dtool Documentation

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18	MIT License	5'

Make your data more resilient, portable and easy to work with by packaging files & metadata into self contained datasets.

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2 Contents

dtool: Manage Scientific Data

Make your data more resilient, portable and easy to work with by packaging files & metadata into self contained datasets.

• Documentation: http://dtool.readthedocs.io

• Paper: https://doi.org/10.7717/peerj.6562

• Free software: MIT License

1.1 Overview

dtool is a suite of software for managing scientific data and making it accessible programatically. It consists of a command line interface dtool and a Python API: dtoolcore.

The dtool command line interface allows one to organise files into datasets and to move datasets between different storage solutions, for example from local disk to remote object storage. Importantly it also provides methods to verify that the transfer has been successful.

The Python API gives complete access to the data and metadata in a dataset. It makes it easy to create scripts for processing the items, or a subset of items, in a dataset. The Python API also allows datasets to be constructed programatically.

dtool is extensible, meaning that it is possible to create plugins both for adding functionality to the command line interface and for creating interfaces to custom storage backends.

The dtool Python package is a meta package that installs the packages:

- dtoolcore core API
- dtool-cli CLI plugin scaffold
- dtool-annotation CLI commands for working with dataset annotations

- dtool-config CLI commands for configuring dtool
- dtool-create CLI commands for creating datasets
- dtool-info CLI commands for getting information about datasets
- dtool-overlay CLI commands for working with per item metadata stored as overlays
- · dtool-symlink storage broker interface allowing symlinking to data
- dtool-http storage broker interface allowing read only access to datasets over HTTP

Installation:

```
$ pip install dtool
```

There are support packages for several object storage solutions:

- dtool-s3 storage broker interface to S3 object storage
- dtool-azure storage broker interface to Azure Storage
- dtool-ecs storage broker interface to ECS S3 object storage
- dtool-irods storage broker interface to iRODS

If you have access to Amazon S3, Microsoft Azure, ECS S3 or iRODS storage you may also want to install support for these:

```
$ pip install dtool-s3 dtool-azure dtool-ecs dtool-irods
```

Usage:

```
$ dtool create my-awesome-dataset
Created proto dataset file:///Users/olssont/my-awesome-dataset
Next steps:
1. Add raw data, eg:
    dtool add item my_file.txt file:///Users/olssont/my-awesome-dataset
    Or use your system commands, e.g:
    mv my_data_directory /Users/olssont/my-awesome-dataset/data/
2. Add descriptive metadata, e.g:
    dtool readme interactive file:///Users/olssont/my-awesome-dataset
3. Convert the proto dataset into a dataset:
    dtool freeze file:///Users/olssont/my-awesome-dataset
```

Installation notes

dtool is a Python package that is pip installable.

Make sure that pip, setputools and wheel are up to date. This is a requirement of one of the dependencies (ruamel.yaml).

```
$ pip install -U pip setuptools wheel
```

dtool can then be installed using pip.

\$ pip install dtool

2.1 Adding support for S3 object storage

Install the dtool-s3 package using pip.

```
$ pip install dtool-s3
```

To configure Amazon S3 credentials see the README file in the dtool-s3 GitHub repository.

2.2 Adding support for Azure storage

Install the dtool-azure package using pip.

```
$ pip install dtool-azure
```

To configure Microsoft Azure credentials see the README file in the dtool-azure GitHub repository.

2.3 Adding support for ECS S3 object storage

Install the dtool-ecs package using pip.

\$ pip install dtool-ecs

To configure ECS S3 object storage credentials see the README file in the dtool-ecs GitHub repository.

2.4 Adding support for iRODS storage

Install the dtool-irods package using pip.

\$ pip install dtool-irods

Warning: In order to be able to use the iRODS backend storage you will need to install the iCommands. Linux packages can be downloaded from irods.org/download. On Mac OSX these can be installed using the brew package manager:

\$ brew install irods

For more details see the dtool-irods GitHub repository.

Philosophy - what is dtool?

3.1 What problem is dtool solving?

Managing data as a collection of individual files is hard. Analysing that data will require that certain sets of files are present, understanding it requires suitable metadata, and copying or moving it while keeping its integrity is difficult.

dtool solves this problem by packaging a collection of files and accompanying metadata into a self contained and unified whole: a dataset.

Having metadata separate from the data, for example in an Excel spread sheet with links to the data files, it becomes difficult to reorganise the data without fear of breaking links between the data and the metadata. By encapsulating both the data files and associated metadata in a dataset one is free to move the dataset around at will. The high level organisation of datasets can therefore evolve over time as data management processes change.

dtool also solves an issue of trust. By including file hashes as metadata it is possible to verify the integrity of a dataset after it has been moved to a new location or when coming back to a dataset after a period of time.

It is possible to discover and access both metadata and data files in a dataset. It is therefore easy to create scripts and pipelines to process the items, or a subset of items, in a dataset.

3.2 What is a "dtool dataset"?

Briefly, a dtool dataset consists of:

- The files added to the dataset, known as the dataset "items"
- Metadata used to describe the dataset as a whole
- Metadata describing the items in the dataset

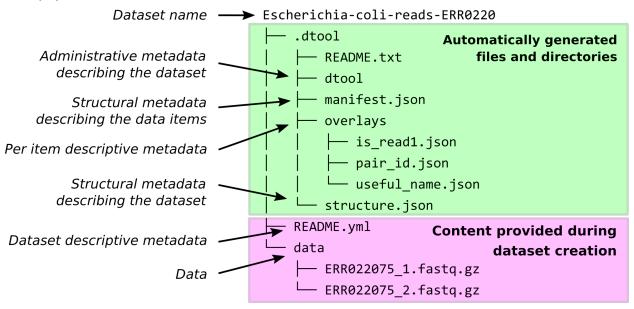
The exact details of how this data and metadata is stored depends on the "backend" (the type of storage used). In other words a dataset is stored differently on local file system disk to how it is stored in Amazon S3 object store. However, the dtool commands and the Python API for interacting with datasets are the same for all backends.

3.3 What does a dtool dataset look like on local disk?

Below is the structure of a fictional dataset containing three items from an RNA sequencing experiment.

The README.yml file is where metadata used to describe the whole dataset is stored. The items of the dataset are stored in the directory named data.

There is also hidden metadata, stored as plain text files, in a directory named .dtool. This should not be edited directly by the user.



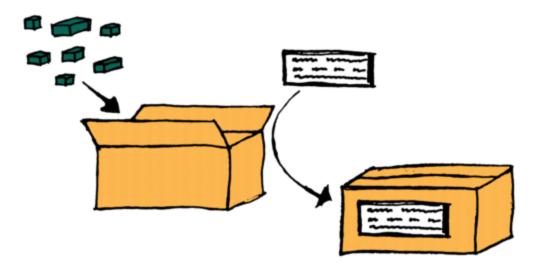
3.4 How does one create a dtool dataset?

This happens in stages:

- 1. One creates a so called "proto dataset"
- 2. One adds data and metadata to this proto dataset
- 3. One converts the proto dataset into a dataset by "freezing" it

Once a proto dataset is "frozen" it is simply referred to as a dataset and it is no longer possible to modify the data in it. In other words it is not possible to add or remove items from a dataset or to alter any of the items in a dataset.

The process can be likened to creating an open box (the proto dataset), putting items (data) into it, sticking a label (metadata) on it, and closing the box (freezing the dataset).



3.5 Give me more details!

An in depth discussion of dtool can be found in the paper Lightweight data management with dtool.

Quick start guide

This quick start guide shows how the dtool command line tool can be used to accomplish some common data management tasks.

4.1 Organising files into a dataset on local disk

In this scenario one simply wants to organise one or more files into a dataset in the file system on the local computer.

When working on local disk a dataset is simply a standardised directory layout combined with some hidden files used to annotate the dataset and its items.

The first step is to create a "proto" dataset. The command below creates a dataset named fishers-iris-data in the current working directory.

```
$ dtool create fishers-iris-data
```

One can now add files to the dataset by moving/copying them to the fisher-iris-data/data directory, or by using the built in dtool add item command. In the example below the file iris.csv is added to the proto dataset.

```
$ touch iris.csv
$ dtool add item iris.csv fishers-iris-data
```

Metadata describing the data is as important as the data itself. Metadata describing the dataset is stored in the file fisers-iris-data/README.yml. An easy way to add content to this file is to use the dtool readme interactive, which will prompt for input regarding the dataset.

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```
name [Your Name]: Tjelvar Olsson
email [olssont@nbi.ac.uk]:
username [olssont]:
creation_date [2017-10-06]:
Updated readme
To edit the readme using your default editor:
dtool readme edit fiser-iris-data
```

Finally, to convert the proto dataset into a dataset one uses the dtool freeze command.

```
$ dtool freeze fishers-iris-data

Generating manifest [######################### 100% iris.csv

Dataset frozen fiser-iris-data
```

4.2 Copying data from an external hard drive to remote storage as a dataset

Genome sequencing generates large volumes of data, which are often sent from the sequencing company to the user by posting an external hard drive. When backing up such data on a remote storage system one does not want to have to reorganise the data before copying it to the remote storage system.

In this case one can create a "symlink" dataset and copy that to the remote storage. A symlink dataset is a dataset where the data directory is a symlink to another location, for example the data directory on the external hard drive.

```
$ dtool create bgi-sequencing-12345 --symlink-path /mnt/external-hard-drive
```

Again, adding metadata to the dataset is vital.

```
$ dtool readme interactive bgi-sequencing-12345
```

One can then convert the proto dataset into a dataset by "freezing" it.

```
$ dtool freeze bgi-sequencing-12345
```

It is now time to copy the dataset to the remote storage. The command below assumes that one has credentials setup to write to the Amazon S3 bucket dtool-demo. The command copies the local dataset to the S3 dtool-demo bucket.

```
$ dtool cp bgi-sequencing-12345 s3://dtool-demo/
```

The command above returns feedback on the URI used to identify the dataset in the remote storage. In this case s3://dtool-demo/1e47c076-2eb0-43b2-b219-fc7d419f1f16.

The URI used to identify the dataset uses the UUID of the dataset rather than the dataset's name. This is to avoid name clashes in the object storage.

Finally, one may want to confirm that the data transfer was successful. This can be achieved using the dtool diff command, which should show no differences if the transfer was successful.

```
\$\  \, dtool\  \, diff\  \, bgi-sequencing-12345\  \, s3://dtool-demo/le47c076-2eb0-43b2-b219-fc7d419f1f16
```

By default only identifiers and file sizes are compared. To check file hashes make use of the --full option.

Warning: When comparing datasets identifiers, sizes and hashes are compared. When checking that the hashes are identical the hashes for the first dataset are recalculated using the hashing algorithm of the reference dataset (the second). If the dataset in S3 had been specified as the first argument then all the files would have had to have been downloaded to the local disk before calculating their hashes, which would have made the command slower.

4.3 Copying a dataset from remote storage to local disk

After having copied a dataset to a remote storage system one may have deleted the copy on the local disk. In this case one may want to be able to get the dataset back onto the local disk.

This can be achieved using the dtool op command. The command below copies the dataset in iRODS to the current working directory.

```
$ dtool cp s3://dtool-demo/1e47c076-2eb0-43b2-b219-fc7d419f1f16 ./
```

Note that on the local disk the dataset will use the name of the dataset rather than the UUID, in this example bgi-sequencing-12345.

Again one can verify the data transfer using the dtool diff command.

\$ dtool diff bgi-sequencing-12345 s3://dtool-demo/1e47c076-2eb0-43b2-b219-fc7d419f1f16

Working with datasets

5.1 Listing datasets

It is possible to list all datasets in a directory or in a S3 bucket using the dtool 1s command.

```
$ dtool ls ~/my_datasets
bgi-sequencing-12345
  file:///Users/olssont/my_datasets/bgi-sequencing-12345
drone-images
  file:///Users/olssont/my_datasets/drone-images
fishers-iris-data
  file:///Users/olssont/my_datasets/fishers-iris-data
my_rnaseq_data
  file:///Users/olssont/my_datasets/my_rnaseq_data
```

Tip: When using this command proto datasets are highlighted in red.

Tip: The dtool ls command takes a URI. As such it can be used to list the datasets in remote storage locations. The example below lists all the datasets in the S3 bucket named dtool-demo:

```
$ dtool ls s3://dtool-demo/
```

5.2 Generating an inventory of datasets

It is possible to generate CSV/TSV/HTML inventories of datasets in a directory or in another base URI such as an Amazon S3 bucket. For example, the command below is used to generate a HTML report of all the datasets in the s3://dtool-demo/ bucket.

```
$ dtool inventory --format html s3://dtool-demo/ > inventory.html
```

5.3 Verifying a dataset has not been modified since freezing it

A dtool dataset has metadata listing its items and their hashes. This information can be used to verify that a dataset is in the same state as it was when it was frozen.

In the example below the dataset has been corrupted in three ways.

- 1. The file rna_seq_reads_4.fq.gz has been added to it
- 2. The file rna_seq_reads_3.fq.gz has been deleted from it
- 3. The content of the file rna_seq_reads_1.fq.gz has been modified

```
$ dtool verify ~/my_datasets/my_rnaseq_data
Unknown item: 49919bdae83011b96bf54d984735e24c4419feb5 rna_seq_reads_4.fq.gz
Missing item: 72b24007759c0086a316d13838021c2571853a16 rna_seq_reads_3.fq.gz
```

By default only identifiers and file sizes are compared. To check file hashes make use of the --full option.

```
$ dtool verify --full ~/my_datasets/my_rnaseq_data
Unknown item: 49919bdae83011b96bf54d984735e24c4419feb5 rna_seq_reads_4.fq.gz
Missing item: 72b24007759c0086a316d13838021c2571853a16 rna_seq_reads_3.fq.gz
Altered item: d4e065787eab480e9cbd2bac6988bc7717464c83 rna_seq_reads_1.fq.gz
```

5.4 Displaying the README descriptive metadata

To display the README metadata used to describe the dataset one can make use of the dtool readme show command.

```
$ dtool readme show ~/my_datasets/chrX-rna-seq
---
description: RNA-seq sample data
creation_date: 2017-11-20
ftp: "ftp://ftp.ccb.jhu.edu/pub/RNAseq_protocol/"
doi: "10.1038/nprot.2016.095"
```

5.5 Reporting summary information about a dataset

One often wants to find out how many items are in a dataset and what their total size is. This can be achieved using the dtool summary command.

```
$ dtool summary ~/my_datasets/drone-images
name: drone-images
uuid: c2542c2b-d149-4f73-84bc-741bf9af918f
creator_username: hartleym
number_of_items: 59
size: 152.5MiB
frozen_at: 2017-09-19
```

5.6 Listing the item identifiers in a dataset

To list all the item identifiers in a dataset one can use the dtool identifiers command.

```
$ dtool identifiers ~/my_datasets/my_rnaseq_data
b0f92a668d24a3015692b0869e2b7590a62a380c
72b24007759c0086a316d13838021c2571853a16
d4e065787eab480e9cbd2bac6988bc7717464c83
```

Tip: Using dtool ls on a dataset URI results in a list of item identifiers and relapths:

```
$ dtool ls ~/my_datasets/my_rnaseq_data
b0f92a668d24a3015692b0869e2b7590a62a380c - rna_seq_reads_2.fq.gz
72b24007759c0086a316d13838021c2571853a16 - rna_seq_reads_3.fq.gz
d4e065787eab480e9cbd2bac6988bc7717464c83 - rna_seq_reads_1.fq.gz
```

5.7 Finding out the size of an item in a dataset

To find the size of a specific item in a dataset one can use the dtool item properties command. The command below accesses the properties of the item with the identifier 58f50508c42a56919376132e36b693e9815dbd0c.

5.8 Accessing the content of an item in a dataset

When all files are on local disk getting access to them is trivial. However, when files are located in some object storage system in the cloud, access may be less trivial.

dtool solves this problem by providing a call to a method that returns an absolute path on local disk with a promise that the file requested will be available from there when the call returns the path.

The dtool command line interface makes this call available as the command dtool item fetch.

Below is an example of this command being used on a local disk file storage.

```
$ dtool item fetch ~/my_datasets/drone-images 58f50508c42a56919376132e36b693e9815dbd0c
/Users/olssont/my_datasets/drone-images/data/IMG_8585.JPG
```

Below is an example of this command being used on a dataset in the S3 bucket dtool-demo.

```
$ dtool item fetch s3://dtool-demo/le47c076-2eb0-43b2-b219-fc7d419f1f16_

$ 3dce23b901709a24cfbb974b70clef132af10a67

/Users/olssont/.cache/dtool/s3/le47c076-2eb0-43b2-b219-fc7d419f1f16/

$ 3dce23b901709a24cfbb974b70clef132af10a67.txt (continues on next page)
```

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5.9 Processing all the items in a dataset

By combining the use of dtool identifiers and dtool item fetch it is possible to create basic Bash scripts to process all the items in a dataset.

```
$ DS_URI=~/my_datasets/my_rnaseq_data
$ for ITEM_ID in `dtool identifiers $DS_URI`;
> do ITEM_FPATH=`dtool item fetch $DS_URI $ITEM_ID`;
> echo $ITEM_FPATH;
> done
/Users/olssont/my_datasets/my_rnaseq_data/data/rna_seq_reads_2.fq.gz
/Users/olssont/my_datasets/my_rnaseq_data/data/rna_seq_reads_3.fq.gz
/Users/olssont/my_datasets/my_rnaseq_data/data/rna_seq_reads_1.fq.gz
```

Tagging datasets

It is possible to tag datasets with labels.

To tag a dataset with the label "rnaseq" one would use the command below:

```
$ dtool tag set <DS_URI> rnaseq
```

It is possible to add more than one tag to a dataset. The command below adds the tag "A.thaliana":

```
$ dtool tag set <DS_URI> A.thaliana
```

To list tags one would use the command below:

\$ dtool tag ls <DS_URI>

This would produce the output:

A.thalina rnaseq

It is possible to delete a tag that has been added to a dataset:

```
$ dtool tag delete <DS_URI> A.thaliana
```

Annotating datasets

It is possible to annotate a dataset with so called key/value pairs. Such key/value annotations are intended to make it easy to add and access specific metadata at a per dataset level.

The difference between annotations and the descriptive metadata is that the former is easier to work with in a programmatic fashion. The descriptive metadata, stored in the dataset's README content, is more free form. It is non-trivial to access specific pieces of information from the descriptive metadata in the dataset's README content, whereas a dtool annotation can be easily accessed by its name (key).

To create an annotation using the dtool CLI one would use the dtool annotation set command. For example to annotate a dataset with a "project" one would use the command:

```
$ dtool annotation set <DS_URI> project world-peace
```

To access the "project" annotation one would use the dtool annotation get command:

```
$ dtool annotation get <DS_URI> project world-peace
```

Annotations set using dtool annotation set are strings by default. It is possible to set the type to int, float, and bool using the —type option. For example to annotate a dataset with a "stars" rating one could use the command:

```
$ dtool annotation set --type int <DS_URI> stars 3
```

For more complex data structures one can set the type to json. For example:

```
$ dtool annotation set --type json <DS_URI> params '{"x": 3.4, "y": 5.6}'
```

It is possible to list all the annotations of a dataset:

```
$ dtool annotation ls
params {"x": 3.4, "y": 5.6}
project world-peace
stars 3
```

To update an annotation one can use the <code>dtool</code> annotation set command again. For example to show that a dataset is really fantastic one could increase its star rating to 5:

```
$ dtool annotation set <DS_URI> stars 5 --type int
$ dtool annotation get <DS_URI> stars
5
```

Warning: There are restrictions on the characters and the length of the keys. They have to match the regular expression [a-zA-Z.-]* and it must be 80 characters or less.

Working with overlays

Overlays provide a means to store and access per item metadata.

8.1 Display table with all per item metadata

It is possible to display all the per item metadata as a CSV table using the command dtool overlays show.

The dataset above has three overlays named: pair_id, is_read1, and useful_name. The columns named identifiers and relpaths are reported for bookkeeping purposes.

8.2 Accessing an overlay value of a specific dataset item

It is possible to get access to the value stored in an overlay for a specific item using the command dtool item overlay.

```
$ dtool item overlay \
   is_read1 \
   http://bit.ly/Ecoli-reads-minified \
   9760280dc6313d3bb598fa03c5931a7f037d7ffc
True
```

8.3 Creating overlays

Overlay creation happens in two steps.

- 1. Create a template overlay CSV file using the format above
- 2. Use the template to write all overlays in the template to the dataset

8.3.1 Creating overlay templates

A starting template can be created using the dtool overlays show command. For a dataset with no overlays this will result in a table with the columns identifiers and relpaths. The table will have one row for each item in the dataset. One can then add columns for the overlays one would wish to create.

However, in many cases one would want to use metadata in the items' relapths to generate a starting CSV template. This can be achieved using the commands:

```
• dtool overlays template parse
```

- dtool overlays template glob
- dtool overlays template pairs

Consider for example the dataset below:

```
$ dtool ls http://bit.ly/Ecoli-reads-minified
8bda245a8cd526673aab775f90206c8b67d196af ERR022075_2.fastq.gz
9760280dc6313d3bb598fa03c5931a7f037d7ffc ERR022075_1.fastq.gz
```

The command below could be used to generate a template for the overlays "useful_name" and "read":

```
$ dtool overlays template parse \
  http://bit.ly/Ecoli-reads-minified \
  '{useful_name}_{read:d}.fastq.gz'
```

Results in the CSV output below:

```
identifiers, read, useful_name, relpaths
8bda245a8cd526673aab775f90206c8b67d196af, 2, ERR022075, ERR022075_2.fastq.gz
9760280dc6313d3bb598fa03c5931a7f037d7ffc, 1, ERR022075, ERR022075_1.fastq.gz
```

To ignore a variable element when parsing one can use unnamed curly braces. The command below for example only generates the overlay "useful_name":

```
$ dtool overlays template parse \
    http://bit.ly/Ecoli-reads-minified \
    '{useful_name}_{:d}.fastq.gz'
identifiers,useful_name,relpaths
8bda245a8cd526673aab775f90206c8b67d196af,ERR022075,ERR022075_2.fastq.gz
9760280dc6313d3bb598fa03c5931a7f037d7ffc,ERR022075,ERR022075_1.fastq.gz
```

Sometimes one simply wants to create a boolean overlay based on weather or not a particular file matches a glob pattern. The command below can be used to create a CSV template for an overlay named is_read1:

```
$ dtool overlays template glob \
  http://bit.ly/Ecoli-reads-minified \
  is_read1 \
  '*1.fastq.gz'
```

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```
identifiers, is_read1, relpaths
8bda245a8cd526673aab775f90206c8b67d196af, False, ERR022075_2.fastq.gz
9760280dc6313d3bb598fa03c5931a7f037d7ffc, True, ERR022075_1.fastq.gz
```

Sometimes it is useful to be able to find pairs of items. For example when dealing with genomic sequencing data that has forward and reverse reads.

One can create a "pair_id" overlay CSV template for this dataset using the command below:

```
$ dtool overlays template pairs http://bit.ly/Ecoli-reads-minified .fastq.gz identifiers,pair_id,relpaths 8bda245a8cd526673aab775f90206c8b67d196af,9760280dc6313d3bb598fa03c5931a7f037d7ffc, 

ERR022075_2.fastq.gz 9760280dc6313d3bb598fa03c5931a7f037d7ffc,8bda245a8cd526673aab775f90206c8b67d196af, 

ERR022075_1.fastq.gz
```

In the above the suffix ".fastq.gz" is used to extract the prefix ERR022075_ that is used to find matching pairs.

8.3.2 Writing an overlay template to a dataset

Once one has a overlay template CSV file one can write this to a dataset:

```
$ dtool overlays write <DS_URI> overlays.csv
```

8.4 Further reading

For more information see the at https://github.com/jic-dtool/dtool-overlay

Configuring user name and email

When running the dtool interactive readme the default name and email address are Your Name and you@example.com.

```
$ dtool readme interactive my_dataset
description [Dataset description]:
project [Project name]:
confidential [False]:
personally_identifiable_information [False]:
name [Your Name]:
email [you@example.com]:
username [olssont]:
creation_date [2017-12-14]:
```

These defaults can be configuring the user name and email address.

```
$ dtool config user name "Care A. Bout-Data"
Care A. Bout-Data
$ dtool config user email researcher@famous.uni.ac.uk
researcher@famous.uni.ac.uk
```

Rerunning the previous dtool readme interactive command now gives updated defaults when prompting for input.

```
$ dtool readme interactive my_dataset
description [Dataset description]:
project [Project name]:
confidential [False]:
personally_identifiable_information [False]:
name [Care A. Bout-Data]:
email [researcher@famous.uni.ac.uk]:
username [olssont]:
creation_date [2017-12-14]:
```

Configuring the dtool cache directory

When fetching a dataset item from a dataset stored in object storage the file get stored in a cache directory. The default cache directory is:

```
~/.cache/dtool
```

You may want to configure this cache to be in a different location. This can be achieved using the dtool config cache command:

```
$ mkdir /tmp/dtool
$ dtool config cache /tmp/dtool
```

It is also possible to override both the default and the configured cache directory by exporting the environment variable DTOOL_CACHE_DIRECTORY. This can be useful when using local SSD on a compute cluster:

```
$ mkdir /local/ssd/dtool
$ export DTOOL_CACHE_DIRECTORY=/local/ssd/dtool
```

Warning: There is no automatic mechanism built into dtool to clear up the cache. It can therefore grow very large if you are working with lots of datasets in object storage.

Configuring a custom README template

When running the dtool interactive readme command one is prompted to enter the default descriptive metadata shown below.

```
$ dtool readme interactive my_dataset
description [Dataset description]:
project [Project name]:
confidential [False]:
personally_identifiable_information [False]:
name [Your Name]:
email [you@example.com]:
username [olssont]:
creation_date [2017-12-14]:
```

It is possible to configure the required metadata prompted for by the dtool readme interactive command. This requires the creation of a README file making use of the YAML file format.

The default template is shown below.

```
description: Dataset description
project: Project name
confidential: False
personally_identifiable_information: False
owners:
    - name: {DTOOL_USER_FULL_NAME}
        email: {DTOOL_USER_EMAIL}
        username: {username}
creation_date: {date}
# links:
# - http://doi.dx.org/your_doi
# - http://github.com/your_code_repository
# budget_codes:
# - E.g. CCBS1H10S
```

To create a custom template that also prompted for a species definition one could create the file \sim /custom_dtool_readme.yml with the content below.

```
description: Dataset description
project: Project name
species: A. thaliana
confidential: False
personally_identifiable_information: False
owners:
   - name: {DTOOL_USER_FULL_NAME}
   email: {DTOOL_USER_EMAIL}
   username: {username}
creation_date: {date}
```

To configure the dtool to make use of this template one can use the dtool config readme-template command:

```
$ dtool config readme-template ~/custom_dtool_readme.yml
```

The dtool config readme-template command sets the DTOOL_README_TEMPLATE_FPATH key in the ~/.config/dtool/dtool.json file. Alternatively one can make use of the DTOOL_README_TEMPLATE_FPATH environment variable:

```
$ export DTOOL_README_TEMPLATE_FPATH=~/custom_dtool_readme.yml
```

Re-running the previous dtool readme interacitve command now includes a prompt for the species and the default value A. thaliana:

```
$ dtool readme interactive my_dataset
description [Dataset description]:
project [Project name]:
species [A. thaliana]:
confidential [False]:
personally_identifiable_information [False]:
name [Your Name]:
email [you@example.com]:
username [olssont]:
creation_date [2017-12-14]:
```

Configuring storage brokers

Some remote storage brokers require extra configuration to enable authentication.

The command below configures access to a Azure storage container named $\verb"jicinformatics":$

```
\ dtool config azure set jicinformatics the-secret-token the-secret-token
```

For information on other storage brokers have a look at their documentation and/or use dtool config --help to get more information.

Publishing a dataset

It is possible to publish a datasets hosted in AWS S3 and Microsoft Azure Storage. A dataset is published by making it accessible via the HTTP(S) protocol.

Warning: A published dataset is accessible by anyone in the world with an internet connection!

```
$ dtool publish s3://dtool-demo/ba92a5fa-d3b4-4f10-bcb9-947f62e652db Dataset accessible at https://dtool-demo.s3.amazonaws.com/ba92a5fa-d3b4-4f10-bcb9-\Rightarrow947f62e652db
```

The URL retuned by the dtool publish command can be used to interact with the dataset.

```
$ dtool summary https://dtool-demo.s3.amazonaws.com/ba92a5fa-d3b4-4f10-bcb9-

$ 947f62e652db
name: hypocoty13
uuid: ba92a5fa-d3b4-4f10-bcb9-947f62e652db
creator_username: olssont
number_of_items: 339
size: 86.7MiB
frozen_at: 2018-09-12
```

Python API

The dtool command line tool is built using the Python API in dtoolcore. This API can also be used to create and interact with datasets directly.

Below is an example showing how to load a dataset from a URI and use it to print out a list of all the data item identifiers in the dataset.

```
>>> from dtoolcore import DataSet
>>> dataset = DataSet.from_uri("bgi-sequencing-12345")
>>> for i in dataset.identifiers:
... print(i)
...
1c10766c4a29536bc648260f456202091e2f57b4
fbcc24bed36128535a263b74b2e138d7cc43e90c
9ca330a84f3dbbdd457a860b5e3c21c917743dd6
3dce23b901709a24cfbb974b70c1ef132af10a67
78e7f1507da598e9f6a02810c1f846cfc24fb8ad
42f43f49b74ef7f901010965aae71170c9fd3ef6
ab069337b0f86cdad899d57e8de63d5b2b680c85
b55ae3fbe6081eb2ed4ed2c4ea316dbeb943ea2c
```

More information on how to make use of the Python API can be found in the dtoolcore documentation.

Creating plugins

It is possible to create plugins to the <code>dtool</code> command line tool. There are two different types of plugins: command line tools and backend storage brokers. The former allows a developer to add custom extensions to the <code>dtool</code> command. The latter allows a developer to create an interface for talking to a new type of storage. One could for example create a storage broker to interface with Amazon S3 object storage.

15.1 Extending the dtool command line tool

Information on how to extend the dtool command line tool is available in the README file of dtool-cli.

Concrete examples making use of this plugin system are:

- · dtool-create
- · dtool-info

15.2 Creating an interface to a new type of storage

Below are the steps required to create a storage broker for allowing dtool to interact with a new backend. A concrete example making use of this plugin system is dtool-irods.

- 1. Examine the code in dtoolcore.storagebroker.DiskStorageBroker.
- 2. Create a Python class for your storage, e.g. MyStorageBroker
- 3. Add a MyStorageBroker.key` attribute to the class, this key is used to lookup an appropriate storage broker when interacting with a dataset
- 4. Add a dtoolcore.FileHasher instance that matches the hashing algorithm used by your storage to your MyStorageBroker.hasher attribute
- 5. Add implementations for all the public functions in dtoolcore.storagebroker. DiskStorageBroker class to MyStorageBroker

6. Expose the MyStorageBroker class as a dtool.storage_broker entrypoint, e.g. add a section along the lines of the below to the setup.py file:

```
entry_points={
    "dtool.storage_brokers": [
         "MyStorageBroker=my_dtool_storage_plugin:MyStorageBroker",
    ],
},
```

Citing dtool

Olsson TSG, Hartley M. 2019. Lightweight data management with dtool. Peer J 7:e6562 https://doi.org/10.7717/peerj. 6562

CHANGELOG

This project uses semantic versioning. This change log uses principles from keep a changelog.

17.1 [Unreleased]

- 17.1.1 Added
- 17.1.2 Changed
- 17.1.3 Deprecated
- **17.1.4 Removed**
- 17.1.5 Fixed
- 17.1.6 Security
- 17.2 [3.25.0] 2020-03-25

Added support for tags from the dtool CLI.

17.2.1 Added

- The CLI command 'dtool tag set'
- The CLI command 'dtool tag Is'
- The CLI command 'dtool tag delete'

17.3 [3.24.0] - 2020-03-23

Added Python API support for tags.

17.3.1 Added

- Added dtoolcore. BaseDataSet.put tag() method
- Added dtoolcore._BaseDataSet.delete_tag() method
- Added dtoolcore. BaseDataSet.list tags() method
- Added dtoolcore.storagebroker.BaseStorageBroker.delete_key() method
- Added dtoolcore.storagebroker.BaseStorageBroker.get_tag_key() method
- Added dtoolcore.storagebroker.BaseStorageBroker.list_tags() method
- Added dtoolcore.storagebroker.BaseStorageBroker.put_tag() method
- Added dtoolcore.storagebroker.BaseStorageBroker.delete_tag() method
- Added dtoolcore.storagebroker.DiskStorageBroker.delete_key() method
- $\bullet \ Added \ {\tt dtoolcore.storagebroker.DiskStorageBroker.get_tag_key()} \ \ {\tt method} \\$
- Added dtoolcore.storagebroker.DiskStorageBroker.list_tags() method
- Default cache directory changed from ~/.cache/dtool/http to ~/.cache/dtool

17.3.2 Fixed

 Cache environment variable changed from DTOOL_HTTP_CACHE_DIRECTORY to DTOOL_CACHE_DIRECTORY

17.4 [3.23.0] - 2020-02-28

17.4.1 Added

- Add dtool readme validate command
- Ability to update descriptive metadata in README of frozen datasets when using dtool redme write

17.4.2 Fixed

• Fixed several defects in how URIs were parsed and generated on Windows.

17.5 [3.22.0] - 2020-02-06

Improved Python API for creating datasets.

17.5.1 Added

- dtoolcore.create_proto_dataset() helper function
- dtoolcore.create_derived_proto_dataset() helper function
- dtoolcore.DataSetCreator helper context manager class
- dtoolcore.DerivedDataSetCreator helper context manager class

17.5.2 Fixed

• Fixed defect where using DTOOL_NUM_PROCESSES > 1 resulted in a cPickle.PicklingError on some storage brokers. Multiprocessing is now only used if the storage broker supports it.

17.6 [3.21.1] - 2020-01-23

• Fixed defect where 'dtool verify' calculated hashes even when the '-f/-full' option was not specified. The 'dtool verify' command now runs more quickly.

17.7 [3.21.0] - 2020-01-21

17.7.1 Added

• Ability to use multiple processes (cores) to generate item properties for manifest files in parallel. Set the environment variable DTOOL_NUM_PROCESSES to specify the number of processes to use.

17.7.2 Fixed

• Included .dtool/annotations directory in DiskStorageBroker self description file

17.8 [3.20.0] - 2019-10-31

New feature: Dataset annotation

Dataset annotations are intended to make it easy to add and access specific metadata at a per dataset level.

The difference between annotations and the descriptive metadata is that the former is easier to work with in a programmatic fashion. The descriptive metadata, stored in the dataset's README content, is more free form. It is non-trivial to access specific pieces of information from the descriptive metadata in the dataset's README content, whereas a dtool annotation can be easily accessed by its name.

17.8.1 Added

- Added dtool annotation set command
- Added dtool annotation get command
- Added dtool annotation ls command

17.9 [3.19.0] - 2019-09-12

17.9.1 Added

• Added sorting of items by relpath to 'dtool ls <DS_URI>'

17.9.2 Fixed

- Fixed formatting of 'dtool ls <DS_URI>' from using two whitespaces to using one tab to make it easier to work with command line tools such as cut
- Fixed ordering of lines in overlay CSV template from being sorted by the identifier to being ordered by the relpath

17.10 [3.18.0] - 2019-09-06

17.10.1 Added

- · Added 'dtool overlays show' command
- · Added 'dtool overlays write' command
- · Added 'dtool overlays template parse' command
- · Added 'dtool overlays template glob' command
- · Added 'dtool overlays template pairs' command

17.10.2 Deprecated

- · Deprecated 'dtool overlay ls'
- Deprecated 'dtool overlay show'

17.11 [3.17.0] - 2019-08-06

17.11.1 Added

- Added support for host name in file URI.
- Added dtool status command for working out if a dataset is frozen or not
- Added dtool uri command for expanding absolute and relative paths into proper URIs

17.12 [3.16.0] - 2019-07-12

17.12.1 Added

· Added more debug logging

- Added dtool config ecs ls command to list ECS base URIs that have been
- · Added support for configuring access to ECS buckets in multiple namespaces

17.12.2 Fixed

• The dtool config azure 1s command now returns base URIs rather than container names

17.13 [3.15.0] - 2019-04-26

17.13.1 Added

- dtool config readme-template CLI command for configuring the path to a custom readme template
- dtoolcore._BaseDataSet.base_uri property
- dtoolcore.storagebroker.BaseStorageBroker.generate_base_uri method
- dtoolcore.utils.DEFAULT_CACHE_PATH global helper variable
- dtoolcore.utils.get_config_value_from_file helper function
- dtoolcore.utils.write_config_value_to_file helper function

17.13.2 Changed

- · dtool config cache now works with one unified cache directory for all storage brokers
- Started using unified environment variable to specify the cache directory DTOOL_CACHE_DIRECTORY
- Default cache directory changed set to ~/.cache/dtool

17.13.3 Fixed

• Fixed defect when username was supplied as two separate strings to dtool config user name in CLI

17.14 [3.14.1] - 2018-12-12

17.14.1 Fixed

• Fixed the dtool config azure set help text

17.15 [3.14.0] - 2018-11-21

17.15.1 Added

- Added dtool publish command
- Added -f/--format option to dtool summary command to enable output in JSON format
- Added sorting of CSV/TSV/HTML inventories by dataset name

17.15.2 Changed

• Changed default output of dtool summary to be human readable YAML

17.16 [3.13.0] - 2018-11-13

17.16.1 Added

- Added support for Windows! :)
- Added dtool config command

17.17 [3.12.0] - 2018-09-25

17.17.1 Added

- Added dtool uuid command
- Added dtool item relpath command

17.18 [3.11.0] - 2018-09-20

17.18.1 Added

- dtool cp to replace dtool copy
- dtool readme write to write readme from file or stdin
- dtool item overlay command

17.18.2 Deprecated

• dtool copy in favour of dtool cp

17.18.3 Removed

• Removed created_at field from default README template

17.18.4 Fixed

- Defect in dtool create when providing a relative path to the --symlink-path option
- Python 2 defect in dealing with unicode in README.yml file when using dtool readme edit

17.19 [3.10.0] - 2018-09-11

17.19.1 Added

- dtoolcore.filehasher.hashsum_digest helper function
- dtoolcore.filehasher.md5sum_digest helper function

17.19.2 Changed

• Improved name from dtoolcore.filehasher.hashsum to dtoolcore.filehasher.hashsum_hexdigest

17.19.3 Fixed

• Deal with issue in how ruamel.yaml deals with float values

17.20 [3.9.0] - 2018-08-03

17.20.1 Added

- Added ability to update the name of a frozen dataset from the dtool CLI
- Added update_name method to DataSet class (previously only available on ProtoDataSet class)

17.21 [3.8.0] - 2018-07-31

Dataset name validation.

17.21.1 Added

- dtoolcore.generate_admin_metadata function raises dtoolcore.

 DtoolCoreInvalidNameError if invalid name is provided
- dtoolcore.utils.name_is_valid utility function for checking sanity of dataset names
- · Validation of dataset name upon creation using dtool CLI
- · Validation of dataset name when updating it using dtool CLI

17.21.2 Fixed

- Fixed defect where dtool ls -q was listing dataset names rather than URIs making it impossible to process datasets in a BASE_URI programatically
- Make SymlinkStorageBroker compatible with dtoolcore 3.4.0

17.22 [3.7.0] - 2018-07-26

Storage broker base class redesign and refactoring.

17.22.1 Added

- Ability to update descriptive metadata in README of frozen datasets
- Validation that the descriptive metadata provided by the dtool readme edit command is valid YAML
- Added dtoolcore.storagebroker.BaseStorageBroker
- Added logging to the reusable BaseStorageBroker methods
- get_text new method on BaseStorageBroker class
- put_text new method on BaseStorageBroker class
- get_admin_metadata_key new method on BaseStorageBroker class
- get_readme_key new method on BaseStorageBroker class
- get_manifest_key new method on BaseStorageBroker class
- get_overlay_key $new\ method\ on\ {\tt BaseStorageBroker}\ class$
- get_structure_key new method on BaseStorageBroker class
- get_dtool_readme_key new method on BaseStorageBroker class
- get_size_in_bytes new method on BaseStorageBroker class
- get_utc_timestamp new method on BaseStorageBroker class
- get_hash new method on BaseStorageBroker class
- ullet get_relpath new method on <code>BaseStorageBroker class</code>
- update_readme new method on BaseStorageBroker class
- DataSet.put_readme method that can be used to update descriptive metadata in (frozen) dataset README whilst keeping a copy of the historical README content
- Add storage_broker_version key to structure parameters

17.22.2 Fixed

- Stop copy_resume function calculating hashes unnecessarily
- Fixed the documentation of the dtool verify command

17.23 [3.6.2] - 2018-07-10

17.23.1 Fixed

• Default config file now set in dtoolcore.utils.get_config_value if not provided in caller

17.24 [3.6.1] - 2018-07-09

17.24.1 Fixed

- Made download to DTOOL_HTTP_CACHE_DIRECTORY more robust
- · Added ability to deal with redirects to enable working with shortened URLs

17.25 [3.6.0] - 2018-07-05

17.25.1 Added

• Bundling of dtool-http package

17.25.2 Removed

- Bundling of dtool-irods package
- Bundling of dtool-s3 package

17.26 [3.5.0] - 2018-06-06

17.26.1 Added

- Pre-checks to 'dtool freeze' command to ensure that there is no rogue content in the base of disk datasets
- Added rogue content validation check to DiskStorageBroker.pre_freeze hook

17.27 [3.4.0] - 2018-05-24

17.27.1 Added

- Pre-checks to 'dtool freeze' command to ensure that the item handles are sane, i.e. that they do not contain newline characters
- Pre-checks to 'dtool freeze' command to ensure that there are not too many items in the proto dataset, default to less than 10000

17.28 [3.3.1] - 2018-05-18

17.28.1 Fixed

• Defect where inventory html template is not included in Python package on PyPi

17.29 [3.3.0] - 2018-05-18

17.29.1 Added

- Add "created_at" key to the administrative metadata
- dtool inventory command for generating csv/tsv/html inventories of collections of datasets
- Added support for -h flag as well as --help
- · Added timestamp to logging output

17.29.2 Fixed

- Improved handling of URIs in validation code
- Fixed defect where running dtool item properties with an invalid identifier resulted in a KeyError exception being propagated to the user
- Fixed defect where dtool verify did not compare file sizes
- · Fixed timestamp defect in DiskStoragBroker

17.30 [3.2.1] - 2018-05-01

17.30.1 Fixed

• Fixed issue arising from a file being put into iRODS and the connection breaking before the appropriate metadata could be set on the file in iRODS. See also: https://github.com/jic-dtool/dtool-irods/issues/7

17.31 [3.2.0] - 2018-02-09

Release to make it easier to create symlink datasets in an automated fashion.

17.31.1 Changed

- Simplified the way to specify the symbolic link path in the SymLinkStorageBroker
- The path to the data when creating a symlink dataset is now specified using the -s/--symlink-path option rather than being something that is prompted for. This makes it easier to create symlink datasets in an automated fashion.

17.32 [3.1.0] - 2018-02-05

17.32.1 Added

- --resume option to dtool copy command
- --quite and --verbose options to dtool 1s and improved formatting

• Add dtoolcore.copy_resume function

17.33 [3.0.0] - 2018-01-18

This release makes use of the dtoolcore version 3.0.0 API, which improves the handling of URIs and adds more metadata describing the structure of datasets.

Another major feature of this release is the addition of an S3 storage broker that can be used to interact with Amazon's S3 object storage.

17.33.1 Added

- AWS S3 object storage broker
- Writing of .dtool/structure.json file to the DiskStorageBroker; a file for describing the structure of the dtool dataset in a computer readable format
- Writing of .dtool/README.txt file to the DiskStorageBroker; a file for describing the structure of the dtool
 dataset in a human readable format
- Writing of .dtool/structure.json file to the IrodsStorageBroker; a file for describing the structure of the dtool dataset in a computer readable format
- Writing of .dtool/README.txt file to the IrodsStorageBroker; a file for describing the structure of the dtool dataset in a human readable format

17.33.2 Changed

• Make use of dtoolcore version 3 API

17.33.3 Fixed

• Removed the historical dtool_readme key/value pair from the administrative metadata (in the .dtool/dtool file)

17.34 [2.4.0] - 2017-12-14

17.34.1 Added

- Ability to specify a custom README.yml template file path.
- Ability to configure the full user name for the README.yml template using DTOOL_USER_FULL_NAME

17.34.2 Fixed

- Made .dtool/manifest.json content created by DiskStorageBroker human readable by adding new lines and indentation to the JSON formatting.
- Made the DiskStorageBroker.list_overlay_names method more robust. It no longer falls over if the .dtool/overlays directory has been lost, i.e. by cloning a dataset with no overlays from a Git repository.

- Fixed defect where an incorrect URI would get set on the dataset when using DataSet.from_path class method on a relative path
- Made the YAML output more pretty by adding more indentation.
- Replaced hardcoded nbi.ac.uk email with configurable DTOOL_USER_EMAIL in the default README.yml template.
- Fixed IrodsStorageBroker.generate_uri class method
- Made .dtool/manifest.json content created by IrodsStorageBroker human readable by adding new lines and indentation to the JSON formatting.
- Added rule to catch CAT_INVALID_USER string for giving a more informative error message when iRODS
 authentication times out

17.35 [2.3.2] - 2017-10-25

17.35.1 Fixed

• Fixed issue where the symbolic link was not fully resolved when creating a symlink dataset that used the terminal to prompt for the data directory

17.36 [2.3.1] - 2017-10-25

17.36.1 Fixed

- More graceful exit if one presses Cancel in file browser when creating a symlink dataset
- Data directory now falls back on click command line prompt if TkInter has issues when creating a symlink dataset

17.37 [2.3.0] - 2017-10-23

17.37.1 Added

- pre_freeze_hoook to the stroage broker interface called at the beginning of ProtoDataSet.freeze method.
- --quiet flag to dtool create command
- dtool overlay is command to list the overlays in dataset
- dtool overlay show command to show the content of a specific overlay

17.37.2 Changed

- Improved speed of freezing a dataset in iRODS by making use of caches to reduce the number of calls made to iRODS during this process
- dtool copy now specifies target location using URI rather than using the --prefix and --storage arguments

17.37.3 Fixed

- Made the DiskStorageBroker.create_structure method more robust
- More informative error message when iRODS has not been configured
- More informative error message when iRODS authentication times out
- · Stopped client hanging when iRODS authentication has timed out
- storagebroker's put_item method now returns relpath
- Made the IrodsStorageBroker.create_structure method more robust by checking if the parent collection exists
- Made error handling in dtool create more specific
- Added propagation of original error message when StorageBrokerOSError captures in dtool create

17.38 [2.2.0] - 2017-10-09

17.38.1 Added

- dtool 1s can now be used to list the relpaths of the items in a dataset
- -f/--full flag to dtool diff command to include checking of file hashes
- -f/--full flag to dtool verify command to include checking of file hashes

17.38.2 Changed

- dtool 1s now works with URIs rather than with prefix and storage arguments
- dtool diff now only compares identifiers and file sizes by default
- dtool verify now only compares identifiers and file sizes by default

17.38.3 Fixed

• Made DiskStorageBroker.list dataset uris class method more robust

17.39 [2.1.2] - 2017-10-05

17.39.1 Fixed

• Set the correct dependency to actually get fix reported in 2.1.1

17.40 [2.1.1] - 2017-10-05

17.40.1 Fixed

Fixed defect in iRODS storage broker where files with white space resulted in broken identifiers

17.41 [2.1.0] - 2017-10-04

17.41.1 Added

- dtool readme show command that returns the readme content
- --quiet flag to dtool copy command

17.41.2 Changed

• Improved the dtool readme --help output

17.41.3 Fixed

- Progress bar now shows information on individual items being processed
- dtool ls now works with relative paths
- Fix defect where IrodsStorageBroker.put_item raised SystemError when trying to overwrite an existing file

17.42 [2.0.2] - 2017-09-25

17.42.1 Fixed

- Better validation of input in terms of base vs proto vs frozen dataset URIs
- Fixed bug where copy creates an intermediate proto dataset that self identifies as a frozen dataset.
- Fixed potential bug where a copy could convert a proto dataset to a dataset before all its overlays had been copied over
- Fixed type of "frozen_at" time stamp in admin metadata: from string to float

17.43 [2.0.1] - 2017-09-20

17.43.1 Fixed

• Made version requirements of dtool sub-packages explicit

17.44 [2.0.0] - 2017-09-14

Initial release of dtool as a meta package.

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