of any given URL, we must first monitor its behavior over time by documenting how it responds to periodic queries. For the context of biodiversity, we consider the case the content that a URL produces is a dataset.

The Data Collection Process

We suggest that digital dataset collection practices have some analogies to well-established physical specimen collection procedures (see figure 1) (Poelen 2019g). If datasets are considered analogous to specimens, then the URLs that locate datasets are analogous to the physical locations of specimens in the natural world; they are where digital datasets were originally found, but not where they should be preserved. Once found, physical specimens are collected by hand; similarly, digital datasets are downloaded by querying their URLs. Once a specimen is collected and deposited to a safe, accessible repository, a record is kept that documents what the specimen is in addition to when, where, and by whom it was collected.

The same can be done for downloaded datasets. When a dataset is downloaded, a record can be kept that details the URL that was queried, the time of query, and who (e.g., a human or software agent) issued the query that initiated the download event; we refer to this record as the dataset's provenance record (Pasquier et al. 2017). Additionally, the dataset itself should be stored in a safe, accessible dataset archive. The final step in the collection process is to link the actual preserved specimen

to its corresponding record (see figure 1(a)) via an assigned unique identifier.

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The identifiers assigned to datasets (or provenance data) must differ only if their contents differ. This can be achieved by deriving the identifiers from the content of their respective datasets. Furthermore, the identifier must be unique to the dataset; a dataset will always be assigned the same identifier and no two datasets (including different versions of a dataset) can share an identifier. With these restrictions in place, it is possible to reliably link each recorded dataset to its provenance record without the need for an intermediate index. That is, the derivation of the content-based identifier from a given dataset can be performed by anyone, anywhere, and at any time, without the need to consult some central authority (Paskin 1999). Cryptographic hashing is one such method for producing content-based identifiers which are both content-derived and unique. A variety of cryptographic hashing algorithms exist hashing algorithms exist some digital file as input and uniquely engles its contents into a fixed-length series of bits called a "has—We use hashes generated by the SHA-256 algorithm (NIST 2001) as unique content-based identifiers.

Data Collection Over Time

By establishing a dedicated data observatory that implements the collection process we have described, we can build a history for each observed URL to capture its long-ter eliability. Such an observatory periodically queries the URLs listed at network's URL registry and produces for each URL two complementary parts: 1) an archived copy of the response to the corresponding query, whether it was a dataset, an error

code, or no reply at all, and 2) a record of its provenance, including the URL itself, the current date, and a content-based identifier of any dataset received. Successive provenance records can be aggregated to construct comprehensive histories for both datasets (when and where they were found) and URLs (which datasets they located over a series of queries over time).

The constructed URL histories can be analyzed to determine whether a link was ever broken, when it was broken, and whether it became responsive again. The logs also identify the content (or lack of that a URL located each time it was queried. Any change in the content identifier fro uery to the next indicates a change in the content of the dataset. These link breakages and content changes correlate to link rot and content drift, respectively, and allow us to determine the responsiveness, stability, and billity of each URL over time.

Data Network Reliability

Our method for monitoring the behavior of a single URL over time can be applied to observe all URLs registered in a biodiversity data network. We also extend the idea of URL reliability to entire data networks and propose that the overall reliability of a data network can be evaluated by monitoring the lower reliability of each inductional URL in the network experience. Whereaver rigidly label individual URLs with binary indicators of responsiveness, stability, and reliably, we grade data networks according to the percentage of registered URLs that are assigned each of the reliability indicators. For example, if a data network contains three distinct URLs and we find that only two out of the three are reliable, then

we say the data network is 67% reliable.

Experiment

The Preston biodiversity dataset tracker (Jorrit Poelen and Patel 2018) implements mech ms for monitoring data networks as we have described. It allows users to deploy a data network observato y observes the entire set of URLs registered in the network, queries each URL for data, then documents data collection and archives the results. All crawl activities, the queries they issue, and the results they produce are met busly recorded in a string of provenance logs.

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We deployed several Preston observatories periodically queried the registered dataset URLs listed by Biodiversity Heritage Library (BHL), Data Observation Network for Earth (DataONE), Global Biodiversity Information Facility (GBIF), and Integrated Digitized Bio Collections (iDigBio). Each of these networks provides online registries of URLs that locate the data in the network. The registered URLs for DataONE, GBIF, and iDigBio were queried monthly from March 2019 through October 2019. 263 BHL was queried monthly from May 2019 through October 2019. The logs taken by each of these observatories describe the URL queries and their results, which were processed to produce the results that follow. A observatory was constructed by aggregating the queries of the data network observatories.

Results

Breakdowns of the overall reliabilities of the data networks are provided in Leville 1. Results are listed as percentages and total counts of URLs in the data network that were assigned each reliability indicator. When analyzing the recorded results of queries to URLs in each data network over a period of self-months, we found that, for each individual network, 5% to 43% of registered URLs were intermittently or consistently unresponsive, 0% to 63% produced unstable content, and 13% to 76% became either unresponsive or unstable over the peri fobservation.

We found that 30% of URLs observed across the networks became unreliable at some point over the period of March 2019 thr October 2019. Of those unreliable URLs, 48% were unstable, 22% became consistently unresponsive, and 70% were at best only intersection to the next query. For 5% of successful queries, the URL failed to respond to the next query. For 4% of successful queries, the URL provided different content the next time it responded when queried.

The changes in reliability over time for each network are visualized in figure 2. Note that because we have defined reliable URLs to be those considered both responsive and stable, they always represent the smallest fraction of URLs in table 1, figure 2, and figure 3. Figure 3 visualizes the cumulative growth of biodiversity data networks during their periods of observation. This growth is illustrated with two metrics: the total number of unique URLs ever registered in each network and the total number of unique contents that hat downloaded from the network at each sampled to time.

The behaviors of the distributions over time of responsive, stable, and

reliable URLs vary notably between data networks. Reasons for these 295 differences might be inferred when cross-examining table 1 and figures 2 296 and 3. For example, although BHL scored relatively low in responsiveness 297 due to frequent link rot, the content that it does provide is more stable 298 than all other networks because content drift within BHL is relatively rare. 299 Conversely, although iDigBio is relatively responsive, it has low stability 300 because the network's near-constant content growth far outpaces its URL 301 growth. GBIF's behavior was characterized by large sporadic swings; a 302 mass URL migration of over 14,000 Plazi-hosted datasets occurred in May, 303 introducing thousands of new URLs over a short period of time, while over 31,000 URLs (60% of URLs that responded to queries that month) 305 suddenly changed contents in October. Even the most reliable network, DataONE, shows a clear downward trend in all three categories, with 13% of URLs becoming unreliable over a period of just seven months. 308 Additionally, DataONE's growth curves indicate that there are far fewer 309 unique contents than unique URLs; the two possibilities: either 310 much of DataONE's URL population is unresponsive, or DataONE lists 311 multiple URLs for many of its datasets. Because DataONE has been 312 shown to be highly responsive, it could be the case that many distinct 313 URLs refer to the same datasets. It's also worth noting that the June and 314 September spikes in BHL's unresponsiveness were largely due to URLs 315 that failed to respond in those particular months but ad ly did respond to future queries. 317

Sources of Potential Numerical Error

We expect that the URL reliability counts generated for the figures and tables are lower than their actual values. When we qualified URLs as being reliable, responsive, and stable, we could not be certain that links did not briefly become unresponsive or change content during the month-long periods between queries. It is therefore likely that some cases of link rot and content drift were not reflected in the results. Additionally, we only URLs that the data networks list in their dataset registries; this means that, after UR as removed from a network's registry, we not detect subsequent instances of reference rot. Therefore, our results represent a very optimistic upper bound on URL and network reliabilities.

The results for DataONE and GBIF in figure 2 are sometimes skewed due to the pagination method that the networks use to supply users with their dataset registries. Registry pages contained set amounts (e 20) of URLs and registry small slices of the actual data network registry. For registries that use pagination, the observatory would keep querying for registry pages until reaching the page or failing to registry. For instance, GBIF's URL and dataset totals in March 2019 (see figure 3(c)) are low because an early query to a GBIF registry page was not answered and, consequently, the URLs of registry pages that should have followed were not discovered. Similar events happened for both the GBIF and DataONE observatories at later points in time, potentially overestimating the reliability of the data network.

In an effort to minimize artificial link rot due to internet access issues in our local network, we deployed the Preston observatories in a large commercial data center in Germany. Discussion 344

We have shown that the reliability of URLs decreases over time in all of the major biodiversity data networks that we monitored. If current trends continue, the extent of reference rot will worsen. Systematic changes in the way we preserve and reference data are needed to reverse these trends and improve the longevity and long-term integrity of the biodiversity data record. Before we propose such changes, it's necessary to first understand why URLs are proving to be ill-suited for referencing data in the long term.

Unreliability of Location-bed Identifiers

The problems related to using URLs for referencing datasets are largely due to the fact that they are location-based identific—they describe where the data is but not necessarily what it is. Also, by definition, data accessed via URLs must be mediated by a central authority, such as the institutional repositories that serve biodiversity datasets, who can match location-based identifiers with data. Interested users are expected to trust the central authority to guarantee long-term access to the referenced data in its original form.

The use of URLs as identifiers violates the requirements of uniqueness and persistence (Paskin 1999). An identifier must only ever identify one entity (uniqueness) and must persist longer than the entity it identifies (persistence) (Paskin 1999). However, as we have shown in our experiments, many URLs do not possess both uniqueness and persistence; unstable URLs forfeit uniqueness in the event of content drift, while unresponsive URLs do not persist as long as the datasets they identify.

At the core of URL instability is the current practice of using URLs to identify evolving datasets rather than fixed dataset versions. If biodiversity data providers were uniformly committed to allocating one URL per dataset version, then content drift might become less common, improving overall URL stability; however, widespread social adoption of such a commitment from all data providers may be unrealistic. Additionally, such a commitment would not address link rot and URL unresponsiveness. Even if a similar commitment were made by data providers to guarantee the long-term responsiveness of URLs, it could not address the case where a data provider either loses authority over a domain name or migrates to another. For example, our deployed Preston observatories recorded the sudden migration of over 14,000 Plazi datasets from the http://plazi.cs.umb.edu/ domain to http://tb.plazi.org/, an event which invalidated any references to URLs within the first domain.

Paskin proposed that "the best way to 'future proof' an identifier scheme is to forego any intelligence within the identifier itself' (Paskin 1999), where the notion of intelligence refers to the inclusion of meaningful information in the textual representation of the identifier. URLs are typically structured according to the Domain Name System specification (though URLs may include an IP address instead of a domain name) and inherently contain some minimum amount of intelligence: the defin that the URL belongs to (Mockapetris 1987). Thus, it is necessary to look to another identification scheme to allow for proper identification and reliable referencing.

An Alternative: Unique Content-Based Identifiers

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Instead of identifying digital datasets by location (e.g., a URL), we can 394 identify datasets by their content. One way to achieve this is to use 395 algorithmically generated content-based identifiers. A variety of 396 cryptographic hashing algorithms are available tell guarantee a tell 397 unique hash, representable as text, for any given dataset (NIST 2001). 398 Because the hash **f** is deterministically derived from the content it 399 identifies, we say that it is a content-based identifier. Because hashes are 400 deterministic, anyone interested inidentifying a dataset can simply 401 compute its hash without the need for some mediating central authority 402 (Paskin 1999). If a change is made to the dataset, then the hash computed 403 from the modified dataset will be different from that of the original. 404 Therefore, if the hash of a dataset is the same as the referenced hash, it 405 must be the originally referenced dataset (figure 4(c)) (NIST 2001). 406 Because hash iden rs can only identify the exact content that was referenced, content drift is impossible; a content hash will never match 408 with either a different version of the content any other content. 409

The shift from location-based to content-based identifiers decouples future dataset accessibility from the original point of access. As long as there exists some discoverable and accessible data repository that serves the desired content can always be retrieved. Such data repositories can be made discoverable through content hash registries such as hash-archive.org (Trask 2015). In response to a user query for a content hash, these content hash registries would provide a list of locators (e.g., URLs), if any, that direct users to the referenced data (e.g., a registry would provide URLs that retrieve data when queried). Even if one

repository becomes inaccessible due to either a temporary outage or permanent retirement, another may be available to provide the referenced data. When several repositories serve referenced datasets, there is no single point of failure for content hash lookups; if a referenced dataset is redundantly located across and within data repositories, access to the dataset will only be lost if all associated locations exhibit link rot. Even if access to a dataset is lost, it can be restored as long as the referenced dataset still exists somewhere and can be made discoverable and accessible. 426

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It is worth noting that the duplication of content across different information platforms does not lead to ambiguous references, but rather to distributed copies of the same reliably addressed content.

Transitioning to Reliable References

Although we propose a change in the fundamental mechanisms used to reference datasets, existing references can be made reliable with only minor modifications. Consider the following citation generated by GBIF according to their citation guidelines (GBIF 2019):

Levatich T, Padilla F (2017). EOD - eBird Observation 435 Dataset. Cornell Lab of Ornithology. Occurrence dataset https://doi.org/10.15468/aomfnb accessed via GBIF.org on 437 2018-09-02. 438

The citation references the eBird dataset hosted at gbif.org as it was 9, 2018. However, at the time of writing, the URL retrieved on Septem https://doi.org/10.15468/aomfnb redirects to a GBIF internal reference es that the eBird dataset was last updated in March of

2019. The dataset made available through the listed URL is different from what was originally referenced in the citation, but it is impossible to determine the extent of the changes without having access to previous versions of the data.

Fortunately, references like the example above can be made more reliable by augmenting them with a content-based identifier for the dataset. Consider the following enriched citation for the eBird dataset that adds a SHA-256 content hash (NIST 2001):

Levatich T, Padilla F (2017). EOD - eBird Observation

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Dataset. Cornell Lab of Ornithology. Occurrence dataset hash:

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//sha256/29d30b566f924355a383b13cd48c3aa239d42cba0a55f4

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ccfc2930289b88b43c accessed at

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https://doi.org/10.15468/aomfnb via GBIF.org on 2018-09-02.

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The content hash is captured in a content address Uniform Resource Identifier (URI) (Berners-Lee et al. 2005) in the form of hash://algo/hash-string proposed by (Trask 2015), where "algo" is a hashing algorithm (e.g., "sha256") and "hash-string" is the content hash generated by the algorithm in hexadecimal format. In the example above, the hashing algorithm in hexadecimal format. In the example above, the hashing algorithm in SHA256 and the hash string starts with "29dillegenerated content hash was derived from and uniquely identifies the exact version of the eBird dataset that was originally referenced. If an interested user knows of and has access to an information retrieval system that has indexed the dataset, finding the desired dataset is as simple as querying for its content hash. With the addition of a content hash, the URL becomes superfluous and is included merely to demonstrate that the URL and content hash are not mutually exclusive (see figure 4(b)).

Note that different hashing algorithms will generate different content hashes from the same data. We use a URI rather than the content hash itself because it allows us to specify the hashing algorithm used to get ate the hash. If the hashing algorithm is not specified, one might mistakenly conclude that a dataset does not match a reference if the wrong hashing algorithm is used to verify the dataset's authenticity. Our proposal to use Trask's content-addressed URIs to reliably reference data is singlet to, and was inspired by, Kuhn & Dumontier's method to make digital content verifiable and permanent using URIs (Kuhn and Dumontier 2015). We chose to use Trask's content hash URIs because they are location- and content-agnostic and easy to read. However, we recognize that URIs can help facilitate content retrieval and processing using a location-based URI prefix and an (optional) extension suffix respectively.

in digital content. For example, the universal numeric fingerprint (UNF) (Altman and King 2007) resists such changes by first prepsissing the input data before generating a content hash. Among other preprocessing techniques used when generating UNFs, numerical data may be rounded to a certain precision before generating a content hash, with the understanding that a dataset may undergo such format changes when translated, for example, between different computing envirionments or hardware configurations. Indeed, on manual examination of the changes between successive versions of the biodiversity datasets we observed, we found that, in two versions of a dataset (determined to be different because they resulted in different content hashes) differed only in formatting, such as the amount of whitespace and the sequential ordering

of observational records. However, for biodiversity data, we expect that 495 such format-specific content-based identification schemes would only prove 496 detrimental in practice. Standard cryptographic hashing algorithms such 497 as SHA-256 are included in most modern software environments and enjoy widespread use across different digital applications, whereas non-standard 499 algorithms such UNF would first need to be installed and may be 500 unknown to most users, presenting a hurdle to their widespread 501 adoption. Additionally, it may be unrealistic to expect preprocessing 502 efforts to filter out non-informative data effectively enough to be able to 503 trust that semantically identical datasets will always result in the same content-based identifiers. This is especially relevant to biodiversity 505 datasets because they consist mostly of text data (whereas UNFs were 506 designed to hash primarily numerica ta), which may be altered in a 507 infinite number of ways without changing the actual 508

Enhancing Dataset References with Provenance

A dataset reference can be given enhanced context by also referencing the record that describes its provenance. The following citation further augments the eBird dataset reference with the content hash of an associated provenance record:

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Levatich T, Padilla F (2017). EOD - eBird Observation 514

Dataset. Cornell Lab of Ornithology. Occurrence dataset hash: 515

//sha256/29d30b566f924355a383b13cd48c3aa239d42cba0a55f4 516

ccfc2930289b88b43c accessed at 517

https://doi.org/10.15468/aomfnb via GBIF.org on 2018-09-02 518

with provenance hash://sha256/b83cf099449dae3f633af618b19d 519

As was the case for the dataset, the provenance itself can be retrieved by querying an information system that has indexed the hash of the referenced provenance record. Note that the provenance hash is not strictly necessary to make a dataset reference reliable; the dataset hash alone is sufficient. However, explicitly referencing the provenance of the dataset is useful because it allows future readers to retrieve the same context that the original researcher referenced the dataset had access to. More generally, the provenance describes the context of the retrieval of any type of content (e.g., datasets, metadata, citation files, etc.). The types of information in the provenance depend on the implementation of the data observatory, but at a minimum include the URLs that were queried to produce the content, the dates of the queries, the format of the content, and the data registries that were searched to find the content.

The use cases for the uded provenance hash are many. For example, if the provenance record of a dataset is found, it may be possible to traverse the provenance and find newer versions of the dataset. This requires that the various versions of the dataset were observed at spoint in time by a provenance-generating data observatory, properly archived, then made publicly accessible.

A provenance record relates to a dataset the way that a map relates to a location: a provenance record provides a context to understand the origin and relations of a dataset. This provenance context may be limited to a small amount meta-data elements related to a single dataset (e.g., web location, data format, author, license), but can also include a comprehensive description of a biodiversity dataset network that sists

of thousands of datasets and their associations. Also, because provenance records are datasets themselves, they can be reliably referenced and 547 embedded in other provenance records using their content URIs. We used such a composition of content URIs and provenance records as part of our monitoring scheme (Jorrit Poelen and Patel 2018) to track the reliability of URLs in biodiveristy data networks over time (see table 1 and figures 2 and 3). The following citation references the history of the entire DataONE 552 network over the period of observation by one of our Preston observatories:

Poelen JH. 2019d. A bio-554 diversity dataset graph: DataONE. doi:10 1/zenodo.3483218. hash://sha256/87 de 0898919 d2212977 a 586965 e 930 a e 45 b dd 1366073591 c 898 c 208 a 635 e 2814 e 208 e

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Dataset Retrieval Using Hash References

The dataset and provenance hashes referenced in the sample references above were produced by our Preston observatori which were set up to 559 monitor the four data networks. Both the referenced dataset and its 560 provenance are available online at zenodo.org (Poelen 2019c,d,f) and 561 archive.org (Poelen 2019b). A query for the provenance hash in the search bar at zenodo.org or hash-archive.org should direct the user to an archived repository of Preston observations that contains both the dataset and its 564 provenance (see figure 5). Given Zenodo's long-term guarantee for data persistence and version availability (Zenodo 2019), the dataset reference is now reliable; it is effectively immune to both link rot and content drift. Future readers can trust that the dataset will stay available and, when downloaded, identically match the version of the eBird dataset we referenced. Note that, to comply with Zenodo's limitations on user uploads

(Zenodo 2019), we only exposed the set of provenance hashes collected by each deployed Preston observatory for search indexing, which are far fewer in number than the dataset hashes. Thus, a query to zenodo.org for the dataset hash above should not produce any results. This is an artificial limitation; ideally, an information system would index the dataset hashes as well. Note that our Zenodo publication for the GBIF/iDigBio/BioCASe observatory (Poelen 2019f) contains only provenance, although the Internet Archive publication (Poelen 2019b) contains the content as well as provenance. Our Zenodo and Internet Archive publications for BHL (Poelen 2019a,c) and DataONE (Poelen 2019d,e) contain both content and provenance.

Several biodiversity data aggregators, such as GBIF and iDigBio, produce a citation file for each user query to allow researchers to simply reference a single citation file rather than each individual dataset (GBIF 2019, iDigBio 2016). A citation file lists the URLs of the datasets (among other things, such as attributions and retrieval dates) that were retrieved by the issued query. We have demonstrated that dataset URLs are unreliable references; thus, citation files that rely on URLs as references are also unreliable. Citation files could be made reliable if they were augmented with the hashes of the retrieved datasets and, optionally, their provenance records. In fact, citation files themselves can be referenced by hash, along with accompanying provenance hashes, as long as they are archived and made accessible.

DOIs for Datasets and Queries

The DOI Handle System (Paskin 2009) associates DOIs with online resources. However, it does not enforce any constraint pe of resource associated with a DOI. When DOIs are used to reference biodiversity datasets, the associated resources are often URLs, and therefore the use of such DOIs as referencing mechal is is just as potentially unreliable as using URLs. In practice, these DOIs identify the evolving dataset (or set of datasets in the case of a query) rather than a fixed version, as demonstrated in the example references above. It is possible that an author would wish to make such a reference to an evolving online digital object. For example, an author promoting use of a published dataset might want future users to be directed to the most up-to-date content. However, such a fluid reference is not appropriate for making published results reproducible.

The Handle System allows for a complex web of redirection and distributed responsibilities. Just as the Domain Name System resolves domain names in URLs to IP addresses, the DOI Handle System allows DOIs to be resolved to URLs. However, the responsibility for resolving DOIs to URLs is divided between the Handle System and DOI registrars. The Handle System serves as the central authority that maps DOI prefixes to DOI registrars, examples of which include BHL, DataONE, GBIF, and

iDigBio. These registrars are then responsible, and indecentral authorities for, associating DOIs that match their designated prefix with URLs, and are free to change the URL associated with any given DOI under their jurisdiction ([IDF] International DOI Foundation 2018, Paskin 2009).

The ability of biodiversity data networks to change the URL associated with a DOI is good for reference reliability in the sense that networks can account for dataset migration without compromising existing references. However, the use of DOIs addresses neither the instability of the URLs they redirect to nor cases of link rot in which no URLs remain responsive to serve the referenced dataset. Additionally, as the number of datasets identified online continues to grow, proper maintenance of all of the DOIs a data network administrates might become more unsustainable over time, potentially increasing the risk of unreliable URLs going undetected.

In an article proposing HTTP-URI-based stable identifiers (e.g., URLs that are resolvable over HTTP) for biological collection objects, Güntsch et al. admit that the use of DOIs does not solve the problem of unreliable referencing but merely deflects the burden of URL maintenance onto institutional repositories (Güntsch et al. 2017). In contrast, we propose a dataset referencing scheme that is reliable and can be supported by existing infrastructures and workflows. If existing workflows require references to be in the form of DOIs, it could be convenient to embed content hashes into DOIs. Such an approach has already been established for ISBNs through the creation of actionable ISBNs, or ISBN-As (Weissberg 2008), which may serve as a model for actionable content hashes.

What It Means to Preserve Data

Our results indicate that reference rot poses an exitial threat to published biodiversity datasets. We have seen that the use of content-based identifiers can effectively address the issue of reference rot. However, identifiers are of little use in a vacuum. An identifier can only be useful for data retrieval when combined with a resolver to associate identifiers with locations and a database to retrieve the dataset at the associated location (Paskin 1999). Thus, we need to address how resolvers and databases might be organized to accommodate content-based identifiers in order to fully realize long-term data preservation. In this context, we define data preservation as the continued capacity for datasets to be reliably referenced and retrieved in their original form even as the global digital biodiversity network evolves over time.

We propose four requirements that must be met to ensure proper data preservation that prevent data loss: 1) datasets must be addressable and retrievable using content-based rather than location-based identifiers; 2) an agent must exist to collect datasets, record their provenance, and deposit both to a dedicated repository; 3) these repositories should archive data that could be used in the future; and 4) content hash registries should be openly accessible to resolve hash identifiers to dataset locations within such repositories. Although openly accessible registries should make archived data discoverable, access to those data can still be restricted. Additionally, for the purposes of appearance, it is important that the recorded provenance records do not nederally describe the datasets themselves, but rather the activities that led to the procurement of those datasets; the primary purposes of provenance in the context of an archive are to

document the fact that evidence (i.e., an observation of a dataset) does exist and to make it discoverable for interested users (Bearman 1995).

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We have shown that software agents such as Preston can be used to 673 collect datasets and their provenance over time while maintaining 674 content-addressability; all that is needed to ensure proper data preservation 675 are a dedicated repository and an openly accessible content hash registry 676 to map content-based identifiers to datasets located in the repository. In 677 practice, repositories and registries (and potentially software agents such as Preston deployments) can be co-ted; examples include Zenodo and the Internet Archive, although they impose some limitations that may restrict file size, number of files, and the amount of information that can be indexed (Internet Archive 2019, Zenodo 2019). These e ng information systems may serve as models for long-term biodiversity information equirements help to ensure that biodiversity data remain FAIR (Findable, Accessible, Interoperable, and Reusable) (Wilkinson et al. 685 2016). Findability is achieved through the publishing of provenance logs 686 thoroughly describe what datasets are and where they originated 687 from. The amenability of the content-based identification paradigm to the 688 operation of independent decentralized repositories strengthens 689 accessibility by preventing the failure of a single data repository from 690 inhibiting future data access (see figure 4). Content-based identification 691 also contributes to interoperability across data networks due to the 692 absence of any central authority to administrate data access; a content 693 hash computed from a dataset is guaranteed to match the hash computed 694 by any other agent using the same dataset. Furthermore, content-based 695 identifiers can be embedded in or referenced by DOIs to maintain 696 compatibility with systems that use DOIs as identifiers. Finally, and particularly relevant to this paper's purpose, reusability is strengthened by enhancing the retrievability of referenced datasets and allowing users to verify that a retrieved dataset exactly matches that which was referenced.

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Conclusions 701

Although reference rot is resulting in a steady decline in the reliability of our digital biodiversity record, realistic solutions are available to address the root causes of the issue. Content drift can be eliminated altogether by changing the way we reference datasets from using location-based identifiers to ones that are content-based. Meanwhile, the online biodiversity data networks can be made more resilient to link rot if decentralized observation, a val, and distribution techniques are used to capture incremental changes to the data record so that references can remain valid even when online datasets are updated, removed, or relocated. 710 The use of content-based identifiers should be considered by biodiversity data aggregators in order to increase the reliability of references to the data they aggregate.

We have demonstrated that data observatories can be deployed to track the growing digital biodiversity data record. Using the dataset provenance collected over a period of seven months, we were able to quantify the change in reliability over time in terms of link rot and content drift exhibited by the URLs registered in major biodiversity data networks. Even if data networks uniformly adopted content-based identification of datasets and maintained versioned datasets, our method of quantifying link rot and content drift in data networks could be used to monitor whether

either of these issues persist in practice due to implementation flaws or non-inical issues.

Biodiversity data observatories can also be used be to increase the longevity of the biodiversity data record. Such observatories can be used to form reliable dataset references as well as recover datasets that would otherwise become inaccessible due to link rot and content drift.

Additionally, the dataset provenance captured by such observatories serves as evidence of the evolution and distribution of the digital biodiversity data record. The combination of archived datasets and provenance can ensure the long-term reproducibility of scholarly works that reference ever-evolving biodiversity datasets.

Furthermore, the establishment of dedicated data repositories and publicly accessible content hash registries are beneficial for making content-addressed biodiversity data discoverable, distributable, and long-lived, by making the datasets a provenance captured by biodiversity data observatories securely archived and publicly available.

Great care has been taken to establish rigorous preservation guidelines for physical specimens, yet there is much that can be done to increase the longevity of our digital data. Our method is not only suited for tracking datasets in biodiversity data networks, but also provides a resilient and reliable way to publish, reference, and preserve scientific digital datasets without having to abandon our existing infrastructures. The method provides a much-needed foundation for constructing digital provenance graphs from an accessible, verifiable, and citable digital scholarly record.

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Figures

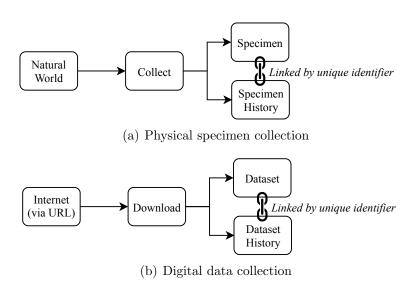


Figure 1. Reliable record keeping for digital datasets (b) can be achieved in an analogous way to current practices in record keeping for physical specimens (a). Biologists collect physical specimens from the natural world, thoroughly document the process, then store the specimens in facilities equipped for long-term preservation. Analogously, digital datasets that are downloaded from the internet can be thoroughly documented and archived in dedicated repositories for long-term preservation. Just as the collection of physical specimens is recorded and identified in specimen history records, the downloading of digital datasets can also be recorded and identified in dataset history records.

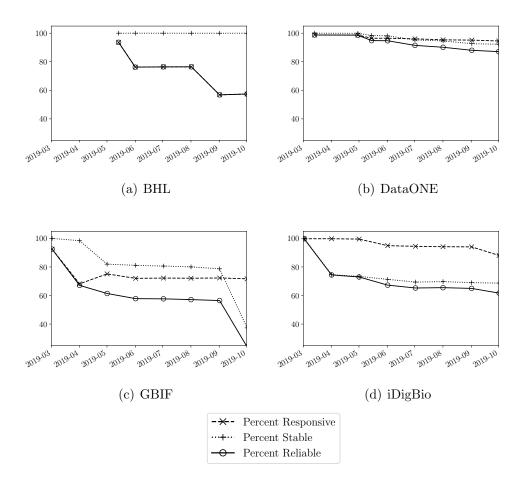


Figure 2. Overall responsiveness, stability, and reliability from March 2019 through October 2019 as percentages of URLs that exhibit each indicator in (a) BHL, (b) DataONE, (c) GBIF, and (d) iDigBio.

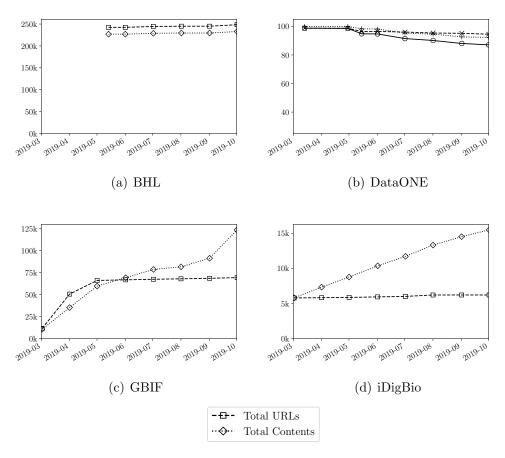


Figure 3. Total number of URLs and unique contents observed from March 2019 through October 2019 in (a) BHL, (b) DataONE, (c) GBIF, and (d) iDigBio.

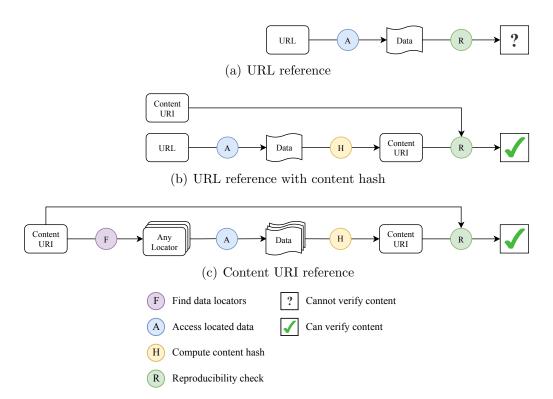


Figure 4. Content resolution and verification for references that use location- versus content-based identifiers. (a) Location-based identifiers (e.g. URLs) cannot verify the authenticity of retrieved content and are vulnerable to link rot due to the use of a fixed locator. (b) If the content hash of the referenced data is known, the authenticity of retrieved data can be verified by comparing the hash of the retrieved data with the provided content hash. However, the fixed locator is still vulnerable to link rot. (c) Content-based identifiers (e.g. Content URIs) can be used to find several locators for the referenced data and contain a content hash to verify the authenticity of retrieved data. The decoupling of the reference from a fixed locator makes the reference resistant to link rot.

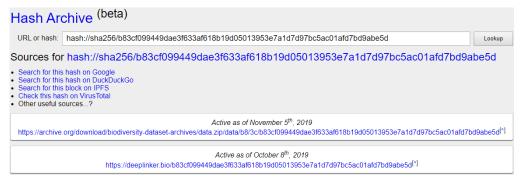


Figure 5. An example of a search index mapping hashes to archives. A search for a content or provenance hash at hash-archive.org will find any associated URLs that have been registered at hash-archive.org.

Tables

Data Network	Responsive URLs	Stable URLs*	Reliable URLs
BHL ^a	57.41% (142,672)	99.97% (232,996)	57.39% (142,633)
$DataONE^{b}$	$94.55\% \ (352,438)$	92.27% (339,109)	87.09% (324,641)
$\mathrm{GBIF^c}$	71.72% (49,707)	37.35% (20,094)	$24.05\% \ (16,669)$
iDigBio ^c	88.04% (5,477)	$68.69\% \ (4,251)$	61.68% (3,837)
All observed URLs**	78.94% (546,645)	90.43% (593,469)	70.07% (485,203)

Table 1. Overall responsiveness, stability, and reliability for URLs observed in each biodiversity data network and for all observed URLs as of October 2019. *URLs that never provided content were omitted from the divisor when calculating Stable URLs percentages. **Because URLs may be registered in more than one data network, the total number of observed URLs is expected to be less than the sum of the URL counts for each network. *Poelen (2019c) *Poelen (2019d) *Poelen (2019f)